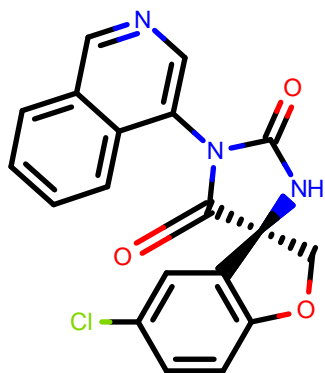
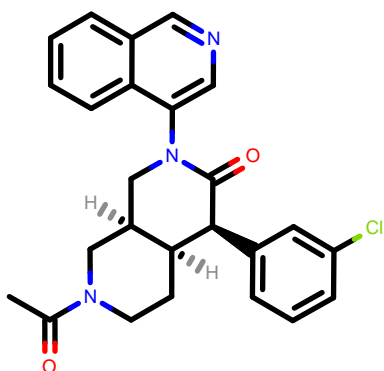


VLA-UNK-83c3754c-1_1



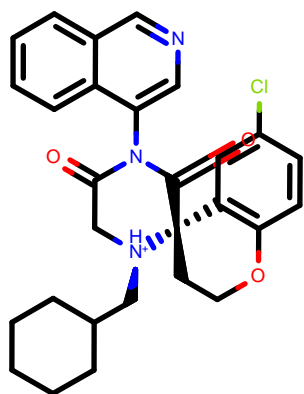
CID:	VLA-UNK-83c3754c-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@@]4(COCc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN2122
DDG (kcal/mol):	-7.04
dDDG (kcal/mol):	0.24

MIC-UNK-9582b2c5-1_6



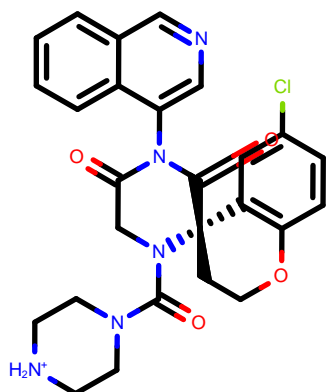
CID:	MIC-UNK-9582b2c5-1_6
SMILES:	<chem>CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3ccc(c3)Cl)c4ncc5c4ccccc5</chem>
RUN:	RUN200
DDG (kcal/mol):	-6.90
dDDG (kcal/mol):	0.24

ADA-UCB-dc2b944c-1_1



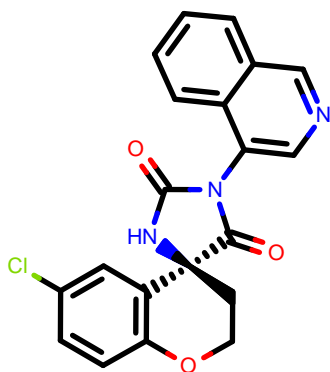
CID:	ADA-UCB-dc2b944c-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[N@@H]([C@@]4(C3=O)COCc5c4cc(cc5)Cl)OC6CCCC6</chem>
RUN:	RUN491
DDG (kcal/mol):	-6.89
dDDG (kcal/mol):	0.44

VLA-UCB-34f3ed0c-18_1



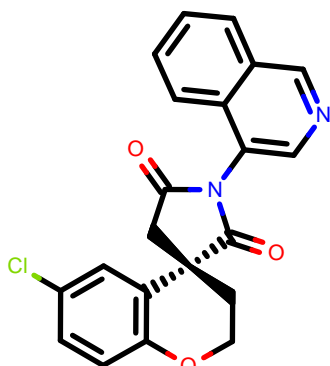
CID:	VLA-UCB-34f3ed0c-18_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)CN([C@@]4(C3=O)COCc5c4cc(cc5)Cl)C(=O)N6CC[NH2+]CC6</chem>
RUN:	RUN546
DDG (kcal/mol):	-6.54
dDDG (kcal/mol):	0.30

VLA-UCB-34f3ed0c-11_1



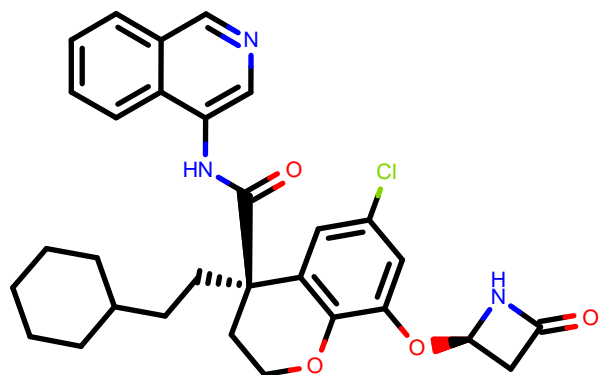
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN539
DDG (kcal/mol):	-6.53
dDDG (kcal/mol):	0.20

VLA-UCB-50c39ae8-2_1



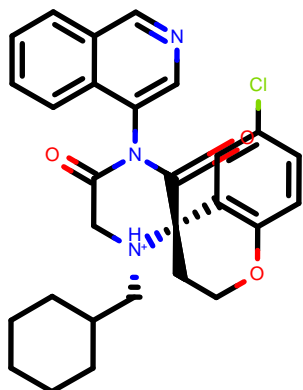
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN274
DDG (kcal/mol):	-6.43
dDDG (kcal/mol):	0.24

VLA-UCB-50c39ae8-9_1_1



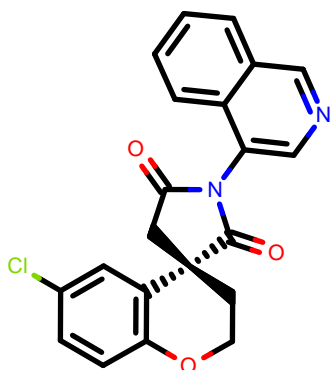
CID:	VLA-UCB-50c39ae8-9_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@]5H5CC(=O)N5)Cl)COC6CCCC6</chem>
RUN:	RUN2706
DDG (kcal/mol):	-6.42
dDDG (kcal/mol):	0.44

ADA-UCB-dc2b944c-1_2



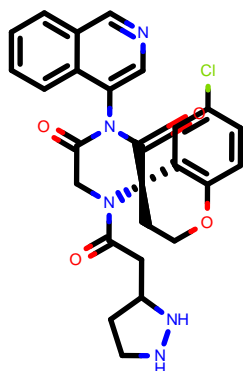
CID:	ADA-UCB-dc2b944c-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@H]([C@@]4(C3=O)CCOc5c4cc(cc5)Cl)COC6CCCC6</chem>
RUN:	RUN464
DDG (kcal/mol):	-6.41
dDDG (kcal/mol):	0.31

BEN-BAS-c2bc0d80-6_1



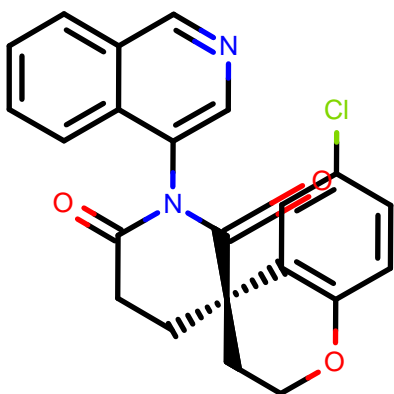
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN1014
DDG (kcal/mol):	-6.18
dDDG (kcal/mol):	0.21

VLA-UCB-34f3ed0c-16_1



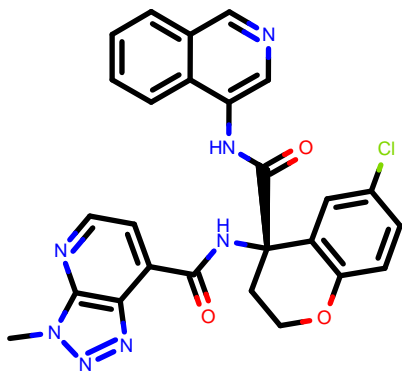
CID:	VLA-UCB-34f3ed0c-16_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)CN[C@@]4(C3=O)CCOc5c4cc(cc5)Cl)C(=O)C6ccn[nH]6</chem>
RUN:	RUN544
DDG (kcal/mol):	-6.15
dDDG (kcal/mol):	0.28

VLA-UCB-50c39ae8-3_1



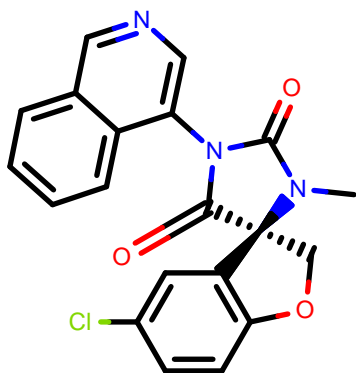
CID:	VLA-UCB-50c39ae8-3_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl</chem>
RUN:	RUN277
DDG (kcal/mol):	-5.84
dDDG (kcal/mol):	0.22

EN300-202106_1_1_1



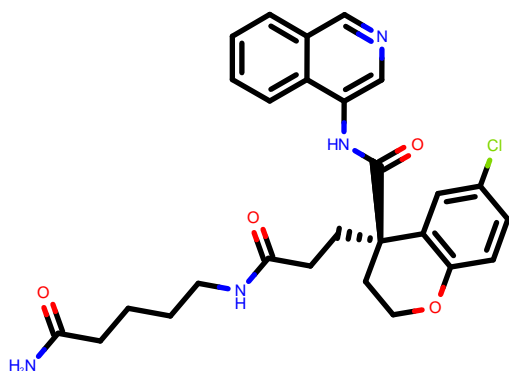
CID:	EN300-202106_1_1_1
SMILES:	<chem>Cn1c2c(c(ccn2)C(=O)N[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccoc6)nn1</chem>
RUN:	RUN2712
DDG (kcal/mol):	-5.77
dDDG (kcal/mol):	0.23

VLA-UNK-83c3754c-2_1



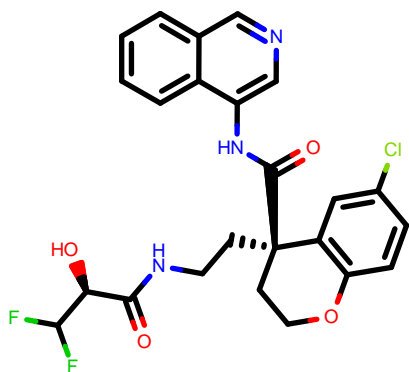
CID:	VLA-UNK-83c3754c-2_1
SMILES:	<chem>CN1C(=O)N(C(=O)[C@@]12COC3c2cc(cc3)Cl)c4cncc5c4cccc5</chem>
RUN:	RUN2133
DDG (kcal/mol):	-5.49
dDDG (kcal/mol):	0.22

EN300-125143_2_1_1



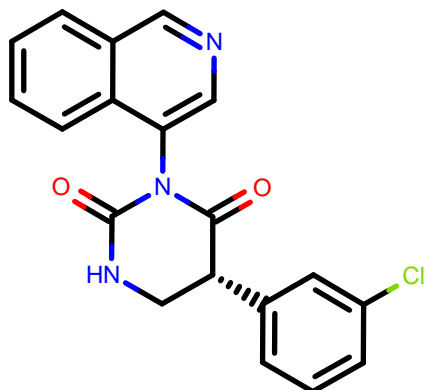
CID:	EN300-125143_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCCC(=O)N</chem>
RUN:	RUN6629
DDG (kcal/mol):	-5.48
dDDG (kcal/mol):	0.29

EN300-1932780_3_1_1



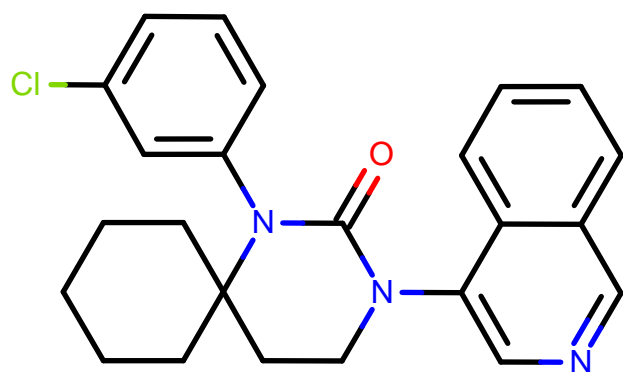
CID:	EN300-1932780_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(F)F</chem>
RUN:	RUN3208
DDG (kcal/mol):	-5.40
dDDG (kcal/mol):	0.20

VLA-UCB-1dbca3b4-18_1



CID:	VLA-UCB-1dbca3b4-18_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]3(CO)C4CCCC(C4)Cl</chem>
RUN:	RUN93
DDG (kcal/mol):	-5.32
dDDG (kcal/mol):	0.28

DAR-DIA-5d6f1b43-10_1



CID: DAR-DIA-5d6f1b43-10_1

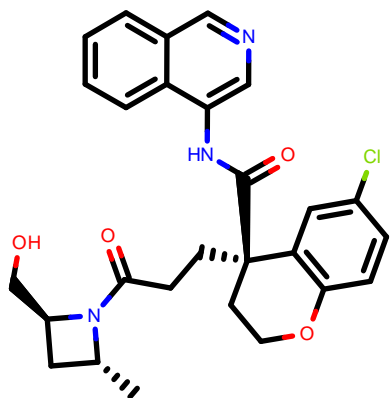
SMILES: c1ccc2c(c1)cncc2N3CCC4(CCCCC4)N(C3=O)c5ccccc(c5)Cl

RUN: RUN395

DDG (kcal/mol): -5.26

dDDG (kcal/mol): 0.24

EN300-1709410_2_3_1



CID: EN300-1709410_2_3_1

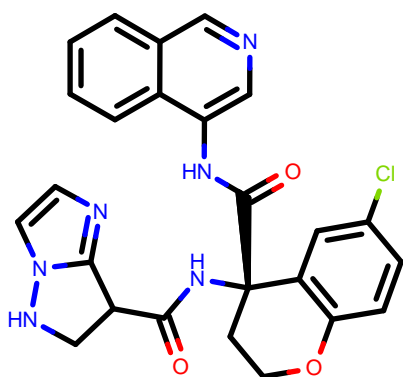
SMILES: C[C@@H]1[C@H](N1C(=O)CC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)N4cnc5c4cccc5)CO

RUN: RUN7095

DDG (kcal/mol): -5.10

dDDG (kcal/mol): 0.26

EDJ-MED-6864a934-3_1



CID: EDJ-MED-6864a934-3_1

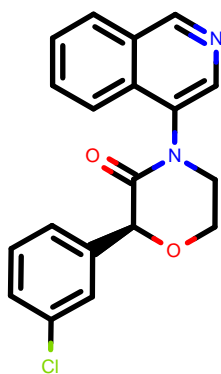
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)c5[nH]p6c5nc6

RUN: RUN2426

DDG (kcal/mol): -5.08

dDDG (kcal/mol): 0.21

PET-UNK-431b3bfb-1_1



CID: PET-UNK-431b3bfb-1_1

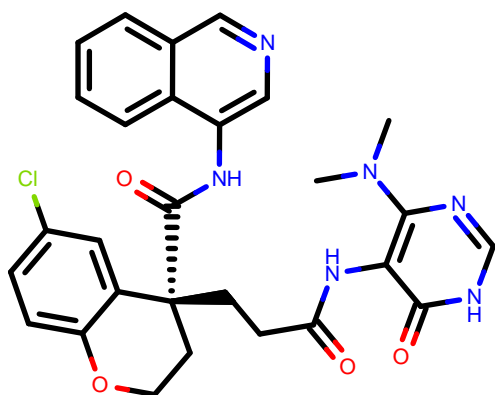
SMILES: c1ccc2c(c1)cncc2N3CCO[C@H](C3=O)c4ccccc(c4)Cl

RUN: RUN174

DDG (kcal/mol): -5.06

dDDG (kcal/mol): 0.22

EN300-106352_2_1_1



CID: EN300-106352_2_1_1

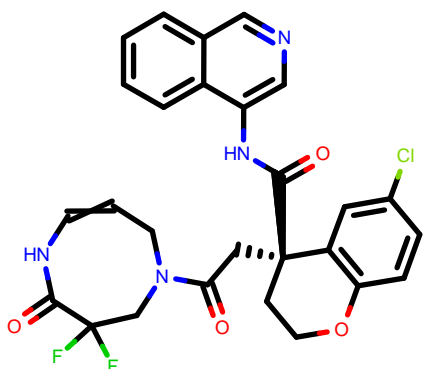
SMILES: CN(C)c1c(c(=O)[nH]cn1)NC(=O)CC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN2744

DDG (kcal/mol): -5.05

dDDG (kcal/mol): 0.37

EN300-1273202_1_1_1



CID: EN300-1273202_1_1_1

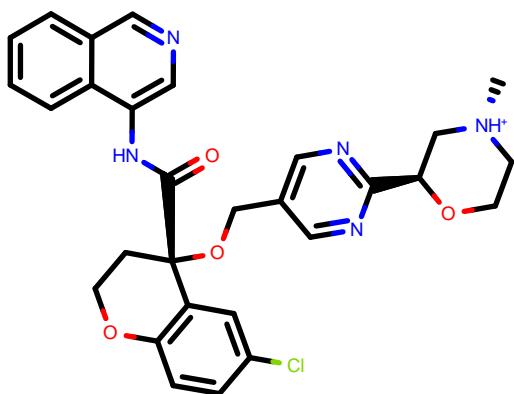
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C(=O)N5CCOCNC(=O)C(C5)F)F

RUN: RUN5510

DDG (kcal/mol): -5.03

dDDG (kcal/mol): 0.34

ED_-GRI-5b13fbe2-66_3



CID: ED_-GRI-5b13fbe2-66_3

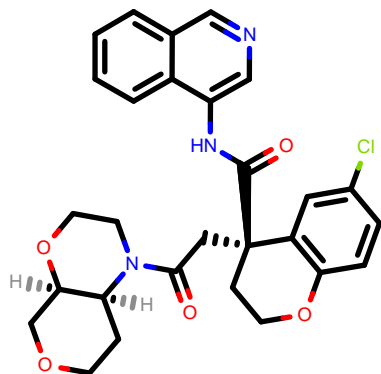
SMILES: C[N+](=O)[C@@H](C1=CN(C)C=C1)C[C@]2(CO)C(CO)C(=O)N5CCOCNC(=O)C(C5)F)F

RUN: RUN1500

DDG (kcal/mol): -5.01

dDDG (kcal/mol): 0.21

EN300-719522_1_1_1



CID: EN300-719522_1_1_1

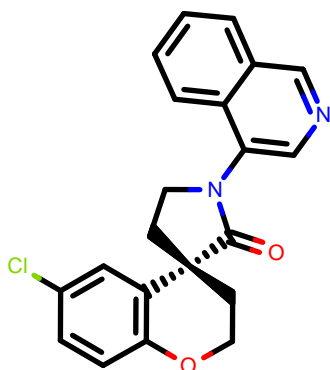
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C(=O)N5CCOCNC(=O)C(C5)F)F

RUN: RUN2714

DDG (kcal/mol): -5.00

dDDG (kcal/mol): 0.21

ALP-POS-477dc5b7-4_1



CID: ALP-POS-477dc5b7-4_1

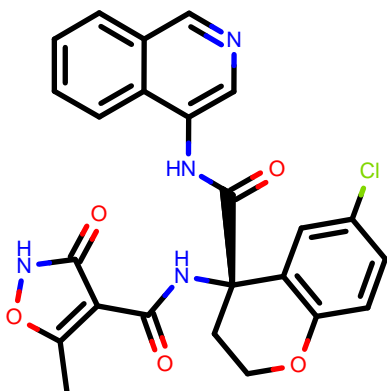
SMILES: c1ccc2c(c1)cncc2N3CC[C@@]4(C(=O)CCOc5c4cc(cc5)Cl

RUN: RUN205

DDG (kcal/mol): -4.98

dDDG (kcal/mol): 0.25

EN300-110423_1_1_1



CID: EN300-110423_1_1_1

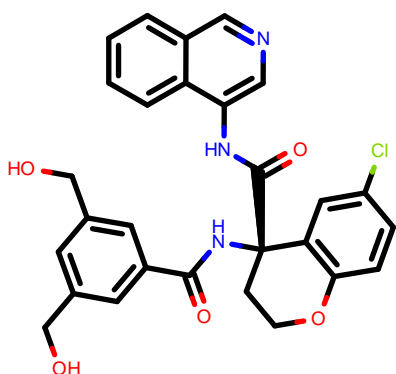
SMILES: Cc1c(c(O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2721

DDG (kcal/mol): -4.96

dDDG (kcal/mol): 0.24

EN300-211158_1_1_1



CID: EN300-211158_1_1_1

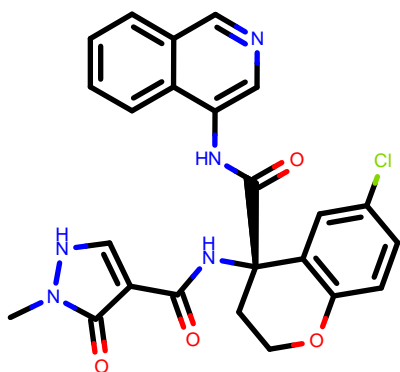
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cc(c5)CO)CO

RUN: RUN3995

DDG (kcal/mol): -4.95

dDDG (kcal/mol): 0.31

EN300-7437779_1_1_1



CID: EN300-7437779_1_1_1

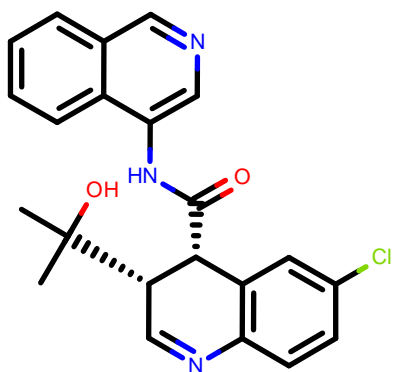
SMILES: Cn1c(=O)c(c[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2700

DDG (kcal/mol): -4.93

dDDG (kcal/mol): 0.24

BEN-BAS-5c03e89e-2_4



CID: BEN-BAS-5c03e89e-2_4

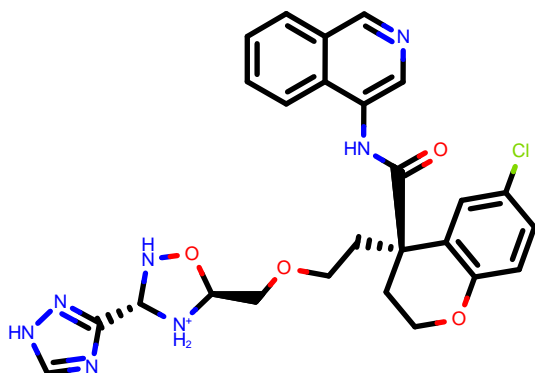
SMILES: CC(C)([C@H]1C=Nc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3ccc4)Cl)O

RUN: RUN1024

DDG (kcal/mol): -4.92

dDDG (kcal/mol): 0.19

EN300-92031_3_1_2



CID: EN300-92031_3_1_2

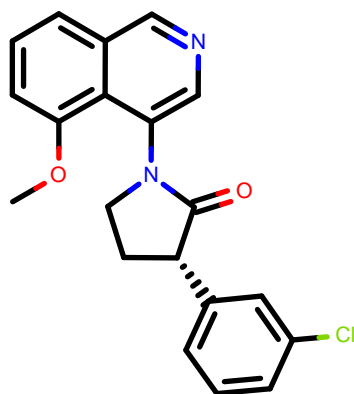
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(C)COCc4ccc(cc4O)COC[C@H]5[NH2+][C@@H]6NOS(=O)(=O)N6

RUN: RUN3267

DDG (kcal/mol): -4.92

dDDG (kcal/mol): 0.58

MIC-UNK-50cce87d-8_2



CID: MIC-UNK-50cce87d-8_2

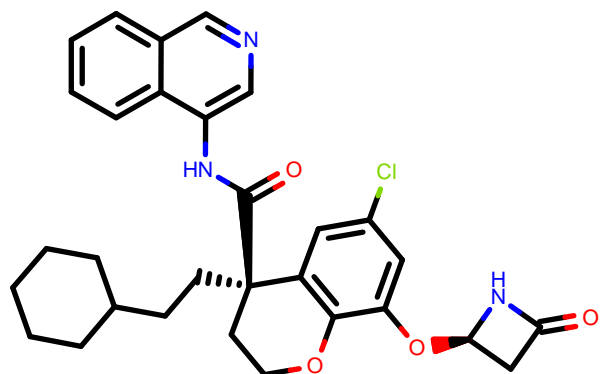
SMILES: COc1cccc2c1c(cnc2)N3CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN554

DDG (kcal/mol): -4.91

dDDG (kcal/mol): 0.26

VLA-UCB-50c39ae8-9_1



CID: VLA-UCB-50c39ae8-9_1

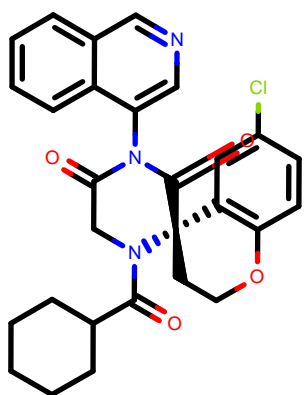
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(C)COCc4ccc(cc4O)[C@@H]5CC(=O)N5)Cl)COC6CCCC6

RUN: RUN432

DDG (kcal/mol): -4.87

dDDG (kcal/mol): 0.37

VLA-UCB-34f3ed0c-17_1



CID: VLA-UCB-34f3ed0c-17_1

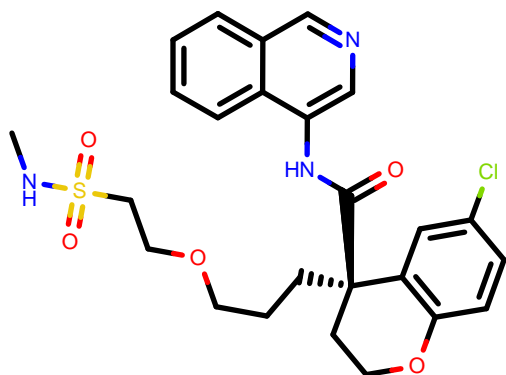
SMILES: c1ccc2c(c1)cncc2N3C(=O)CN(C@@H)4(C3=O)CCOCc5c4cc(cc5)Cl)C(=O)C6CCCCC6

RUN: RUN526

DDG (kcal/mol): -4.86

dDDG (kcal/mol): 0.26

EN300-6482967_4_1_1



CID: EN300-6482967_4_1_1

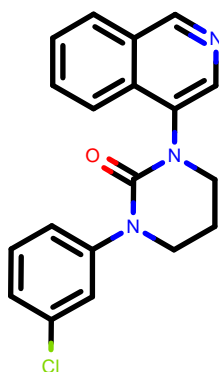
SMILES: CNS(=O)(=O)CCOCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6726

DDG (kcal/mol): -4.83

dDDG (kcal/mol): 0.41

PET-UNK-7be94445-1_1



CID: PET-UNK-7be94445-1_1

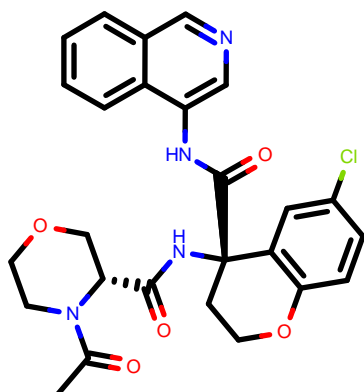
SMILES: c1ccc2c(c1)cncc2N3CCCN(C3=O)c4cccc(c4)Cl

RUN: RUN39

DDG (kcal/mol): -4.83

dDDG (kcal/mol): 0.19

EN300-116313_1_1_1



CID: EN300-116313_1_1_1

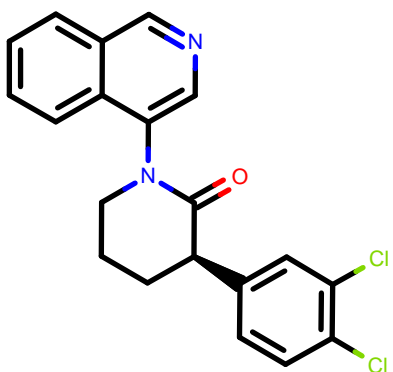
SMILES: CC(=O)N1CCOC[C@@H]1C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3010

DDG (kcal/mol): -4.80

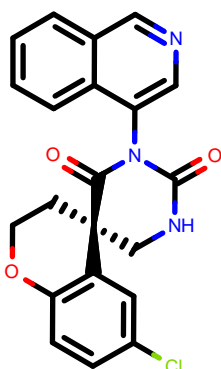
dDDG (kcal/mol): 0.23

ALP-POS-e0fe77e5-1_1



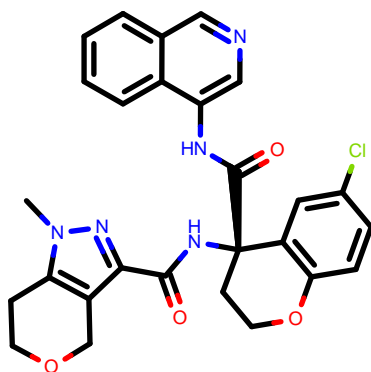
CID:	ALP-POS-e0fe77e5-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCC[C@H](C3=O)c4ccc(c(c4)Cl)Cl</chem>
RUN:	RUN2126
DDG (kcal/mol):	-4.78
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-12_1



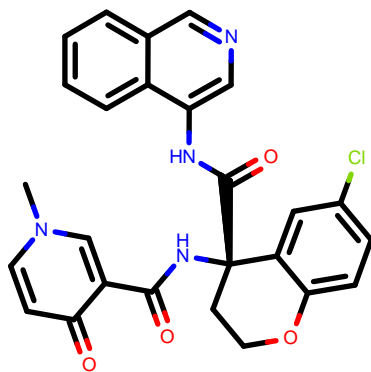
CID:	VLA-UCB-34f3ed0c-12_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CNC3=O</chem>
RUN:	RUN531
DDG (kcal/mol):	-4.65
dDDG (kcal/mol):	0.23

EN300-1681046_1_1_1



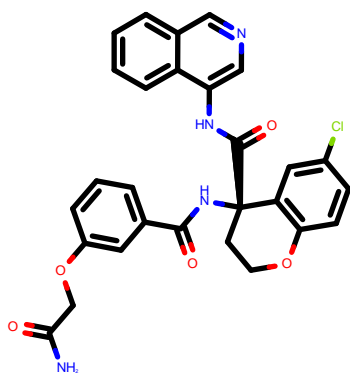
CID:	EN300-1681046_1_1_1
SMILES:	<chem>Cn1c2c(c(n1)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)COC2</chem>
RUN:	RUN2908
DDG (kcal/mol):	-4.62
dDDG (kcal/mol):	0.25

EN300-171522_1_1_1



CID:	EN300-171522_1_1_1
SMILES:	<chem>Cn1ccc(=O)c(c1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5</chem>
RUN:	RUN3055
DDG (kcal/mol):	-4.56
dDDG (kcal/mol):	0.29

EN300-30687_1_1_1



CID: EN300-30687_1_1_1

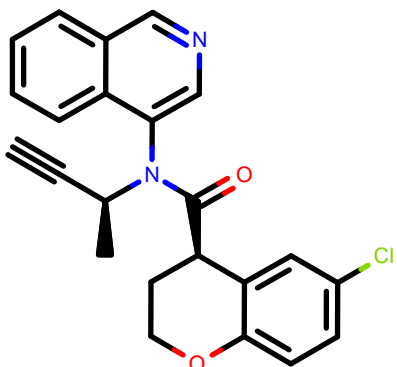
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5)OCC(=O)N

RUN: RUN4309

DDG (kcal/mol): -4.52

dDDG (kcal/mol): 0.32

DAR-DIA-5ff57136-16_1_1



CID: DAR-DIA-5ff57136-16_1_1

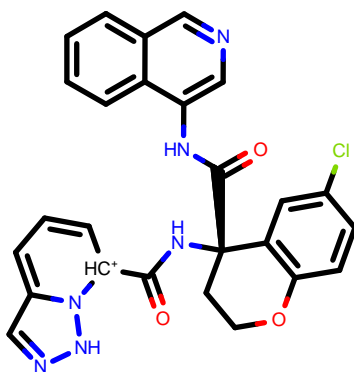
SMILES: C[C@@H](C#C)N(C1cnc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN2730

DDG (kcal/mol): -4.46

dDDG (kcal/mol): 0.14

EDJ-MED-6864a934-8_1



CID: EDJ-MED-6864a934-8_1

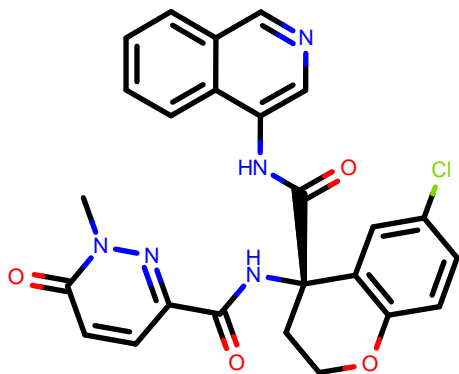
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc6n5nnc6

RUN: RUN2447

DDG (kcal/mol): -4.45

dDDG (kcal/mol): 0.25

EN300-05798_1_1_1



CID: EN300-05798_1_1_1

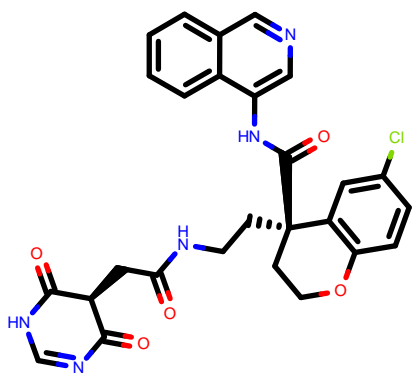
SMILES: Cn1c(=O)ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3657

DDG (kcal/mol): -4.41

dDDG (kcal/mol): 0.21

EN300-86205_3_1_1



CID: EN300-86205_3_1_1

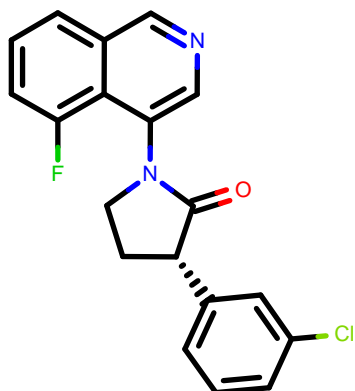
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4ccc(cc4)C)CCNC(=O)C@H5C1=O)NC=O)C5=O

RUN: RUN5616

DDG (kcal/mol): -4.38

dDDG (kcal/mol): 0.30

MIC-UNK-50cce87d-5_1



CID: MIC-UNK-50cce87d-5_1

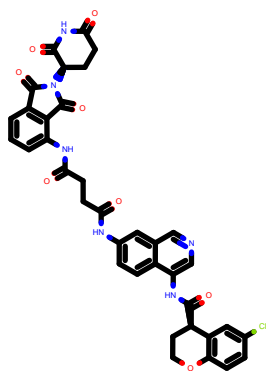
SMILES: c1cc(cc(c1)Cl)[C@@H]2CCN(C2=O)c3cncc4c3c(ccc4)F

RUN: RUN552

DDG (kcal/mol): -4.37

dDDG (kcal/mol): 0.24

DAR-DIA-9e4459de-15_3



CID: DAR-DIA-9e4459de-15_3

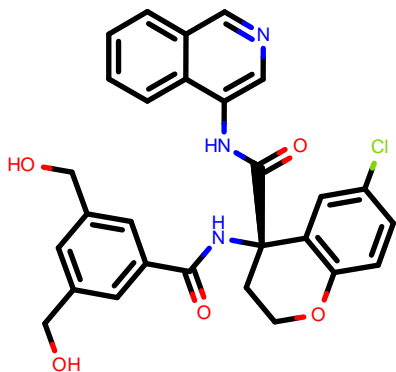
SMILES: c1ccc2c(c1)NC(=O)C(CO)Nc3ccc4c(c3)ncnc4NC(=O)C@@3(CCOc4ccc(cc4)C)C1=O)C@H7C(CO)C1=O)NC7=O)O

RUN: RUN1327

DDG (kcal/mol): -4.36

dDDG (kcal/mol): 0.25

EDJ-MED-6864a934-1_1



CID: EDJ-MED-6864a934-1_1

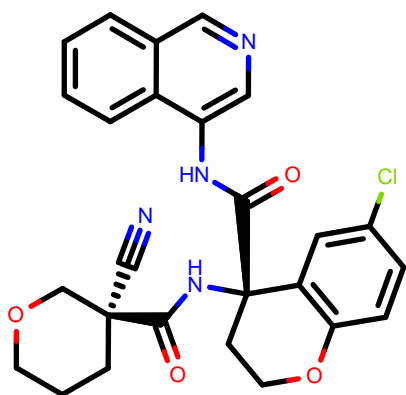
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4ccc(cc4)C)NC(=O)c5ccc(cc5)CO)CO

RUN: RUN2422

DDG (kcal/mol): -4.33

dDDG (kcal/mol): 0.25

EN300-301925_1_2_1



CID: EN300-301925_1_2_1

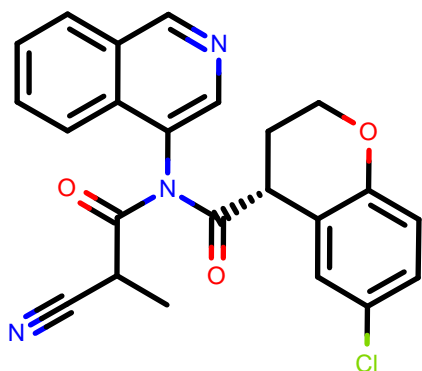
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN3762

DDG (kcal/mol): -4.33

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-1_1



CID: VLA-UCB-34f3ed0c-1_1

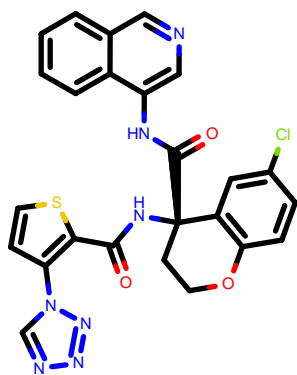
SMILES: C=C(C#N)C(=O)N(c1cnc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN592

DDG (kcal/mol): -4.32

dDDG (kcal/mol): 0.14

EN300-36731_1_1_1



CID: EN300-36731_1_1_1

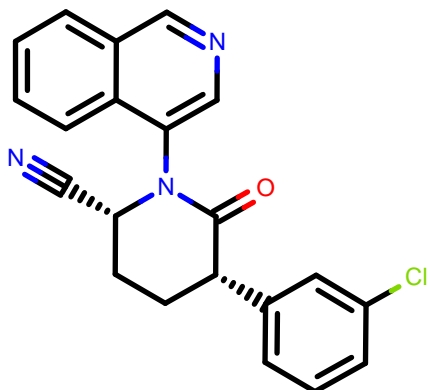
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ccs5)n6cnm6

RUN: RUN2750

DDG (kcal/mol): -4.31

dDDG (kcal/mol): 0.24

PET-UNK-3e354a91-1_1



CID: PET-UNK-3e354a91-1_1

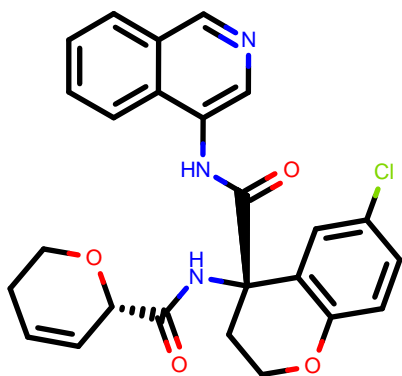
SMILES: c1ccc2c(c1)ncnc2N3[C@H](CC[C@H](C3=O)c4cccc(c4)Cl)C#N

RUN: RUN48

DDG (kcal/mol): -4.30

dDDG (kcal/mol): 0.28

EN300-378044_1_1_1



CID: EN300-378044_1_1_1

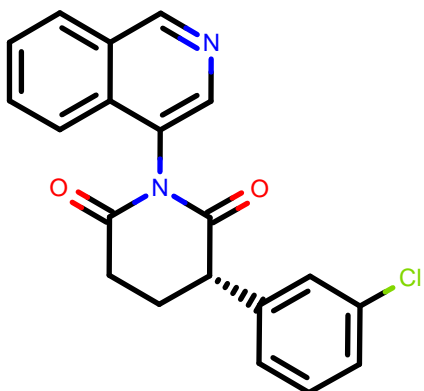
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC=CCO5

RUN: RUN2705

DDG (kcal/mol): -4.30

dDDG (kcal/mol): 0.25

VLA-UCB-1dbca3b4-10_2



CID: VLA-UCB-1dbca3b4-10_2

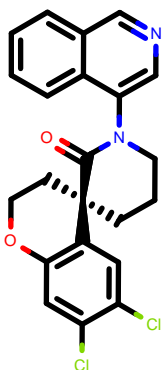
SMILES: c1ccc2c(c1)cncc2N3C(=O)CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN74

DDG (kcal/mol): -4.28

dDDG (kcal/mol): 0.28

ALP-POS-e0fe77e5-4_1



CID: ALP-POS-e0fe77e5-4_1

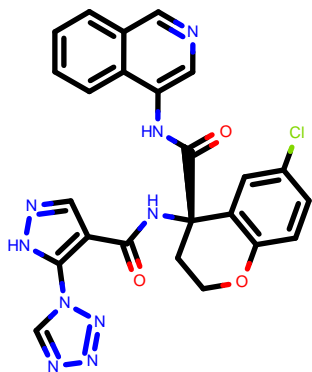
SMILES: c1ccc2c(c1)cncc2N3CCC[C@]4(C3=O)CCOc5c4cc(c(c5)Cl)Cl

RUN: RUN2141

DDG (kcal/mol): -4.27

dDDG (kcal/mol): 0.24

EN300-7549839_1_1_1



CID: EN300-7549839_1_1_1

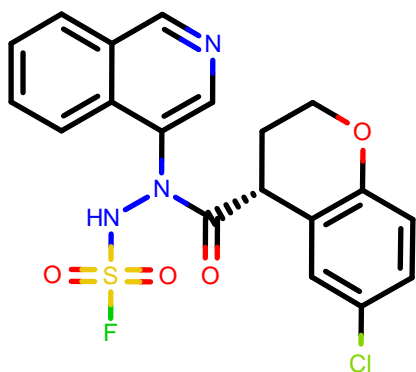
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn[nH]c5n6nnn6

RUN: RUN2740

DDG (kcal/mol): -4.25

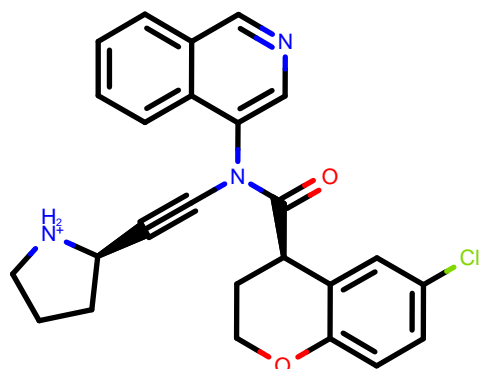
dDDG (kcal/mol): 0.28

JOH-UNI-ea72002d-7_1



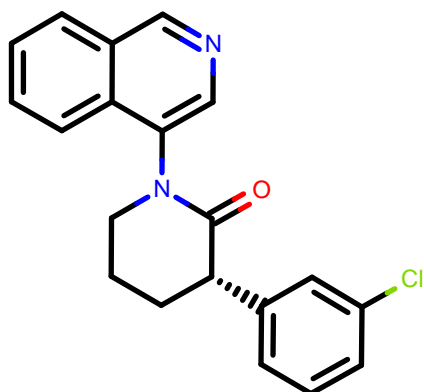
CID:	JOH-UNI-ea72002d-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOCc4ccc(cc4)Cl)NS(=O)(=O)F</chem>
RUN:	RUN2320
DDG (kcal/mol):	-4.24
dDDG (kcal/mol):	0.20

DAR-DIA-5ff57136-12_2



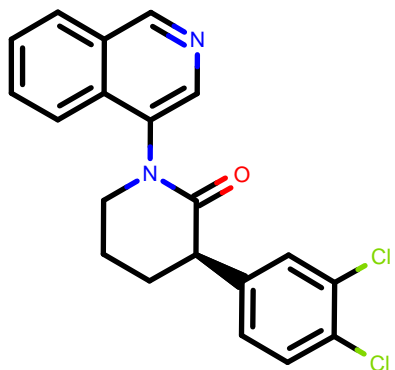
CID:	DAR-DIA-5ff57136-12_2
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#C[C@H]3CC[C@H]3)C(=O)[C@@H]4CCOCc5ccc(cc5)Cl</chem>
RUN:	RUN1259
DDG (kcal/mol):	-4.20
dDDG (kcal/mol):	0.22

PET-UNK-c9c1e0d8-3_2



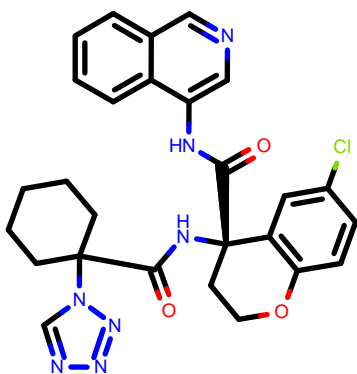
CID:	PET-UNK-c9c1e0d8-3_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCCC[C@H](C3=O)c4ccc(cc4)Cl</chem>
RUN:	RUN33
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.31

ALP-UNI-3735e77e-1_1



CID:	ALP-UNI-3735e77e-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCCC[C@H](C3=O)c4ccc(cc4)Cl</chem>
RUN:	RUN1763
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.23

EN300-186536_1_1_1



CID: EN300-186536_1_1_1

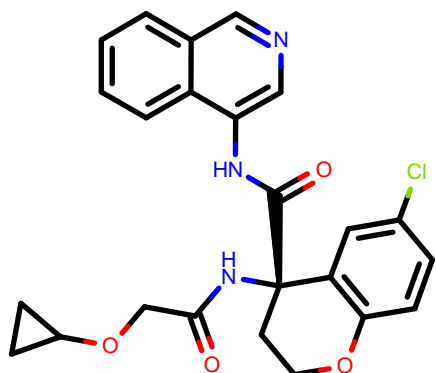
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)n6nnn6

RUN: RUN2760

DDG (kcal/mol): -4.17

dDDG (kcal/mol): 0.26

EN300-378373_1_1_1



CID: EN300-378373_1_1_1

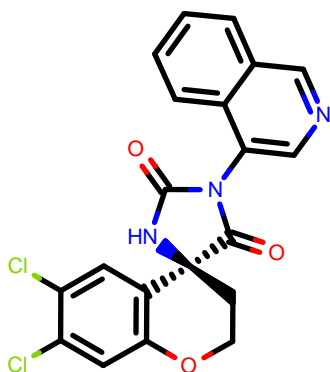
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC5CC5

RUN: RUN2794

DDG (kcal/mol): -4.17

dDDG (kcal/mol): 0.18

VLA-UNK-56836b69-2_1



CID: VLA-UNK-56836b69-2_1

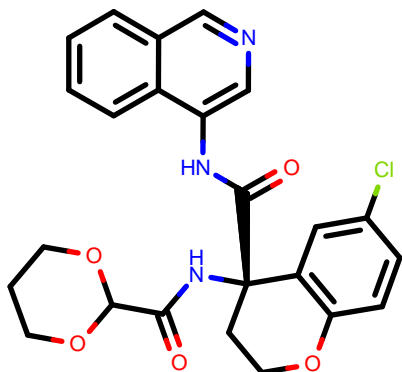
SMILES: c1ccc2c(c1)ncnc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O

RUN: RUN2096

DDG (kcal/mol): -4.15

dDDG (kcal/mol): 0.22

EN300-170985_1_1_1



CID: EN300-170985_1_1_1

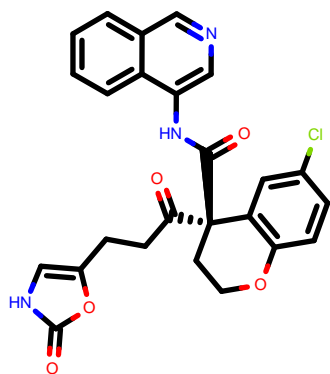
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCCO5

RUN: RUN2765

DDG (kcal/mol): -4.14

dDDG (kcal/mol): 0.24

VLA-UCB-34f3ed0c-9_1_1



CID: VLA-UCB-34f3ed0c-9_1_1

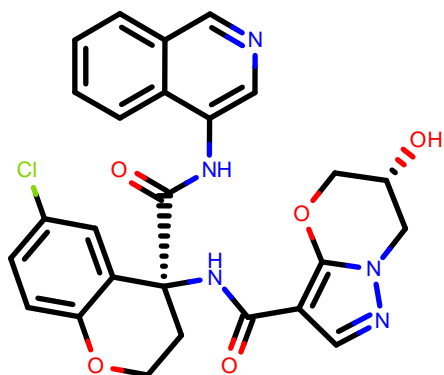
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5

RUN: RUN3111

DDG (kcal/mol): -4.14

dDDG (kcal/mol): 0.20

EN300-6497444_1_1_1



CID: EN300-6497444_1_1_1

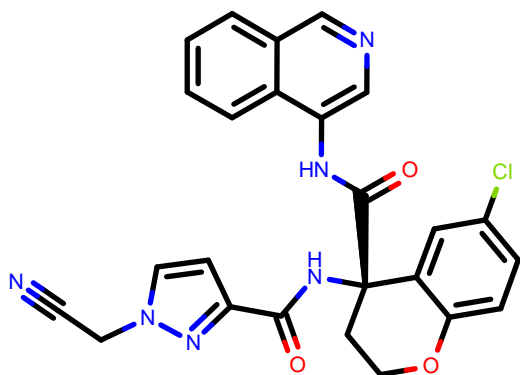
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnc6sOC[C@@]H(C6)O

RUN: RUN2775

DDG (kcal/mol): -4.13

dDDG (kcal/mol): 0.25

EDJ-MED-6864a934-9_1



CID: EDJ-MED-6864a934-9_1

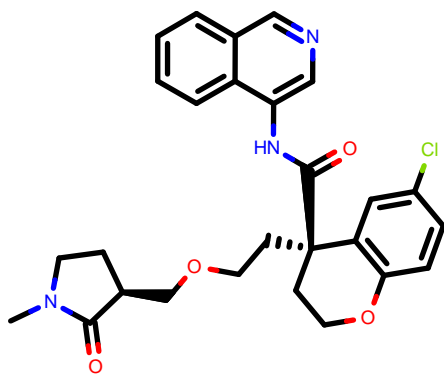
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(c5)CC#N

RUN: RUN2455

DDG (kcal/mol): -4.13

dDDG (kcal/mol): 0.28

EN300-260816_3_2_1



CID: EN300-260816_3_2_1

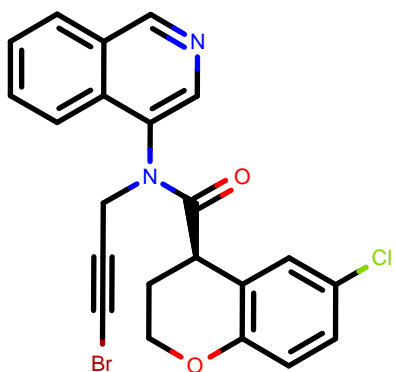
SMILES: CN1CC[C@H](C1=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN3127

DDG (kcal/mol): -4.12

dDDG (kcal/mol): 0.29

DAR-DIA-5ff57136-17_1_1



CID: DAR-DIA-5ff57136-17_1_1

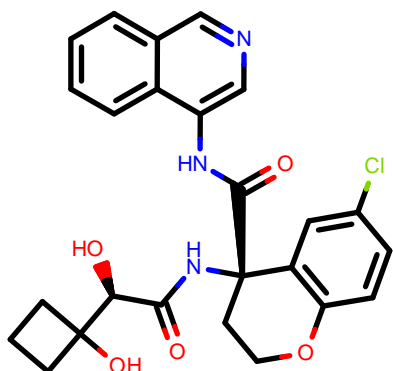
SMILES: c1ccc2c(c1)cncc2N(CC#CCBr)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl

RUN: RUN3438

DDG (kcal/mol): -4.10

dDDG (kcal/mol): 0.18

EN300-1073320_1_1_1



CID: EN300-1073320_1_1_1

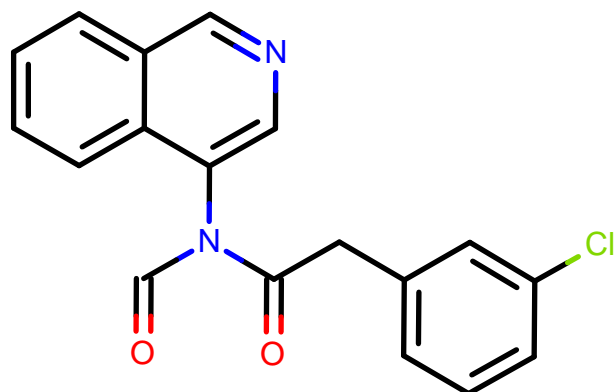
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)NC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN2833

DDG (kcal/mol): -4.09

dDDG (kcal/mol): 0.22

PET-UNK-12d8d43f-1_1



CID: PET-UNK-12d8d43f-1_1

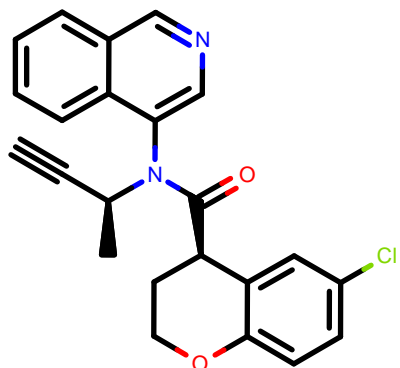
SMILES: c1ccc2c(c1)cncc2N(C(=O)C(=O)CCc3cccc(c3)Cl)C=O

RUN: RUN1319

DDG (kcal/mol): -4.08

dDDG (kcal/mol): 0.22

DAR-DIA-5ff57136-16_1



CID: DAR-DIA-5ff57136-16_1

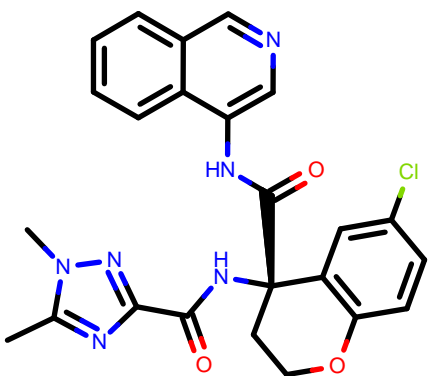
SMILES: C[C@@H](C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl

RUN: RUN1228

DDG (kcal/mol): -4.07

dDDG (kcal/mol): 0.14

EN300-1709101_1_1_1



CID: EN300-1709101_1_1_1

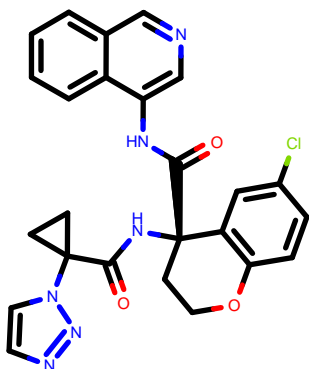
SMILES: Cc1nc(nn1C)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2737

DDG (kcal/mol): -4.02

dDDG (kcal/mol): 0.22

EN300-658559_1_1_1



CID: EN300-658559_1_1_1

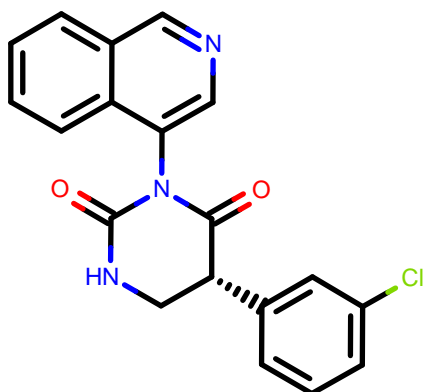
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)n6cnm6

RUN: RUN3087

DDG (kcal/mol): -3.99

dDDG (kcal/mol): 0.28

PET-UNK-abc197b8-1_1



CID: PET-UNK-abc197b8-1_1

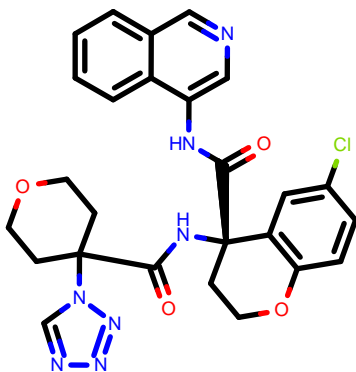
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C)NC(=O)c4cccc(c4)Cl

RUN: RUN334

DDG (kcal/mol): -3.98

dDDG (kcal/mol): 0.27

EN300-254908_1_1_1



CID: EN300-254908_1_1_1

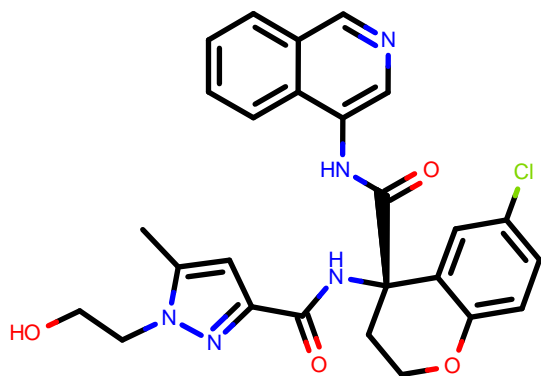
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)n6cnm6

RUN: RUN2738

DDG (kcal/mol): -3.97

dDDG (kcal/mol): 0.26

EN300-6739934_1_1_1



CID: EN300-6739934_1_1_1

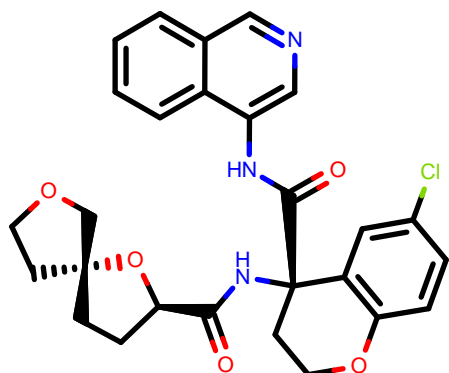
SMILES: Cc1cc(nn1CCO)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2798

DDG (kcal/mol): -3.97

dDDG (kcal/mol): 0.29

EN300-3031933_1_2_1



CID: EN300-3031933_1_2_1

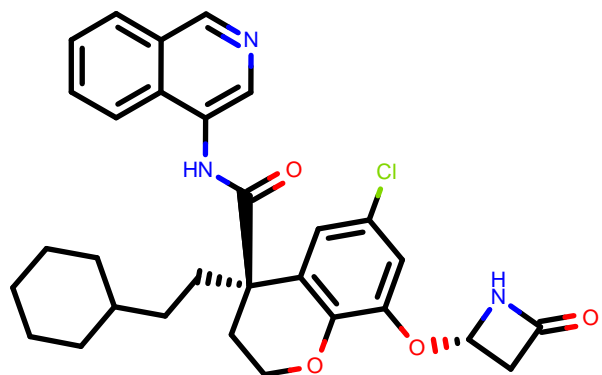
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)N[C@@H]5CC[C@@]6(O)OCCCC6

RUN: RUN2768

DDG (kcal/mol): -3.97

dDDG (kcal/mol): 0.26

VLA-UCB-50c39ae8-9_2_1



CID: VLA-UCB-50c39ae8-9_2_1

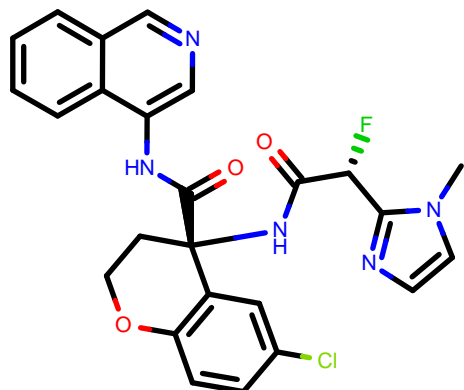
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)[C@@H]5CC(=O)N5)Cl)CC6CCCCC6

RUN: RUN4459

DDG (kcal/mol): -3.96

dDDG (kcal/mol): 0.37

EDG-MED-90036822-19_2



CID: EDG-MED-90036822-19_2

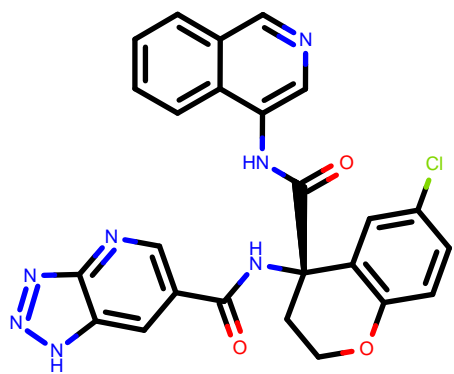
SMILES: Cn1ccnc1[C@@H](C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F

RUN: RUN1568

DDG (kcal/mol): -3.95

dDDG (kcal/mol): 0.24

EN300-124555_1_1_1



CID: EN300-124555_1_1_1

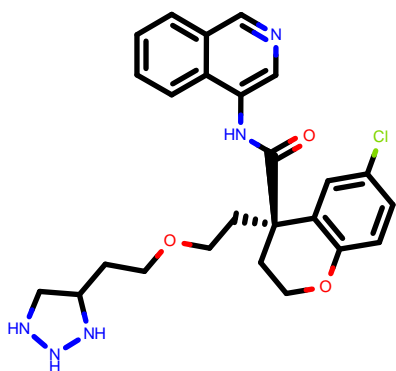
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(nc5)[nH]n6

RUN: RUN2829

DDG (kcal/mol): -3.94

dDDG (kcal/mol): 0.22

EN300-222357_3_1_1



CID: EN300-222357_3_1_1

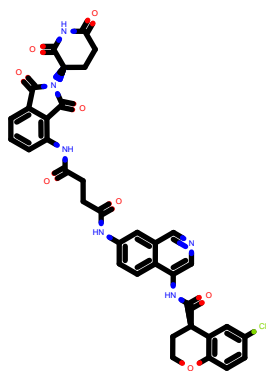
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5cn[nH]n5

RUN: RUN2719

DDG (kcal/mol): -3.93

dDDG (kcal/mol): 0.27

DAR-DIA-9e4459de-15_4



CID: DAR-DIA-9e4459de-15_4

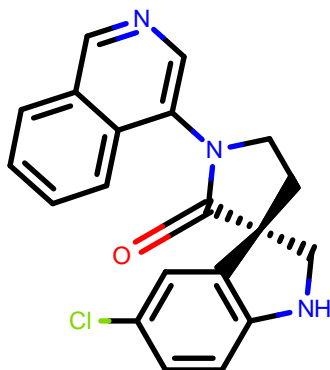
SMILES: c1cc2c(c1)NC(=O)CCCl=O)Nc3ccc4c(c3)ncnc4NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C1c[nH]c2O[C@@]3H7CCCl=O)NC7=O)O

RUN: RUN1321

DDG (kcal/mol): -3.93

dDDG (kcal/mol): 0.36

DAR-DIA-6be260fc-1_1



CID: DAR-DIA-6be260fc-1_1

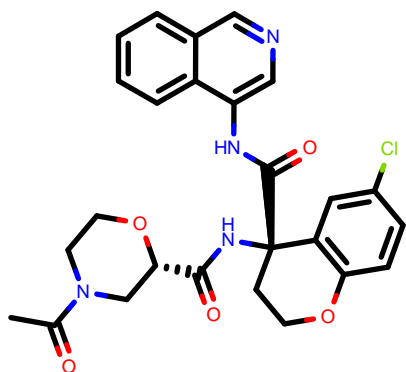
SMILES: c1ccc2c(c1)ncnc2N3CC[C@@]4(C3=O)CNc5c4cc(cc5)Cl

RUN: RUN1932

DDG (kcal/mol): -3.91

dDDG (kcal/mol): 0.27

EN300-100689_1_1_1



CID: EN300-100689_1_1_1

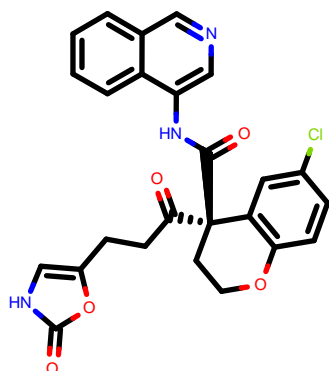
SMILES: CC(=O)N1CCO[C@@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN2763

DDG (kcal/mol): -3.90

dDDG (kcal/mol): 0.25

VLA-UCB-34f3ed0c-9_1



CID: VLA-UCB-34f3ed0c-9_1

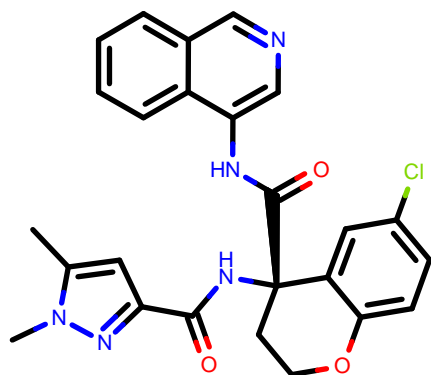
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5

RUN: RUN597

DDG (kcal/mol): -3.89

dDDG (kcal/mol): 0.20

EN300-1600312_1_1_1



CID: EN300-1600312_1_1_1

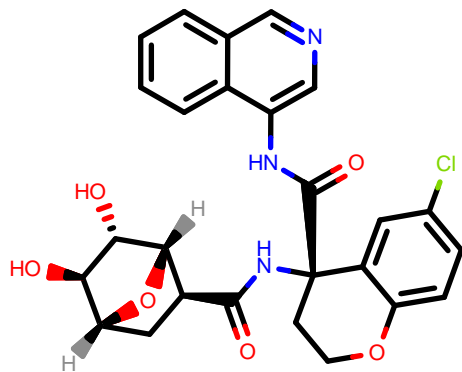
SMILES: Cc1cc(nn1C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN2698

DDG (kcal/mol): -3.88

dDDG (kcal/mol): 0.24

EN300-6764836_1_4_1



CID: EN300-6764836_1_4_1

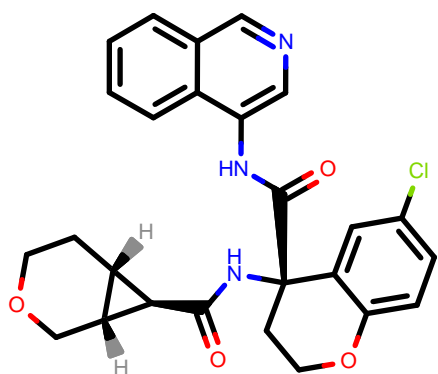
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5(C)C(O)C(O)C5

RUN: RUN4714

DDG (kcal/mol): -3.87

dDDG (kcal/mol): 0.28

EN300-1644723_1_5_1



CID: EN300-1644723_1_5_1

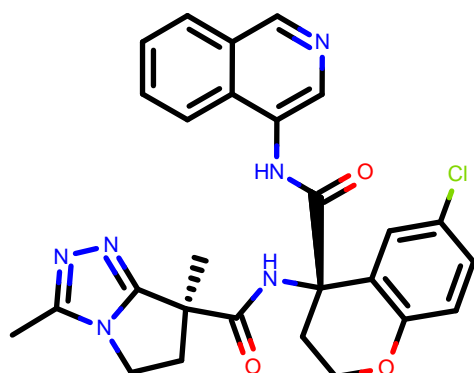
SMILES: c1ccc2c(c1)nnc2NC(=O)C@@3(C)CCOC4C3C(C4)C(NC(=O)C@@H5[C@@H]6CCCC6

RUN: RUN2832

DDG (kcal/mol): -3.87

dDDG (kcal/mol): 0.22

EN300-7431629_1_2_1



CID: EN300-7431629_1_2_1

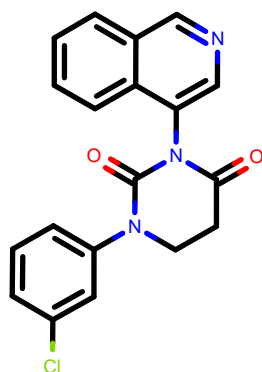
SMILES: Cc1nc2n1CC[C@@2](C)C(=O)N[C@@3](C)COC4C3C(C4)C(=O)Nc5ccc6c5ccc6

RUN: RUN2803

DDG (kcal/mol): -3.86

dDDG (kcal/mol): 0.34

VLA-UCB-1dbca3b4-13_1



CID: VLA-UCB-1dbca3b4-13_1

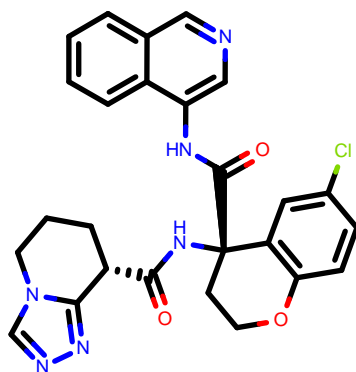
SMILES: c1ccc2c(c1)cncc2N3C(=O)CCN(C3=O)c4cccc(c4)Cl

RUN: RUN77

DDG (kcal/mol): -3.85

dDDG (kcal/mol): 0.34

EN300-748981_1_2_1



CID: EN300-748981_1_2_1

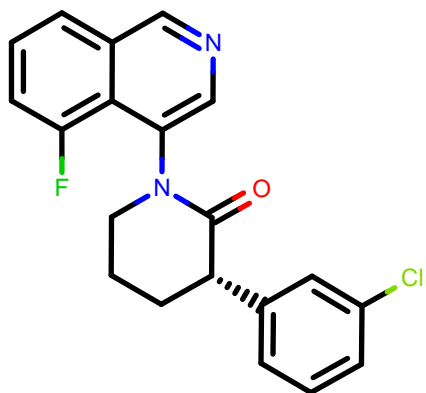
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(C)COC4C3C(C4)C(NC(=O)C@@H5[C@@H]6CCCC6

RUN: RUN2733

DDG (kcal/mol): -3.82

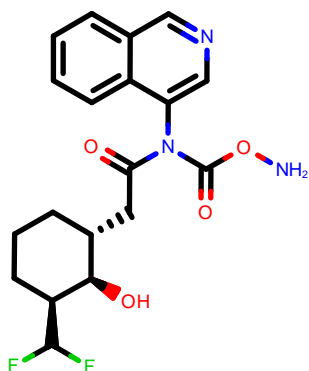
dDDG (kcal/mol): 0.35

MIC-UNK-50cce87d-9_1



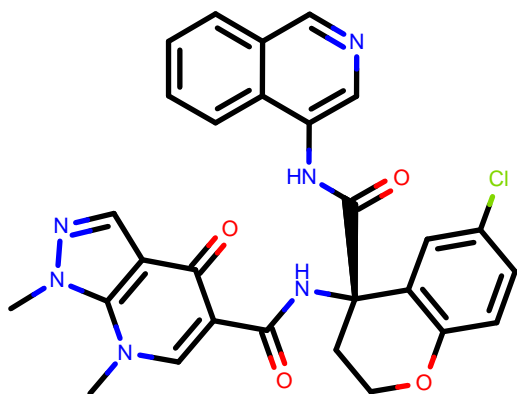
CID:	MIC-UNK-50cce87d-9_1
SMILES:	<chem>c1cc(cc(c1)Cl)[C@@H]2CCCN(C2=O)c3cncc4c3c(ccc4)F</chem>
RUN:	RUN547
DDG (kcal/mol):	-3.81
dDDG (kcal/mol):	0.27

MAK-UNK-c749d764-29_2



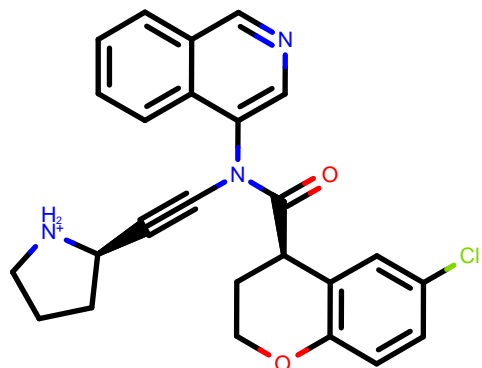
CID:	MAK-UNK-c749d764-29_2
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)C[C@@H]3CC[C@@H](C[C@@H]3O)C(F)F)C(=O)ON</chem>
RUN:	RUN1093
DDG (kcal/mol):	-3.81
dDDG (kcal/mol):	0.26

EN300-128324_1_1_1



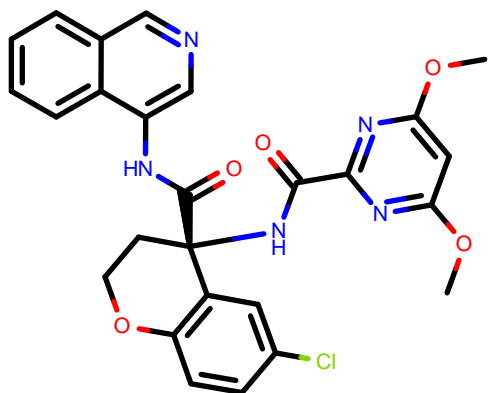
CID:	EN300-128324_1_1_1
SMILES:	<chem>Cn1cc(c(O)c2c1n(nc2)C(=O)N(C)[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5ccc6</chem>
RUN:	RUN2935
DDG (kcal/mol):	-3.80
dDDG (kcal/mol):	0.30

DAR-DIA-5ff57136-12_2_1



CID:	DAR-DIA-5ff57136-12_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#C[C@@H]3CC[C@H](N3)C(=O)C[C@@H]4CCOC5c4cc(cc5)Cl</chem>
RUN:	RUN2946
DDG (kcal/mol):	-3.79
dDDG (kcal/mol):	0.19

EN300-393341_1_1_1



CID: EN300-393341_1_1_1

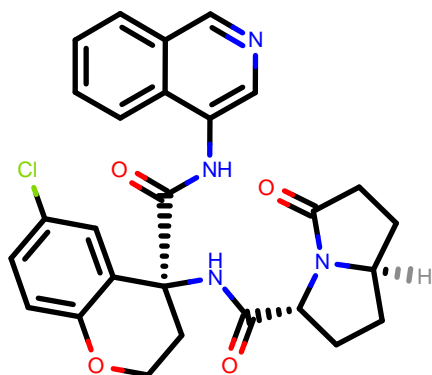
SMILES: COc1cc(nc(n1)C(=O)N[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5)OC

RUN: RUN4559

DDG (kcal/mol): -3.79

dDDG (kcal/mol): 0.25

EN300-6479181_1_4_1



CID: EN300-6479181_1_4_1

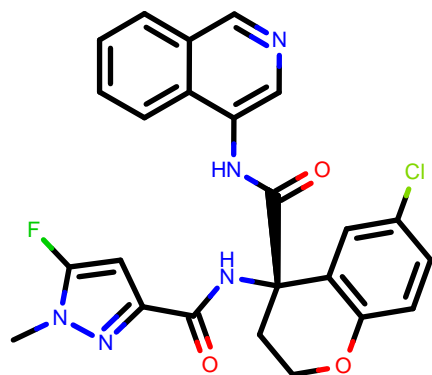
SMILES: c1ccc2c(c1)ncoc2N(c1=O)[C@@]3(C)CCOC4c3cc(cc4)N(c1=O)C@H5CC[C@@H]6NSC[C@O]C6

RUN: RUN2723

DDG (kcal/mol): -3.78

dDDG (kcal/mol): 0.41

EN300-243465_1_1_1



CID: EN300-243465_1_1_1

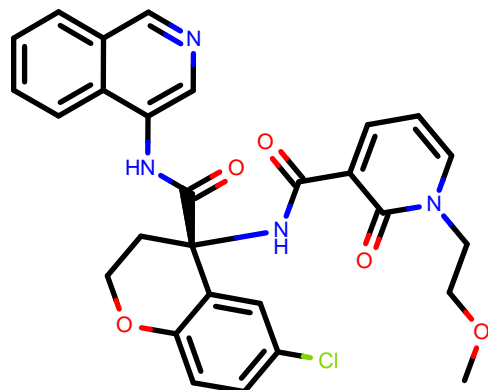
SMILES: Cn1c(cc(n1)C(=O)N[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5)F

RUN: RUN2753

DDG (kcal/mol): -3.77

dDDG (kcal/mol): 0.21

EN300-685077_1_1_1



CID: EN300-685077_1_1_1

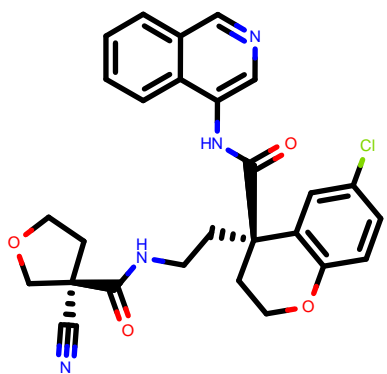
SMILES: COCc1cccc(c1=O)C(=O)N[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5

RUN: RUN2877

DDG (kcal/mol): -3.75

dDDG (kcal/mol): 0.32

EN300-261210_3_1_1



CID: EN300-261210_3_1_1

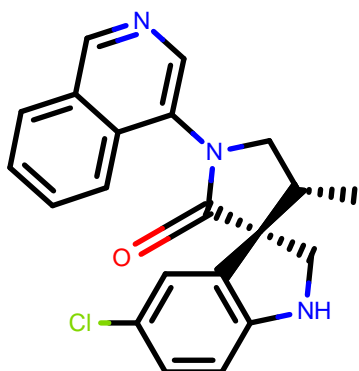
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN4146

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.32

DAR-DIA-6be260fc-3_1



CID: DAR-DIA-6be260fc-3_1

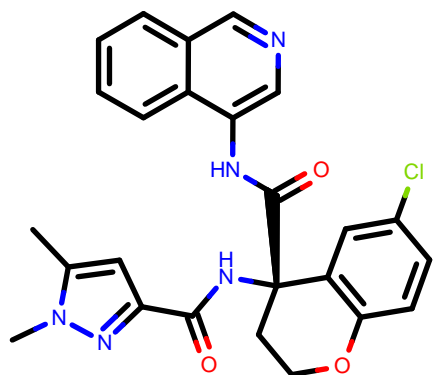
SMILES: C[C@H]1CN(C(=O)[C@@]2[C@@]12CNc3c2cc(cc3)C)c4cncc5c4cccc5

RUN: RUN1934

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.34

EN300-1600312_1_1_1



CID: EN300-1600312_1_1_1

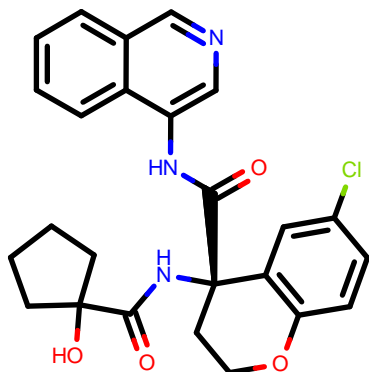
SMILES: Cc1cc(nn1C)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN2677

DDG (kcal/mol): -3.73

dDDG (kcal/mol): 0.23

EN300-25960_1_1_1



CID: EN300-25960_1_1_1

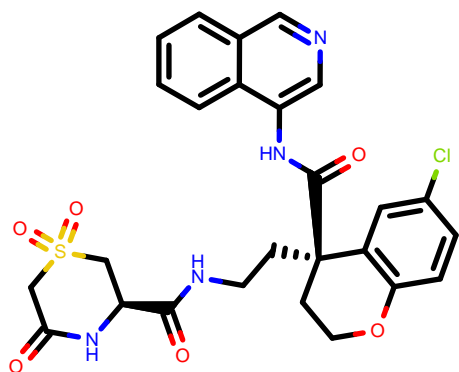
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCCC5)O

RUN: RUN3171

DDG (kcal/mol): -3.73

dDDG (kcal/mol): 0.36

EN300-702756_3_1_1



CID: EN300-702756_3_1_1

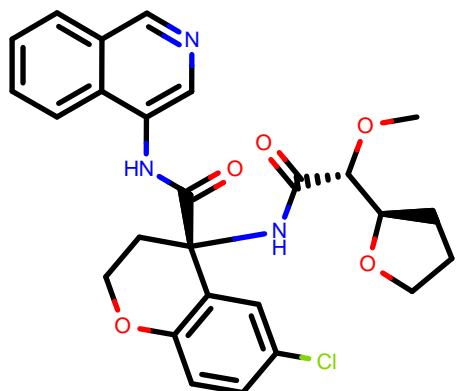
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOc4c3ccc4O)CNC(=O)C@@H5CS(=O)(=O)CC1=O)NS

RUN: RUN4313

DDG (kcal/mol): -3.72

dDDG (kcal/mol): 0.21

EN300-6277108_1_4_1



CID: EN300-6277108_1_4_1

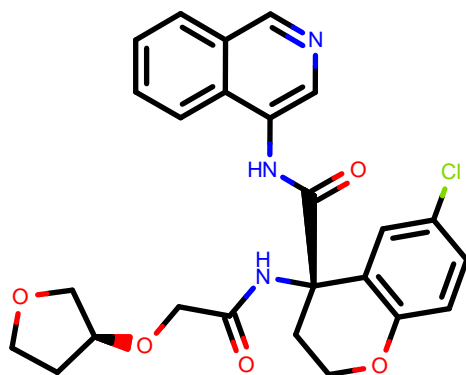
SMILES: CO[C@H]([C@H]1CCO1)C(=O)N(C@@2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3230

DDG (kcal/mol): -3.71

dDDG (kcal/mol): 0.25

EN300-99391_1_2_1



CID: EN300-99391_1_2_1

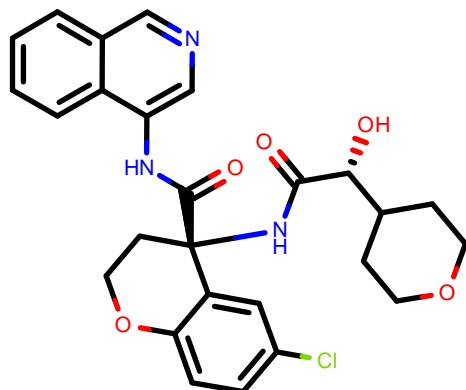
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOc4c3ccc(cc4)C)NC(=O)CO[C@H]5CCOC5

RUN: RUN2870

DDG (kcal/mol): -3.68

dDDG (kcal/mol): 0.21

EN300-79180_1_1_1



CID: EN300-79180_1_1_1

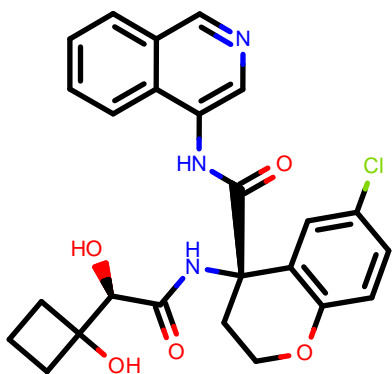
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOc4c3ccc(cc4)C)NC(=O)C@@H]C5CCOCC5)O

RUN: RUN3187

DDG (kcal/mol): -3.67

dDDG (kcal/mol): 0.27

EDJ-MED-6864a934-10_1



CID: EDJ-MED-6864a934-10_1

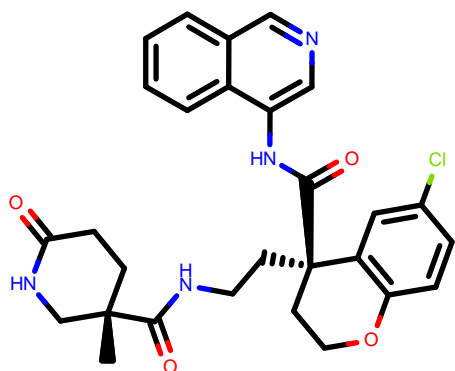
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN2454

DDG (kcal/mol): -3.67

dDDG (kcal/mol): 0.25

EN300-195924_3_1_1



CID: EN300-195924_3_1_1

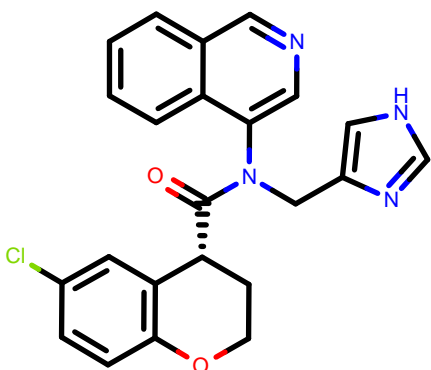
SMILES: C[C@@]1(CCC(=O)NC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4401

DDG (kcal/mol): -3.66

dDDG (kcal/mol): 0.29

ALP-UNI-44c99a80-2_1_1



CID: ALP-UNI-44c99a80-2_1_1

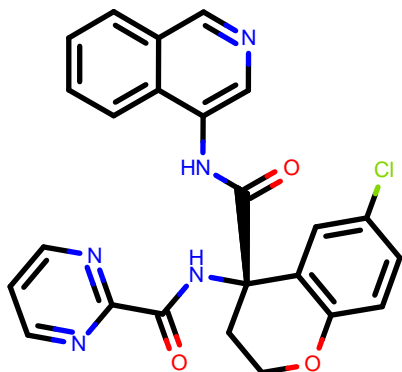
SMILES: c1ccc2c(c1)cncc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN: RUN2949

DDG (kcal/mol): -3.66

dDDG (kcal/mol): 0.19

EN300-80230_1_1_1



CID: EN300-80230_1_1_1

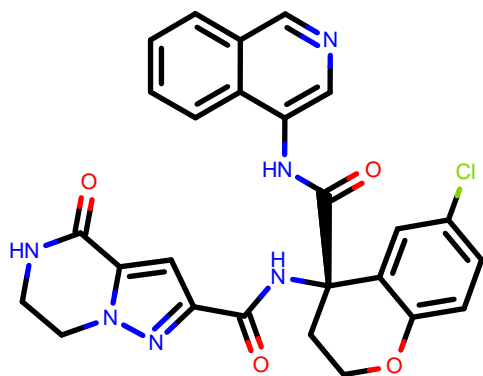
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccc5

RUN: RUN3124

DDG (kcal/mol): -3.65

dDDG (kcal/mol): 0.20

EN300-200426_1_1_1



CID: EN300-200426_1_1_1

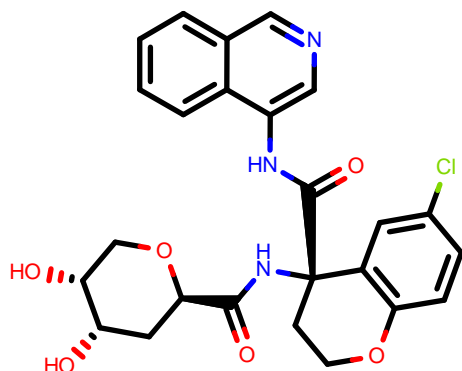
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCNC6=O

RUN: RUN2796

DDG (kcal/mol): -3.64

dDDG (kcal/mol): 0.20

EN300-7352736_1_1_1



CID: EN300-7352736_1_1_1

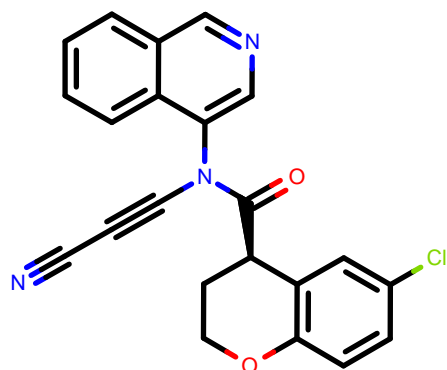
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H](O)[C@H](O)CO5

RUN: RUN2862

DDG (kcal/mol): -3.64

dDDG (kcal/mol): 0.29

DAR-DIA-5ff57136-10_1_1



CID: DAR-DIA-5ff57136-10_1_1

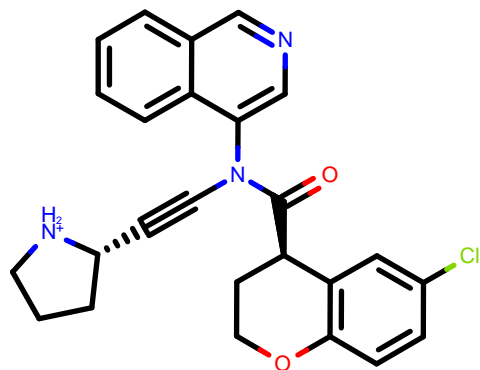
SMILES: c1ccc2c(c1)cncc2N(C#CC#N)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN2801

DDG (kcal/mol): -3.64

dDDG (kcal/mol): 0.13

DAR-DIA-5ff57136-12_1



CID: DAR-DIA-5ff57136-12_1

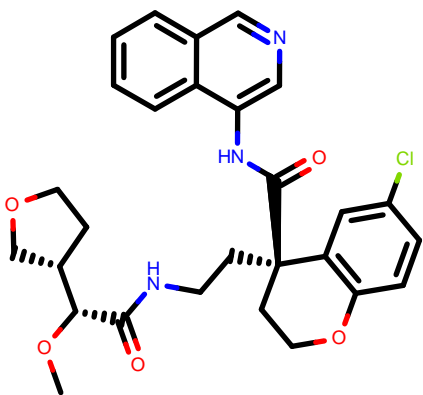
SMILES: c1ccc2c(c1)cncc2N(C#C[C@@H]3CC[C@H](N3)C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)

RUN: RUN1270

DDG (kcal/mol): -3.63

dDDG (kcal/mol): 0.20

EN300-298552_3_4_1



CID: EN300-298552_3_4_1

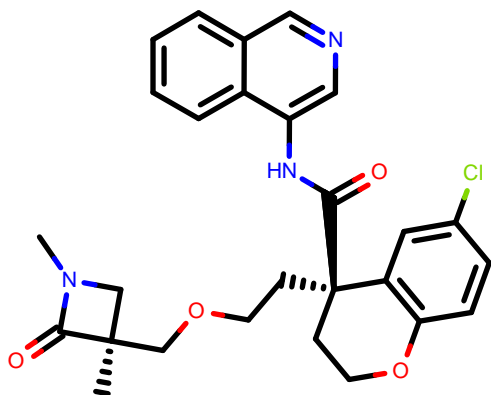
SMILES: CO[C@H]([C@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5290

DDG (kcal/mol): -3.63

dDDG (kcal/mol): 0.23

EN300-1273362_3_2_1



CID: EN300-1273362_3_2_1

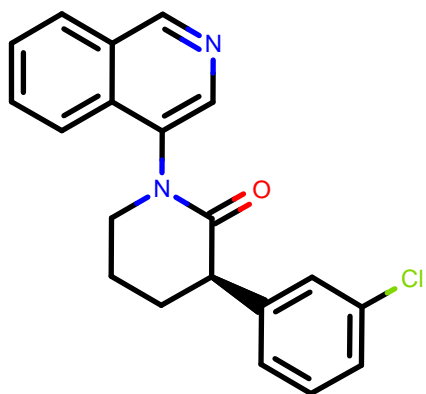
SMILES: C[C@]1(CN(C1=O)C)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2779

DDG (kcal/mol): -3.62

dDDG (kcal/mol): 0.37

PET-UNK-c9c1e0d8-3_1



CID: PET-UNK-c9c1e0d8-3_1

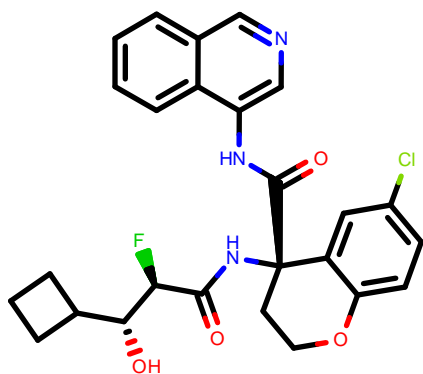
SMILES: c1ccc2c(c1)cncc2N3CCCC[C@]([C@H]3C=O)c4cccc(c4)Cl

RUN: RUN35

DDG (kcal/mol): -3.62

dDDG (kcal/mol): 0.17

EDG-MED-90036822-99_1



CID: EDG-MED-90036822-99_1

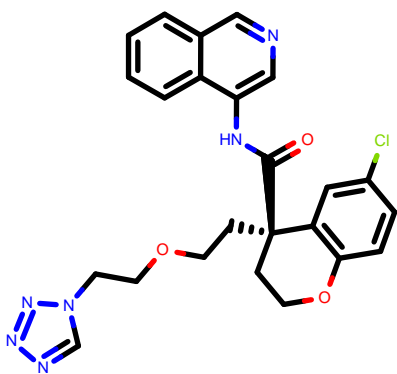
SMILES: c1ccc2c(c1)cncc2N[C@@]([C@]3([C@@H]4CC[C@]4)C)C(=O)N[C@@]([C@]5([C@@H]6C5CCO6)O)F

RUN: RUN1705

DDG (kcal/mol): -3.61

dDDG (kcal/mol): 0.27

EN300-364679_3_1_1



CID: EN300-364679_3_1_1

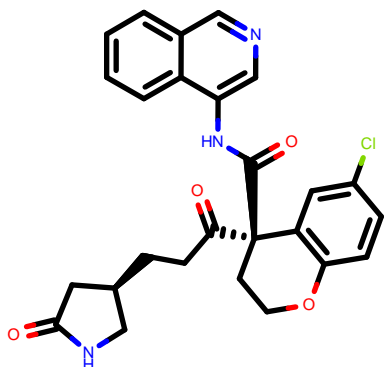
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnnn5

RUN: RUN2878

DDG (kcal/mol): -3.61

dDDG (kcal/mol): 0.29

VLA-UCB-34f3ed0c-21_1



CID: VLA-UCB-34f3ed0c-21_1

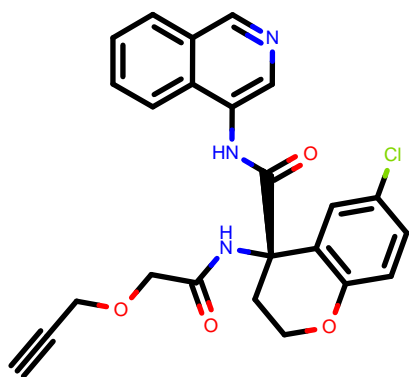
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@]4H5CC(=O)N45

RUN: RUN589

DDG (kcal/mol): -3.60

dDDG (kcal/mol): 0.35

EN300-106432_1_1_1



CID: EN300-106432_1_1_1

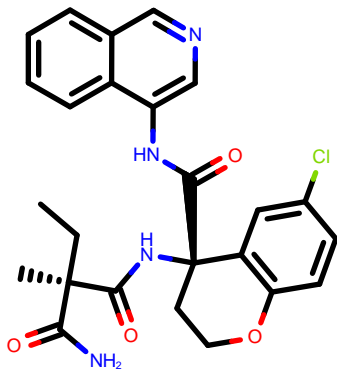
SMILES: C#CCOCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4022

DDG (kcal/mol): -3.60

dDDG (kcal/mol): 0.19

EN300-2908024_1_2_1



CID: EN300-2908024_1_2_1

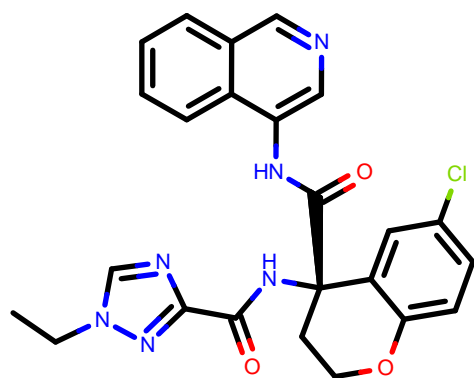
SMILES: CC[C@@]1(C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3388

DDG (kcal/mol): -3.59

dDDG (kcal/mol): 0.31

EN300-1719160_1_1_1



CID: EN300-1719160_1_1_1

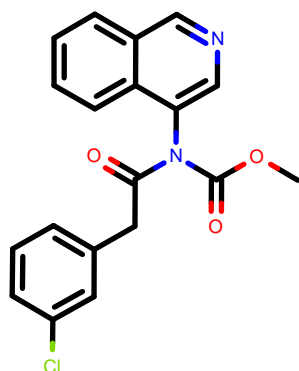
SMILES: CCn1cnc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2826

DDG (kcal/mol): -3.58

dDDG (kcal/mol): 0.23

PET-UNK-12d8d43f-2_1



CID: PET-UNK-12d8d43f-2_1

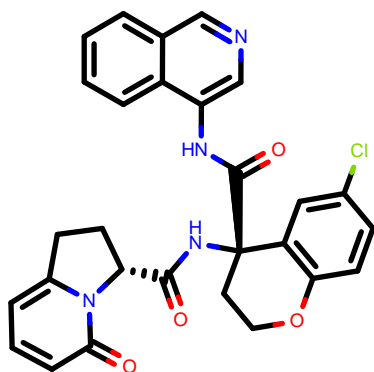
SMILES: COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl

RUN: RUN1313

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.26

EN300-332002_1_2_1



CID: EN300-332002_1_2_1

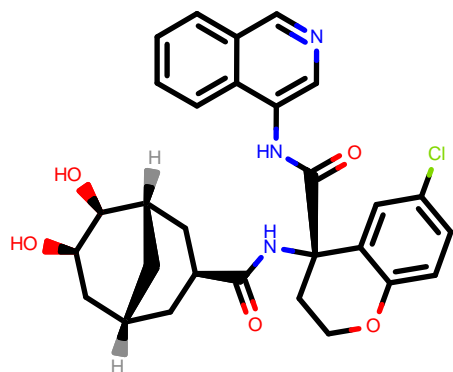
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCc6n5c(=O)ccc6

RUN: RUN2761

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.33

EN300-6487755_1_1_1



CID: EN300-6487755_1_1_1

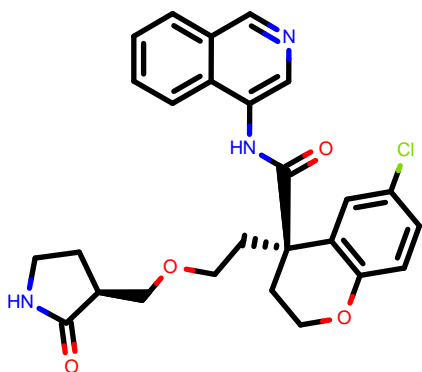
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@@H](C)C[C@@H]6[C@H](C5)C[C@@H]6CO

RUN: RUN3399

DDG (kcal/mol): -3.56

dDDG (kcal/mol): 0.29

EN300-246248_3_1_1



CID: EN300-246248_3_1_1

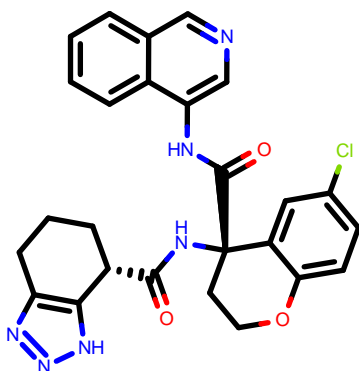
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN3701

DDG (kcal/mol): -3.55

dDDG (kcal/mol): 0.23

EDJ-MED-6864a934-6_1



CID: EDJ-MED-6864a934-6_1

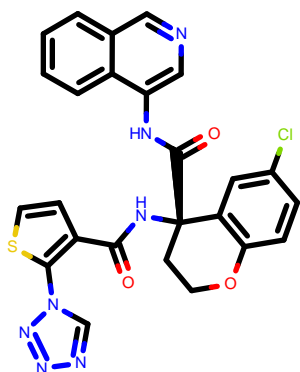
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCc6c5n[nH]n6

RUN: RUN2440

DDG (kcal/mol): -3.55

dDDG (kcal/mol): 0.31

EN300-6744029_1_1_1



CID: EN300-6744029_1_1_1

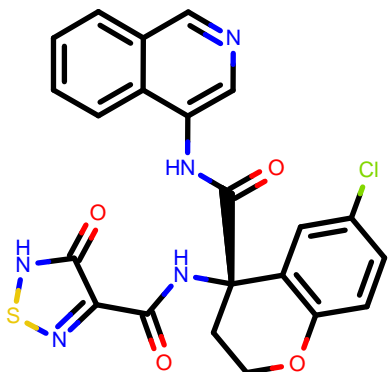
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)NC(=O)c5ccsc5n6nnn6

RUN: RUN2735

DDG (kcal/mol): -3.54

dDDG (kcal/mol): 0.26

EN300-261859_1_1_1



CID: EN300-261859_1_1_1

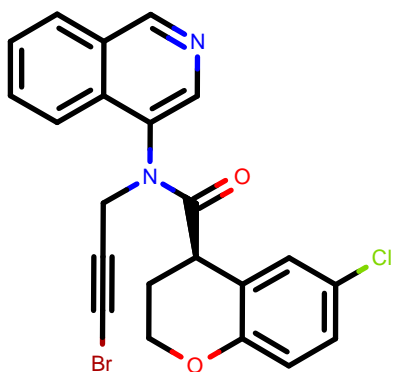
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)NC(=O)c5c(-O)[nH]s5

RUN: RUN2804

DDG (kcal/mol): -3.53

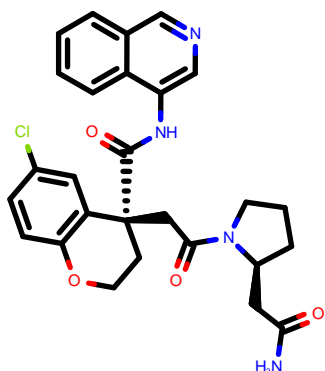
dDDG (kcal/mol): 0.20

DAR-DIA-5ff57136-17_1



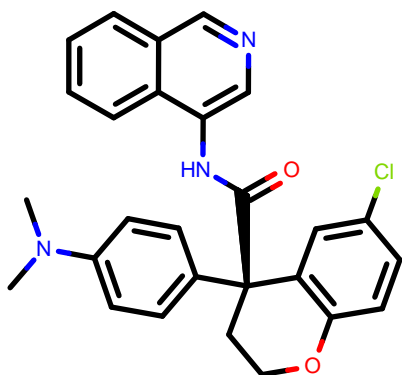
CID:	DAR-DIA-5ff57136-17_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(CC#CBr)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl</chem>
RUN:	RUN1248
DDG (kcal/mol):	-3.53
dDDG (kcal/mol):	0.17

EN300-124652_1_2_1



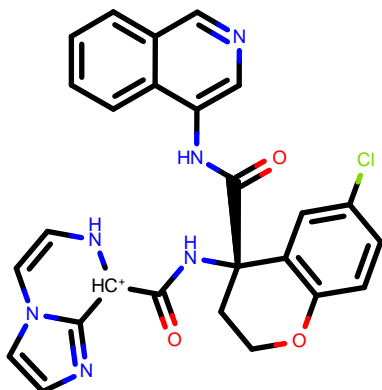
CID:	EN300-124652_1_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4ccc(cc4)Cl)CC(=O)N5CCCC[C@H]5CC(=O)N</chem>
RUN:	RUN6717
DDG (kcal/mol):	-3.53
dDDG (kcal/mol):	0.20

VLA-UCB-551c2366-1_1_1



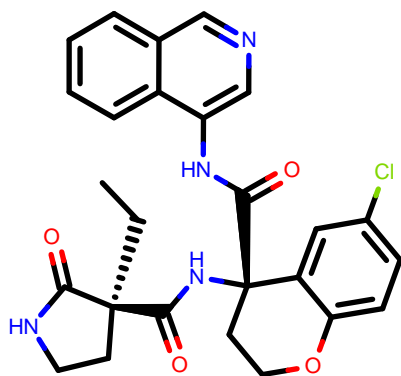
CID:	VLA-UCB-551c2366-1_1_1
SMILES:	<chem>CN(C)c1ccc(cc1)[C@@H]2(CCOc3ccc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN2982
DDG (kcal/mol):	-3.52
dDDG (kcal/mol):	0.21

EDJ-MED-6864a934-4_1



CID:	EDJ-MED-6864a934-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4ccc(cc4)Cl)NC(=O)c5c6nccn6ccn5</chem>
RUN:	RUN2448
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.24

EN300-304135_1_1_1



CID: EN300-304135_1_1_1

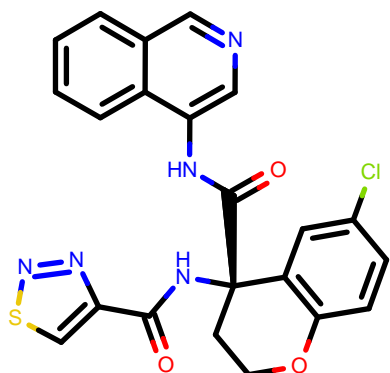
SMILES: CC[C@@]1(CCN1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN2985

DDG (kcal/mol): -3.49

dDDG (kcal/mol): 0.31

EN300-24297_1_1_1



CID: EN300-24297_1_1_1

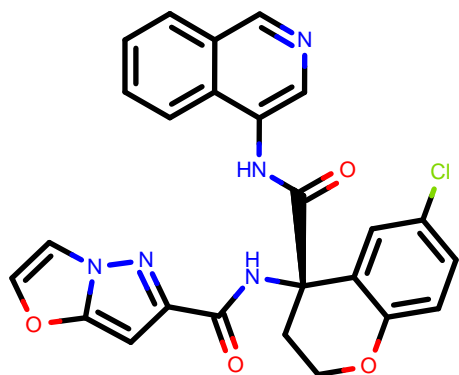
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)c5csnn5)

RUN: RUN2795

DDG (kcal/mol): -3.49

dDDG (kcal/mol): 0.18

EDJ-MED-6864a934-2_1



CID: EDJ-MED-6864a934-2_1

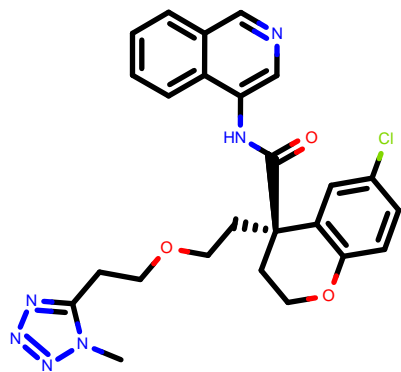
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)c5cc6n(n5)CCO6)

RUN: RUN2429

DDG (kcal/mol): -3.47

dDDG (kcal/mol): 0.19

EN300-365398_3_1_1



CID: EN300-365398_3_1_1

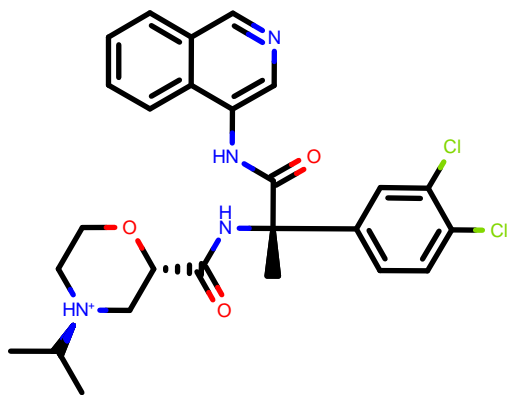
SMILES: Cn1c(nnn1)CCOCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2792

DDG (kcal/mol): -3.47

dDDG (kcal/mol): 0.25

MAT-POS-e9e99895-2_2



CID: MAT-POS-e9e99895-2_2

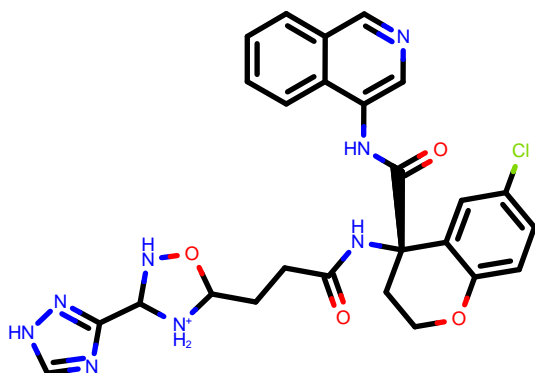
SMILES: CC(C)[N@H]1CCOC(C@H)(C1C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN2124

DDG (kcal/mol): -3.47

dDDG (kcal/mol): 0.26

EN300-61140_1_1_1



CID: EN300-61140_1_1_1

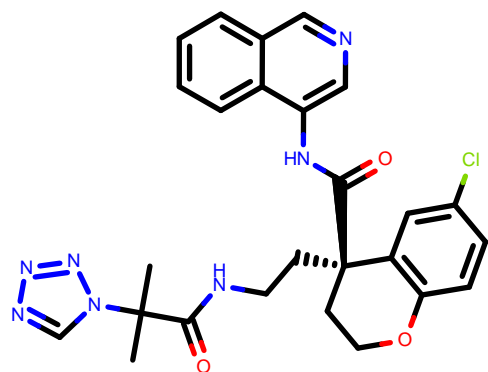
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5nc(n5)c6[nH]n6

RUN: RUN4161

DDG (kcal/mol): -3.47

dDDG (kcal/mol): 0.26

EN300-1248064_3_1_1



CID: EN300-1248064_3_1_1

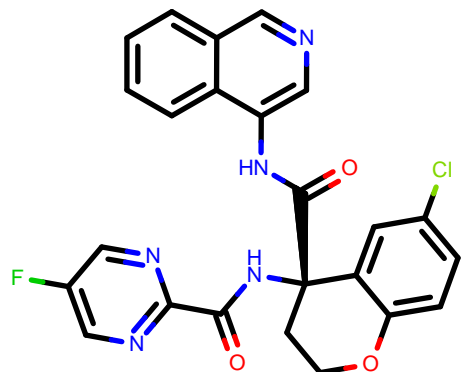
SMILES: CC(C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)Cl)NC(=O)Nc3ncc4c3ccc4[nH]5nn5

RUN: RUN2988

DDG (kcal/mol): -3.46

dDDG (kcal/mol): 0.31

EN300-149296_1_1_1



CID: EN300-149296_1_1_1

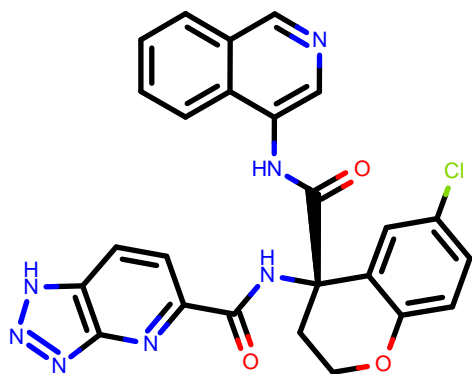
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncc(cn5)F

RUN: RUN2857

DDG (kcal/mol): -3.45

dDDG (kcal/mol): 0.18

EN300-133058_1_1_1



CID: EN300-133058_1_1_1

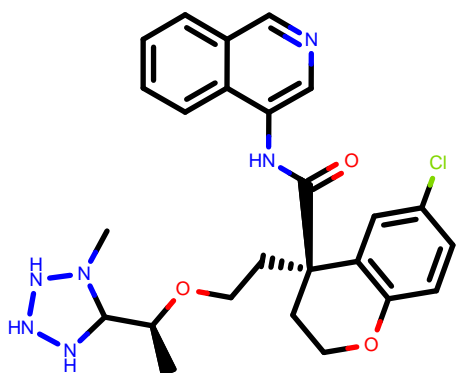
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc6c(n5)n[nH]6

RUN: RUN2918

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.21

EN300-173006_3_1_1



CID: EN300-173006_3_1_1

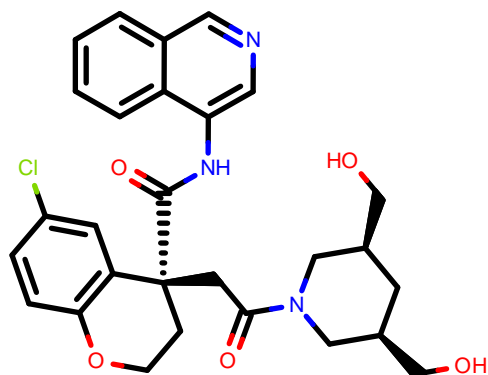
SMILES: C[C@@H](c1nnn1C)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3655

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.24

EN300-2007627_1_1_1



CID: EN300-2007627_1_1_1

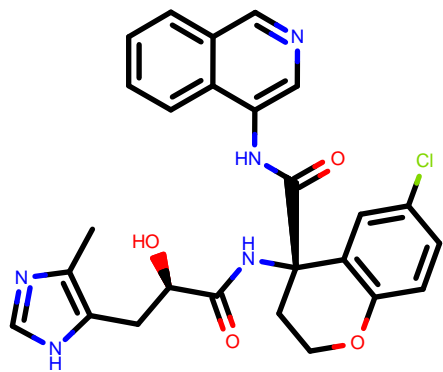
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5C[C@@H](C)C[C@@H](C5)CO

RUN: RUN3253

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.34

EN300-7494324_1_2_1



CID: EN300-7494324_1_2_1

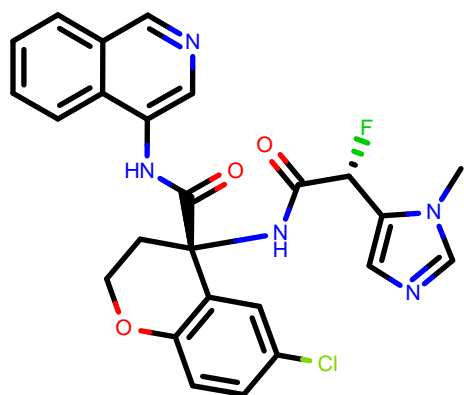
SMILES: Cc1c(nc[nH]1)C[C@@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN4567

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.25

EDG-MED-90036822-26_2



CID: EDG-MED-90036822-26_2

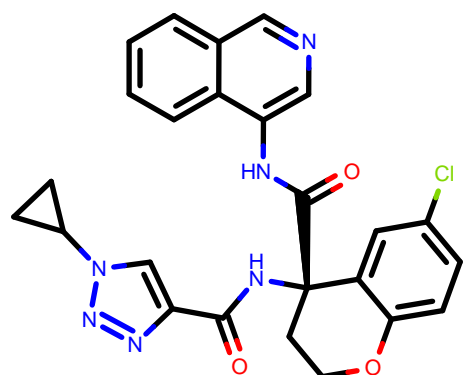
SMILES: Cn1ccc1[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)F

RUN: RUN1582

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.24

EN300-210110_1_1_1



CID: EN300-210110_1_1_1

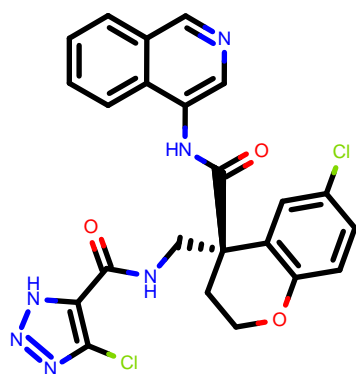
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nc5)C6CC6

RUN: RUN5972

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.23

EN300-149013_2_1_1



CID: EN300-149013_2_1_1

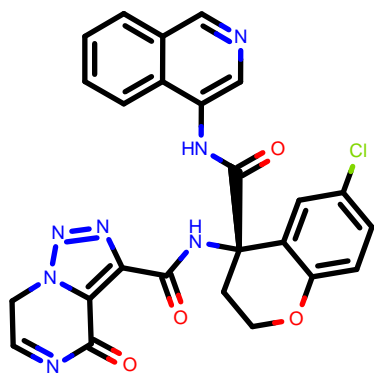
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(n[nH]n5)Cl

RUN: RUN3099

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.23

EN300-176023_1_1_1



CID: EN300-176023_1_1_1

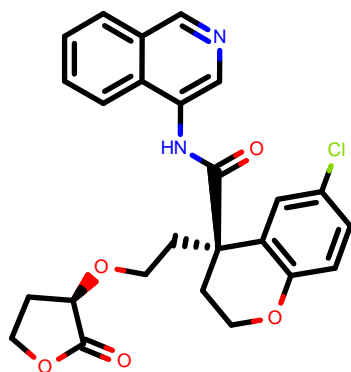
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6n(nc5)CCNC6=O

RUN: RUN2788

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.24

EN300-20496_3_1_1



CID: EN300-20496_3_1_1

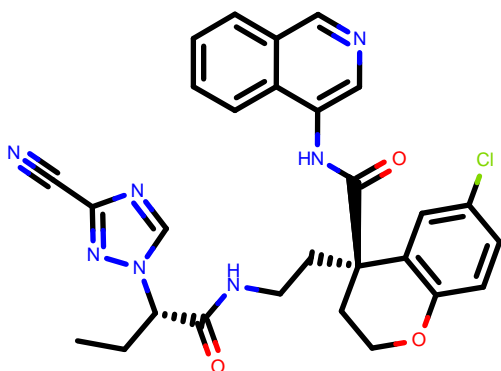
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCOC5=O

RUN: RUN2834

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.22

EN300-245264_3_1_1



CID: EN300-245264_3_1_1

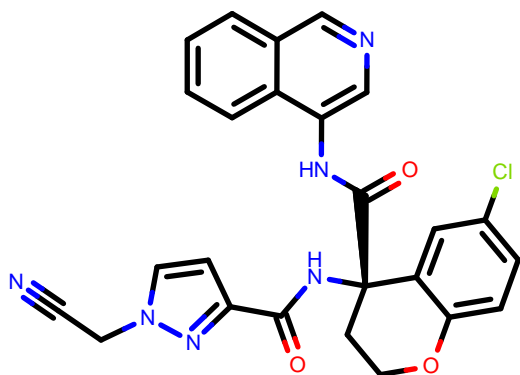
SMILES: CC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4)n5nc(n5)C#N

RUN: RUN4065

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.34

EN300-1251424_1_1_1



CID: EN300-1251424_1_1_1

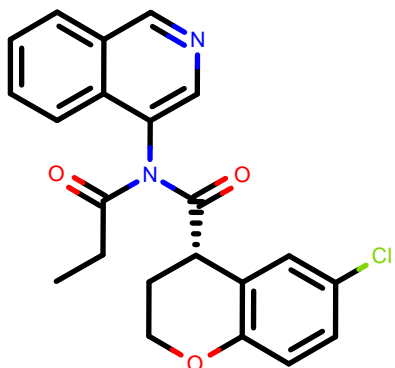
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(c5)C#N

RUN: RUN2711

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.25

VLA-UCB-05e51b3f-10_1



CID: VLA-UCB-05e51b3f-10_1

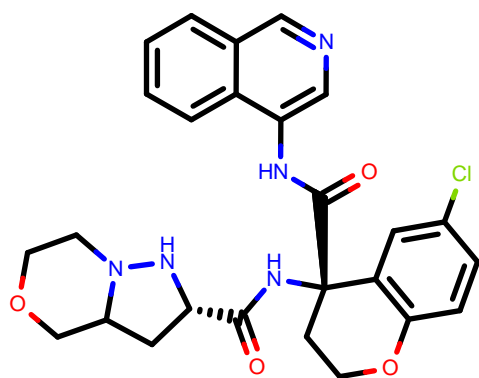
SMILES: C=CC(=O)N(c1ncnc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN260

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.34

EN300-244278_1_1_1



CID: EN300-244278_1_1_1

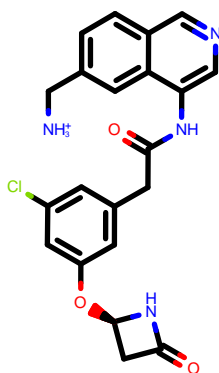
SMILES: c1ccc2(c1)ncnc2NC(=O)C@3[C@@H](COC4C3cc(c4)C)NC(=O)C@H5[C@@H]5C=C6COC6N@7[8]9

RUN: RUN2961

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.34

ALF-EVA-0b412456-5_1



CID: ALF-EVA-0b412456-5_1

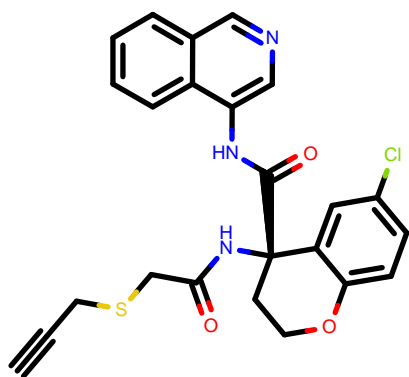
SMILES: c1cc2cnc(c2cc1C[NH3+])NC(=O)Cc3ccc(cc3)C)O[C@@H]4CC(=O)N4

RUN: RUN2582

DDG (kcal/mol): -3.41

dDDG (kcal/mol): 0.59

EN300-86878_1_1_1



CID: EN300-86878_1_1_1

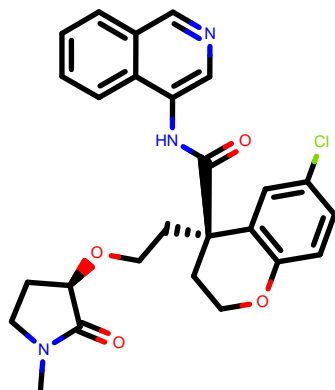
SMILES: C#CCSCC(=O)N[C@@]1(COC2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN2762

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.24

EN300-98648_3_2_1



CID: EN300-98648_3_2_1

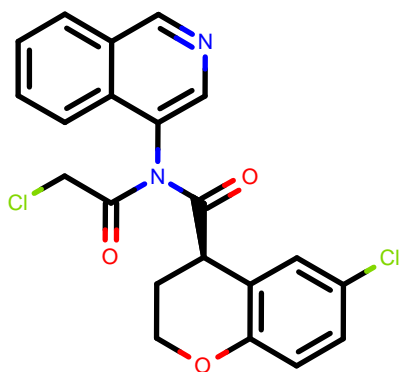
SMILES: CN1CC[C@H](C1=O)OCC[C@@]2(COC3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2844

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.28

VLA-UCB-50c39ae8-6_1



CID: VLA-UCB-50c39ae8-6_1

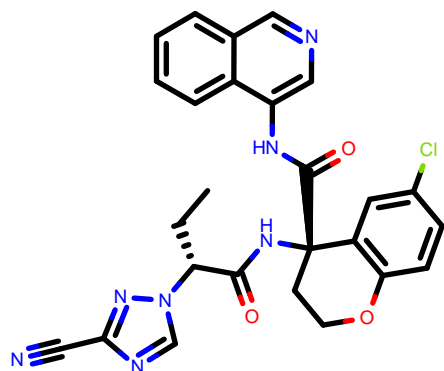
SMILES: c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN329

DDG (kcal/mol): -3.38

dDDG (kcal/mol): 0.21

EN300-245264_1_2_1



CID: EN300-245264_1_2_1

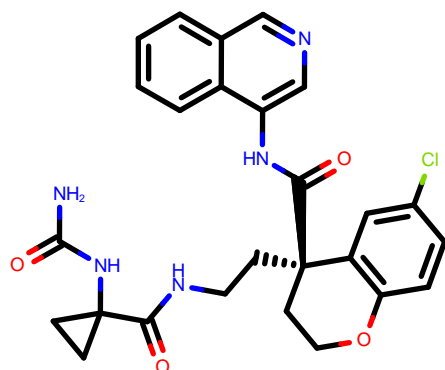
SMILES: CC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccc4)n5ncn(n5)C#N

RUN: RUN3233

DDG (kcal/mol): -3.38

dDDG (kcal/mol): 0.27

EN300-123614_3_1_1



CID: EN300-123614_3_1_1

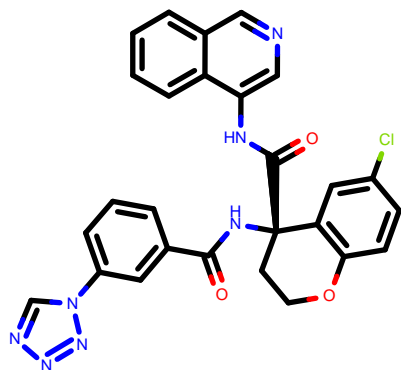
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(C)C5N(C)C(=O)N

RUN: RUN5741

DDG (kcal/mol): -3.37

dDDG (kcal/mol): 0.31

EN300-09239_1_1_1



CID: EN300-09239_1_1_1

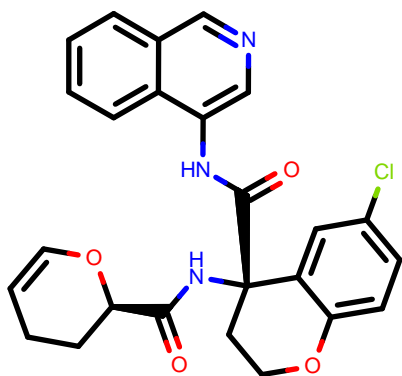
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(c5)n6cnnn6

RUN: RUN2899

DDG (kcal/mol): -3.37

dDDG (kcal/mol): 0.27

EN300-378044_1_2_1



CID: EN300-378044_1_2_1

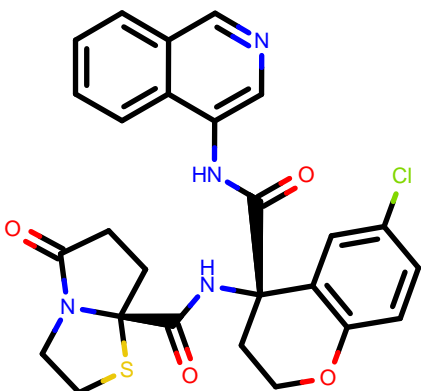
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC=CCO5

RUN: RUN3525

DDG (kcal/mol): -3.36

dDDG (kcal/mol): 0.24

EN300-10334_1_2_1



CID: EN300-10334_1_2_1

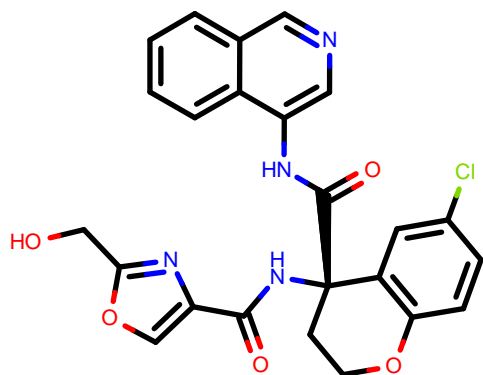
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@]56CCCC(=O)N5CCS6

RUN: RUN2728

DDG (kcal/mol): -3.35

dDDG (kcal/mol): 0.34

EN300-7549555_1_1_1



CID: EN300-7549555_1_1_1

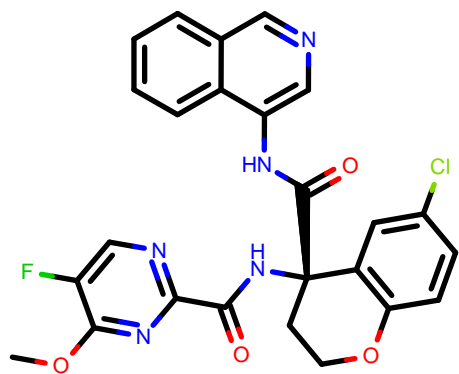
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5occn5CO

RUN: RUN3756

DDG (kcal/mol): -3.35

dDDG (kcal/mol): 0.18

EN300-1703711_1_1_1



CID: EN300-1703711_1_1_1

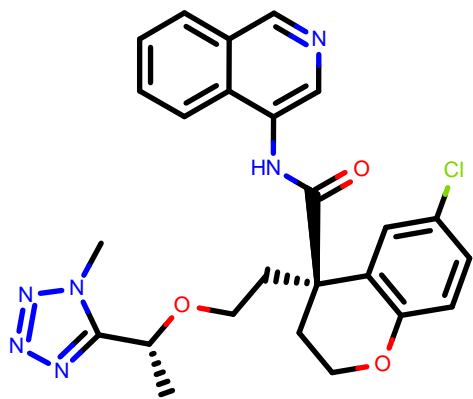
SMILES: COc1c(ncn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccoc5F

RUN: RUN2813

DDG (kcal/mol): -3.34

dDDG (kcal/mol): 0.23

EN300-173006_3_2_1



CID: EN300-173006_3_2_1

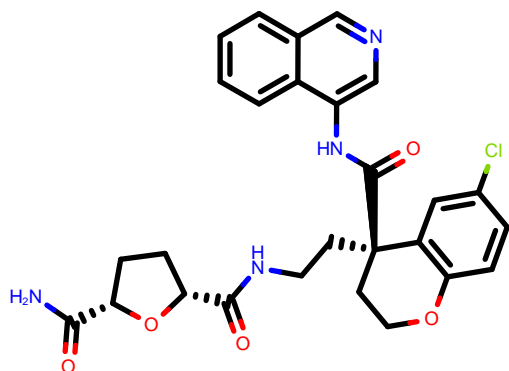
SMILES: C[C@@H](c1nnnn1C)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2855

DDG (kcal/mol): -3.34

dDDG (kcal/mol): 0.27

EN300-315238_3_1_1



CID: EN300-315238_3_1_1

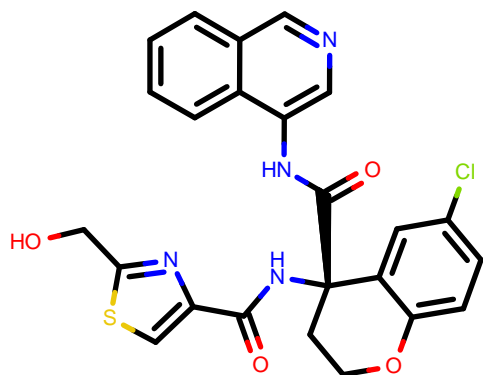
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[C@@H](O5)C(=O)N

RUN: RUN3079

DDG (kcal/mol): -3.34

dDDG (kcal/mol): 0.29

EN300-250112_1_1_1



CID: EN300-250112_1_1_1

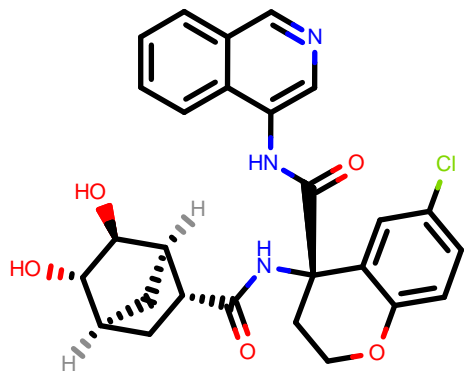
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5scn(n5)CO

RUN: RUN3289

DDG (kcal/mol): -3.32

dDDG (kcal/mol): 0.24

EN300-6744028_1_5_1



CID: EN300-6744028_1_5_1

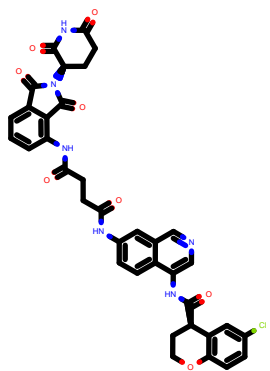
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H](O5)C(=O)N[C@@H]6C[C@@H](O)C6

RUN: RUN2872

DDG (kcal/mol): -3.32

dDDG (kcal/mol): 0.32

DAR-DIA-9e4459de-15_1



CID: DAR-DIA-9e4459de-15_1

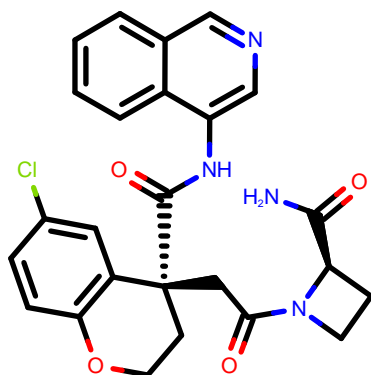
SMILES: c1cc2c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)nc4NC(=O)C(C)C(=O)Nc5cc6c5c(c6)C1=C(C)C(=O)Nc7c(c1)NC7=O

RUN: RUN1382

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.26

EN300-862094_1_1_1



CID: EN300-862094_1_1_1

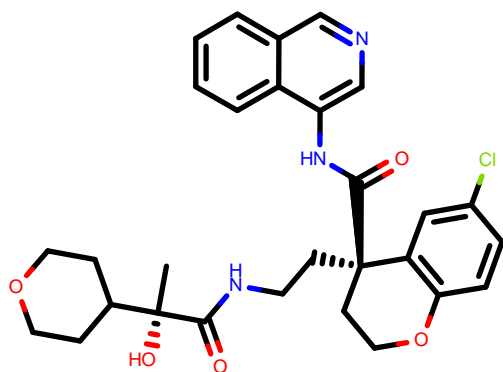
SMILES: c1ccc2c(c1)cncc2NC(=O)C(C)C(=O)Nc3cc4c3cc(cc4)C1CC(=O)N5CC(C)C@H5C1=O

RUN: RUN2836

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.26

EN300-217499_3_2_1



CID: EN300-217499_3_2_1

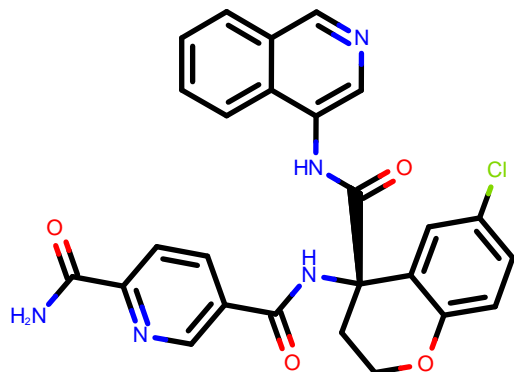
SMILES: C(C)C(=O)Nc1cc2c(c1)ncoc2C(=O)Nc3cc4c3cc(cc4)C1CC(=O)Nc5cc6c5c(c6)C1=C(C)C(=O)Nc7c(c1)NC7=O

RUN: RUN4777

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.44

EN300-58864_1_1_1



CID: EN300-58864_1_1_1

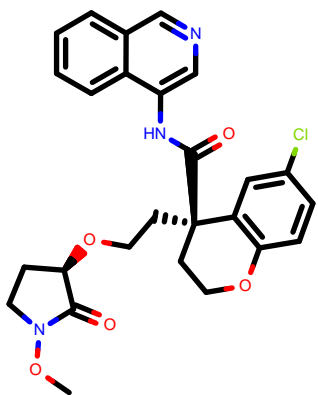
SMILES: c1ccc2c(c1)cncc2NC(=O)C(C)C(=O)Nc3cc4c3cc(cc4)C1CC(=O)Nc5cc6c5c(c6)C1=C(C)C(=O)Nc7c(c1)NC7=O

RUN: RUN2950

DDG (kcal/mol): -3.30

dDDG (kcal/mol): 0.27

EN300-302058_3_2_1



CID: EN300-302058_3_2_1

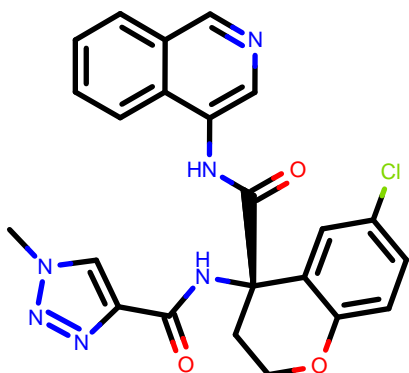
SMILES: CON1CC[C@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3418

DDG (kcal/mol): -3.30

dDDG (kcal/mol): 0.30

EN300-86357_1_1_1



CID: EN300-86357_1_1_1

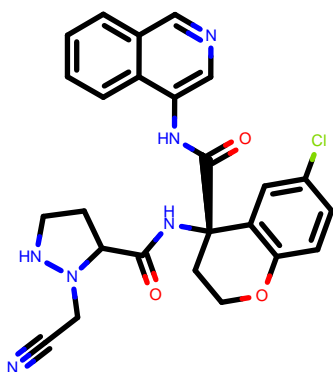
SMILES: Cn1cc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4674

DDG (kcal/mol): -3.30

dDDG (kcal/mol): 0.22

EN300-373791_1_1_1



CID: EN300-373791_1_1_1

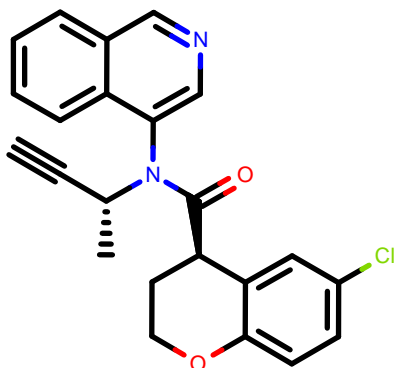
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C)C(=O)c5ccnn5C@H#N

RUN: RUN3483

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.27

DAR-DIA-5ff57136-16_2



CID: DAR-DIA-5ff57136-16_2

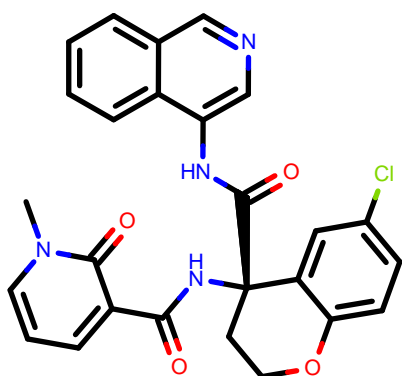
SMILES: C[C@H](C#C)N(c1ncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)C)C

RUN: RUN1231

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.13

EN300-69811_1_1_1



CID: EN300-69811_1_1_1

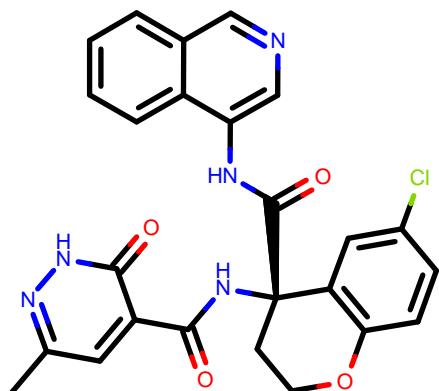
SMILES: Cn1cccc(c1=O)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3117

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.32

EN300-147499_1_1_1



CID: EN300-147499_1_1_1

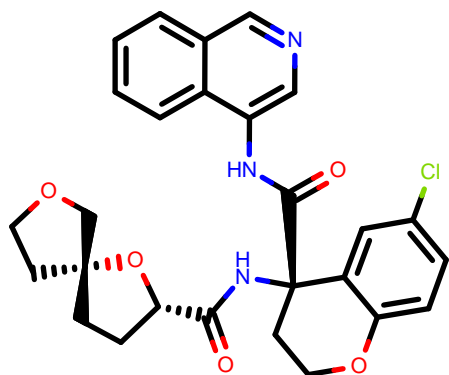
SMILES: Cc1cc(c(=O)[nH]n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2722

DDG (kcal/mol): -3.27

dDDG (kcal/mol): 0.26

EN300-3031933_1_1_1



CID: EN300-3031933_1_1_1

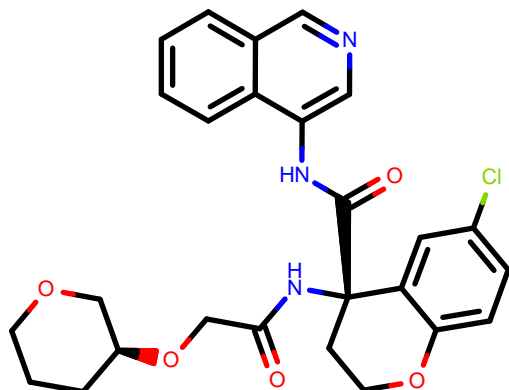
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(COC4c3cc(cc4)Cl)NC(=O)C@@H5CC[C@@]3(O)O5CCCC6

RUN: RUN2710

DDG (kcal/mol): -3.26

dDDG (kcal/mol): 0.34

EN300-1627945_1_2_1



CID: EN300-1627945_1_2_1

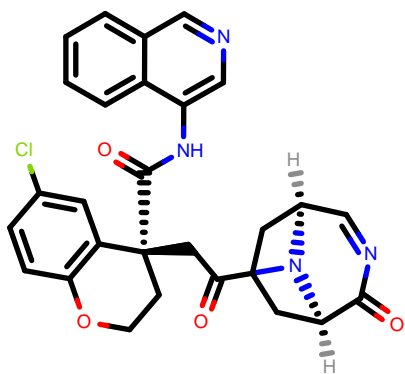
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(COC4c3cc(cc4)Cl)NC(=O)CO[C@@H]5CCCC5

RUN: RUN3348

DDG (kcal/mol): -3.26

dDDG (kcal/mol): 0.19

EN300-6740329_1_1_1



CID: EN300-6740329_1_1_1

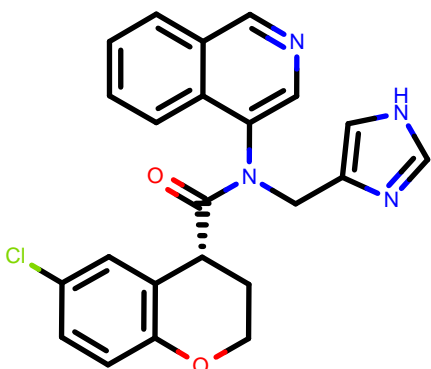
SMILES: c1ccc2c(c1)nccc2N(C(=O)C@H)(C3CCOC4CC(=O)C(C)C(=O)N5[C@@H](C)C[C@@H]5C)C@H5(C)O)N6

RUN: RUN4866

DDG (kcal/mol): -3.25

dDDG (kcal/mol): 0.41

ALP-UNI-44c99a80-2_1



CID: ALP-UNI-44c99a80-2_1

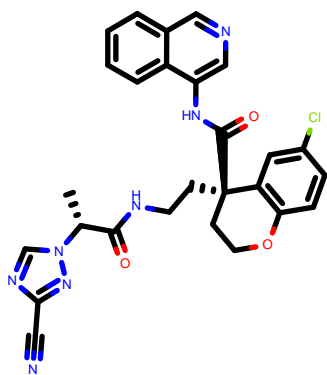
SMILES: c1ccc2c(c1)nccc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOC5C4cc(cc5)Cl

RUN: RUN447

DDG (kcal/mol): -3.25

dDDG (kcal/mol): 0.16

EN300-198515_3_2_1



CID: EN300-198515_3_2_1

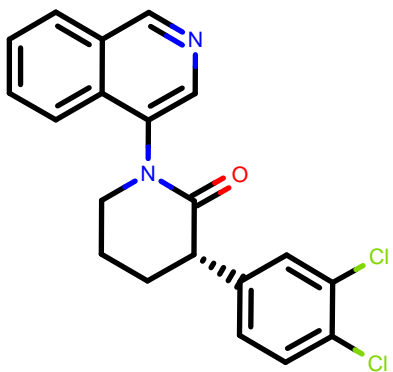
SMILES: C[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)n5nc(n5)C#N

RUN: RUN3001

DDG (kcal/mol): -3.25

dDDG (kcal/mol): 0.33

ALP-UNI-3735e77e-1_2



CID: ALP-UNI-3735e77e-1_2

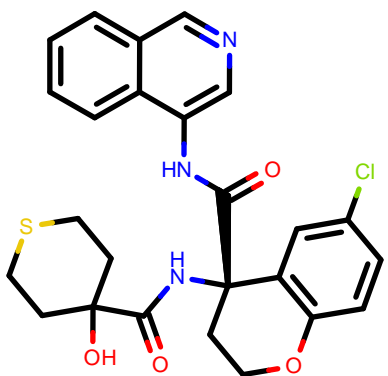
SMILES: c1ccc2c(c1)nccc2N3CCCC[C@H](C3=O)c4ccc(c(c4)Cl)Cl

RUN: RUN1750

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.28

EN300-122340_1_1_1



CID: EN300-122340_1_1_1

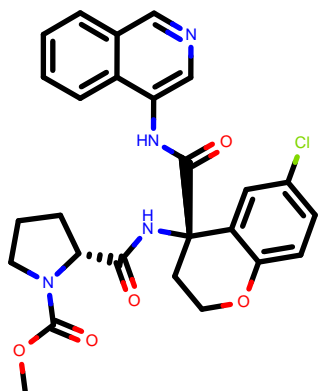
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)C5(CCSCC5)O

RUN: RUN2895

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.28

EN300-66845_1_1_1



CID: EN300-66845_1_1_1

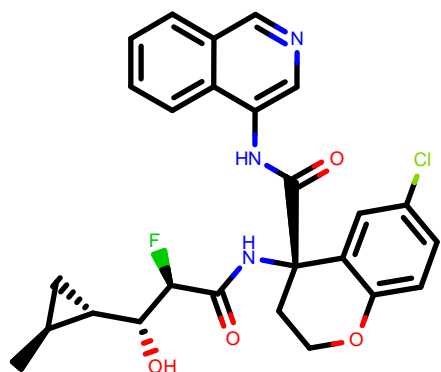
SMILES: COC(=O)N1CCC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3509

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.33

EDG-MED-90036822-94_14



CID: EDG-MED-90036822-94_14

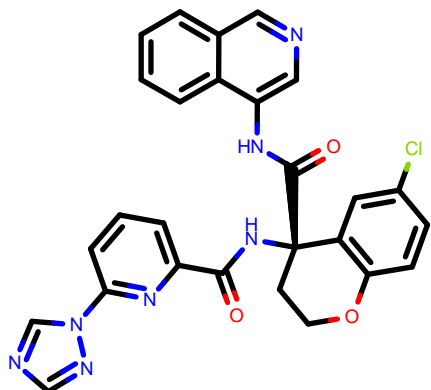
SMILES: C1C@H1[C@@]2([C@@H]1)[C@@H]3(CO)N[C@@]2(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6F

RUN: RUN1733

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.25

EN300-123712_1_1_1



CID: EN300-123712_1_1_1

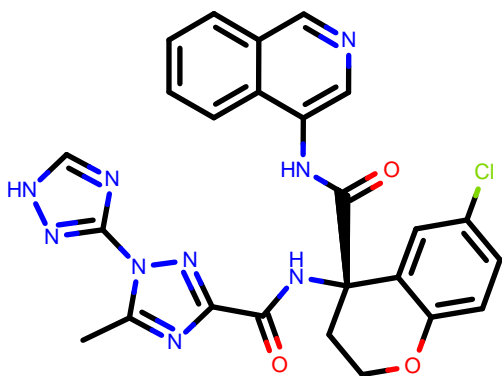
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)n6cnc6

RUN: RUN2865

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.24

EN300-26973_1_1_1



CID: EN300-26973_1_1_1

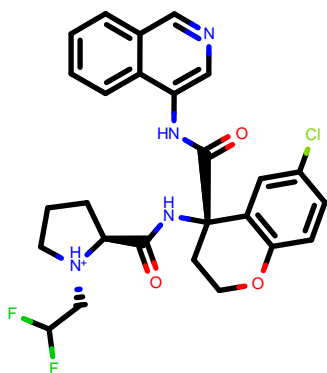
SMILES: Cc1nc(m1c2[nH]jcn2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccc6

RUN: RUN2940

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.24

EDG-MED-90036822-98_1



CID: EDG-MED-90036822-98_1

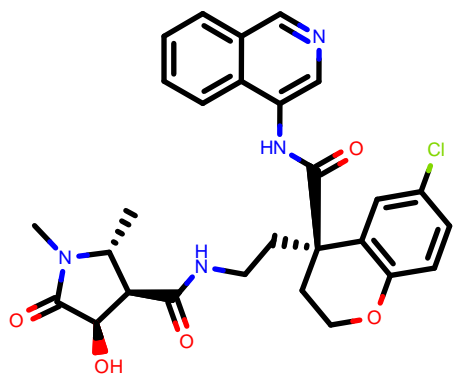
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C[C@@]6N(C)C(F)(F)F

RUN: RUN1724

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.28

EN300-378828_3_1_1



CID: EN300-378828_3_1_1

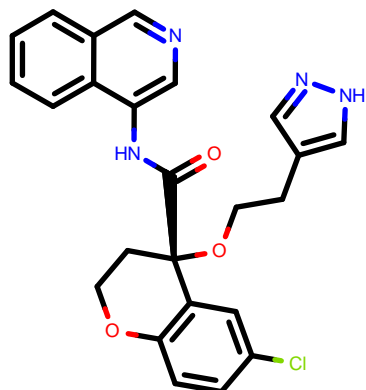
SMILES: C[C@@]1(C)C(=O)N(C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN3599

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.46

EDJ-MED-28ec730d-5_1



CID: EDJ-MED-28ec730d-5_1

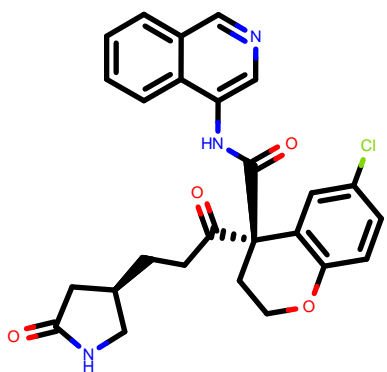
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]jnc5

RUN: RUN582

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-21_1_1



CID: VLA-UCB-34f3ed0c-21_1_1

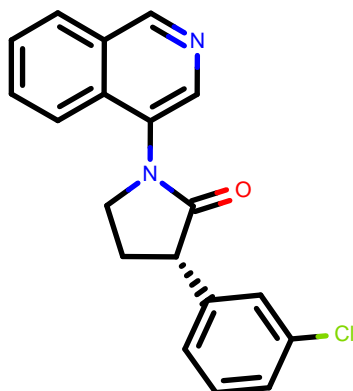
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NCS

RUN: RUN3528

DDG (kcal/mol): -3.22

dDDG (kcal/mol): 0.32

GIA-UNK-80c9bc96-1_2



CID: GIA-UNK-80c9bc96-1_2

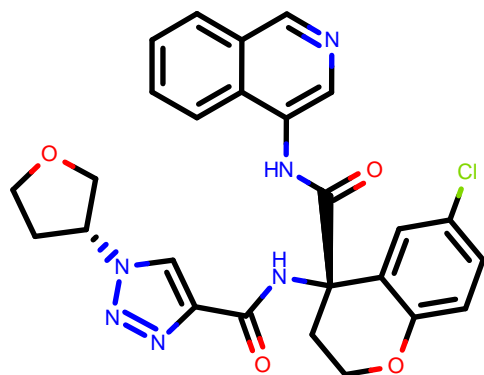
SMILES: c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN962

DDG (kcal/mol): -3.22

dDDG (kcal/mol): 0.27

EN300-151461_1_1_1



CID: EN300-151461_1_1_1

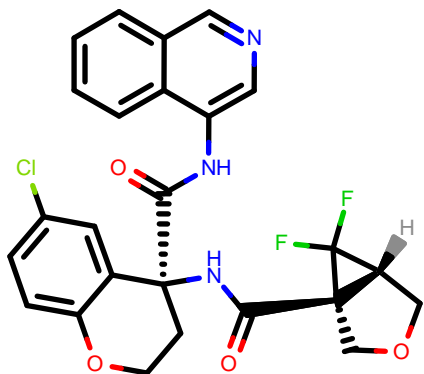
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)NC(=O)c5cn(n5)[C@@H]6CCOC6

RUN: RUN3284

DDG (kcal/mol): -3.22

dDDG (kcal/mol): 0.25

EN300-6738732_1_1_1



CID: EN300-6738732_1_1_1

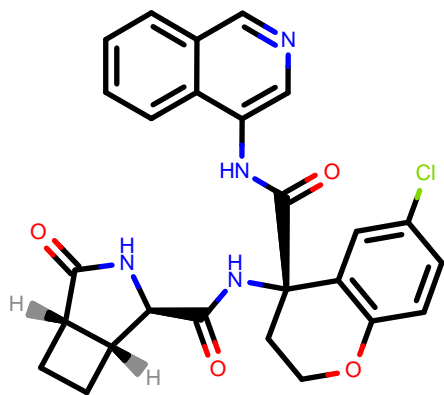
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)NC(=O)[C@@]56COC[C@@H]5C6(F)F

RUN: RUN2783

DDG (kcal/mol): -3.21

dDDG (kcal/mol): 0.21

EN300-6735902_1_1_1



CID: EN300-6735902_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C1NC(=O)[C@H]5[C@@H]6CC[C@@H]6C1=O)NS

RUN:

RUN2828

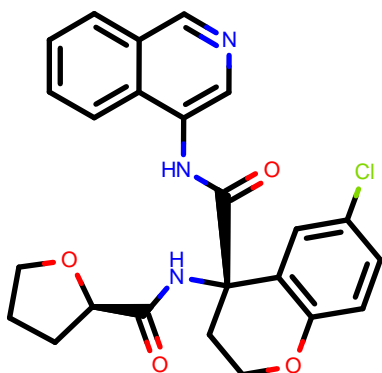
DDG (kcal/mol):

-3.20

dDDG (kcal/mol):

0.25

EN300-21009_1_2_1



CID: EN300-21009_1_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C1NC(=O)[C@H]5CCCCO5

RUN:

RUN3145

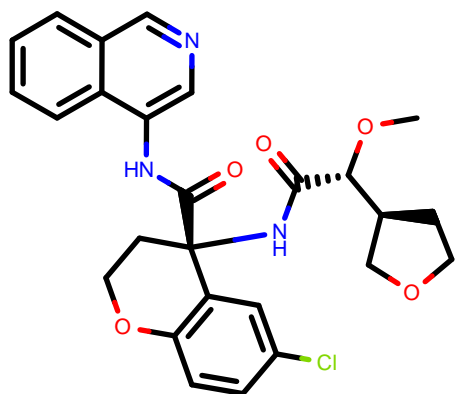
DDG (kcal/mol):

-3.20

dDDG (kcal/mol):

0.25

EN300-298552_1_4_1



CID: EN300-298552_1_4_1

SMILES:

CO[C@H]([C@H]1CCOC1)C(=O)N[C@@]2(C)CCOC3C2C(=O)C1C(=O)Nc4ccc5c4ccc5

RUN:

RUN2827

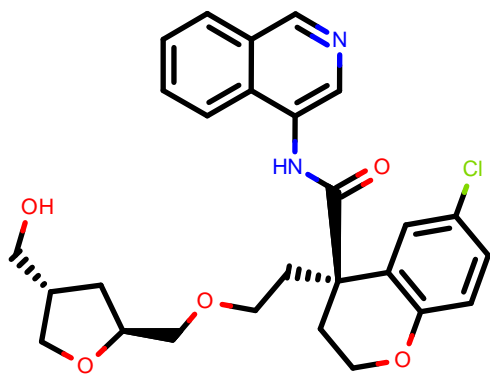
DDG (kcal/mol):

-3.20

dDDG (kcal/mol):

0.26

EN300-6494158_3_3_1



CID: EN300-6494158_3_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C1CCOC[C@@H]5[C@H]C[C@H]C(O)5)CO

RUN:

RUN7125

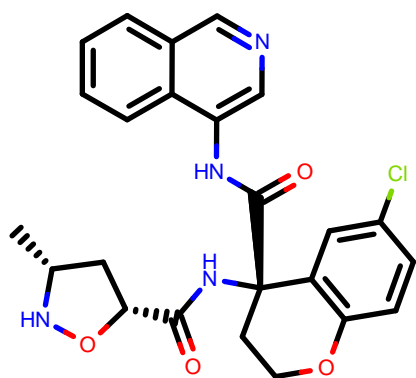
DDG (kcal/mol):

-3.20

dDDG (kcal/mol):

0.32

EN300-92447_1_2_1



CID: EN300-92447_1_2_1

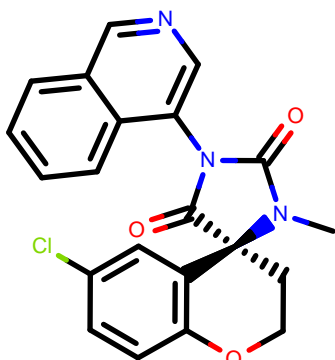
SMILES: C[C@@H]1C[C@@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3464

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.26

BEN-BAS-c2bc0d80-7_1



CID: BEN-BAS-c2bc0d80-7_1

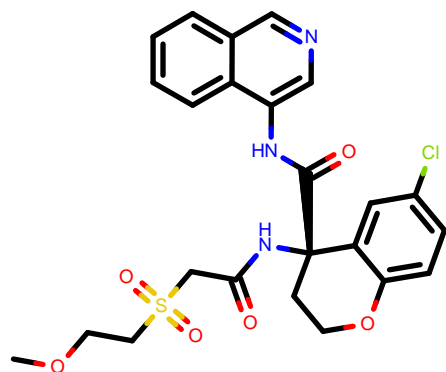
SMILES: CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4ncoc5c4ccoc5

RUN: RUN1000

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.28

EN300-39501_1_1_1



CID: EN300-39501_1_1_1

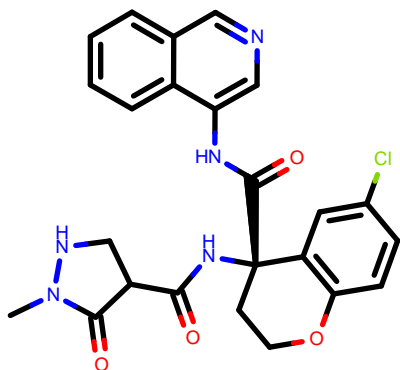
SMILES: COCCS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3300

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.41

EN300-7437779_1_1_1



CID: EN300-7437779_1_1_1

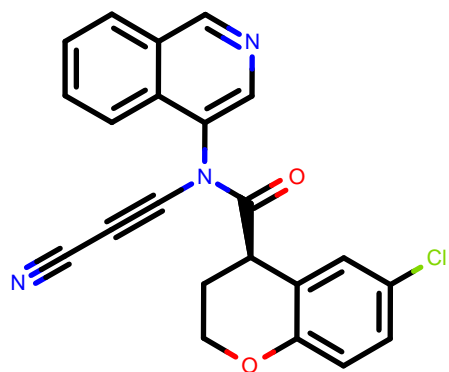
SMILES: Cn1c(=O)c(c[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2685

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.26

DAR-DIA-5ff57136-10_1



CID: DAR-DIA-5ff57136-10_1

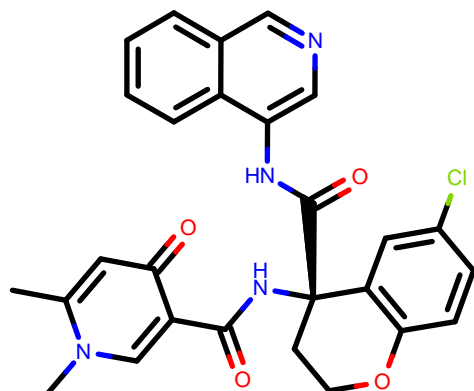
SMILES: c1ccc2c(e1)cncc2N(C#CC#N)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN1249

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.14

EN300-199991_1_1_1



CID: EN300-199991_1_1_1

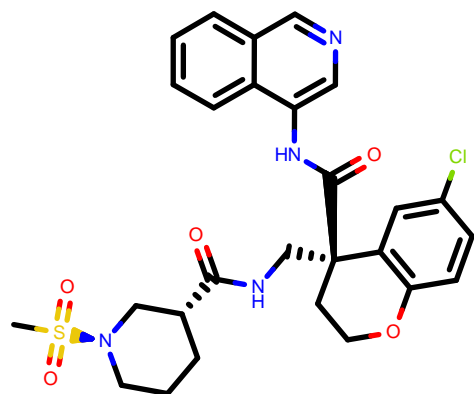
SMILES: Cc1cc(=O)c(en1C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN3446

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.32

EN300-27341_2_2_1



CID: EN300-27341_2_2_1

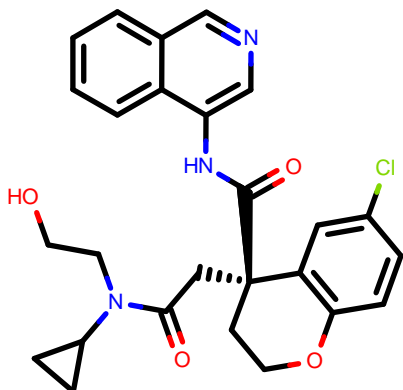
SMILES: CS(=O)(=O)N1CCCC1[C@@H]2(C)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccccc6

RUN: RUN2754

DDG (kcal/mol): -3.17

dDDG (kcal/mol): 0.31

EN300-37102_1_1_1



CID: EN300-37102_1_1_1

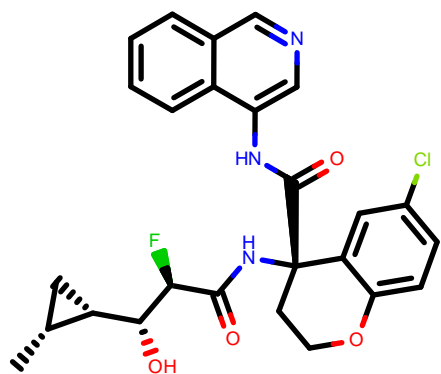
SMILES: c1ccc2c(e1)cncc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5CC5

RUN: RUN2923

DDG (kcal/mol): -3.15

dDDG (kcal/mol): 0.37

EDG-MED-90036822-94_13



CID: EDG-MED-90036822-94_13

SMILES:

C[C@@H]1C[C@@H]2[C@@H]3[C@@H]4[C@@H]5[C@@H]6[C@@H]7[C@@H]8[C@@H]9[C@@H]10[C@@H]11[C@@H]12[C@@H]13[C@@H]14[C@@H]15[C@@H]16[C@@H]17[C@@H]18[C@@H]19[C@@H]20[C@@H]21[C@@H]22[C@@H]23[C@@H]24[C@@H]25[C@@H]26[C@@H]27[C@@H]28[C@@H]29[C@@H]30[C@@H]31[C@@H]32[C@@H]33[C@@H]34[C@@H]35[C@@H]36[C@@H]37[C@@H]38[C@@H]39[C@@H]40[C@@H]41[C@@H]42[C@@H]43[C@@H]44[C@@H]45[C@@H]46[C@@H]47[C@@H]48[C@@H]49[C@@H]50[C@@H]51[C@@H]52[C@@H]53[C@@H]54[C@@H]55[C@@H]56[C@@H]57[C@@H]58[C@@H]59[C@@H]60[C@@H]61[C@@H]62[C@@H]63[C@@H]64[C@@H]65[C@@H]66[C@@H]67[C@@H]68[C@@H]69[C@@H]70[C@@H]71[C@@H]72[C@@H]73[C@@H]74[C@@H]75[C@@H]76[C@@H]77[C@@H]78[C@@H]79[C@@H]80[C@@H]81[C@@H]82[C@@H]83[C@@H]84[C@@H]85[C@@H]86[C@@H]87[C@@H]88[C@@H]89[C@@H]90[C@@H]91[C@@H]92[C@@H]93[C@@H]94[C@@H]95[C@@H]96[C@@H]97[C@@H]98[C@@H]99[C@@H]100[C@@H]101[C@@H]102[C@@H]103[C@@H]104[C@@H]105[C@@H]106[C@@H]107[C@@H]108[C@@H]109[C@@H]110[C@@H]111[C@@H]112[C@@H]113[C@@H]114[C@@H]115[C@@H]116[C@@H]117[C@@H]118[C@@H]119[C@@H]120[C@@H]121[C@@H]122[C@@H]123[C@@H]124[C@@H]125[C@@H]126[C@@H]127[C@@H]128[C@@H]129[C@@H]130[C@@H]131[C@@H]132[C@@H]133[C@@H]134[C@@H]135[C@@H]136[C@@H]137[C@@H]138[C@@H]139[C@@H]140[C@@H]141[C@@H]142[C@@H]143[C@@H]144[C@@H]145[C@@H]146[C@@H]147[C@@H]148[C@@H]149[C@@H]150[C@@H]151[C@@H]152[C@@H]153[C@@H]154[C@@H]155[C@@H]156[C@@H]157[C@@H]158[C@@H]159[C@@H]160[C@@H]161[C@@H]162[C@@H]163[C@@H]164[C@@H]165[C@@H]166[C@@H]167[C@@H]168[C@@H]169[C@@H]170[C@@H]171[C@@H]172[C@@H]173[C@@H]174[C@@H]175[C@@H]176[C@@H]177[C@@H]178[C@@H]179[C@@H]180[C@@H]181[C@@H]182[C@@H]183[C@@H]184[C@@H]185[C@@H]186[C@@H]187[C@@H]188[C@@H]189[C@@H]190[C@@H]191[C@@H]192[C@@H]193[C@@H]194[C@@H]195[C@@H]196[C@@H]197[C@@H]198[C@@H]199[C@@H]200[C@@H]201[C@@H]202[C@@H]203[C@@H]204[C@@H]205[C@@H]206[C@@H]207[C@@H]208[C@@H]209[C@@H]210[C@@H]211[C@@H]212[C@@H]213[C@@H]214[C@@H]215[C@@H]216[C@@H]217[C@@H]218[C@@H]219[C@@H]220[C@@H]221[C@@H]222[C@@H]223[C@@H]224[C@@H]225[C@@H]226[C@@H]227[C@@H]228[C@@H]229[C@@H]230[C@@H]231[C@@H]232[C@@H]233[C@@H]234[C@@H]235[C@@H]236[C@@H]237[C@@H]238[C@@H]239[C@@H]240[C@@H]241[C@@H]242[C@@H]243[C@@H]244[C@@H]245[C@@H]246[C@@H]247[C@@H]248[C@@H]249[C@@H]250[C@@H]251[C@@H]252[C@@H]253[C@@H]254[C@@H]255[C@@H]256[C@@H]257[C@@H]258[C@@H]259[C@@H]260[C@@H]261[C@@H]262[C@@H]263[C@@H]264[C@@H]265[C@@H]266[C@@H]267[C@@H]268[C@@H]269[C@@H]270[C@@H]271[C@@H]272[C@@H]273[C@@H]274[C@@H]275[C@@H]276[C@@H]277[C@@H]278[C@@H]279[C@@H]280[C@@H]281[C@@H]282[C@@H]283[C@@H]284[C@@H]285[C@@H]286[C@@H]287[C@@H]288[C@@H]289[C@@H]290[C@@H]291[C@@H]292[C@@H]293[C@@H]294[C@@H]295[C@@H]296[C@@H]297[C@@H]298[C@@H]299[C@@H]300[C@@H]301[C@@H]302[C@@H]303[C@@H]304[C@@H]305[C@@H]306[C@@H]307[C@@H]308[C@@H]309[C@@H]310[C@@H]311[C@@H]312[C@@H]313[C@@H]314[C@@H]315[C@@H]316[C@@H]317[C@@H]318[C@@H]319[C@@H]320[C@@H]321[C@@H]322[C@@H]323[C@@H]324[C@@H]325[C@@H]326[C@@H]327[C@@H]328[C@@H]329[C@@H]330[C@@H]331[C@@H]332[C@@H]333[C@@H]334[C@@H]335[C@@H]336[C@@H]337[C@@H]338[C@@H]339[C@@H]340[C@@H]341[C@@H]342[C@@H]343[C@@H]344[C@@H]345[C@@H]346[C@@H]347[C@@H]348[C@@H]349[C@@H]350[C@@H]351[C@@H]352[C@@H]353[C@@H]354[C@@H]355[C@@H]356[C@@H]357[C@@H]358[C@@H]359[C@@H]360[C@@H]361[C@@H]362[C@@H]363[C@@H]364[C@@H]365[C@@H]366[C@@H]367[C@@H]368[C@@H]369[C@@H]370[C@@H]371[C@@H]372[C@@H]373[C@@H]374[C@@H]375[C@@H]376[C@@H]377[C@@H]378[C@@H]379[C@@H]380[C@@H]381[C@@H]382[C@@H]383[C@@H]384[C@@H]385[C@@H]386[C@@H]387[C@@H]388[C@@H]389[C@@H]390[C@@H]391[C@@H]392[C@@H]393[C@@H]394[C@@H]395[C@@H]396[C@@H]397[C@@H]398[C@@H]399[C@@H]400[C@@H]401[C@@H]402[C@@H]403[C@@H]404[C@@H]405[C@@H]406[C@@H]407[C@@H]408[C@@H]409[C@@H]410[C@@H]411[C@@H]412[C@@H]413[C@@H]414[C@@H]415[C@@H]416[C@@H]417[C@@H]418[C@@H]419[C@@H]420[C@@H]421[C@@H]422[C@@H]423[C@@H]424[C@@H]425[C@@H]426[C@@H]427[C@@H]428[C@@H]429[C@@H]430[C@@H]431[C@@H]432[C@@H]433[C@@H]434[C@@H]435[C@@H]436[C@@H]437[C@@H]438[C@@H]439[C@@H]440[C@@H]441[C@@H]442[C@@H]443[C@@H]444[C@@H]445[C@@H]446[C@@H]447[C@@H]448[C@@H]449[C@@H]450[C@@H]451[C@@H]452[C@@H]453[C@@H]454[C@@H]455[C@@H]456[C@@H]457[C@@H]458[C@@H]459[C@@H]460[C@@H]461[C@@H]462[C@@H]463[C@@H]464[C@@H]465[C@@H]466[C@@H]467[C@@H]468[C@@H]469[C@@H]470[C@@H]471[C@@H]472[C@@H]473[C@@H]474[C@@H]475[C@@H]476[C@@H]477[C@@H]478[C@@H]479[C@@H]480[C@@H]481[C@@H]482[C@@H]483[C@@H]484[C@@H]485[C@@H]486[C@@H]487[C@@H]488[C@@H]489[C@@H]490[C@@H]491[C@@H]492[C@@H]493[C@@H]494[C@@H]495[C@@H]496[C@@H]497[C@@H]498[C@@H]499[C@@H]500[C@@H]501[C@@H]502[C@@H]503[C@@H]504[C@@H]505[C@@H]506[C@@H]507[C@@H]508[C@@H]509[C@@H]510[C@@H]511[C@@H]512[C@@H]513[C@@H]514[C@@H]515[C@@H]516[C@@H]517[C@@H]518[C@@H]519[C@@H]520[C@@H]521[C@@H]522[C@@H]523[C@@H]524[C@@H]525[C@@H]526[C@@H]527[C@@H]528[C@@H]529[C@@H]530[C@@H]531[C@@H]532[C@@H]533[C@@H]534[C@@H]535[C@@H]536[C@@H]537[C@@H]538[C@@H]539[C@@H]540[C@@H]541[C@@H]542[C@@H]543[C@@H]544[C@@H]545[C@@H]546[C@@H]547[C@@H]548[C@@H]549[C@@H]550[C@@H]551[C@@H]552[C@@H]553[C@@H]554[C@@H]555[C@@H]556[C@@H]557[C@@H]558[C@@H]559[C@@H]560[C@@H]561[C@@H]562[C@@H]563[C@@H]564[C@@H]565[C@@H]566[C@@H]567[C@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RUN:

RUN1697

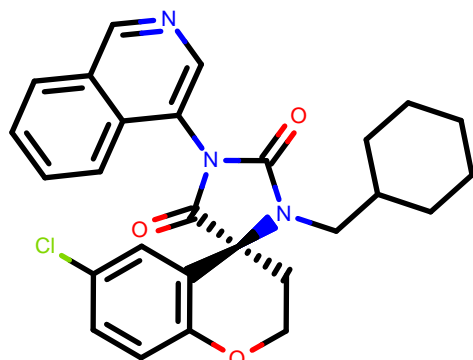
DDG (kcal/mol):

-3.15

dDDG (kcal/mol):

0.26

VLA-UCB-34f3ed0c-14_1



CID: VLA-UCB-34f3ed0c-14_1

SMILES:

c1ccc2c(c1)cnc2N3C(=O)C@@H4(CCOc5c4cc(c5)Cl)N(C3=O)CC6CCCC6

RUN:

RUN517

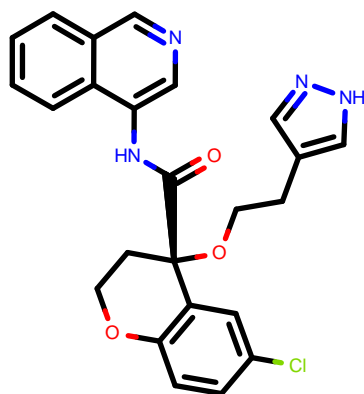
DDG (kcal/mol):

-3.15

dDDG (kcal/mol):

0.35

CHO-MSK-5891c1ff-12_1



CID: CHO-MSK-5891c1ff-12_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)C@@H3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5

RUN:

RUN1735

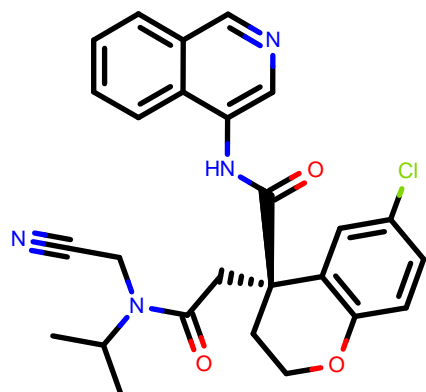
DDG (kcal/mol):

-3.14

dDDG (kcal/mol):

0.22

EDG-MED-ba1ac7b9-6_2



CID: EDG-MED-ba1ac7b9-6_2

SMILES:

CC(C)N(CC#N)C(=O)C[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN:

RUN2483

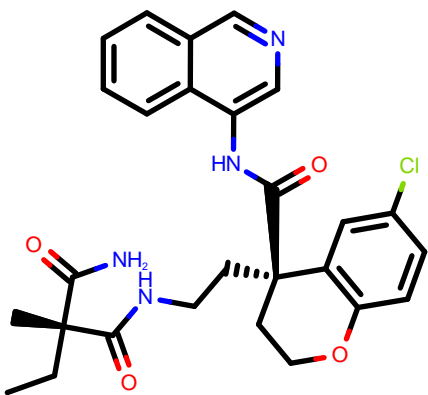
DDG (kcal/mol):

-3.14

dDDG (kcal/mol):

0.27

EN300-2908024_3_2_1



CID: EN300-2908024_3_2_1

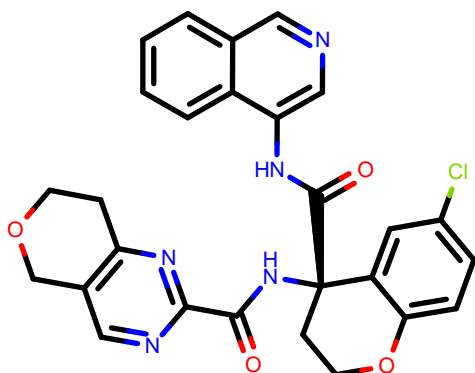
SMILES: CC[C@](C)(C(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4298

DDG (kcal/mol): -3.13

dDDG (kcal/mol): 0.29

EN300-7435929_1_1_1



CID: EN300-7435929_1_1_1

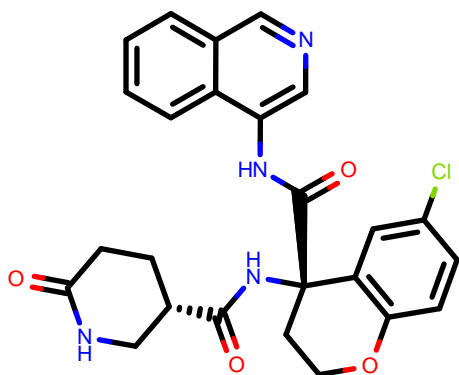
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6c(n5)CCOC6

RUN: RUN3106

DDG (kcal/mol): -3.13

dDDG (kcal/mol): 0.27

EN300-42819_1_2_1



CID: EN300-42819_1_2_1

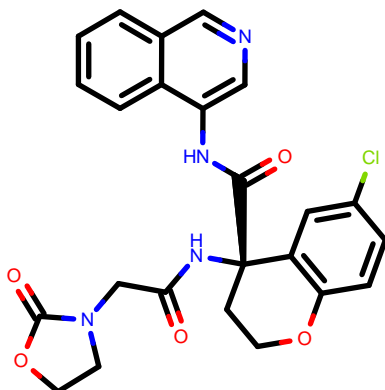
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCN(C=O)N5

RUN: RUN2680

DDG (kcal/mol): -3.12

dDDG (kcal/mol): 0.24

EN300-172179_1_1_1



CID: EN300-172179_1_1_1

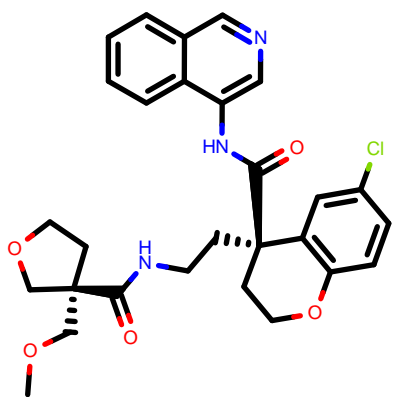
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)N5CCOC5=O

RUN: RUN3218

DDG (kcal/mol): -3.12

dDDG (kcal/mol): 0.29

EN300-248883_3_2_1



CID: EN300-248883_3_2_1

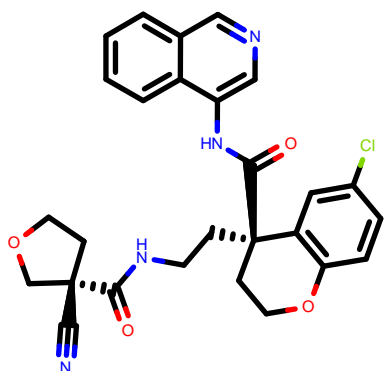
SMILES: COC[C@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3256

DDG (kcal/mol): -3.12

dDDG (kcal/mol): 0.35

EN300-261210_3_2_1



CID: EN300-261210_3_2_1

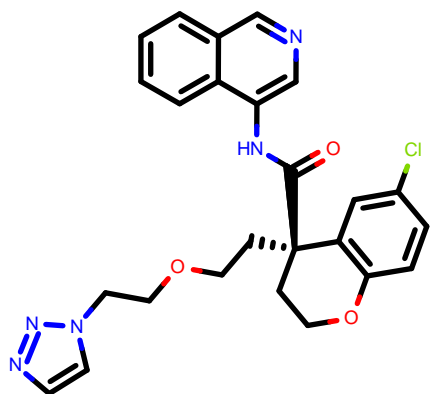
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOc5)C#N

RUN: RUN2894

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.32

EN300-1715993_3_1_1



CID: EN300-1715993_3_1_1

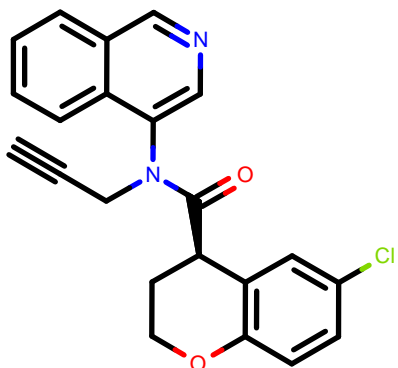
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnn5

RUN: RUN2879

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.22

DAR-DIA-5ff57136-13_1



CID: DAR-DIA-5ff57136-13_1

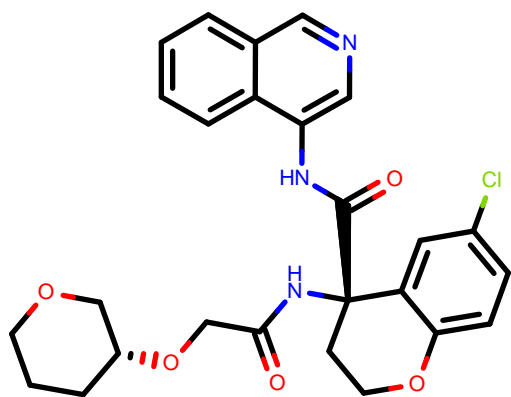
SMILES: C#CCN(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN1252

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.12

EN300-1627945_1_1_1



CID: EN300-1627945_1_1_1

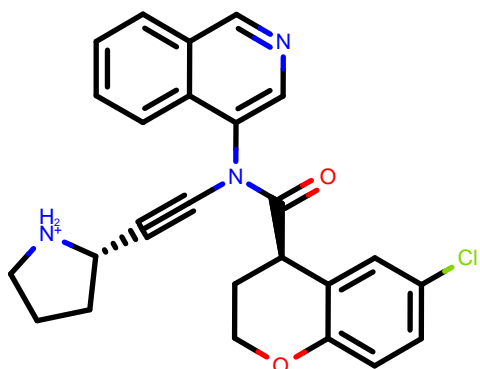
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@]5H5CCOC5

RUN: RUN3035

DDG (kcal/mol): -3.10

dDDG (kcal/mol): 0.21

DAR-DIA-5ff57136-12_1_1



CID: DAR-DIA-5ff57136-12_1_1

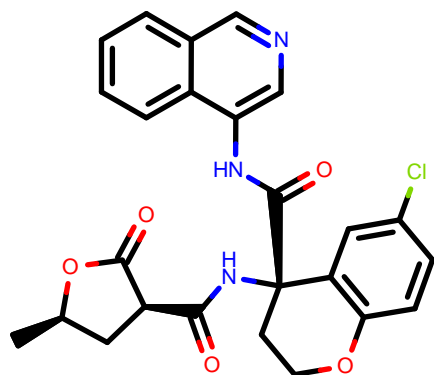
SMILES: c1ccc2c(c1)ncnc2N(C#C[C@@]3C[C@@H]3)C(=O)[C@@]4COCc5cc(Cl)cc5

RUN: RUN3987

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.19

EN300-7444533_1_1_1



CID: EN300-7444533_1_1_1

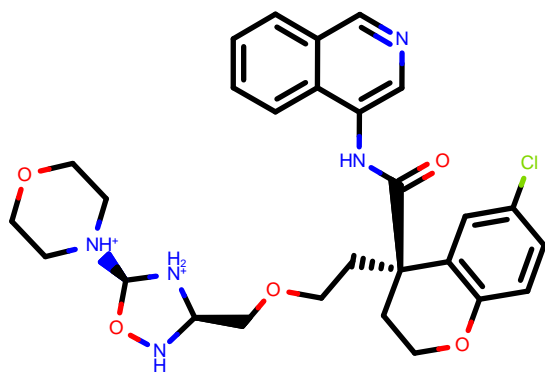
SMILES: C[C@@]1[C@@]2[C@@]3(C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3936

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.27

EN300-1608590_3_1_1



CID: EN300-1608590_3_1_1

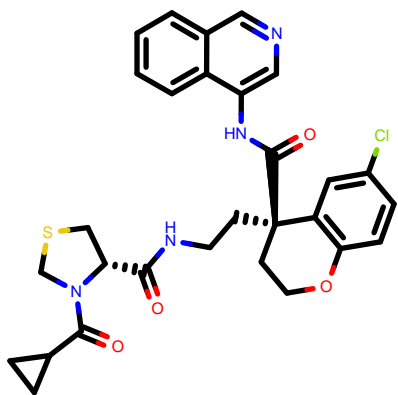
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@]5C[C@@H](O5)N+KCCOC6

RUN: RUN4648

DDG (kcal/mol): -3.08

dDDG (kcal/mol): 0.42

EN300-18928_3_2_1



CID: EN300-18928_3_2_1

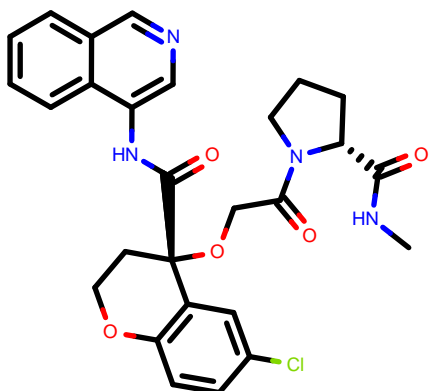
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(C)CCOC4C3C(=O)C(C)CCN(C1=O)[C@H]5C5CN(C1=O)C6CC6

RUN: RUN4466

DDG (kcal/mol): -3.08

dDDG (kcal/mol): 0.44

EN300-48902_1_2_1



CID: EN300-48902_1_2_1

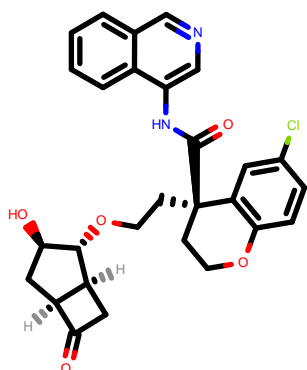
SMILES: CNC(=O)[C@H]1CCCN1C(=O)CO[C@@H]2(C)CCOC3C2C(=O)C(C)C(=O)Nc4ccc5c4ccc5

RUN: RUN6056

DDG (kcal/mol): -3.07

dDDG (kcal/mol): 0.34

EN300-6481287_3_1_1



CID: EN300-6481287_3_1_1

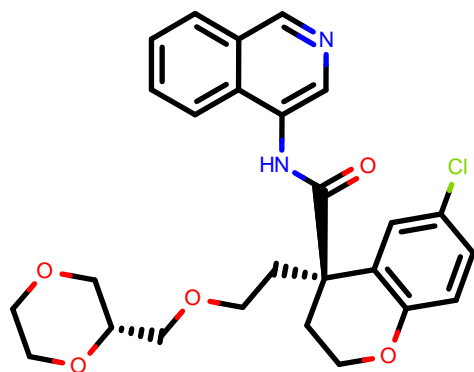
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(C)CCOC4C3C(=O)C(C)CCO[C@H]5[C@@H](C)C[C@H]6[C@@H]5COC6=O

RUN: RUN3042

DDG (kcal/mol): -3.07

dDDG (kcal/mol): 0.25

EN300-139167_3_2_1



CID: EN300-139167_3_2_1

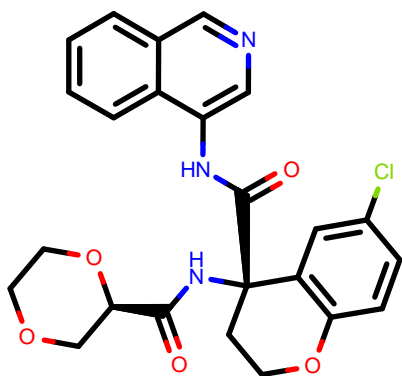
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(C)CCOC4C3C(=O)C(C)CCOC[C@H]5COC6CO5

RUN: RUN4951

DDG (kcal/mol): -3.07

dDDG (kcal/mol): 0.27

EN300-36158_1_2_1



CID: EN300-36158_1_2_1

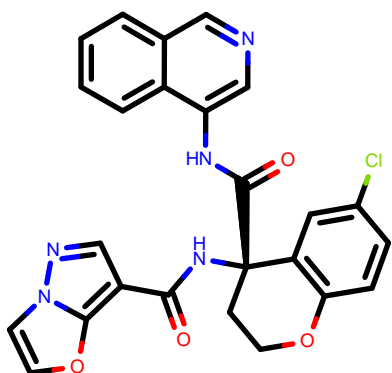
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COCCO5

RUN: RUN3137

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.23

EN300-303519_1_1_1



CID: EN300-303519_1_1_1

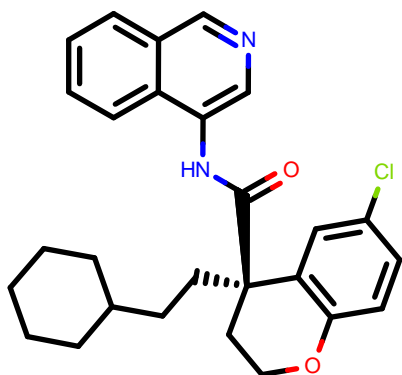
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnc6c5OCC6

RUN: RUN3842

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.20

VLA-UCB-50c39ae8-10_1



CID: VLA-UCB-50c39ae8-10_1

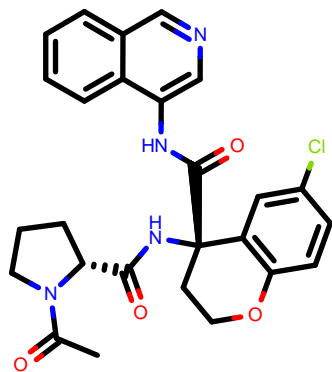
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCC5CCCC5

RUN: RUN315

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.26

EN300-12587_1_1_1



CID: EN300-12587_1_1_1

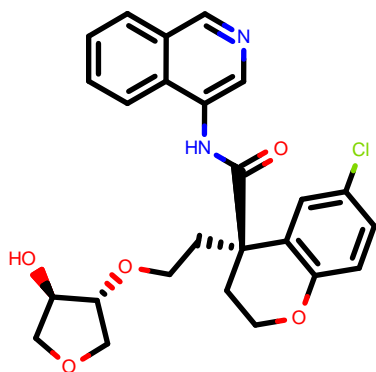
SMILES: CC(=O)N1CCC[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4ncc5c4ccccc5

RUN: RUN2785

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.34

EN300-331828_3_1_1



CID: EN300-331828_3_1_1

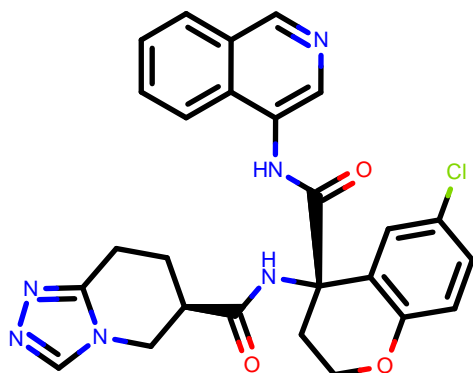
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCO[C@@H]5COC[C@H]5O

RUN: RUN4515

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.25

EN300-51350_1_1_1



CID: EN300-51350_1_1_1

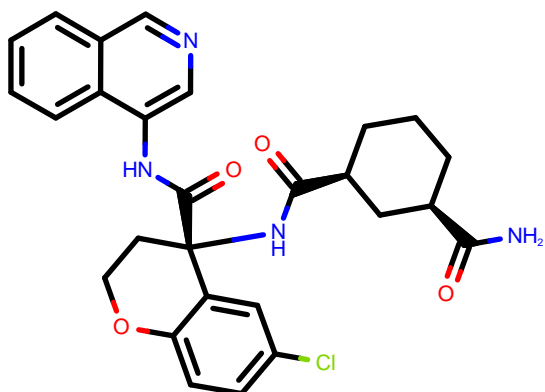
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@@H]5COC6nncn6C5

RUN: RUN3377

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.31

EN300-90142_1_4_1



CID: EN300-90142_1_4_1

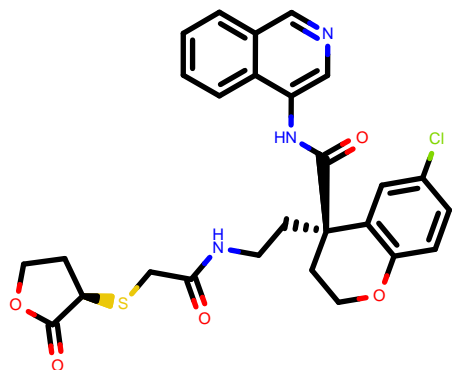
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@@H]5CC[C@H]5C(=O)N

RUN: RUN2959

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.24

EN300-113218_3_1_1



CID: EN300-113218_3_1_1

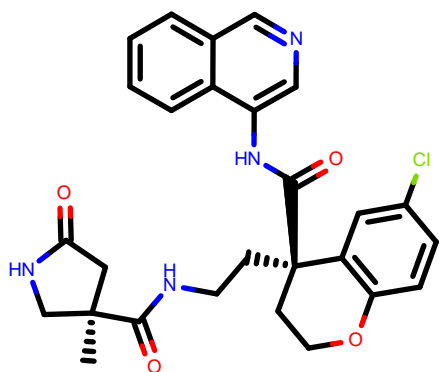
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCNC(=O)CS[C@@H]5CCOC5=O

RUN: RUN3263

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.36

EN300-132157_3_2_1



CID: EN300-132157_3_2_1

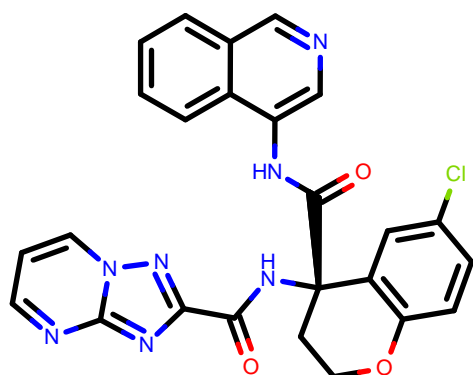
SMILES: C[C@]1(CC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN4724

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.34

EN300-83529_1_1_1



CID: EN300-83529_1_1_1

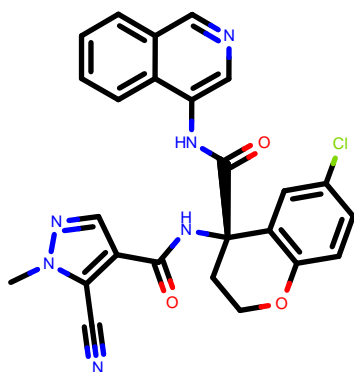
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6nccn6n5

RUN: RUN3795

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.24

EN300-140837_1_1_1



CID: EN300-140837_1_1_1

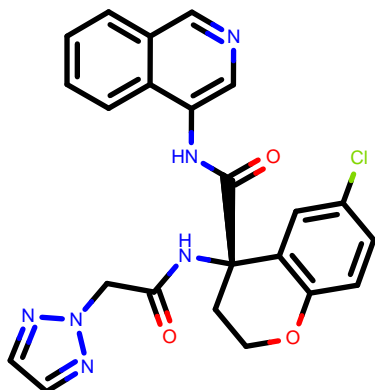
SMILES: Cn1c(c(en1)C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5C#N

RUN: RUN2789

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.23

EN300-100916_1_1_1



CID: EN300-100916_1_1_1

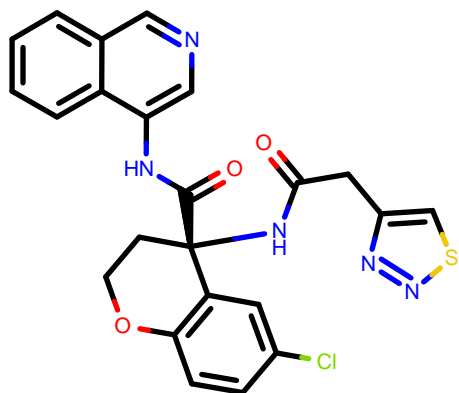
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5nccn5

RUN: RUN3609

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.22

EN300-300519_1_1_1



CID: EN300-300519_1_1_1

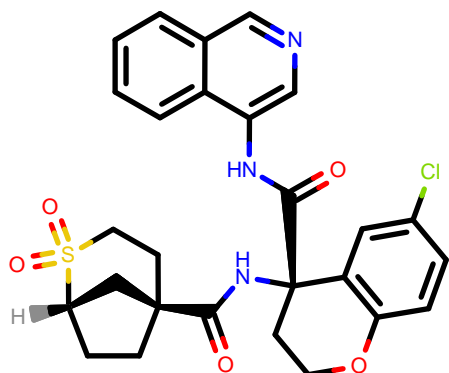
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5csnn5

RUN: RUN3407

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.20

EN300-6503702_1_1_1



CID: EN300-6503702_1_1_1

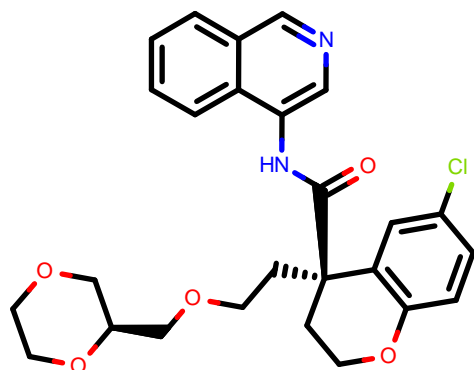
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5=CC(=O)N(S(=O)(=O)O)C6

RUN: RUN5125

DDG (kcal/mol): -3.03

dDDG (kcal/mol): 0.31

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

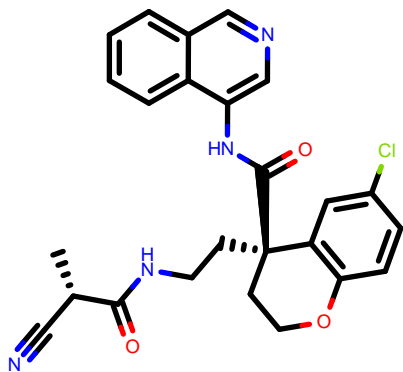
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(C)OCCO5

RUN: RUN3916

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.27

EN300-72730_3_1_1



CID: EN300-72730_3_1_1

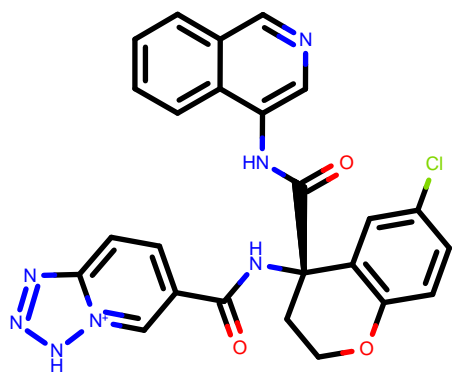
SMILES: C[C@@]1(C#N)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN3703

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.22

EN300-102853_1_1_1



CID: EN300-102853_1_1_1

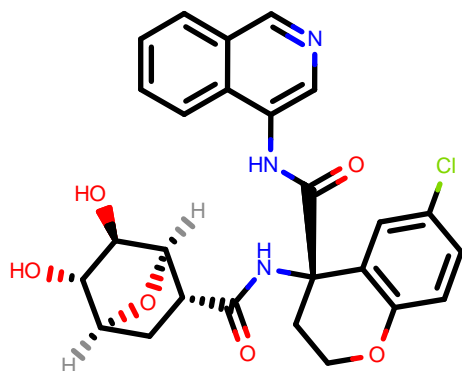
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6n[n-][n+]6c5

RUN: RUN3863

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.22

EN300-6764836_1_5_1



CID: EN300-6764836_1_5_1

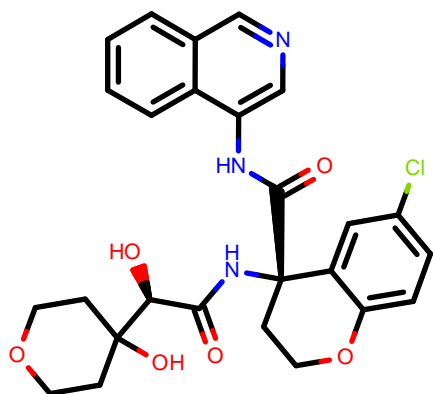
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(CO)COC4O

RUN: RUN2755

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.27

EN300-749499_1_1_1



CID: EN300-749499_1_1_1

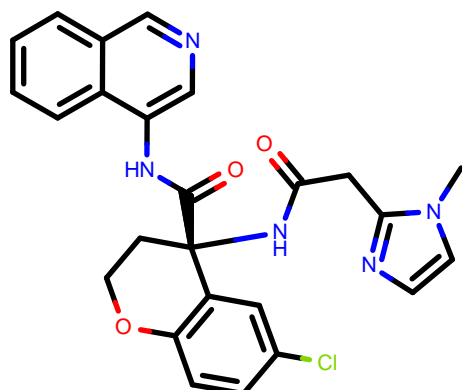
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(CO)COC4O

RUN: RUN2912

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.24

EDG-MED-90036822-41_1



CID: EDG-MED-90036822-41_1

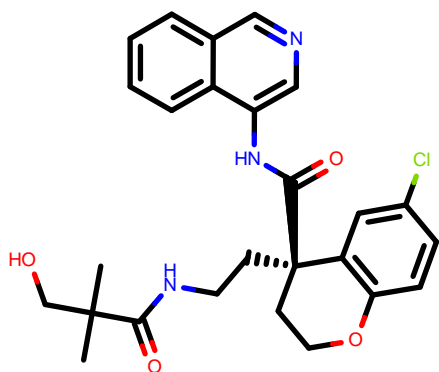
SMILES: Cn1cnc1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1566

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.23

EN300-65050_3_1_1



CID: EN300-65050_3_1_1

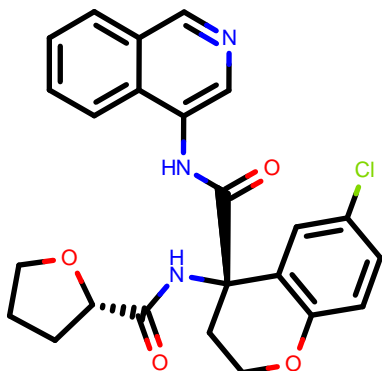
SMILES: CC(C)(CO)C(=O)NCC[C@]1(C)C(CO)C2c1cc(cc2)C(C=O)Nc3cncc4c3cccc4

RUN: RUN3707

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.26

EN300-104395_1_1_1



CID: EN300-104395_1_1_1

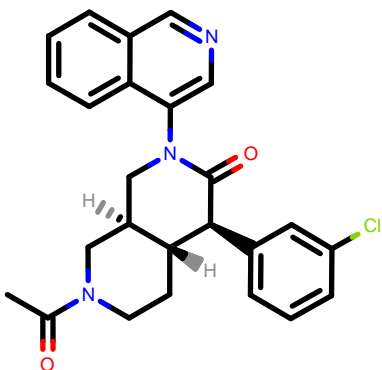
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(C=O)N[C@@H]5CCCCO5

RUN: RUN2897

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.22

MIC-UNK-9582b2c5-1_5



CID: MIC-UNK-9582b2c5-1_5

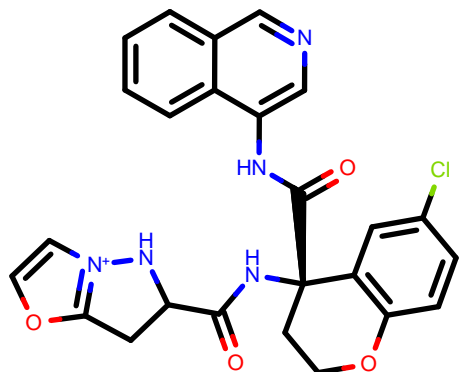
SMILES: CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)C)C4c5cncc5c4cccc5

RUN: RUN193

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.36

EN300-181688_1_1_1



CID: EN300-181688_1_1_1

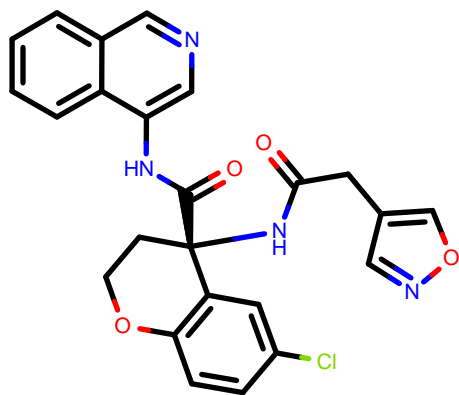
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(C=O)Nc5cc6n(n5)CCO6

RUN: RUN2937

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.22

EN300-315963_1_1_1



CID: EN300-315963_1_1_1

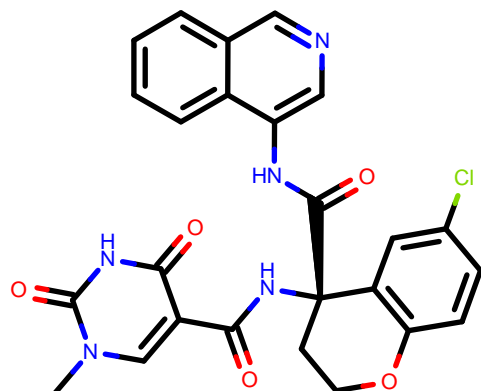
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5cnoc5

RUN: RUN2929

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.20

EN300-37123_1_1_1



CID: EN300-37123_1_1_1

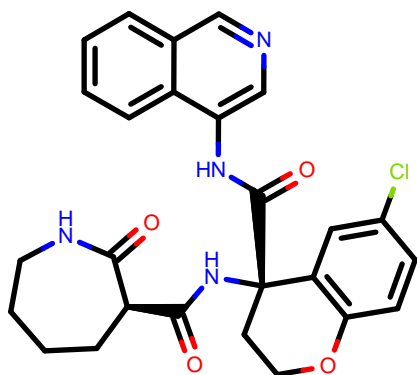
SMILES: Cn1cc(c(O)[nH]c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN3579

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.30

EN300-6737762_1_2_1



CID: EN300-6737762_1_2_1

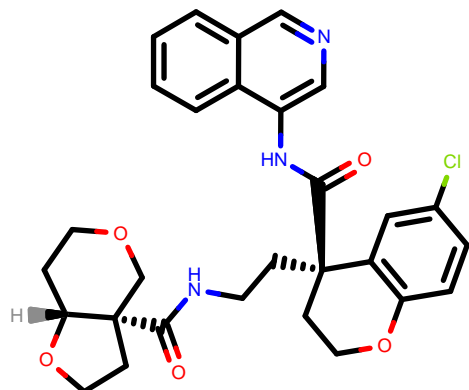
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCCNC5=O

RUN: RUN2883

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.28

EN300-341337_3_2_1



CID: EN300-341337_3_2_1

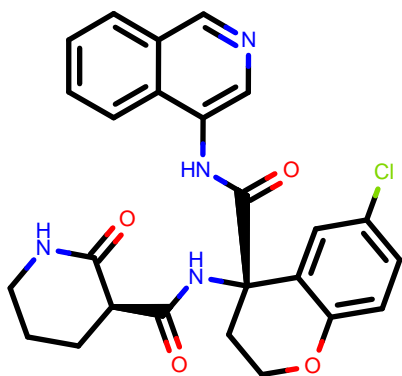
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]56CCO[C@@]5H5CCO6

RUN: RUN4909

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.38

EN300-82616_1_2_1



CID: EN300-82616_1_2_1

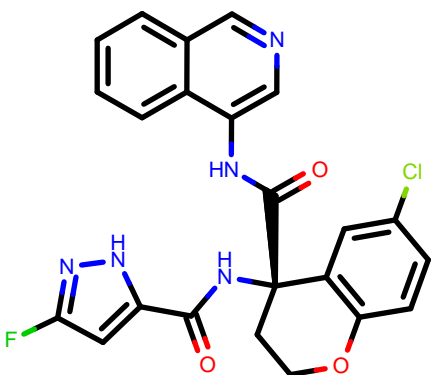
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3[C@@]3(CCOC4C3CC(Cc4)C)NC(=O)[C@@H]5CCNC5=O

RUN: RUN4123

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.30

EN300-150212_1_1_1



CID: EN300-150212_1_1_1

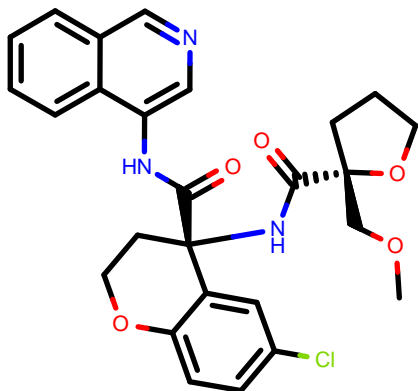
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3[C@@]3(CCOC4C3CC(Cc4)C)NC(=O)[nH]n5F

RUN: RUN3165

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.19

EN300-1301381_1_2_1



CID: EN300-1301381_1_2_1

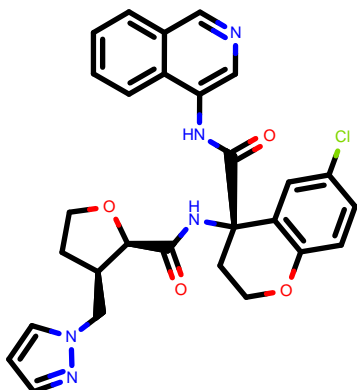
SMILES: COC[C@@]1(CCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3062

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.27

EN300-304627_1_1_1



CID: EN300-304627_1_1_1

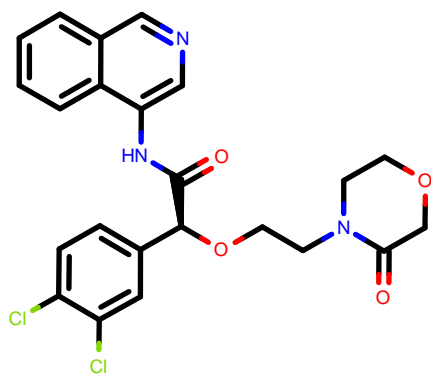
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3[C@@]3(CCOC4C3CC(Cc4)C)NC(=O)[C@@H]5[C@@H]5C[C@@H]6COC6=O

RUN: RUN2864

DDG (kcal/mol): -2.99

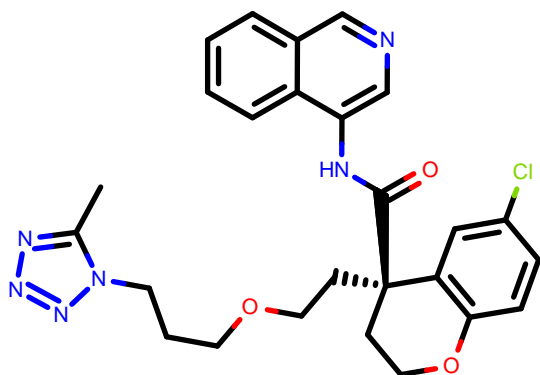
dDDG (kcal/mol): 0.33

MAT-POS-de59a476-3_2



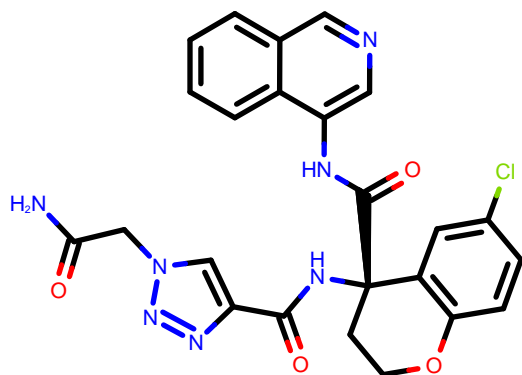
CID:	MAT-POS-de59a476-3_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)OCCN4CCOCC4=O</chem>
RUN:	RUN2070
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.45

EN300-197715_3_1_1



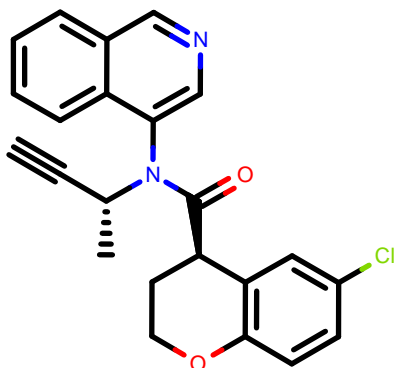
CID:	EN300-197715_3_1_1
SMILES:	<chem>Cc1nnnn1CCCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN2860
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.33

EN300-52380_1_1_1



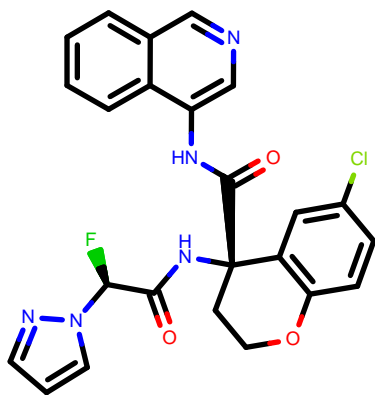
CID:	EN300-52380_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)CC(=O)N</chem>
RUN:	RUN3402
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.26

DAR-DIA-5ff57136-16_2_1



CID:	DAR-DIA-5ff57136-16_2_1
SMILES:	<chem>C[C@H](C#C)N(c1ncnc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN4314
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.14

EN300-1726277_1_1_1



CID: EN300-1726277_1_1_1

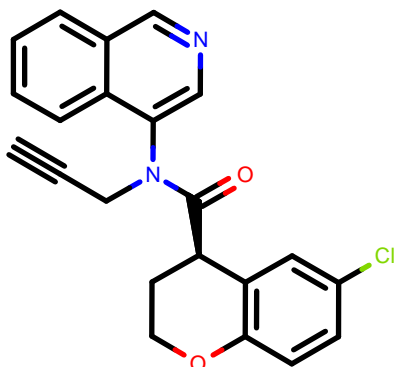
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H[n5ccc5]F

RUN: RUN3606

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.20

DAR-DIA-5ff57136-13_1_1



CID: DAR-DIA-5ff57136-13_1_1

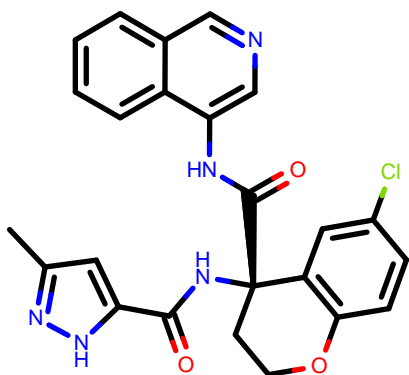
SMILES: C#CCN(C1CNC2C1CCCC2)C(=O)[C@@]3H3CCOC4c3cc(cc4)Cl

RUN: RUN2998

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.13

EN300-41425_1_1_1



CID: EN300-41425_1_1_1

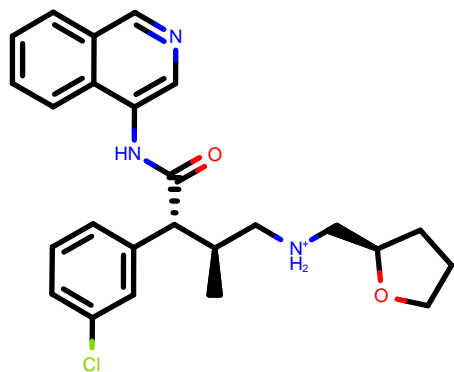
SMILES: Cc1cc[nH]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4838

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.18

MAK-UNK-c749d764-22_8



CID: MAK-UNK-c749d764-22_8

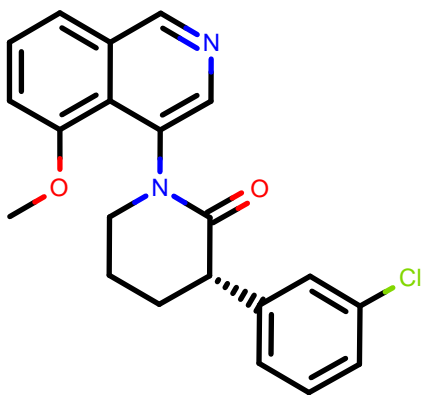
SMILES: C[C@@]H[C](NH2+)[C@@]H1CCCCO1[C@@]H(c2ccccc2)C(=O)Nc3nccc4c3cccc4

RUN: RUN963

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.45

MIC-UNK-50cce87d-12_2



CID: MIC-UNK-50cce87d-12_2

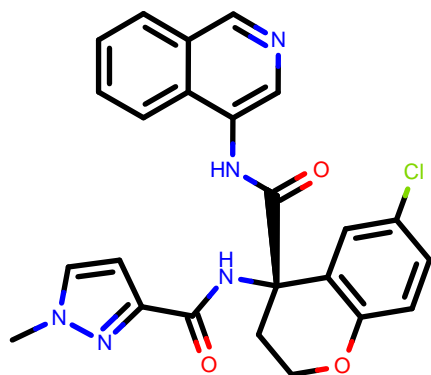
SMILES: COc1cccc2c1c(cnc2)N3CCC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN556

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.32

EN300-66976_1_1_1



CID: EN300-66976_1_1_1

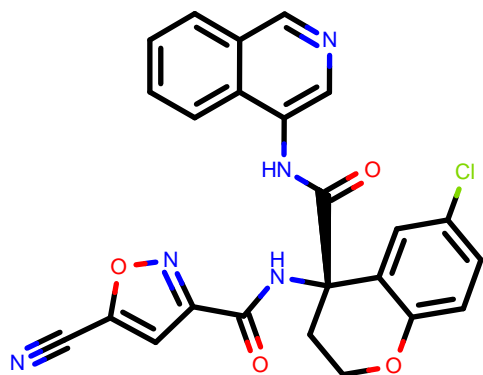
SMILES: Cn1ccc(n1)C(=O)N[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN2809

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.21

EN300-1178005_1_1_1



CID: EN300-1178005_1_1_1

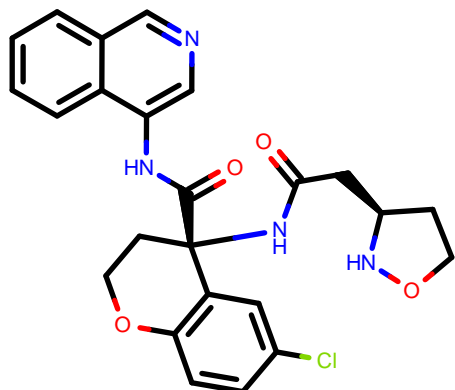
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(oc5)C#N

RUN: RUN3118

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.23

EN300-82037_1_1_1



CID: EN300-82037_1_1_1

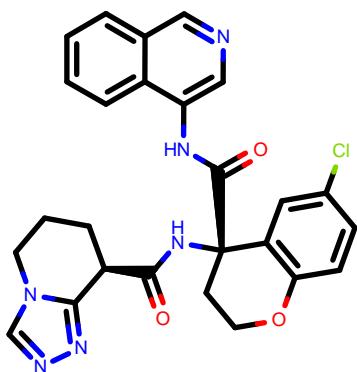
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5C=CON5

RUN: RUN4075

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.18

EN300-748981_1_1_1



CID: EN300-748981_1_1_1

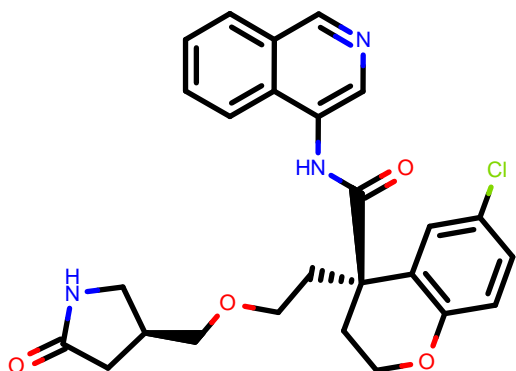
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CCc6c5nn6

RUN: RUN2913

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.27

EN300-246747_3_2_1



CID: EN300-246747_3_2_1

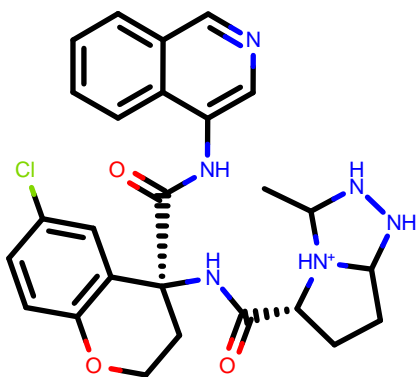
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5CC(=O)N5

RUN: RUN3844

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.28

EN300-6489289_1_2_1



CID: EN300-6489289_1_2_1

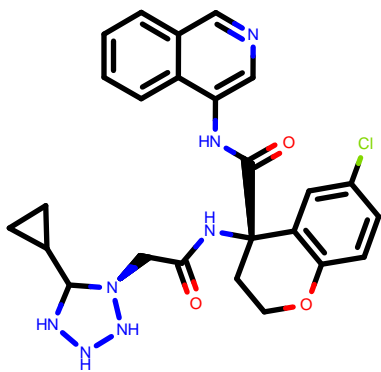
SMILES: Cc1nc2n1[C@@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN2920

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.30

EN300-872798_1_1_1



CID: EN300-872798_1_1_1

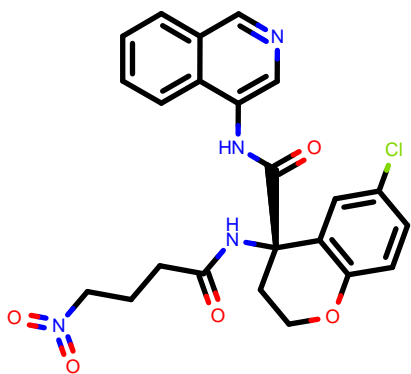
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(mn5)C6CC6

RUN: RUN4129

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.34

EN300-143449_1_1_1



CID: EN300-143449_1_1_1

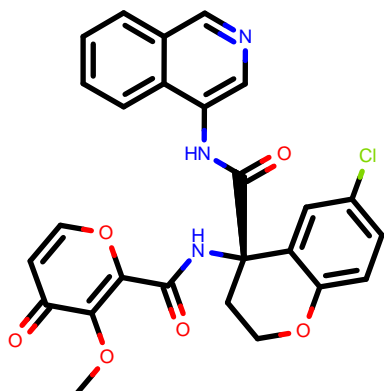
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCN(=O)=O

RUN: RUN3645

DDG (kcal/mol): -2.95

dDDG (kcal/mol): 0.21

EN300-7465954_1_1_1



CID: EN300-7465954_1_1_1

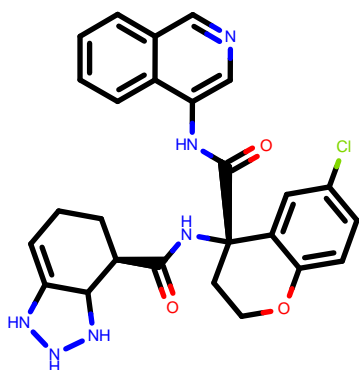
SMILES: COc1c(O)cccc1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccccc5

RUN: RUN3744

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.25

EN300-208236_1_1_1



CID: EN300-208236_1_1_1

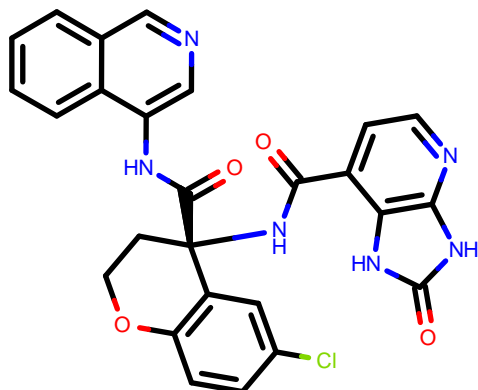
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5CNC6c6c5n[nH]n6

RUN: RUN2736

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.23

EN300-189901_1_1_1



CID: EN300-189901_1_1_1

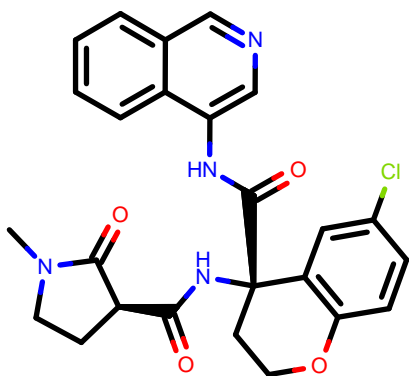
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc6c5[nH]c1=O[nH]6

RUN: RUN2758

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.24

EN300-141695_1_1_1



CID: EN300-141695_1_1_1

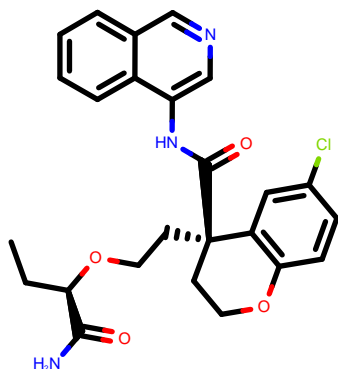
SMILES: CN1CC[C@@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN2815

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.26

EN300-65839_3_2_1



CID: EN300-65839_3_2_1

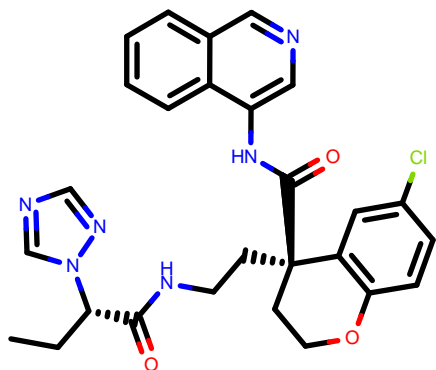
SMILES: CC[C@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN2746

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.32

EN300-651307_3_1_1



CID: EN300-651307_3_1_1

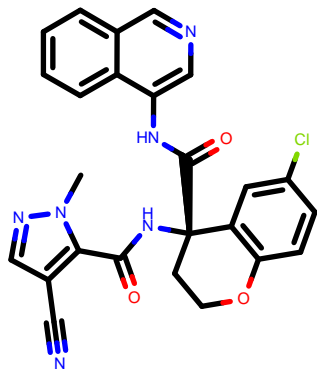
SMILES: CC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)n5cnnc5

RUN: RUN3173

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.27

EN300-2983057_1_1_1



CID: EN300-2983057_1_1_1

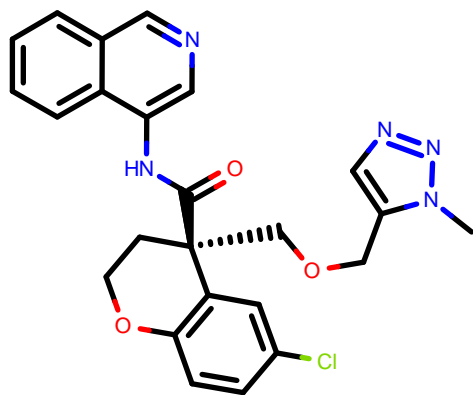
SMILES: Cn1c(c(en1)C#N)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3463

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.23

EN300-216673_2_1_1



CID: EN300-216673_2_1_1

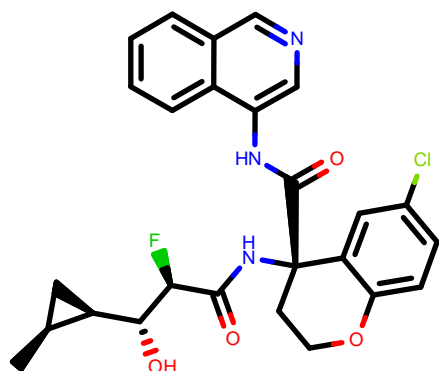
SMILES: Cn1c(cnn1)COC[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3492

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.25

EDG-MED-90036822-94_16



CID: EDG-MED-90036822-94_16

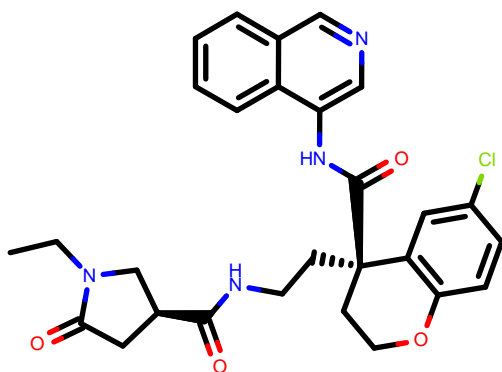
SMILES: C[C@H]1[C@@H]2[C@H]3[C@@H]4[C@H]5[C@@H]6[C@@]2(CCOC3c2cc(cc3)C)C1=O)Nc4cncc5c4cccc5F)O

RUN: RUN1700

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.22

EN300-33478_3_2_1



CID: EN300-33478_3_2_1

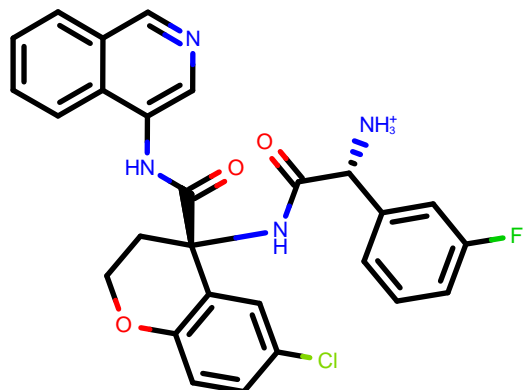
SMILES: CCN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4628

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.44

EDG-MED-90036822-91_1



CID: EDG-MED-90036822-91_1

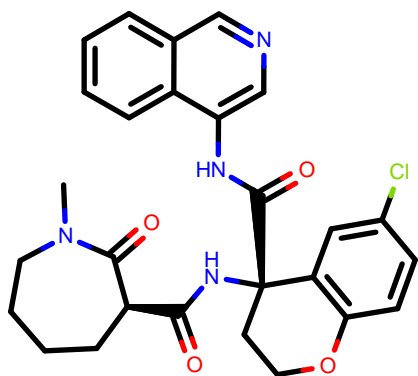
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)[C@]5[H](c5cccc(c5)F)[NH3+]

RUN: RUN1652

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.25

EN300-304695_1_1_1



CID: EN300-304695_1_1_1

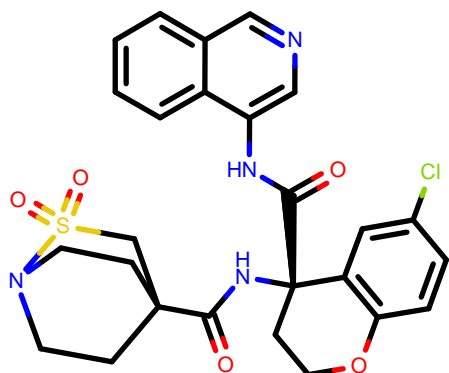
SMILES: CN1CCCC[C@@H](C1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN2814

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.22

EN300-6731334_1_1_1



CID: EN300-6731334_1_1_1

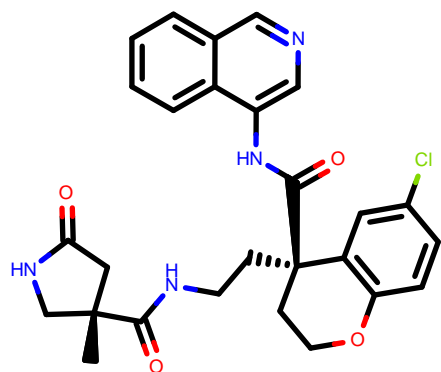
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C56CCN(CC5)S(=O)(=O)C6

RUN: RUN2780

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.36

EN300-132157_3_1_1



CID: EN300-132157_3_1_1

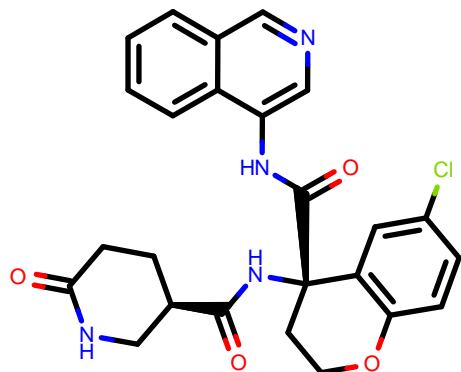
SMILES: ClC@@]1(CC(=O)NC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN4262

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.29

EN300-42819_1_1_1



CID: EN300-42819_1_1_1

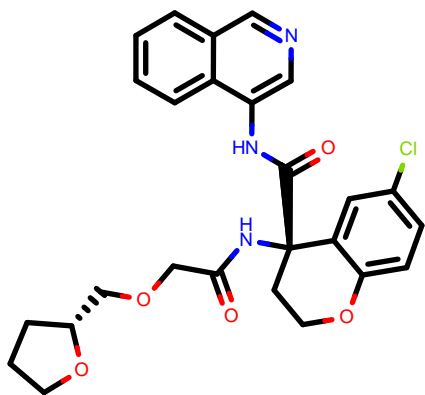
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@]5CCCC(=O)NCS

RUN: RUN2715

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.23

EN300-60033_1_2_1



CID: EN300-60033_1_2_1

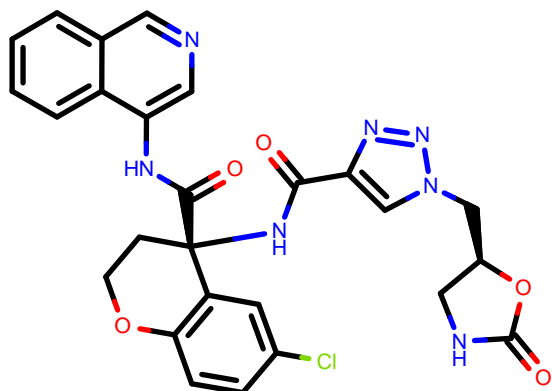
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COC[C@H]5CCOC5

RUN: RUN3481

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.29

EN300-379219_1_1_1



CID: EN300-379219_1_1_1

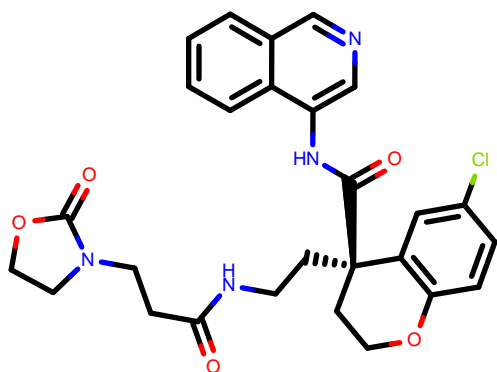
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CN(C)C5=O

RUN: RUN5085

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.28

EN300-53918_3_1_1



CID: EN300-53918_3_1_1

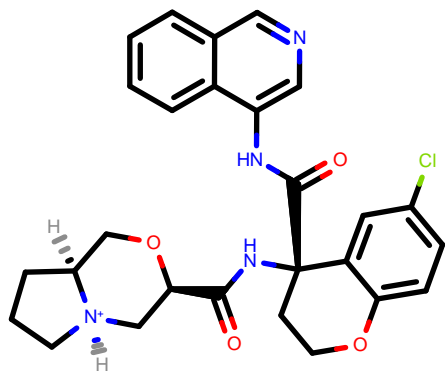
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCN5CCOC5=O

RUN: RUN4781

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.27

EN300-7437385_1_1_1



CID: EN300-7437385_1_1_1

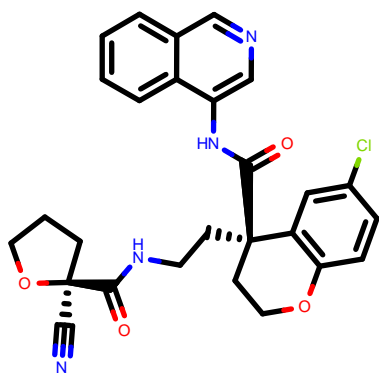
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[NH+]5CC[C@H]6CCOC6

RUN: RUN3255

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.42

EN300-3710141_3_1_1



CID: EN300-3710141_3_1_1

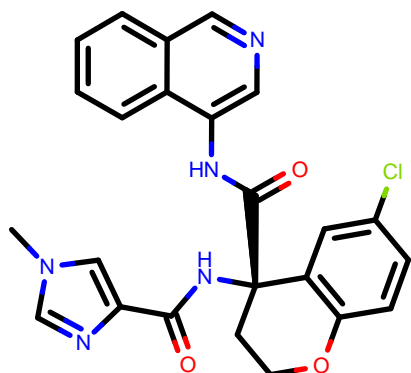
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN4633

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.27

EN300-97847_1_1_1



CID: EN300-97847_1_1_1

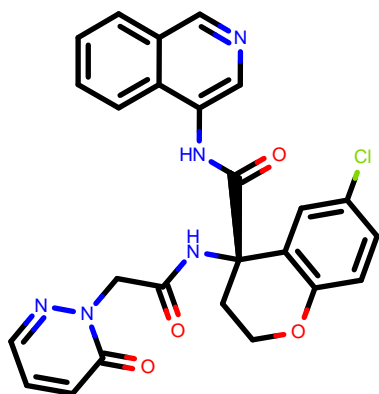
SMILES: Cn1cc(nc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3059

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.21

EN300-237561_1_1_1



CID: EN300-237561_1_1_1

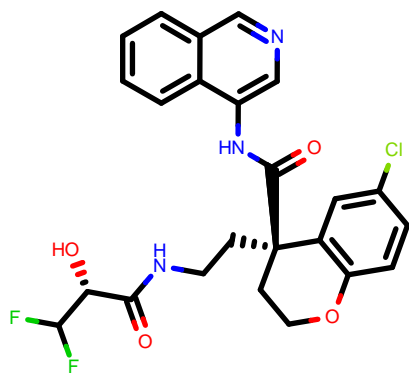
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c(c=O)cccn5

RUN: RUN3129

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.33

EN300-1932780_3_2_1



CID: EN300-1932780_3_2_1

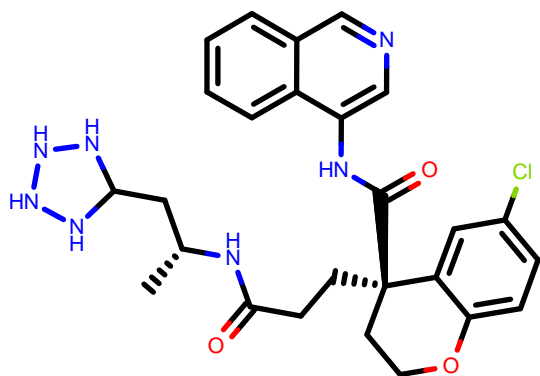
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H](C(F)F)O

RUN: RUN3065

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.31

EN300-76387_2_2_1



CID: EN300-76387_2_2_1

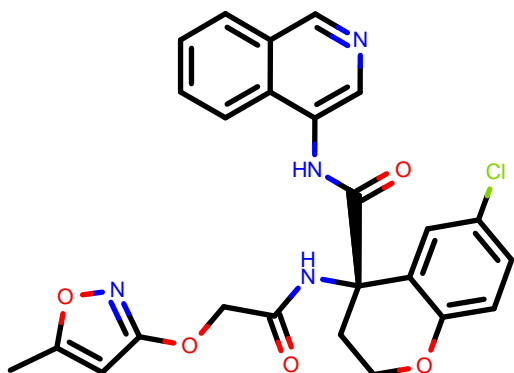
SMILES: C[C@H](CC1N[NH2+][NH2+][N1]NC(=O)CC[C@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN5099

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.24

EN300-12929_1_1_1



CID: EN300-12929_1_1_1

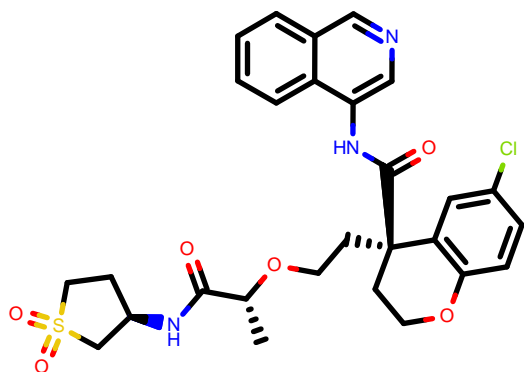
SMILES: Cc1cc(no1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3696

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.26

EN300-23318_3_2_1



CID: EN300-23318_3_2_1

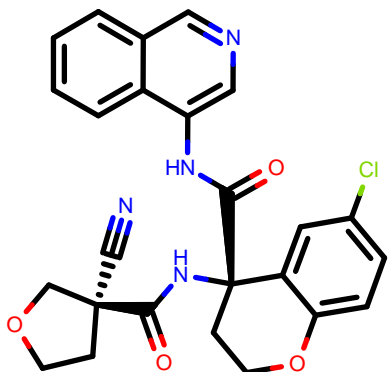
SMILES: C[C@H](Cl)O[N]C@]H1[CC]S(=O)(=O)C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN4305

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.38

EN300-261210_1_2_1



CID: EN300-261210_1_2_1

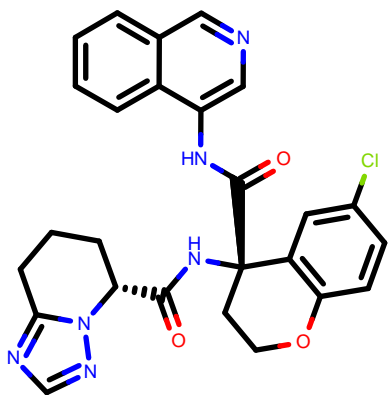
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)C#N

RUN: RUN3033

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.23

EN300-1273016_1_2_1



CID: EN300-1273016_1_2_1

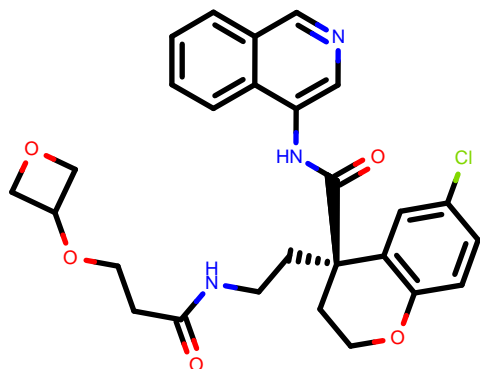
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC6n5nc6

RUN: RUN2791

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.31

EN300-321703_3_1_1



CID: EN300-321703_3_1_1

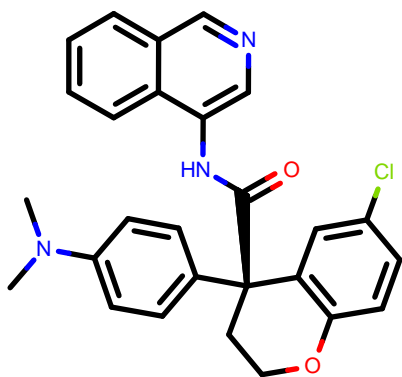
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCOC5OC5

RUN: RUN3973

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.31

VLA-UCB-551c2366-1_1



CID: VLA-UCB-551c2366-1_1

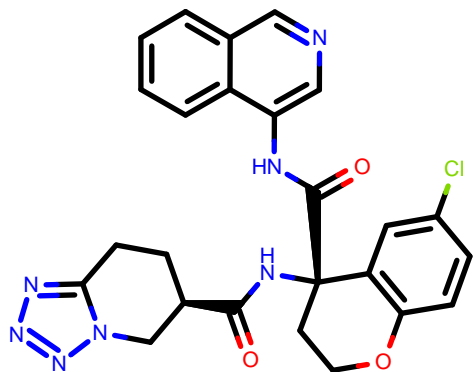
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5

RUN: RUN995

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.20

EN300-269453_1_1_1



CID: EN300-269453_1_1_1

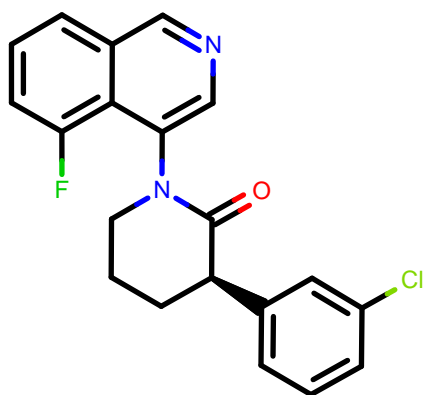
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC6n6nn6C5

RUN: RUN2793

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.27

MIC-UNK-50cce87d-9_2



CID: MIC-UNK-50cce87d-9_2

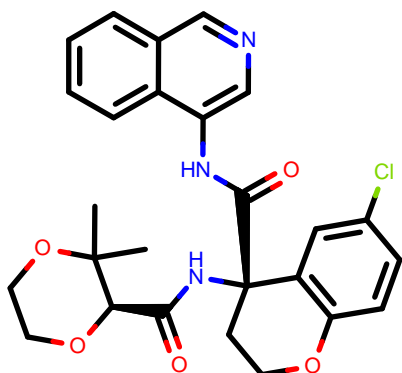
SMILES: c1cc(cc(c1)Cl)[C@H]2CCCN(C2=O)c3cncc4c3c(ccc4)F

RUN: RUN562

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.20

EN300-1601684_1_2_1



CID: EN300-1601684_1_2_1

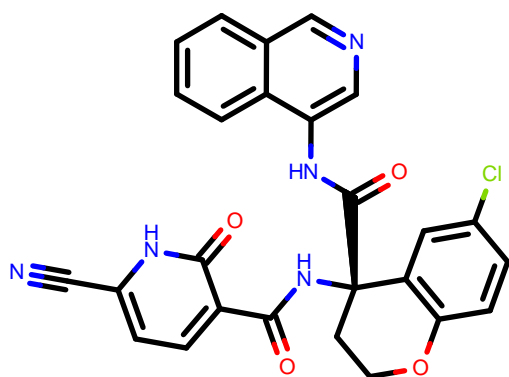
SMILES: CC1([C@H](OCCO1)C(=O)N)C@2(COCOC3C2C(C3)Cl)C(=O)Nc4cncc5c4ccoc5)C

RUN: RUN2849

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.25

EN300-640698_1_1_1



CID: EN300-640698_1_1_1

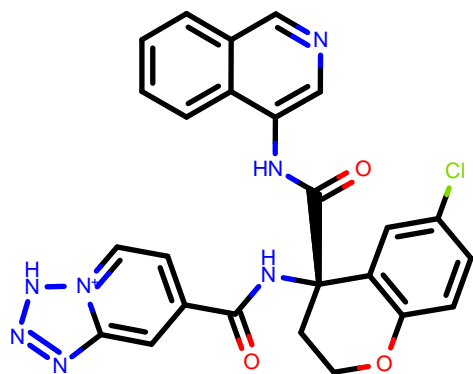
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc([nH]c5=O)[C#N

RUN: RUN2874

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.24

EN300-305567_1_1_1



CID: EN300-305567_1_1_1

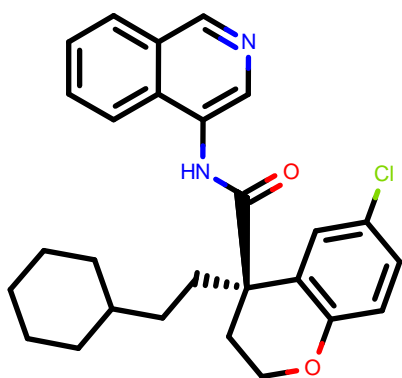
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc[nH]c5nn[nH]6

RUN: RUN4823

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.27

DAR-DIA-6a508060-9_1_1



CID: DAR-DIA-6a508060-9_1_1

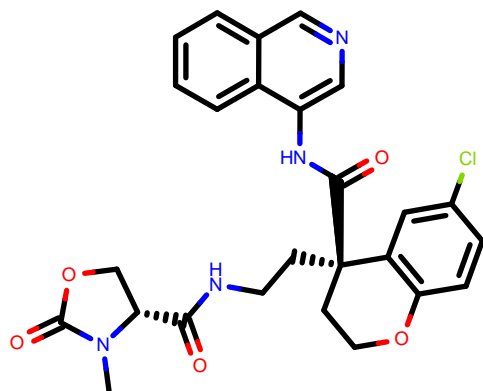
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCS5CCCC5

RUN: RUN4136

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.31

EN300-332838_3_2_1



CID: EN300-332838_3_2_1

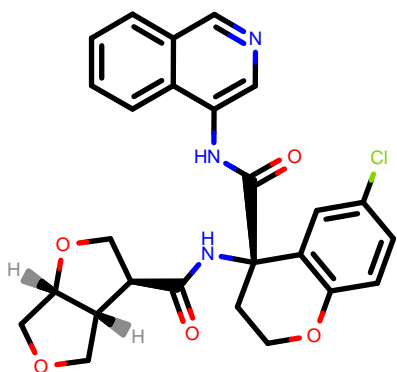
SMILES: CN1[C@H](COC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4168

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.27

EN300-6482296_1_5_1



CID: EN300-6482296_1_5_1

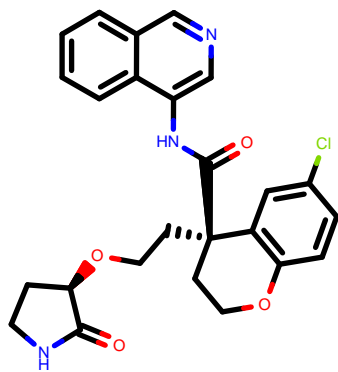
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@]5(CO)C[C@H]5COC6

RUN: RUN3499

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.26

EN300-6736413_3_1_1



CID: EN300-6736413_3_1_1

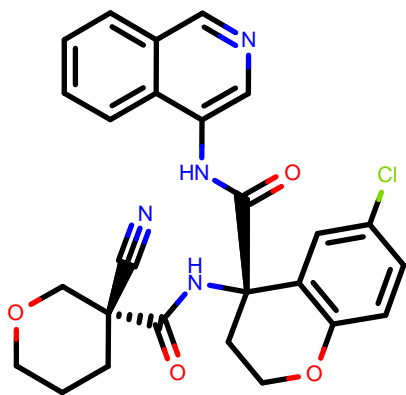
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(C)CNC5=O

RUN: RUN3545

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.26

EN300-301925_1_1_1



CID: EN300-301925_1_1_1

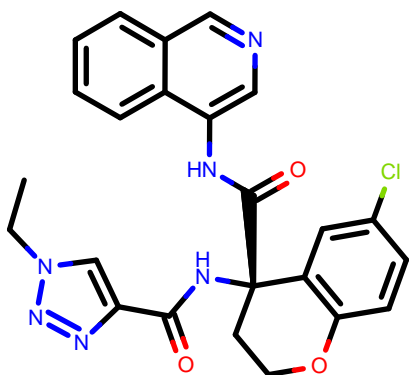
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN3044

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.29

EN300-262745_1_1_1



CID: EN300-262745_1_1_1

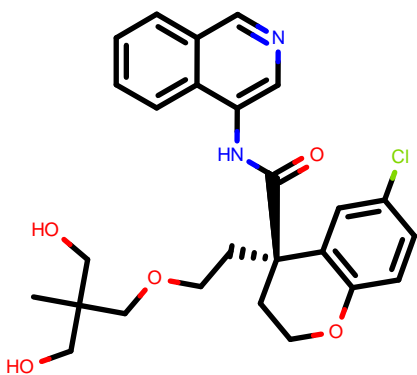
SMILES: CCn1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4404

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.22

EN300-218116_3_1_1



CID: EN300-218116_3_1_1

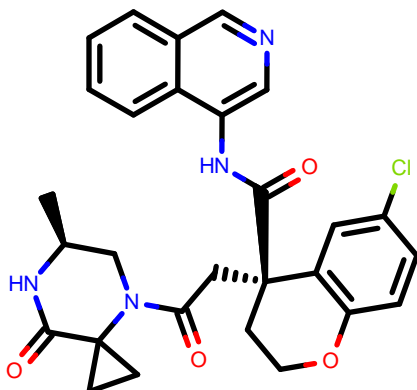
SMILES: CC(CO)(CO)COCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN4937

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.42

EN300-7542429_1_2_1



CID: EN300-7542429_1_2_1

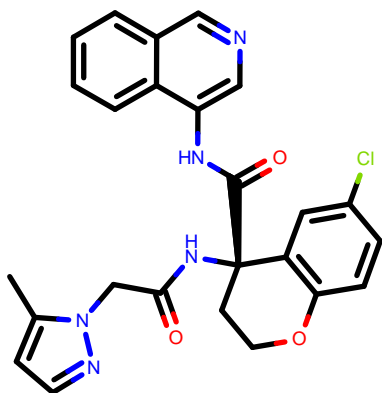
SMILES: C[C@@H]1CN(C2(CC2)C(=O)N1)C(=O)C[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cncc6c5cccc6

RUN: RUN2887

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.27

EN300-83558_1_1_1



CID: EN300-83558_1_1_1

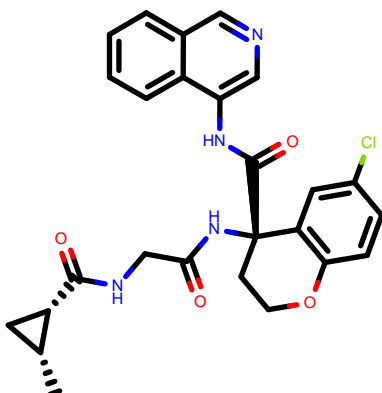
SMILES: Cc1ccnn1CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3688

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.24

EN300-30768_1_1_1



CID: EN300-30768_1_1_1

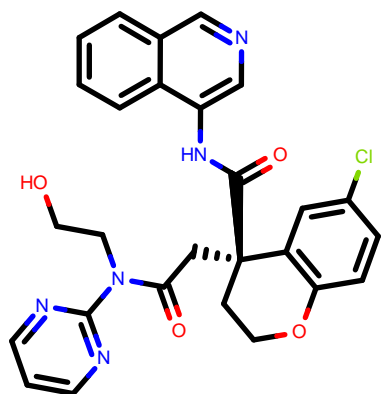
SMILES: C[C@@H]1C[C@@H]1C(=O)NCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3950

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.31

EN300-65352_1_1_1



CID: EN300-65352_1_1_1

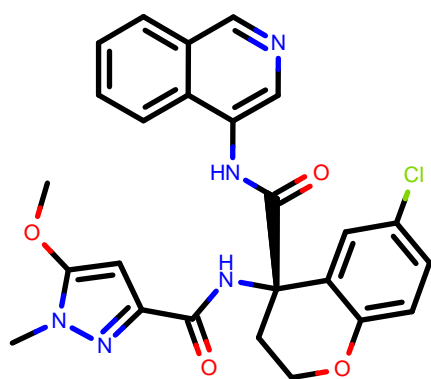
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N(CCO)c5ncccc5

RUN: RUN2934

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.27

EN300-142240_1_1_1



CID: EN300-142240_1_1_1

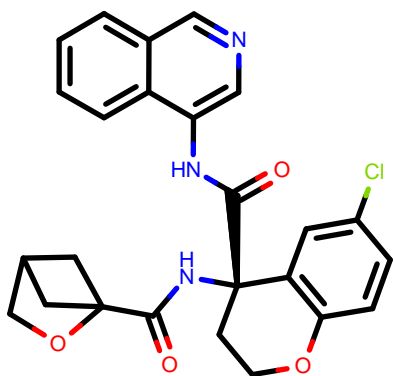
SMILES: Cn1c(cc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC

RUN: RUN2843

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.28

EN300-2007648_1_1_1



CID: EN300-2007648_1_1_1

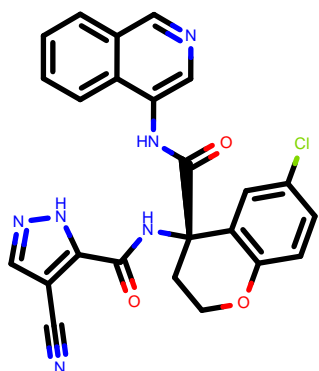
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C56CC(C5)CO6

RUN: RUN2741

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.22

EN300-1267109_1_1_1



CID: EN300-1267109_1_1_1

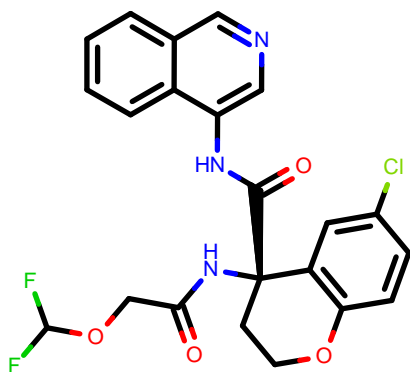
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(c[nH]5)C#N

RUN: RUN3472

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.18

EN300-179091_1_1_1



CID: EN300-179091_1_1_1

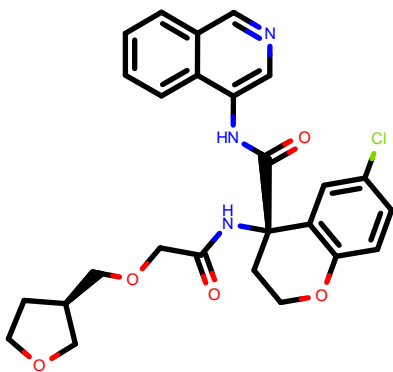
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COC(F)F

RUN: RUN5288

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.18

EN300-80522_1_1_1



CID: EN300-80522_1_1_1

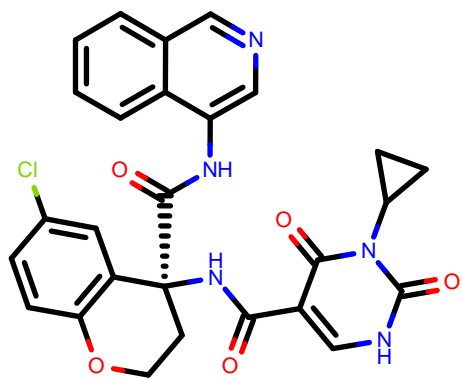
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COC[C@@H]5CCOC5

RUN: RUN4408

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.24

EN300-7433864_1_1_1



CID: EN300-7433864_1_1_1

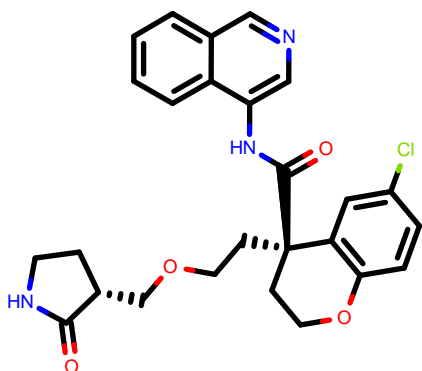
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]c(=O)n(c5=O)C6CC6

RUN: RUN3214

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.33

EN300-246248_3_2_1



CID: EN300-246248_3_2_1

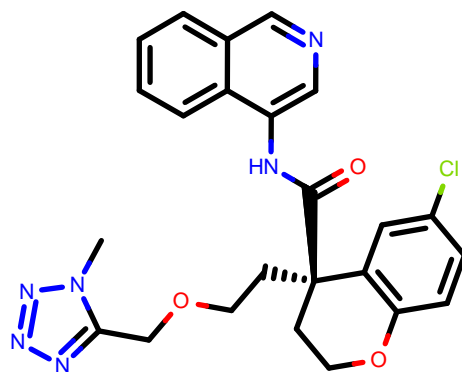
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5CCNC5=O

RUN: RUN3788

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.27

EN300-62574_3_1_1



CID: EN300-62574_3_1_1

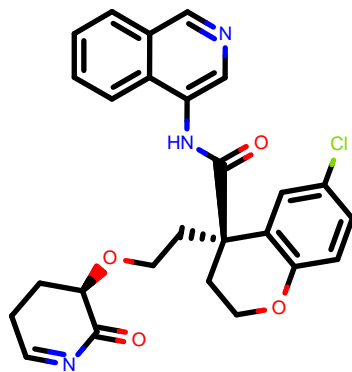
SMILES: Cn1c(nnn1)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3282

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.27

EN300-107267_3_1_1



CID: EN300-107267_3_1_1

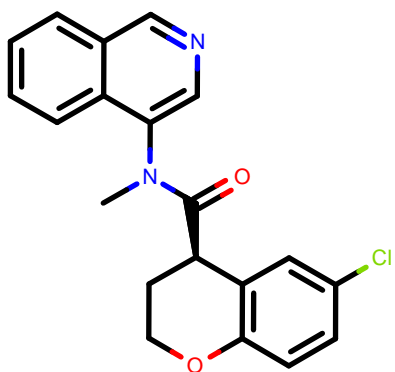
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@]5CCNC5=O

RUN: RUN3143

DDG (kcal/mol): -2.85

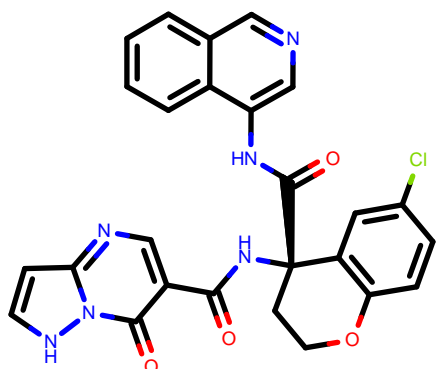
dDDG (kcal/mol): 0.21

MAK-UNK-3875bbc8-2_1_1



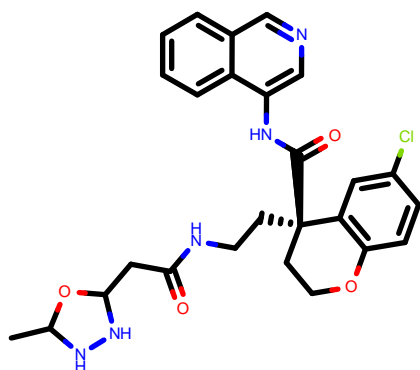
CID:	MAK-UNK-3875bbc8-2_1_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN3363
DDG (kcal/mol):	-2.85
dDDG (kcal/mol):	0.09

EN300-220228_1_1_1



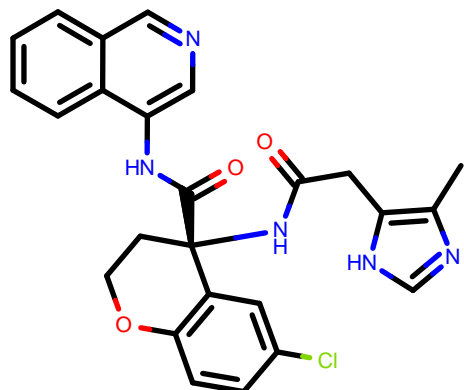
CID:	EN300-220228_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6cc[nH]n6c5=O</chem>
RUN:	RUN3935
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.25

EN300-64193_3_1_1



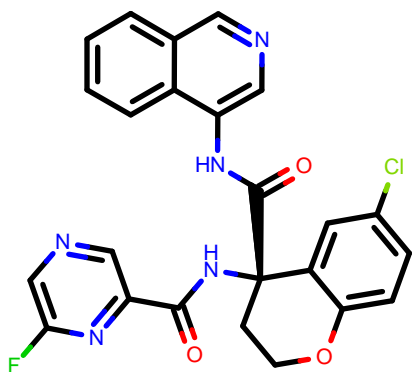
CID:	EN300-64193_3_1_1
SMILES:	<chem>Cc1nnc(o1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN3141
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.26

EN300-186929_1_1_1



CID:	EN300-186929_1_1_1
SMILES:	<chem>Cc1c(nc[nH]1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN2980
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.24

EN300-373552_1_1_1



CID: EN300-373552_1_1_1

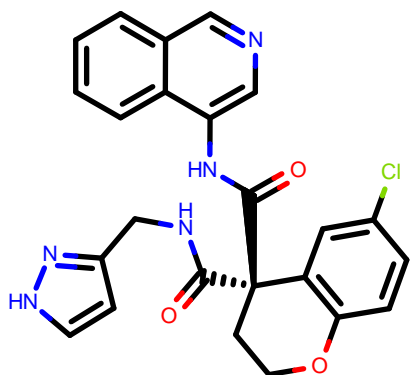
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc[n5]F

RUN: RUN2996

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.19

VLA-UCB-34f3ed0c-3_1_1



CID: VLA-UCB-34f3ed0c-3_1_1

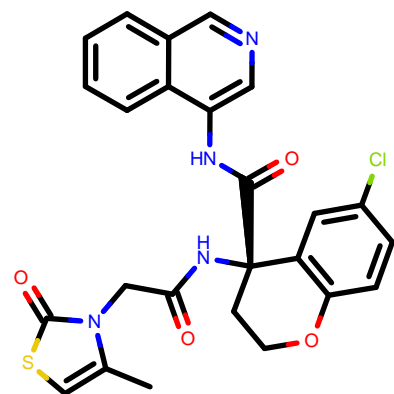
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)NC5c[nH]5

RUN: RUN2909

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.26

EN300-12067_1_1_1



CID: EN300-12067_1_1_1

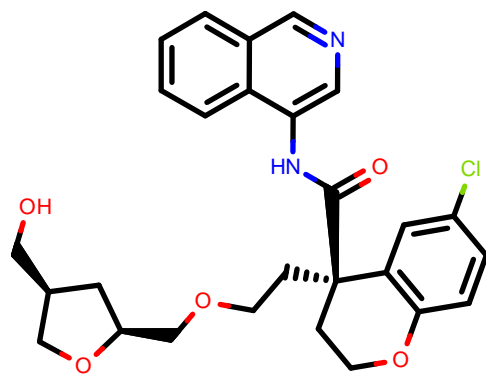
SMILES: Cc1csc(=O)n1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN2987

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.28

EN300-6494158_3_1_1



CID: EN300-6494158_3_1_1

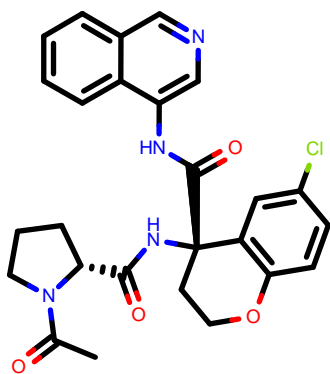
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5C[C@@H](CO)CO

RUN: RUN3537

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.32

EN300-211777_1_1_1



CID: EN300-211777_1_1_1

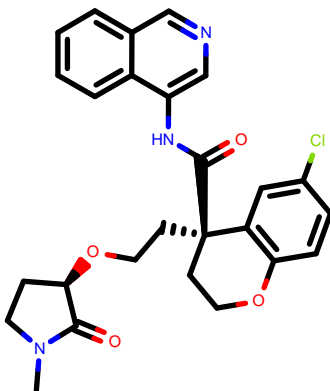
SMILES: CC(=O)N1CCC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2810

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.33

EN300-98648_3_2_1



CID: EN300-98648_3_2_1

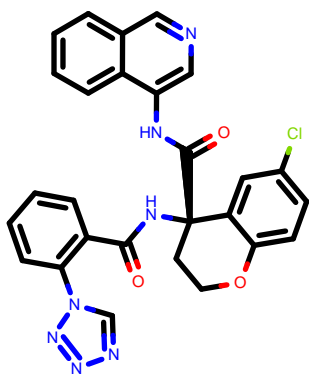
SMILES: CN1CC[C@H](C1=O)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2936

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.28

EN300-09325_1_1_1



CID: EN300-09325_1_1_1

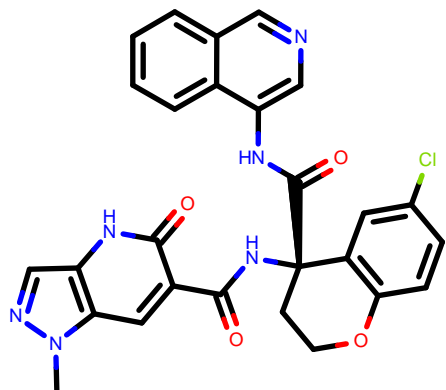
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5n6cnnn6

RUN: RUN2925

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.26

EN300-805037_1_1_1



CID: EN300-805037_1_1_1

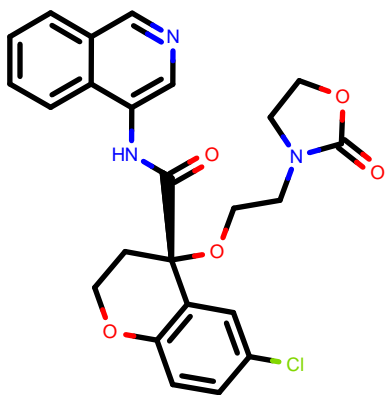
SMILES: Cn1c2cc(c(=O)[nH]c2cn1)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cncoc5ccoc6

RUN: RUN3274

DDG (kcal/mol): -2.83

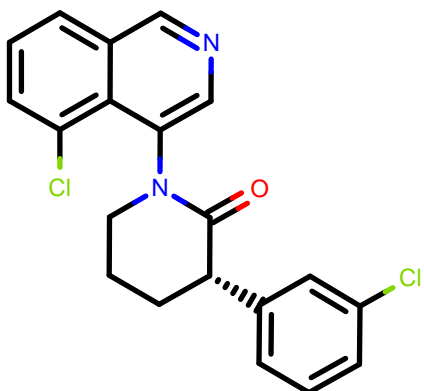
dDDG (kcal/mol): 0.33

CHO-MSK-5891c1ff-3_1



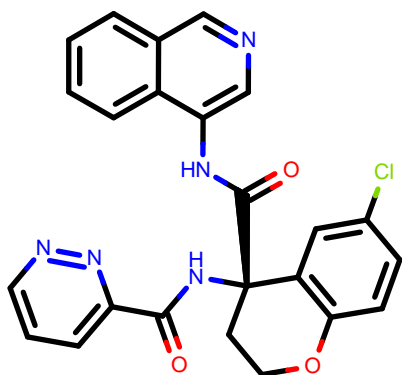
CID:	CHO-MSK-5891c1ff-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O</chem>
RUN:	RUN1726
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.22

MIC-UNK-50cce87d-10_1



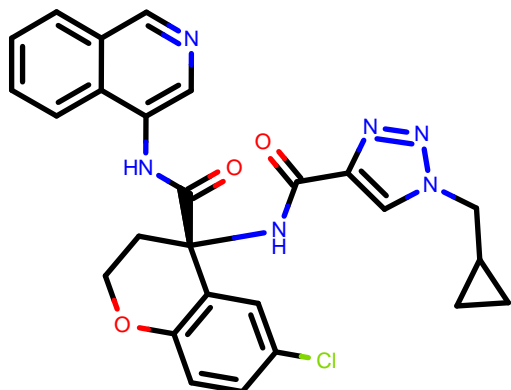
CID:	MIC-UNK-50cce87d-10_1
SMILES:	<chem>c1cc(cc(c1)Cl)C(=O)N[C@@H]2CCCCN(C2=O)c3cncc4c3c(ccc4)Cl</chem>
RUN:	RUN559
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.34

EN300-79022_1_1_1



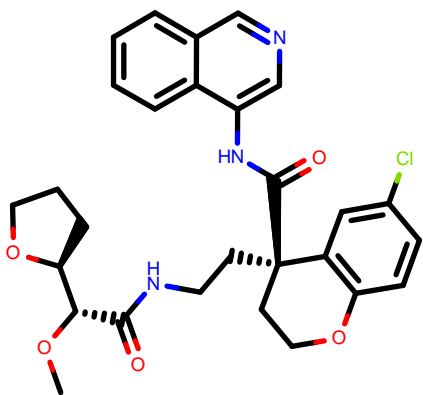
CID:	EN300-79022_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5</chem>
RUN:	RUN4376
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.19

EN300-247428_1_1_1



CID:	EN300-247428_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]5C6CC6</chem>
RUN:	RUN3302
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.25

EN300-6277108_3_2_1



CID: EN300-6277108_3_2_1

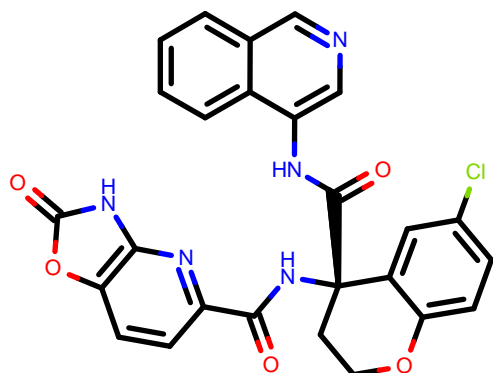
SMILES: CO[C@H]([C@@H]1CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3O)C(=O)Nc4ccc5c4ccc5

RUN: RUN4244

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.35

EN300-188174_1_1_1



CID: EN300-188174_1_1_1

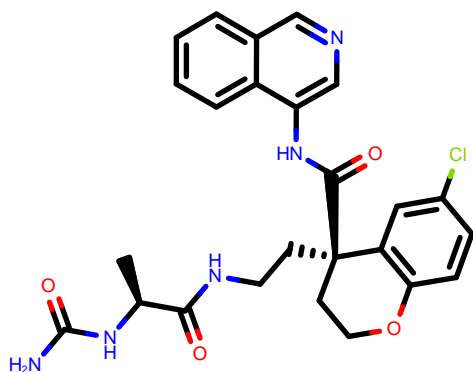
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C)NC(=O)c5ccc6c(n5)[nH]c(=O)o6

RUN: RUN3210

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.23

EN300-00271_3_1_1



CID: EN300-00271_3_1_1

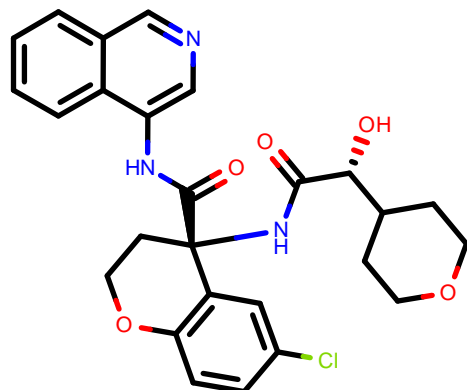
SMILES: C[C@@H]([C@@H]1CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3O)C)NC(=O)Nc3ccc4c3ccc4NC(=O)N

RUN: RUN5617

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.33

EN300-7443878_1_1_1



CID: EN300-7443878_1_1_1

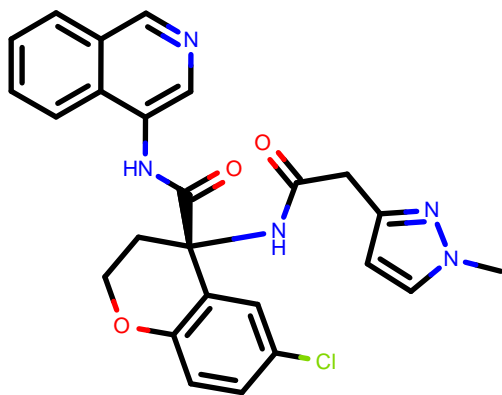
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C)NC(=O)[C@@H]5C5COCC5O

RUN: RUN3403

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.24

EN300-258702_1_1_1



CID: EN300-258702_1_1_1

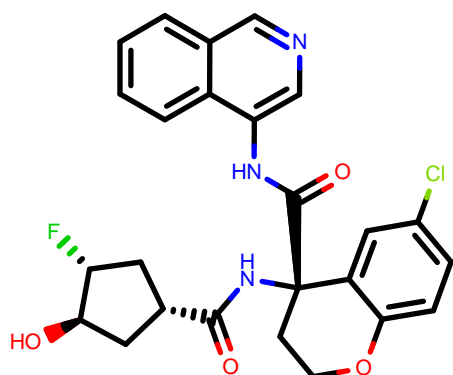
SMILES: Cn1ccc(n1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3103

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.23

EN300-7461217_1_1_1



CID: EN300-7461217_1_1_1

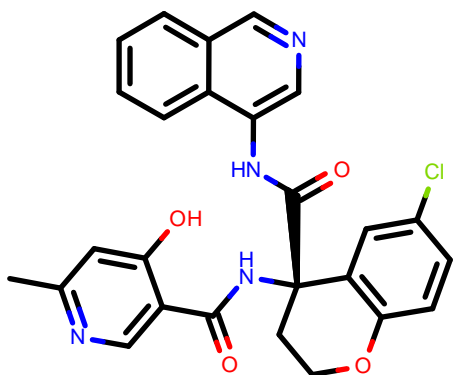
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(COCOC4c3cc(cc4)Cl)N(C)C(=O)Nc5cnc(C)nc5F

RUN: RUN3199

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.25

EN300-85853_1_1_1



CID: EN300-85853_1_1_1

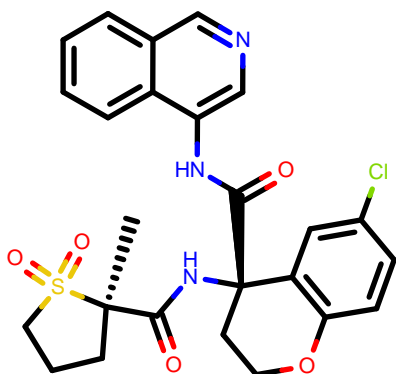
SMILES: Cc1cc(=O)c(c[nH]1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3700

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.30

EN300-373476_1_1_1



CID: EN300-373476_1_1_1

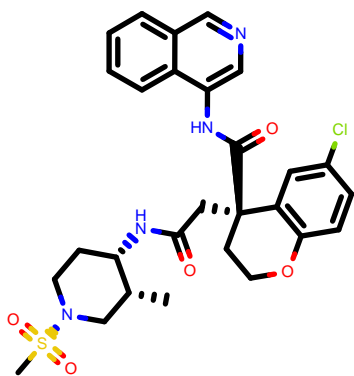
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2818

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.32

ALP-POS-5bb456a5-1_9



CID: ALP-POS-5bb456a5-1_9

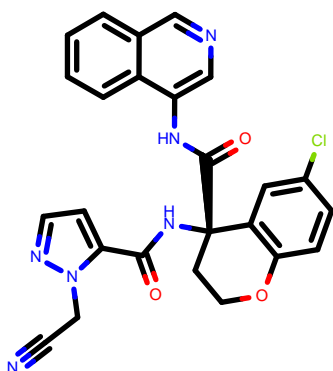
SMILES: C[C@@H]1CN[C@@H]2C[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5S(=O)(=O)C

RUN: RUN2301

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.41

EDJ-MED-6864a934-5_1



CID: EDJ-MED-6864a934-5_1

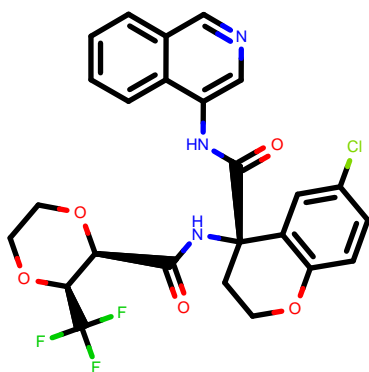
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn5CC#N

RUN: RUN2427

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.24

EN300-322400_1_1_1



CID: EN300-322400_1_1_1

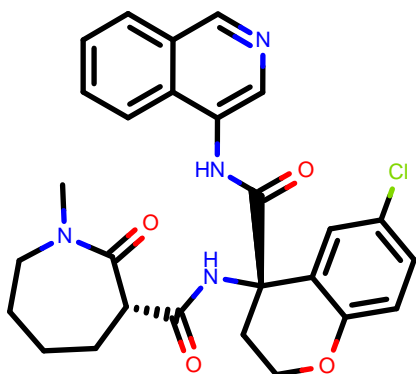
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5H5[C@@H](OCOC5)C(F)F

RUN: RUN2731

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.24

EN300-304695_1_2_1



CID: EN300-304695_1_2_1

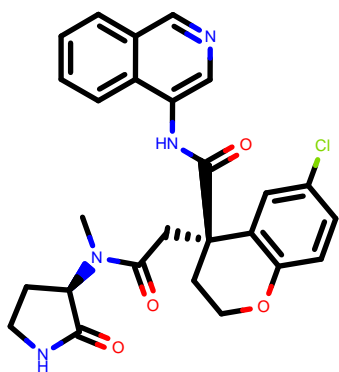
SMILES: CN1CCCC[C@@H](C1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5S

RUN: RUN3374

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.27

EN300-120119_1_1_1



CID: EN300-120119_1_1_1

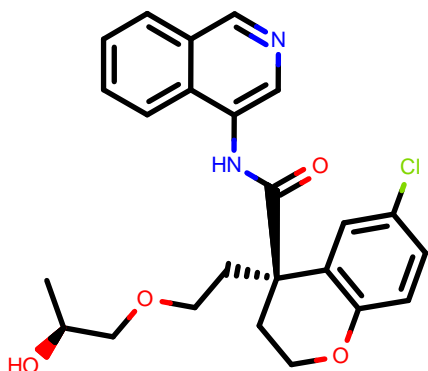
SMILES: CN[C@@H]1CCNC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN2824

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.24

EN300-185378_3_1_1



CID: EN300-185378_3_1_1

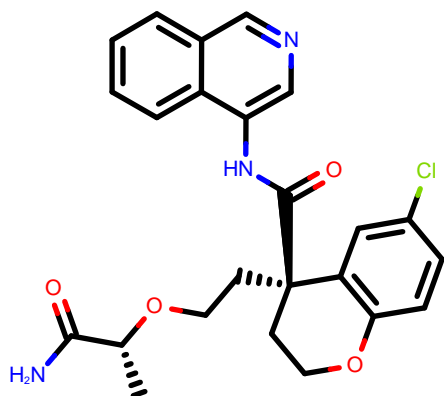
SMILES: C[C@@H](COCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN3277

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.30

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

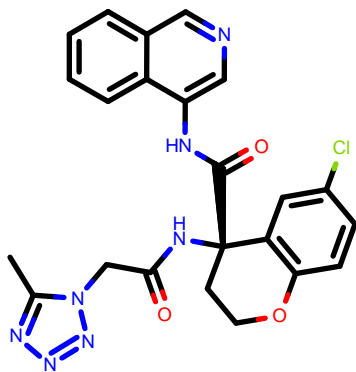
SMILES: C[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN2992

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.22

EN300-1244816_1_1_1



CID: EN300-1244816_1_1_1

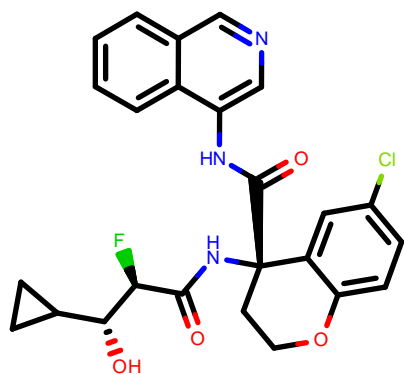
SMILES: Cc1nnn1CC(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3046

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.25

EDG-MED-90036822-78_1



CID: EDG-MED-90036822-78_1

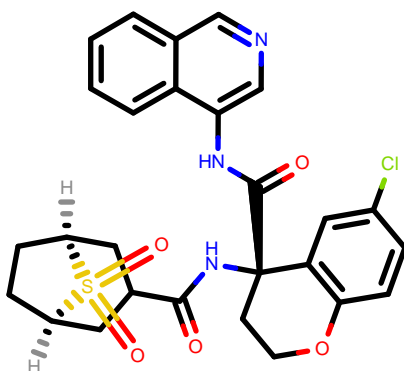
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H(C5CC5)O)F

RUN: RUN1672

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.21

EN300-373435_1_1_1



CID: EN300-373435_1_1_1

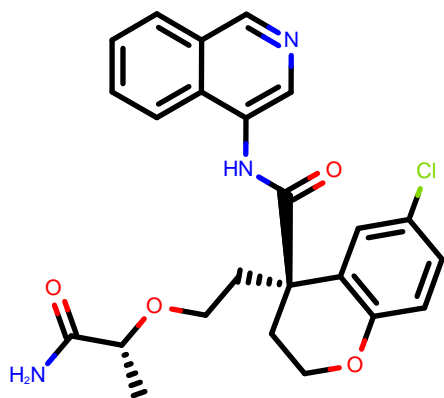
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5C[C@@H]N(C)C5=O

RUN: RUN6704

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.30

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

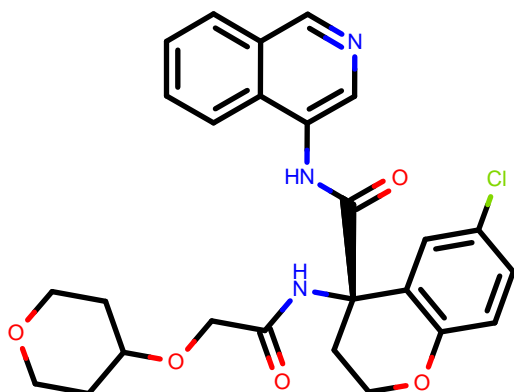
SMILES: C[C@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN2896

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.24

EN300-77520_1_1_1



CID: EN300-77520_1_1_1

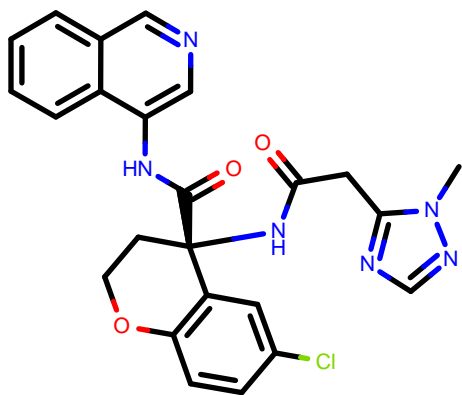
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC5COCC5

RUN: RUN2786

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.21

EN300-209316_1_1_1



CID: EN300-209316_1_1_1

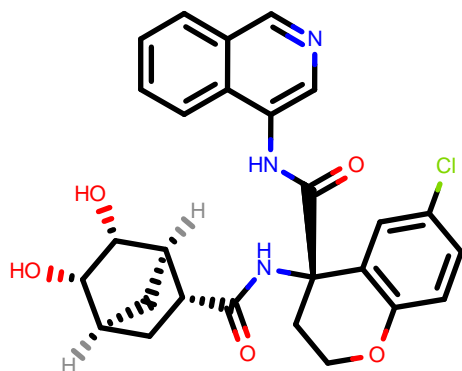
SMILES: Cn1c(ncn1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN2979

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.21

EN300-6744028_1_7_1



CID: EN300-6744028_1_7_1

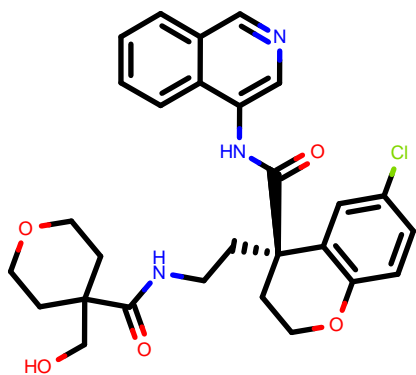
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5H5C[C@@]H6[C@@]H5[C@@]H6[C@@]H5O

RUN: RUN3462

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.26

EN300-244909_3_1_1



CID: EN300-244909_3_1_1

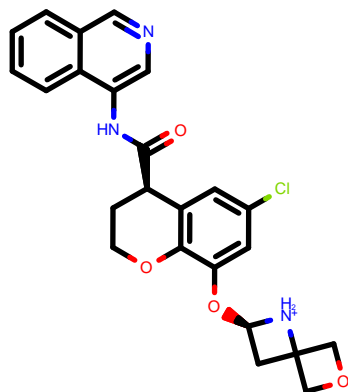
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCOCC5)CO

RUN: RUN2854

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.33

DAR-DIA-23e5a6a0-3_1_1



CID: DAR-DIA-23e5a6a0-3_1_1

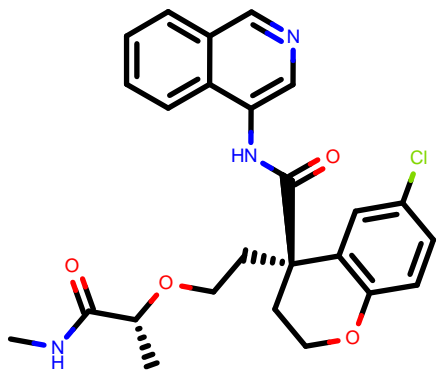
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)[C@@]5H5CC6([NH2+][5]COC6)Cl

RUN: RUN6482

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.30

EN300-211482_3_2_1



CID: EN300-211482_3_2_1

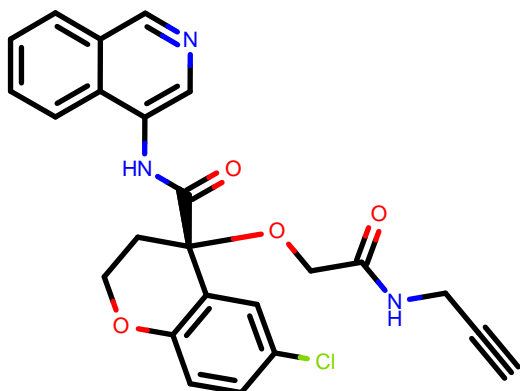
SMILES: C[C@H](C(=O)NC)OCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2964

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.32

EN300-1659582_1_1_1



CID: EN300-1659582_1_1_1

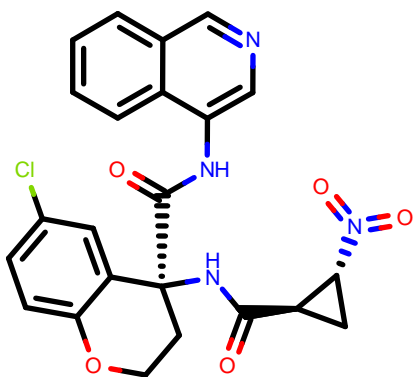
SMILES: C#CCNC(=O)CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5419

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.21

EN300-254854_1_1_1



CID: EN300-254854_1_1_1

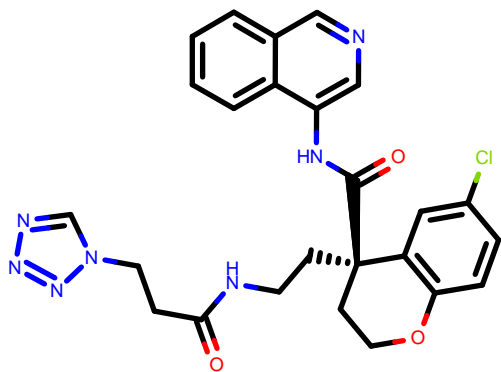
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5[C@@]5N(=O)=O

RUN: RUN2805

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.18

EN300-191904_3_1_1



CID: EN300-191904_3_1_1

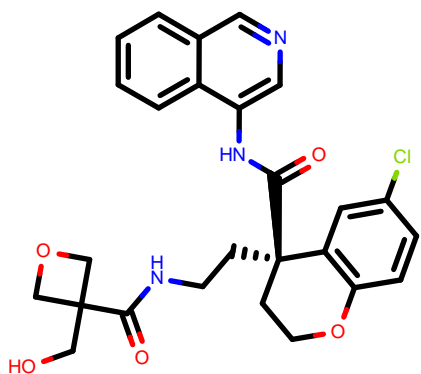
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5nnn5

RUN: RUN2819

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.35

EN300-105693_3_1_1



CID: EN300-105693_3_1_1

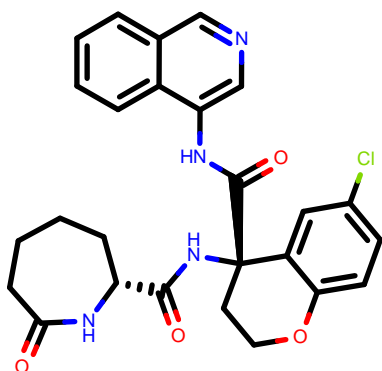
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)CCNC(=O)C5(COC5)CO

RUN: RUN3459

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.31

EN300-80083_1_2_1



CID: EN300-80083_1_2_1

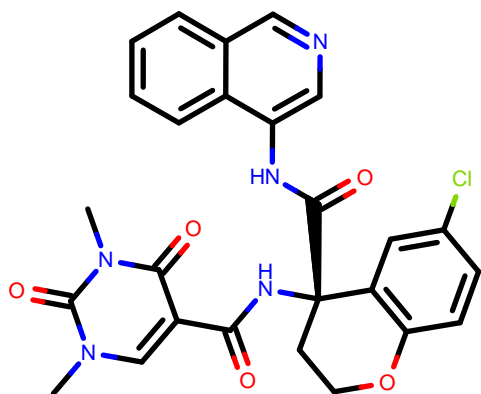
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)NC(=O)[C@H]5CCCCC(=O)N5

RUN: RUN3529

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.26

EN300-79497_1_1_1



CID: EN300-79497_1_1_1

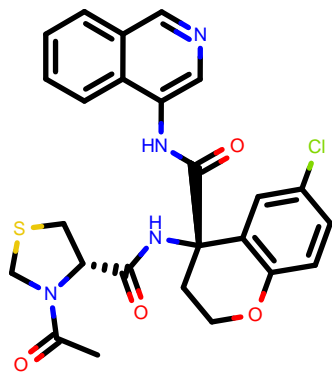
SMILES: Cn1cc(c(=O)n(c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3O)C(=O)Nc4nccc5c4cccc5

RUN: RUN4734

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.37

EN300-56202_1_1_1



CID: EN300-56202_1_1_1

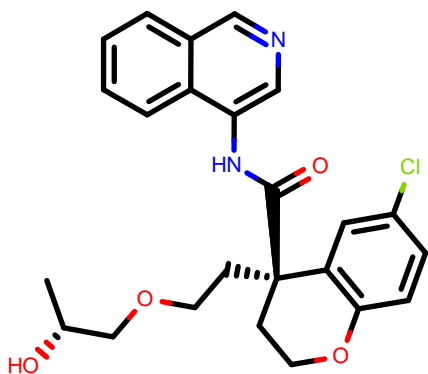
SMILES: CC(=O)N1CSC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3O)C(=O)Nc4nccc5c4cccc5

RUN: RUN2873

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.39

EN300-185378_3_2_1



CID: EN300-185378_3_2_1

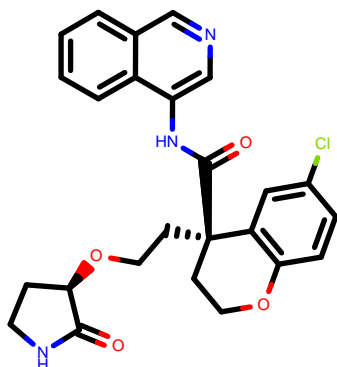
SMILES: C[C@H](COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)O

RUN: RUN4676

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.31

EN300-6736413_3_1_1



CID: EN300-6736413_3_1_1

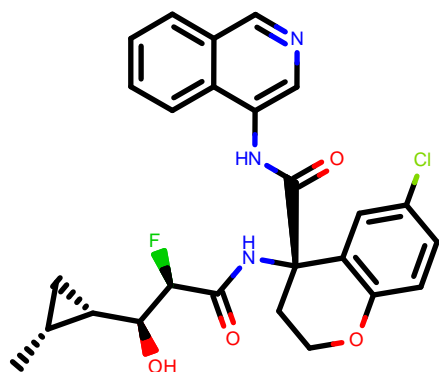
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O

RUN: RUN2766

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.25

EDG-MED-90036822-94_9



CID: EDG-MED-90036822-94_9

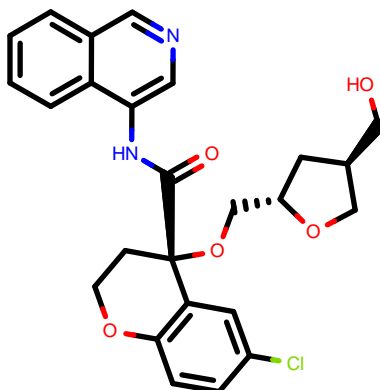
SMILES: C[C@@H]1[C@@H]2[C@@H]3[C@@H]4[C@@H]5C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4c5ccc6c4cccc6)F)O

RUN: RUN1696

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.23

CHO-MSK-5891c1ff-1_1



CID: CHO-MSK-5891c1ff-1_1

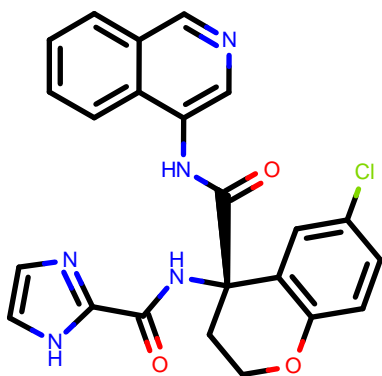
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[C@H](CO)CO5

RUN: RUN1779

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.29

EN300-315836_1_1_1



CID: EN300-315836_1_1_1

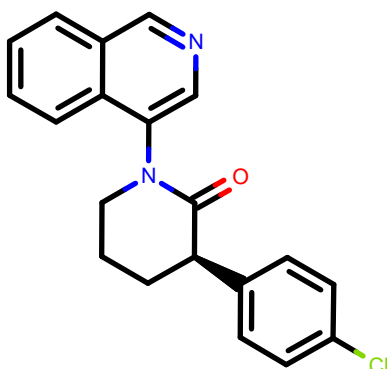
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]jcn5

RUN: RUN3201

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.19

ALP-POS-ce760d3f-8_1



CID: ALP-POS-ce760d3f-8_1

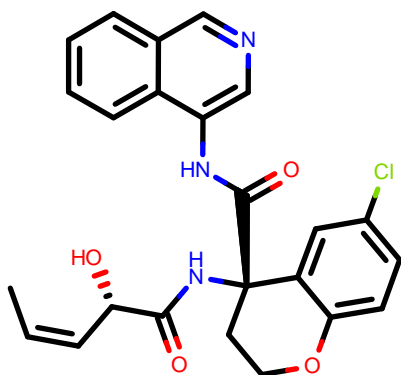
SMILES: c1ccc2c(c1)cncc2N3CCCC[C@@H](C3=O)c4ccc(cc4)Cl

RUN: RUN1278

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.23

EN300-300217_1_1_1



CID: EN300-300217_1_1_1

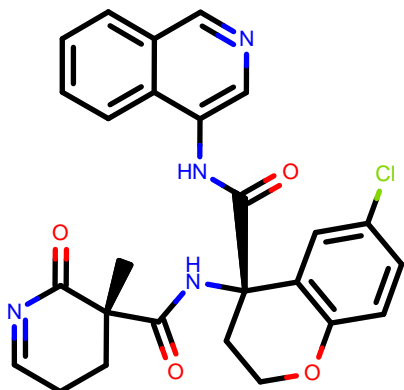
SMILES: C/C=C/[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN3409

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.30

EN300-178876_1_2_1



CID: EN300-178876_1_2_1

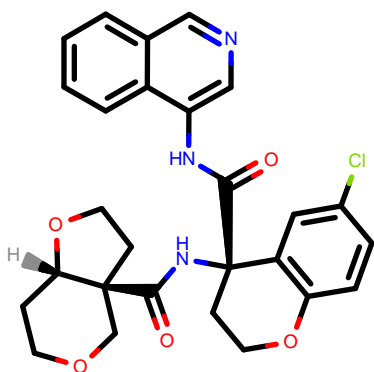
SMILES: C[C@@]1(CCCNC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7412

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.36

EN300-341337_1_4_1



CID: EN300-341337_1_4_1

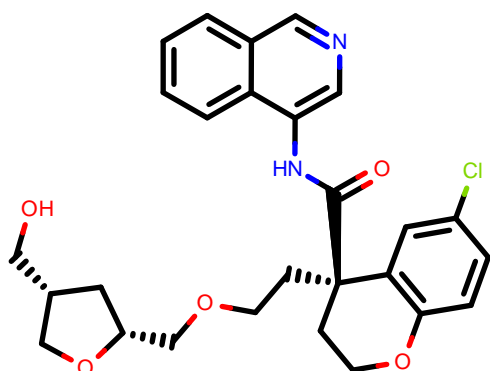
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCO[C@H]5CCOC6

RUN: RUN3512

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.28

EN300-6494158_3_4_1



CID: EN300-6494158_3_4_1

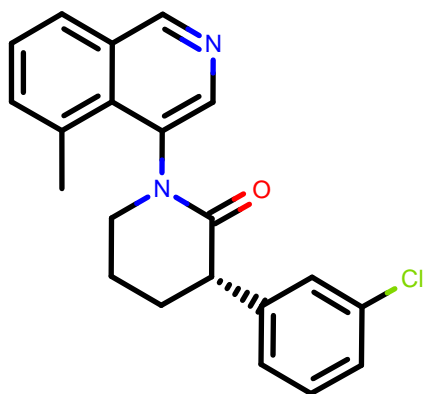
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C[C@H](CO)CO

RUN: RUN7359

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.34

MIC-UNK-50cce87d-11_2



CID: MIC-UNK-50cce87d-11_2

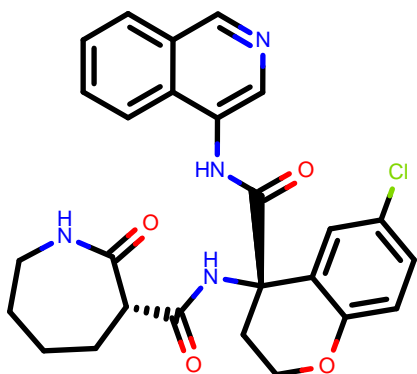
SMILES: Cc1cccc2c1c(cnc2)N3CCCC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN550

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.27

EN300-6737762_1_1_1



CID: EN300-6737762_1_1_1

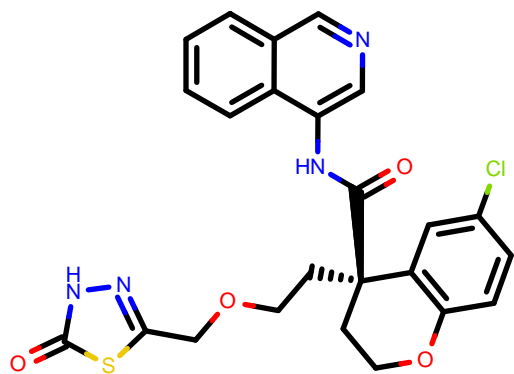
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CCOCCN5=O

RUN: RUN3636

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.24

EN300-171766_3_1_1



CID: EN300-171766_3_1_1

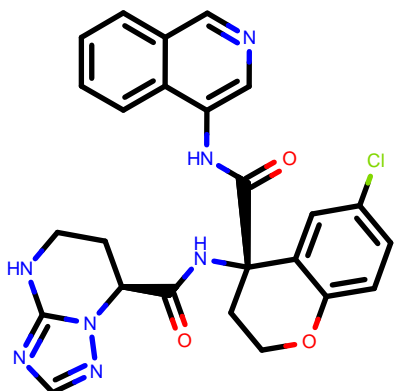
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC5n[nH]c(=O)S5

RUN: RUN3186

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.22

EN300-28262_1_1_1



CID: EN300-28262_1_1_1

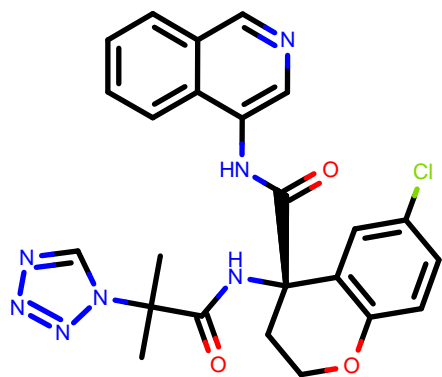
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5CNC(=O)Nc6n5ncn6

RUN: RUN6494

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.33

EN300-1248064_1_1_1



CID: EN300-1248064_1_1_1

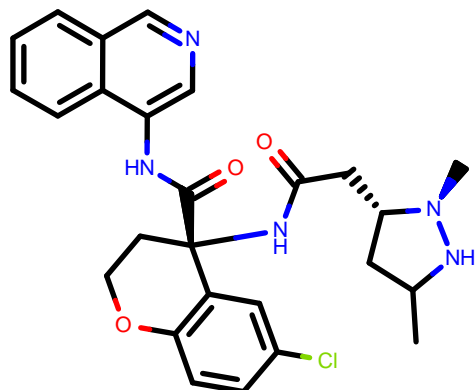
SMILES: CC(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)n5cncn5

RUN: RUN3138

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.23

EN300-6499639_1_1_2



CID: EN300-6499639_1_1_2

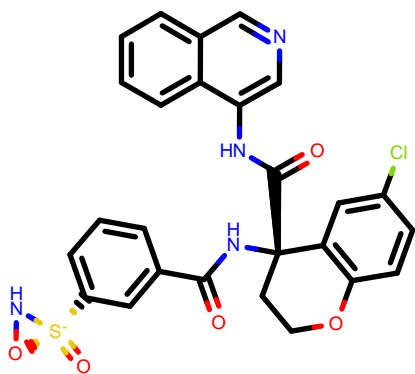
SMILES: CC1=N[N@@]([C@@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)C

RUN: RUN5605

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.19

EN300-04520_1_1_1



CID: EN300-04520_1_1_1

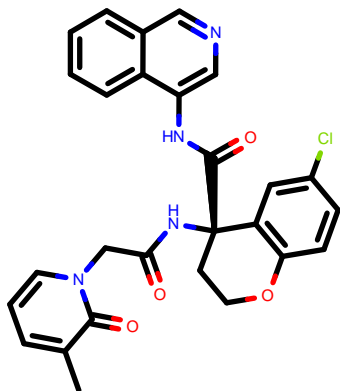
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5S(=O)(=O)N

RUN: RUN2963

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.26

EN300-126104_1_1_1



CID: EN300-126104_1_1_1

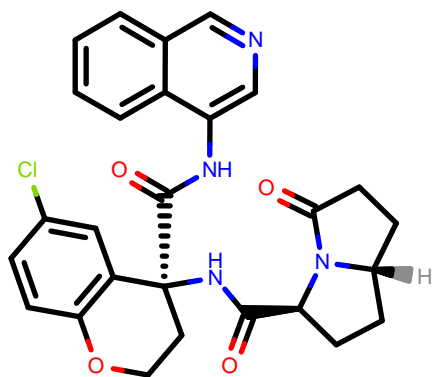
SMILES: Cc1cccn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN3219

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.29

EN300-6479181_1_1_1



CID: EN300-6479181_1_1_1

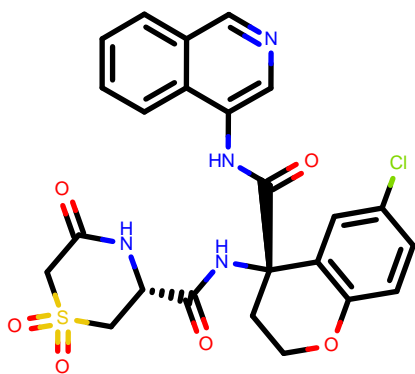
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C)C(=O)C@@H5C[C@@]3(H)N5C(=O)OCC6

RUN: RUN2960

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.42

EN300-702756_1_1_1



CID: EN300-702756_1_1_1

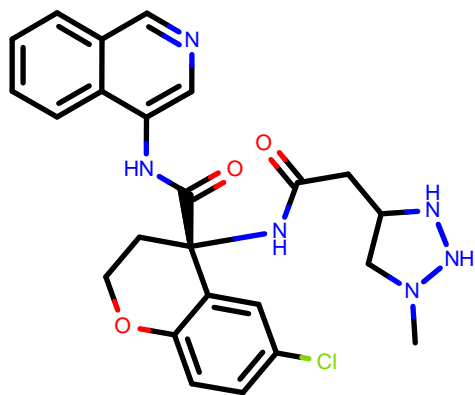
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C)C(=O)C@@H5C[S(=O)(=O)O]C1=O)N5

RUN: RUN3154

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.27

EN300-1073264_1_1_1



CID: EN300-1073264_1_1_1

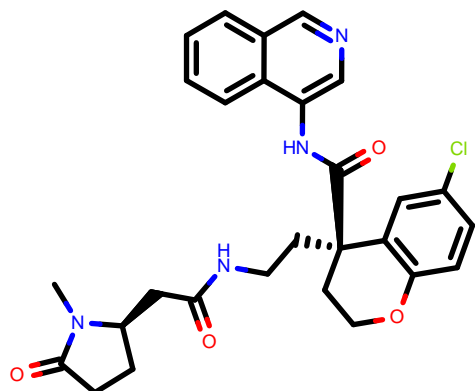
SMILES: Cn1cc(nn1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3347

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.23

EN300-207765_3_2_1



CID: EN300-207765_3_2_1

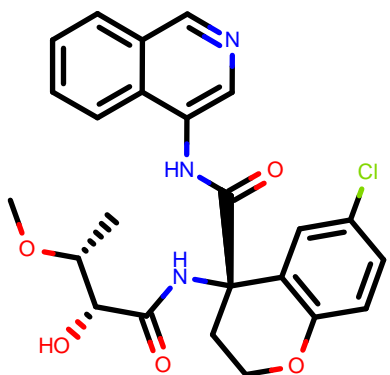
SMILES: CN1C@H](CCC1=O)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5599

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.21

EN300-220194_1_4_1



CID: EN300-220194_1_4_1

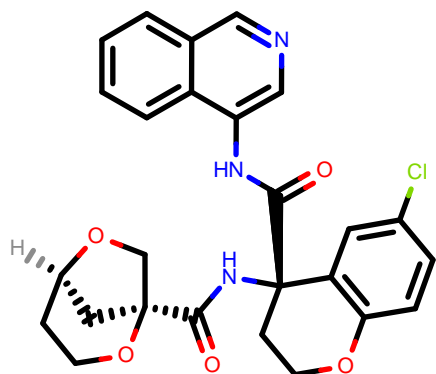
SMILES: CC@H(C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC

RUN: RUN3131

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.26

EN300-6736394_1_1_1



CID: EN300-6736394_1_1_1

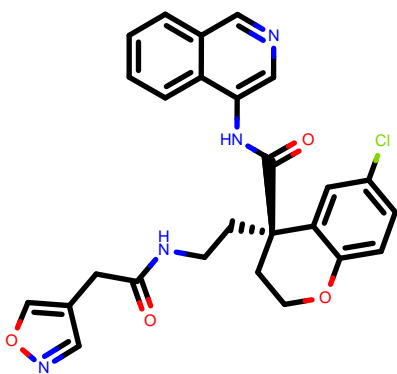
SMILES: c1cc2c(c1)cncc2N[C@@]3(C(=O)N[C@@]4(CCOC5c4cc(cc5)Cl)N[C@@]6(C(=O)Nc7cncc8c7cccc8)O)O)O

RUN: RUN3425

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.30

EN300-315963_3_1_1



CID: EN300-315963_3_1_1

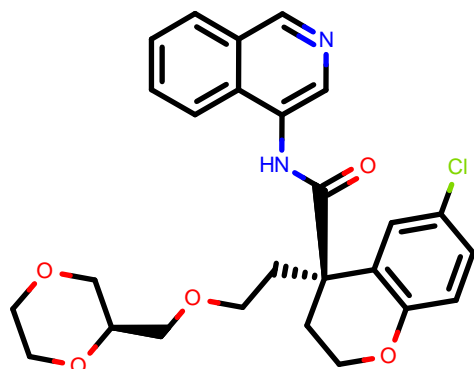
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnoc5

RUN: RUN3602

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.30

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

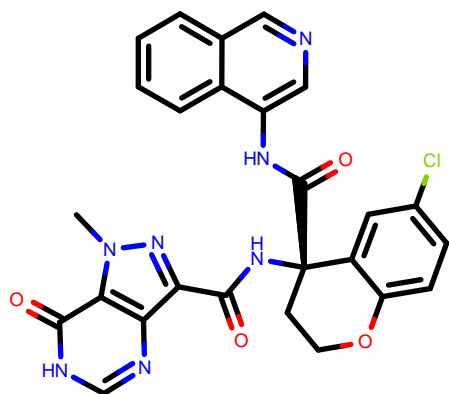
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5H5COCOC5

RUN: RUN4110

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.27

EN300-7355981_1_1_1



CID: EN300-7355981_1_1_1

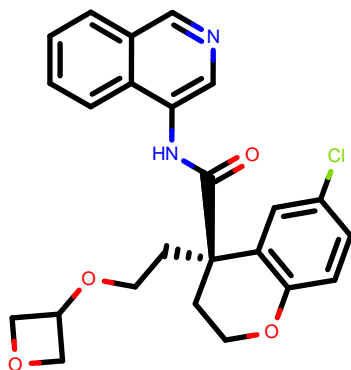
SMILES: Cn1c2c(c(n1)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncnc6c5ccccc6)nc[nH]e2=O

RUN: RUN3625

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.30

EN300-317082_3_1_1



CID: EN300-317082_3_1_1

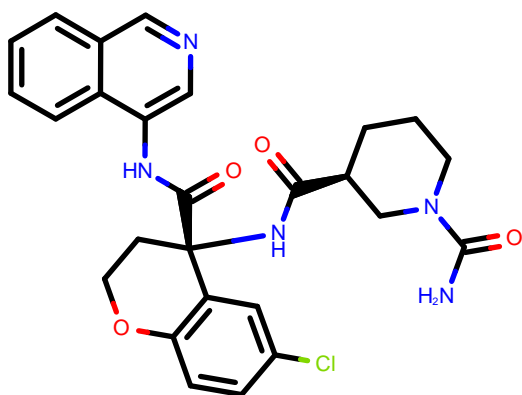
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5COC5

RUN: RUN2907

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.21

EN300-14767_1_2_1



CID: EN300-14767_1_2_1

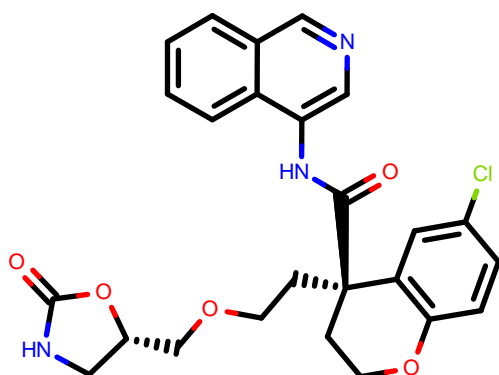
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCN(C5)C(=O)N

RUN: RUN5106

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.38

EN300-203293_3_1_1



CID: EN300-203293_3_1_1

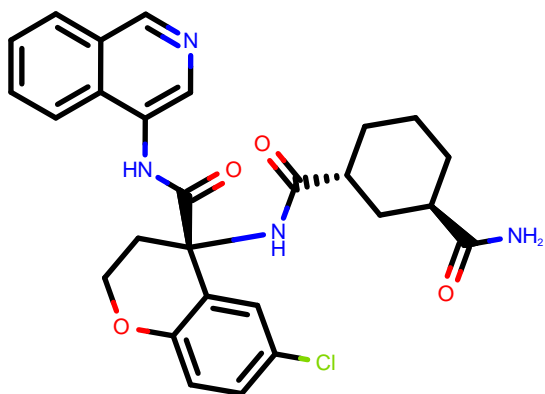
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CNC(=O)O5

RUN: RUN3419

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.32

EN300-90142_1_3_1



CID: EN300-90142_1_3_1

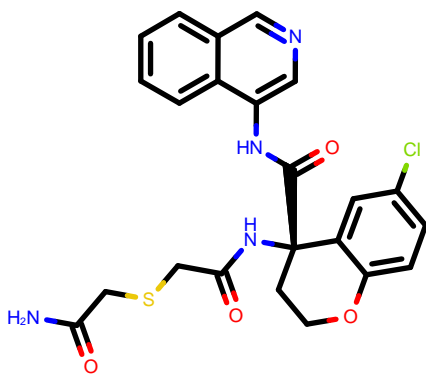
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@@H](C5)Cl=O

RUN: RUN4183

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.27

EN300-33513_1_1_1



CID: EN300-33513_1_1_1

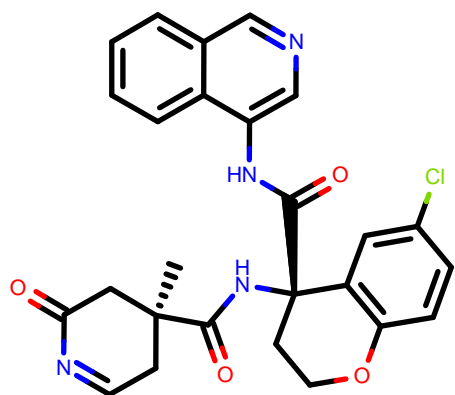
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CSCC(=O)N

RUN: RUN3871

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.22

EN300-315854_1_1_1



CID: EN300-315854_1_1_1

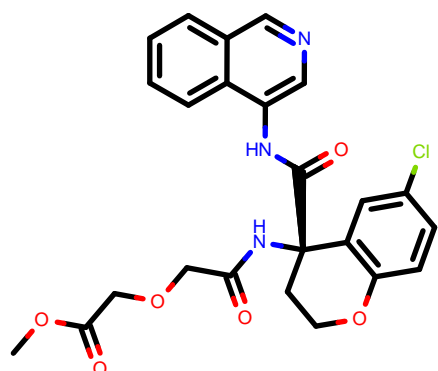
SMILES: C[C@@]1(CCN(C=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2726

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.29

EN300-205635_1_1_1



CID: EN300-205635_1_1_1

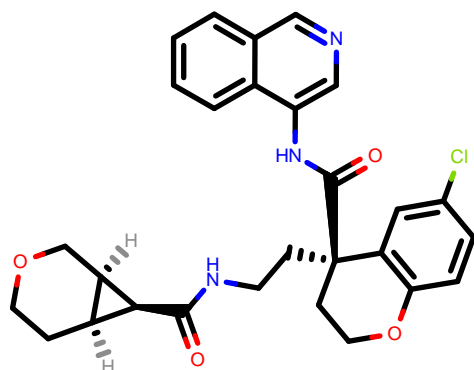
SMILES: COC(=O)COCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN3334

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.23

EN300-1644723_3_6_1



CID: EN300-1644723_3_6_1

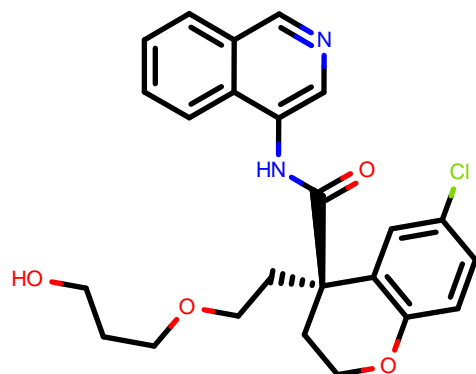
SMILES: c1ccc2c(c1)ncc2N[C@@]1(C)[C@@]3(CCOc4c3cc(cc4)Cl)CNC1=O[C@@]H2[C@@]3H[C@@]H3COCCO

RUN: RUN3497

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.30

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

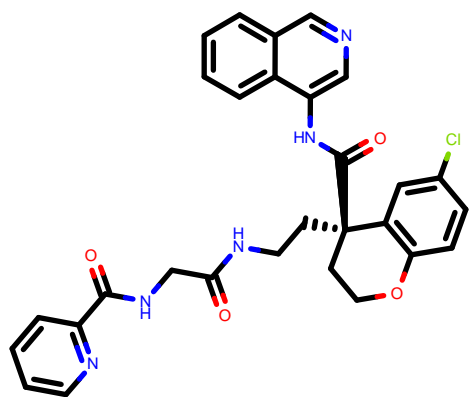
SMILES: c1ccc2c(c1)ncc2N[C@@]1(C)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN3306

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.25

EN300-83280_3_1_1



CID: EN300-83280_3_1_1

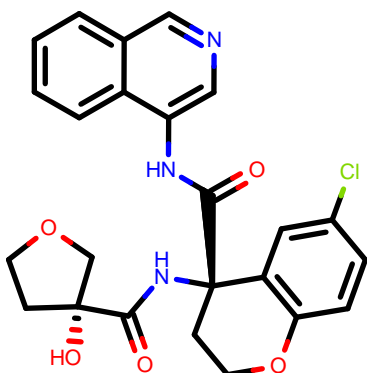
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CNC(=O)c5ccccc5

RUN: RUN5966

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.28

EN300-148421_1_2_1



CID: EN300-148421_1_2_1

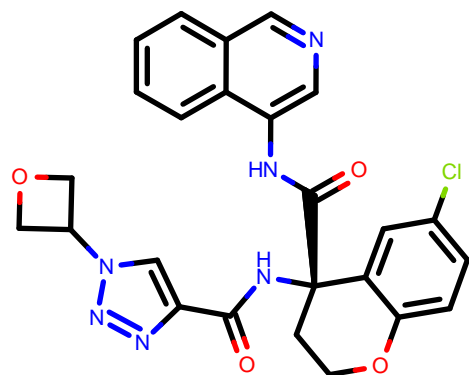
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@]5(CCOCS)O

RUN: RUN3115

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.36

EN300-1696043_1_1_1



CID: EN300-1696043_1_1_1

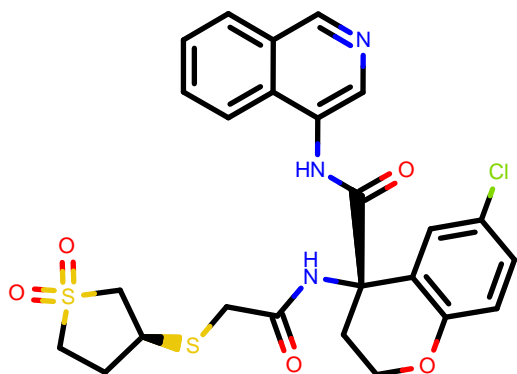
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn1nn5C6OC6

RUN: RUN4925

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.24

EN300-13890_1_2_1



CID: EN300-13890_1_2_1

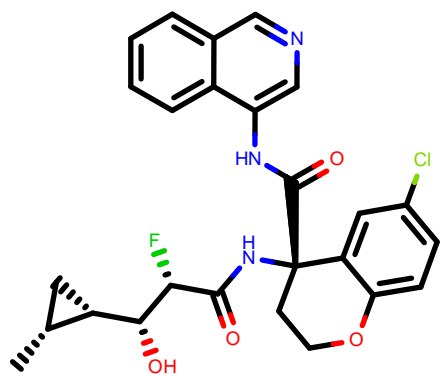
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@H]5CCS(=O)(=O)C5

RUN: RUN4216

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.32

EDG-MED-90036822-94_5



CID: EDG-MED-90036822-94_5

SMILES:

C[C@@H](C[C@@H](C@H)[C@@H](C)C(=O)N[C@@]2(COC3C2C(C3)C)C(=O)N4CCCC5F4O

RUN:

RUN1663

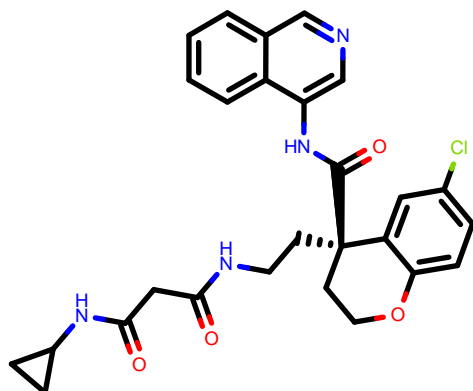
DDG (kcal/mol):

-2.69

dDDG (kcal/mol):

0.28

EN300-128464_3_1_1



CID: EN300-128464_3_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC(=O)NC5CC5

RUN:

RUN5993

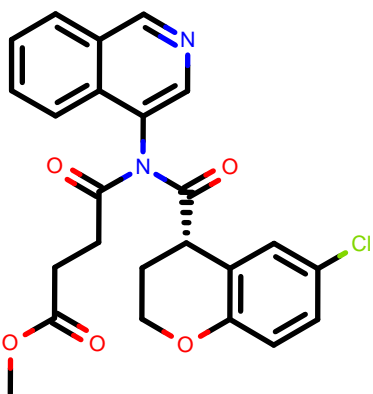
DDG (kcal/mol):

-2.69

dDDG (kcal/mol):

0.38

MAT-POS-9db1e783-3_1



CID: MAT-POS-9db1e783-3_1

SMILES:

COC(=O)/C=C/C(=O)N(c1nccc2c1cccc2)C(=O)[C@H]3CCOC4c3cc(cc4)Cl

RUN:

RUN2639

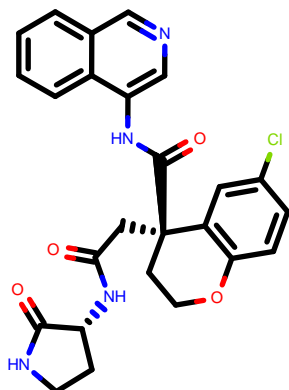
DDG (kcal/mol):

-2.69

dDDG (kcal/mol):

0.38

EDJ-MED-d203f206-29_1



CID: EDJ-MED-d203f206-29_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5CCNC5=O

RUN:

RUN2405

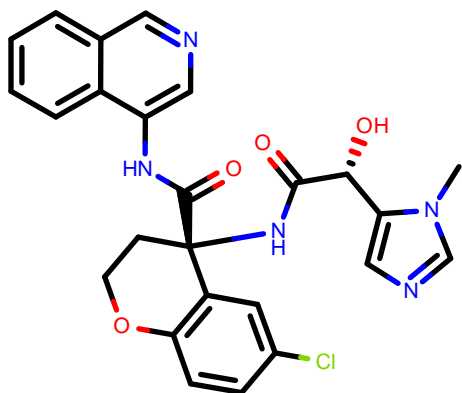
DDG (kcal/mol):

-2.69

dDDG (kcal/mol):

0.32

EN300-190283_1_2_1



CID: EN300-190283_1_2_1

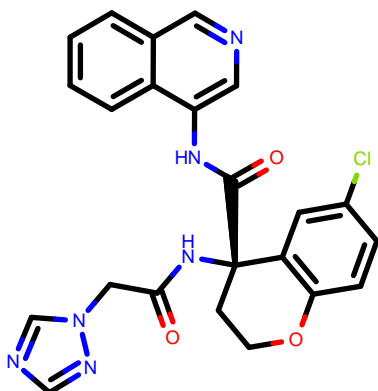
SMILES: Cn1cncc1[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN3011

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.35

EN300-06654_1_1_1



CID: EN300-06654_1_1_1

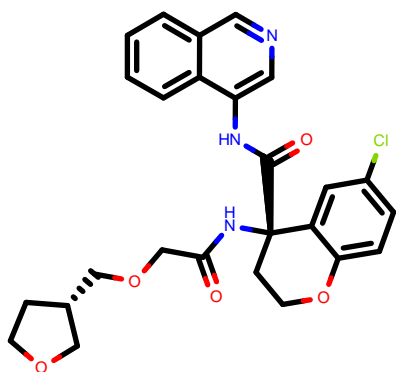
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncc5

RUN: RUN3164

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.20

EN300-80522_1_2_1



CID: EN300-80522_1_2_1

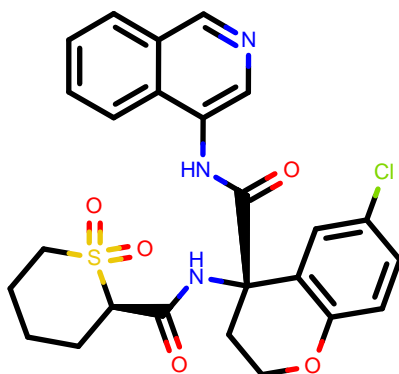
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@H]5COC5

RUN: RUN5498

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.23

EN300-107435_1_2_1



CID: EN300-107435_1_2_1

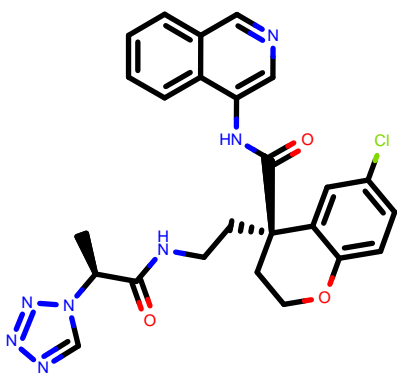
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCCS5(=O)=O

RUN: RUN6407

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.29

EN300-191915_3_1_1



CID: EN300-191915_3_1_1

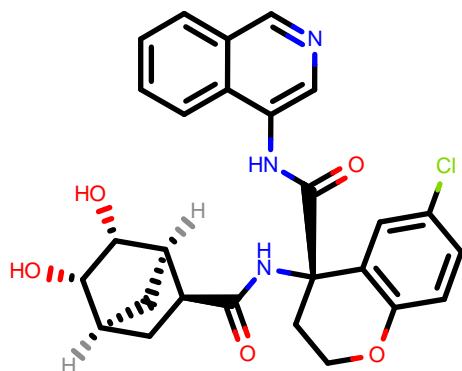
SMILES: C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)n5nnn5

RUN: RUN5855

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.29

EN300-6744028_1_8_1



CID: EN300-6744028_1_8_1

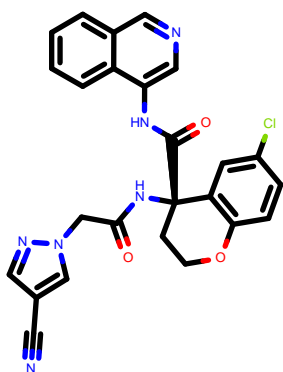
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)[C@@H]5[C@@H]6[C@@H]5[C@@H]6O

RUN: RUN5239

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.32

EN300-1590388_1_1_1



CID: EN300-1590388_1_1_1

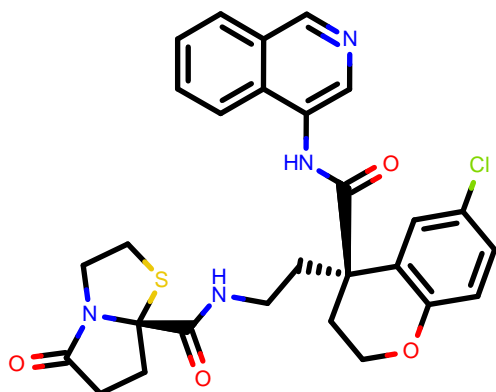
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)Cn5ccn5C#N

RUN: RUN3506

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.24

EN300-10334_3_1_1



CID: EN300-10334_3_1_1

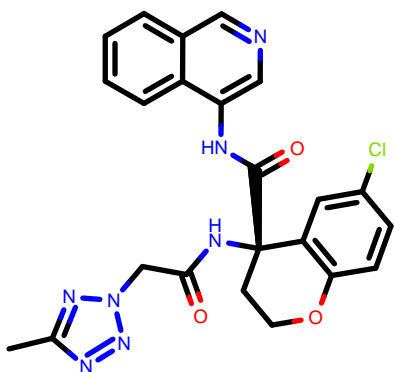
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCNC(=O)[C@@]56CCC(=O)N5CCS6

RUN: RUN3228

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.38

EN300-6487680_1_1_1



CID: EN300-6487680_1_1_1

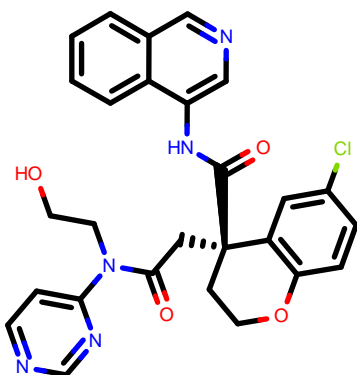
SMILES: Cc1nnn(n1)CC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3608

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.21

EDJ-MED-d203f206-5_1



CID: EDJ-MED-d203f206-5_1

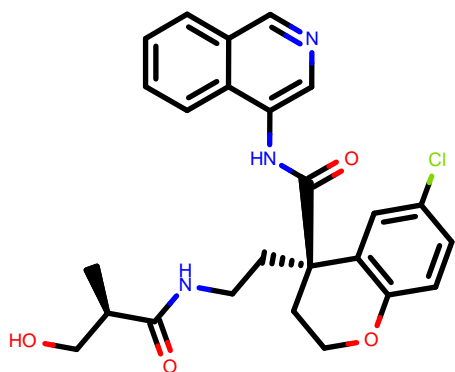
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N(CCO)c5ccncc5

RUN: RUN2439

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.39

EN300-55072_3_2_1



CID: EN300-55072_3_2_1

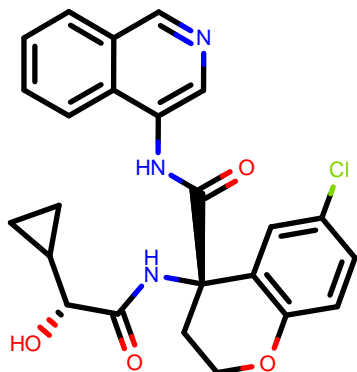
SMILES: C[C@H](CO)C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4429

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.26

EN300-72211_1_1_1



CID: EN300-72211_1_1_1

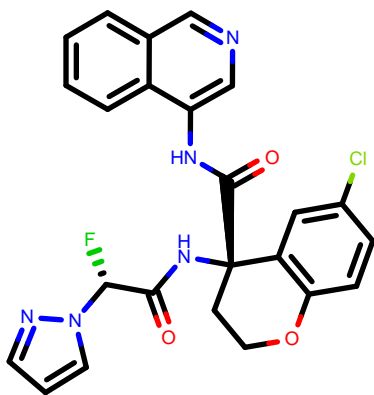
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)[C@@H](C5CC5)O

RUN: RUN3030

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.25

EN300-1726277_1_2_1



CID: EN300-1726277_1_2_1

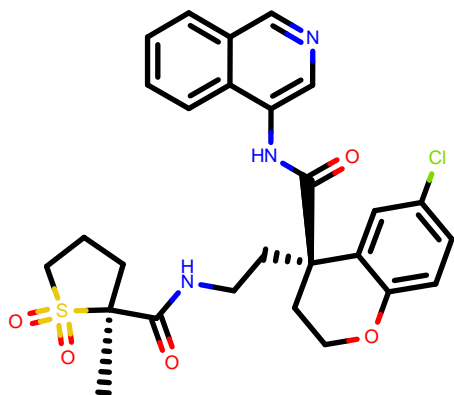
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](n5cccn5)F

RUN: RUN3178

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.21

EN300-373476_3_2_1



CID: EN300-373476_3_2_1

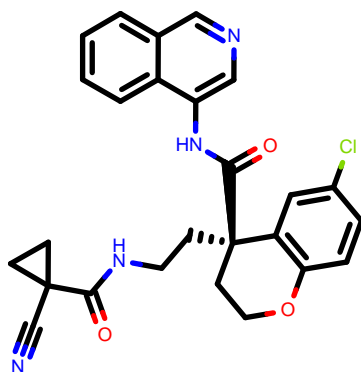
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN5971

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.35

EN300-114082_3_1_1



CID: EN300-114082_3_1_1

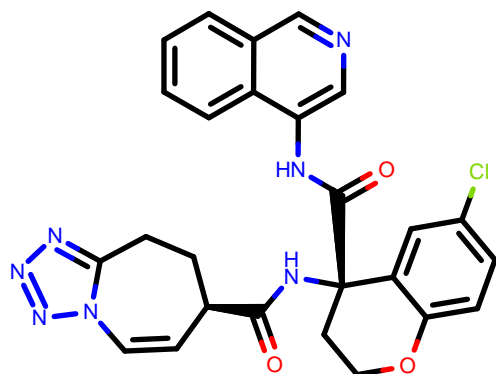
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5/C#N

RUN: RUN3027

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.31

EN300-253571_1_1_1



CID: EN300-253571_1_1_1

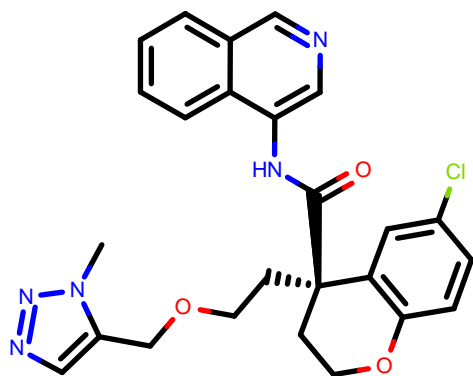
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6nmm6CC5

RUN: RUN3803

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.24

EN300-216673_3_1_1



CID: EN300-216673_3_1_1

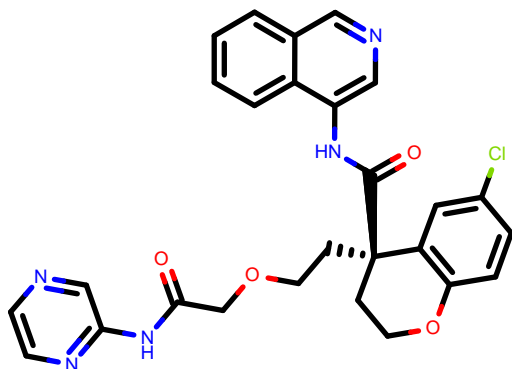
SMILES: Cn1c(cnn1)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3375

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.27

EN300-105267_3_1_1



CID: EN300-105267_3_1_1

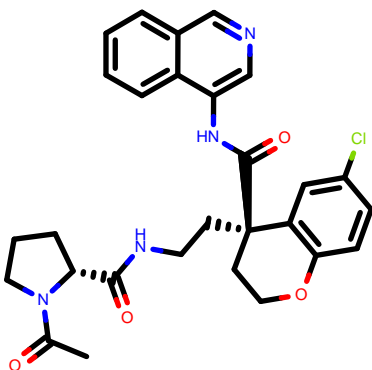
SMILES: c1ccc2c(c1)cnc2N[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5cncn5

RUN: RUN5219

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.26

EN300-211777_3_1_1



CID: EN300-211777_3_1_1

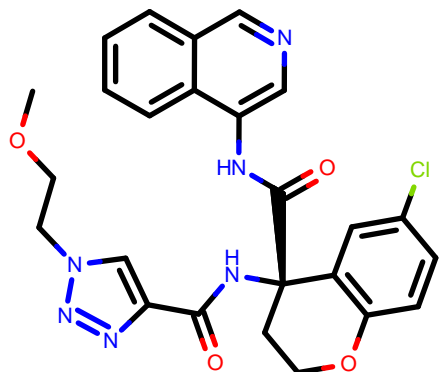
SMILES: CC(=O)N1CCCC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN7271

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.35

EN300-251867_1_1_1



CID: EN300-251867_1_1_1

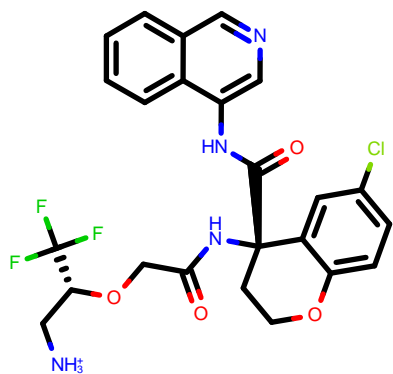
SMILES: COCc1c(cc(nn1)C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3780

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.24

EDG-MED-90036822-27_2



CID: EDG-MED-90036822-27_2

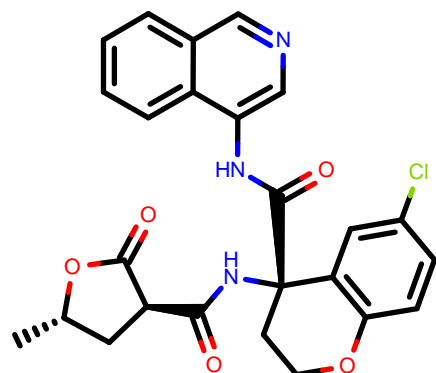
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@H](CN)C(F)(F)F

RUN: RUN1576

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.50

EN300-7444533_1_2_1



CID: EN300-7444533_1_2_1

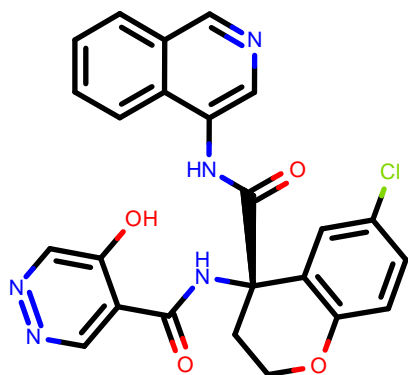
SMILES: C[C@H]1C[C@@H](C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncnc4ccoc5

RUN: RUN2924

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.25

EN300-243828_1_1_1



CID: EN300-243828_1_1_1

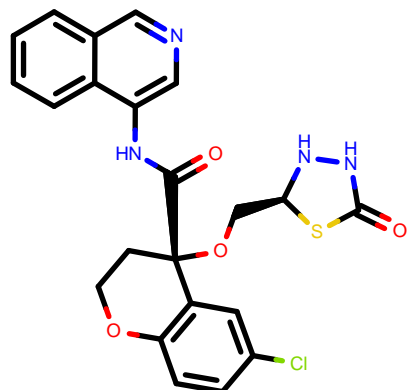
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]nc5=O

RUN: RUN2852

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.26

EN300-171766_1_1_2



CID: EN300-171766_1_1_2

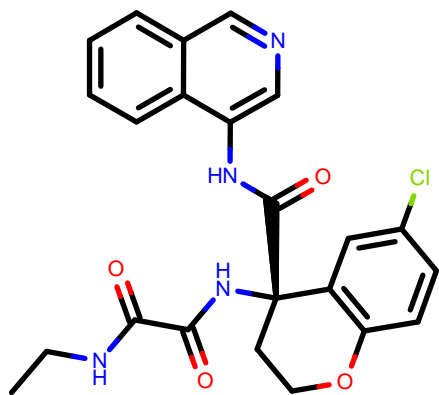
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5NNC(=O)S5

RUN: RUN3570

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.21

EN300-1262608_1_1_1



CID: EN300-1262608_1_1_1

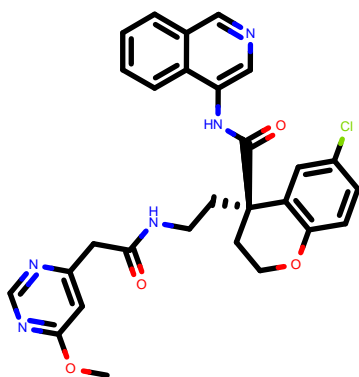
SMILES: CCNC(=O)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2871

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.24

EN300-7444950_3_1_1



CID: EN300-7444950_3_1_1

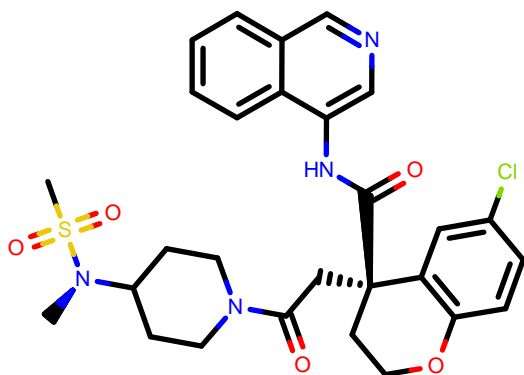
SMILES: COc1cc(ncn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3232

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.32

KAD-UNI-80f122c8-5_3



CID: KAD-UNI-80f122c8-5_3

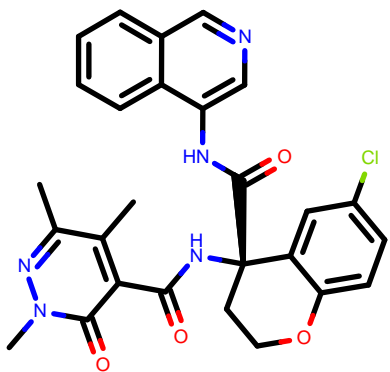
SMILES: CN(C)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5S(=O)(=O)C

RUN: RUN2205

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.27

EN300-28894_1_1_1



CID: EN300-28894_1_1_1

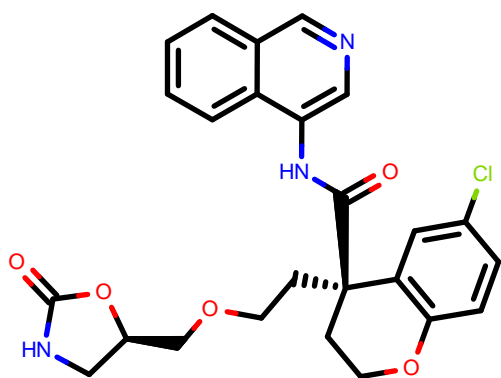
SMILES: Cc1c(nn(c(=O)c1C(=O)N)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C)C

RUN: RUN3122

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.28

EN300-203293_3_2_1



CID: EN300-203293_3_2_1

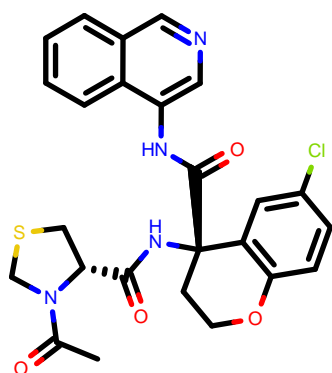
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CNC(=O)O5

RUN: RUN2850

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.31

EN300-761220_1_1_1



CID: EN300-761220_1_1_1

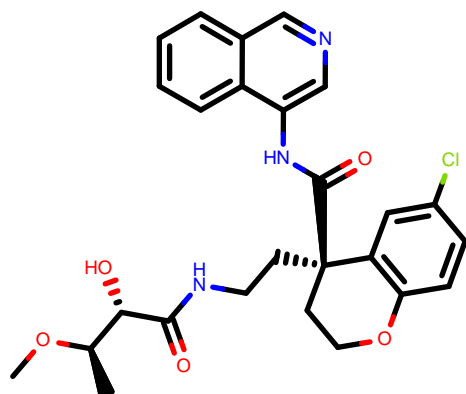
SMILES: CC(=O)N1CSC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2840

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.27

EN300-220194_3_2_1



CID: EN300-220194_3_2_1

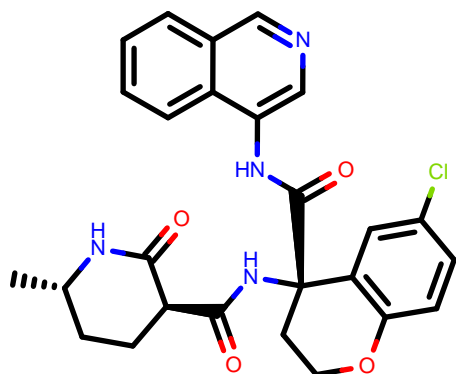
SMILES: C[C@@H](C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)O)OC

RUN: RUN6435

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.28

EN300-6505003_1_2_1



CID: EN300-6505003_1_2_1

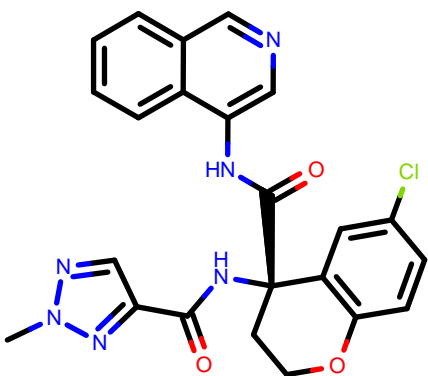
SMILES: C[C@@H]1CC[C@@H](C(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3066

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.33

EN300-61694_1_1_1



CID: EN300-61694_1_1_1

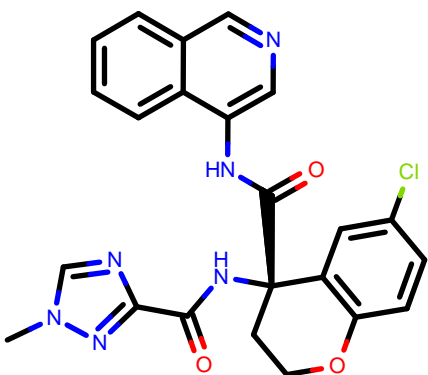
SMILES: Cn1ncc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3532

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.17

EN300-214172_1_1_1



CID: EN300-214172_1_1_1

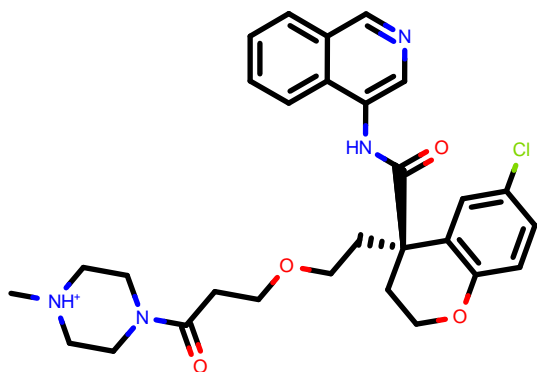
SMILES: Cn1ncc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2991

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.18

EN300-178293_3_1_1



CID: EN300-178293_3_1_1

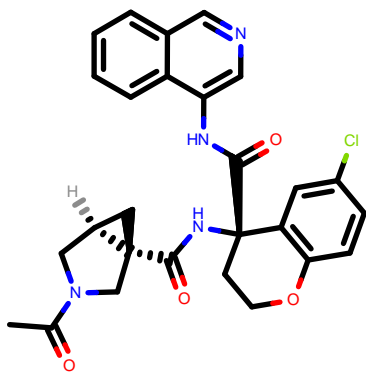
SMILES: [CnH+][1]CCN(CC1)C(=O)CCOC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5145

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.38

EN300-313062_1_4_1



CID: EN300-313062_1_4_1

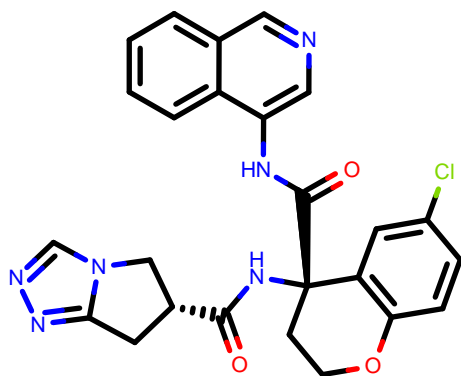
SMILES: CC(=O)N1C[C@H]2C[C@@]3(C1)C(=O)N[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6

RUN: RUN3009

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.29

EN300-6745453_1_1_1



CID: EN300-6745453_1_1_1

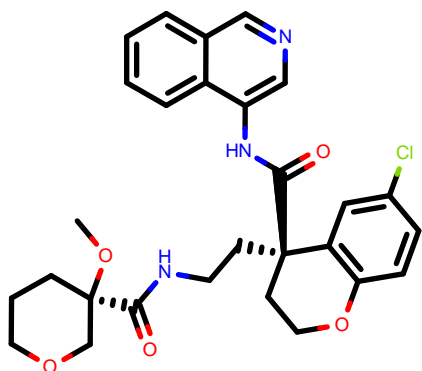
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C6nncn6C5

RUN: RUN3064

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.22

EN300-1072199_3_1_1



CID: EN300-1072199_3_1_1

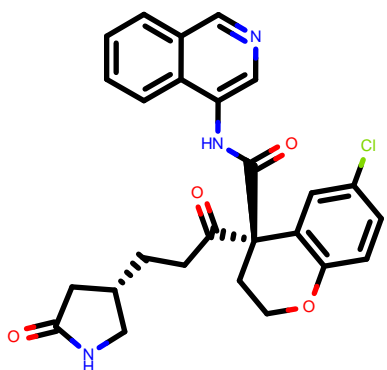
SMILES: CO[C@@]1(CCCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN2884

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.35

VLA-UCB-34f3ed0c-21_2



CID: VLA-UCB-34f3ed0c-21_2

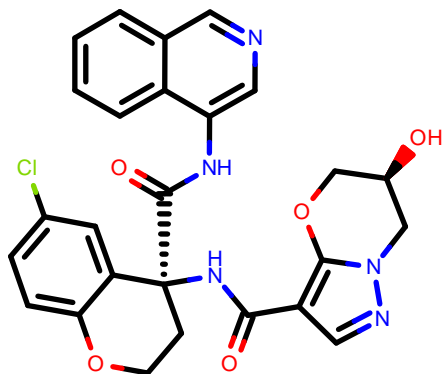
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)CC[C@@H]5CC(=O)NCS

RUN: RUN631

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.29

EN300-6497444_1_2_1



CID: EN300-6497444_1_2_1

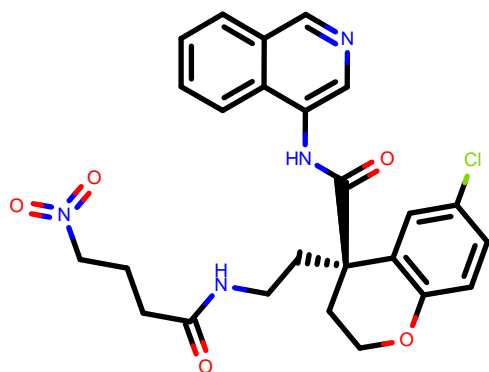
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn6c5OC[C@@H](C6)O

RUN: RUN3562

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.24

EN300-143449_3_1_1



CID: EN300-143449_3_1_1

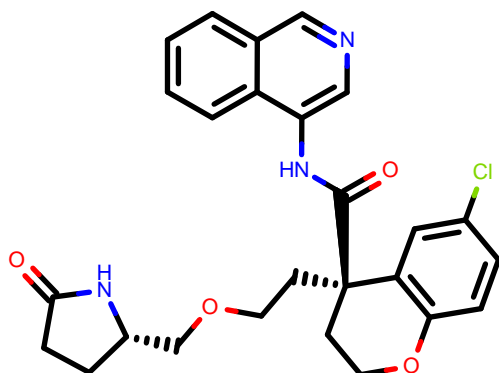
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CCCN(=O)=O

RUN: RUN3157

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.31

EN300-264301_3_1_1



CID: EN300-264301_3_1_1

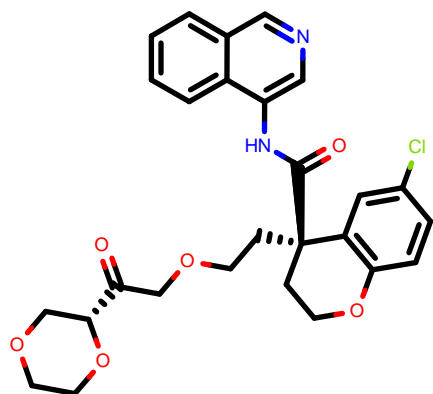
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H]5CCCC(=O)N5

RUN: RUN4573

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.23

EN300-6238494_3_2_1



CID: EN300-6238494_3_2_1

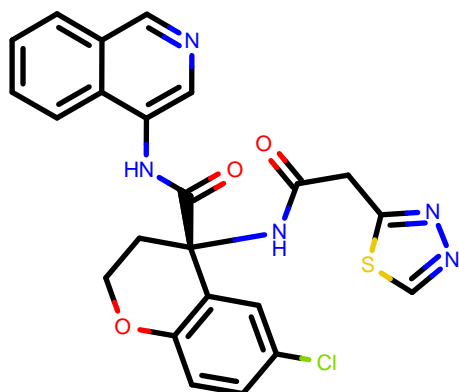
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCOCC(=O)[C@@H]5COCOC5

RUN: RUN4511

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.27

EN300-6488240_1_1_1



CID: EN300-6488240_1_1_1

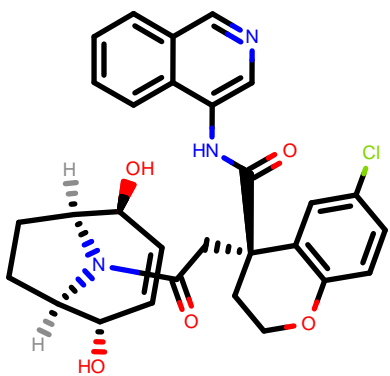
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C5nncs5

RUN: RUN2831

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.24

EN300-6738887_1_2_1



CID: EN300-6738887_1_2_1

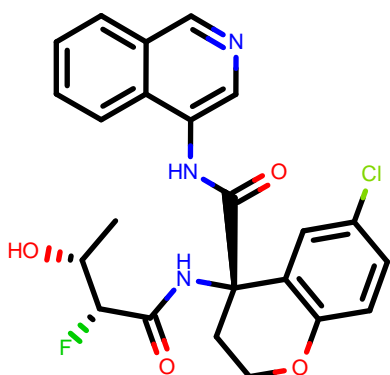
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C(=O)N[C@@H]5C[C@@H]6C[C@@H]7C[C@@H]6O

RUN: RUN3340

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.27

EDG-MED-90036822-37_4



CID: EDG-MED-90036822-37_4

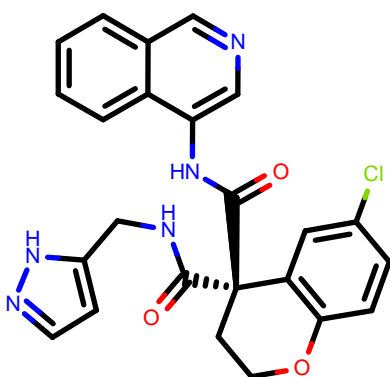
SMILES: C[C@@H]([C@@H](C(=O)N[C@@]1(C)CCOC2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)F)O

RUN: RUN1578

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.21

VLA-UCB-34f3ed0c-3_1



CID: VLA-UCB-34f3ed0c-3_1

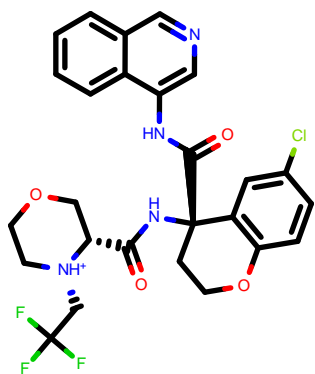
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C(=O)N[C@@]5cnc[nH]5

RUN: RUN610

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.23

EN300-201551_1_2_1



CID: EN300-201551_1_2_1

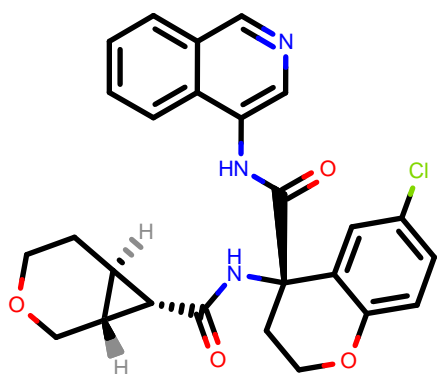
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C(=O)N[C@@H]5COCQ[N@@]5C(F)(F)F

RUN: RUN3098

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.28

EN300-1644723_1_8_1



CID: EN300-1644723_1_8_1

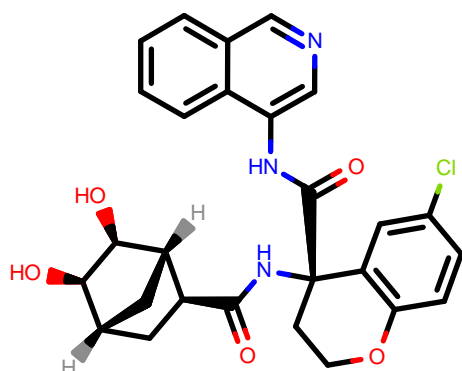
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(c4)C1N(C1=O)C@H5[C@@H]6[C@@H]5COC6=O

RUN: RUN3023

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.20

EN300-6744028_1_2_1



CID: EN300-6744028_1_2_1

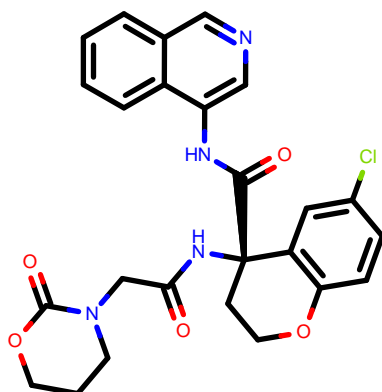
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(c4)C1N(C1=O)C@H5[C@@H]6[C@@H]5COC6=O

RUN: RUN3395

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.29

EN300-103638_1_1_1



CID: EN300-103638_1_1_1

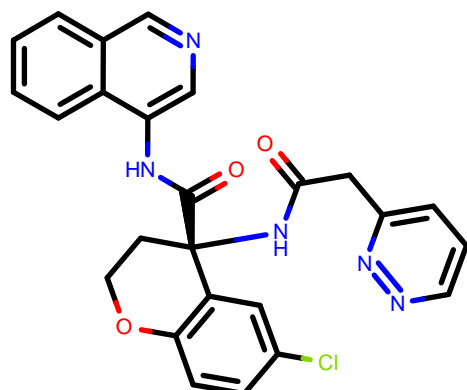
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(c4)C1N(C1=O)CN5CCCC5=O

RUN: RUN3712

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.32

EN300-7456948_1_1_1



CID: EN300-7456948_1_1_1

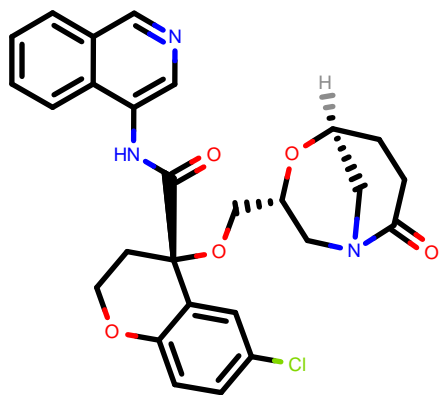
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(c4)C1N(C1=O)C5ccnccn5

RUN: RUN3029

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.22

EN300-2008102_1_2_1



CID: EN300-2008102_1_2_1

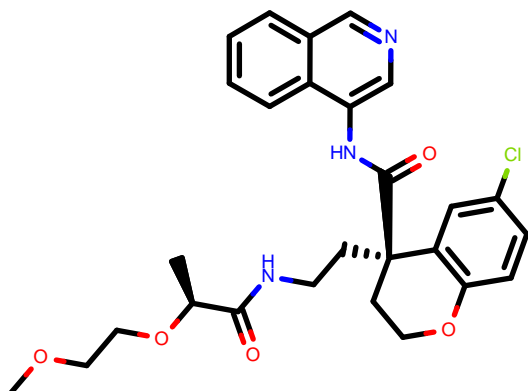
SMILES: c1ccc2c(c1)ncnc2N(C(=O)O)C@@H3(COCOC4C3CC(=O)C)OC(C@@H5CN6C(C@@H)O5)CCOC6=O

RUN: RUN3293

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.33

EN300-77359_3_1_1



CID: EN300-77359_3_1_1

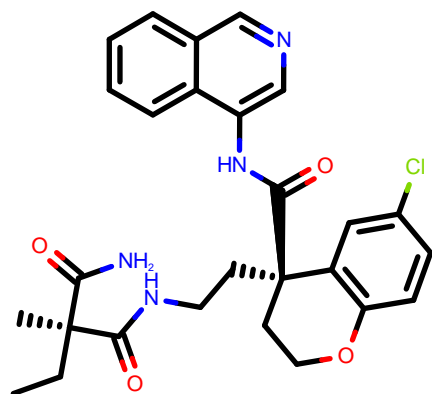
SMILES: C(C@@H)(C(=O)N)C(C(=O)O)C@1(COCOC2C1CC(=O)C)C(=O)Nc3ncoc4c3ccoc4)OCCOC

RUN: RUN5465

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.30

EN300-2908024_3_1_1



CID: EN300-2908024_3_1_1

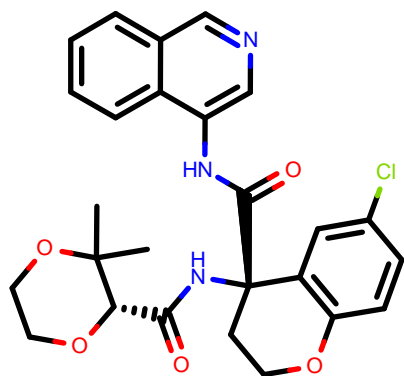
SMILES: CC(C@@H)(C(=O)N)C(=O)NCC(C@1(COCOC2C1CC(=O)C)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3633

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.28

EN300-1601684_1_1_1



CID: EN300-1601684_1_1_1

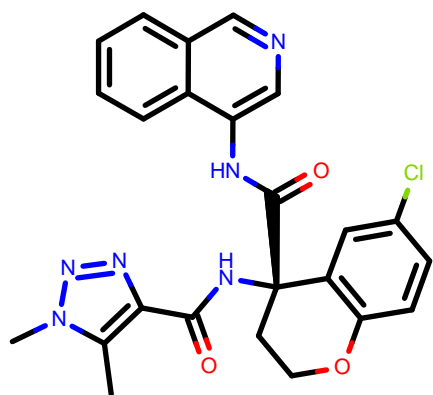
SMILES: CC1(C@@H)(OCCO1)C(=O)N(C@2(COCOC3C2CC(=O)C)C(=O)Nc4ncoc5c4ccoc5)C

RUN: RUN2971

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.28

EN300-85473_1_1_1



CID: EN300-85473_1_1_1

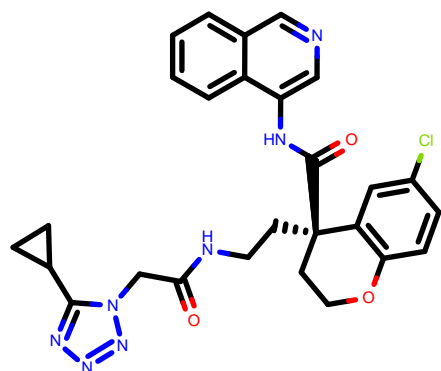
SMILES: Cc1c(nnn1C)C(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN6014

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.23

EN300-872798_3_1_1



CID: EN300-872798_3_1_1

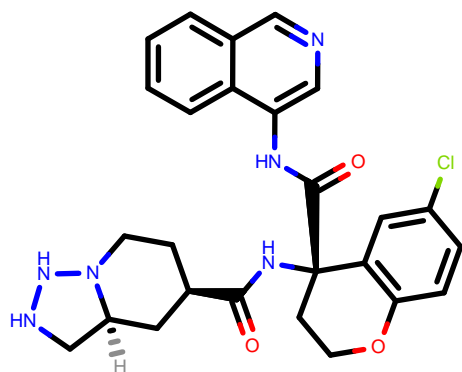
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5c(nnn5)C6CC6

RUN: RUN3775

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.31

EN300-7430501_1_1_1



CID: EN300-7430501_1_1_1

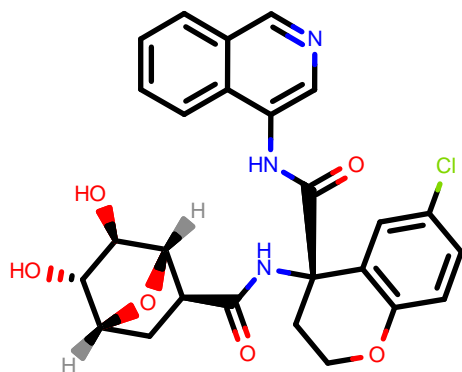
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5Cn6c(nnn6)C5

RUN: RUN3146

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.28

EN300-6764836_1_6_1



CID: EN300-6764836_1_6_1

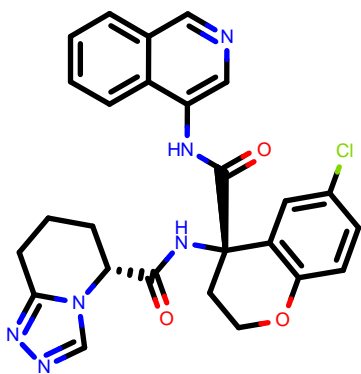
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5Cn6c(nnn6)C5

RUN: RUN3369

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.27

EN300-6478631_1_2_1



CID: EN300-6478631_1_2_1

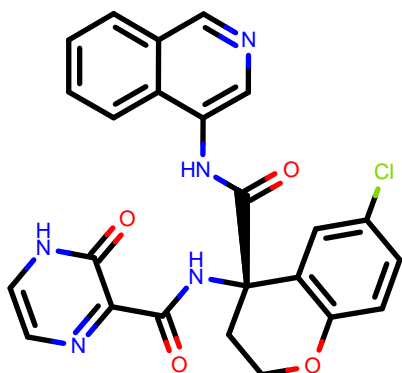
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6n5cnn6

RUN: RUN2947

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.24

EN300-97055_1_1_1



CID: EN300-97055_1_1_1

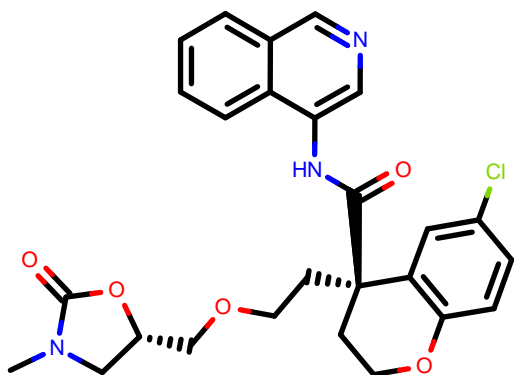
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(=O)[nH]cnn5

RUN: RUN3746

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.21

EN300-222969_3_2_1



CID: EN300-222969_3_2_1

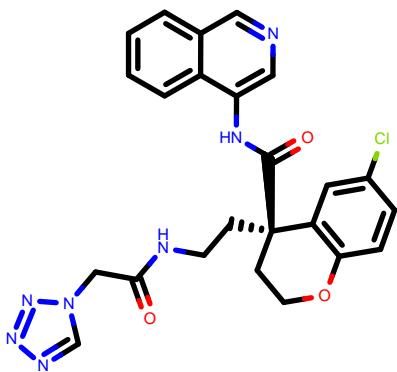
SMILES: CN1C[C@H](OC1=O)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5o4ccccc5

RUN: RUN2898

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.30

EN300-20980_3_1_1



CID: EN300-20980_3_1_1

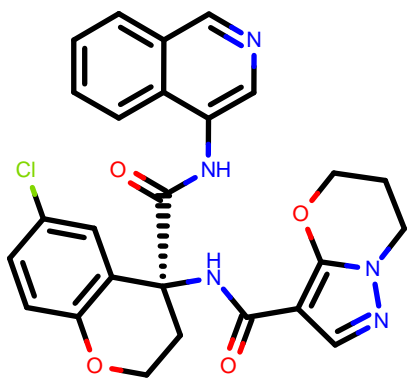
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cnnn5

RUN: RUN2903

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.26

EN300-103722_1_1_1



CID: EN300-103722_1_1_1

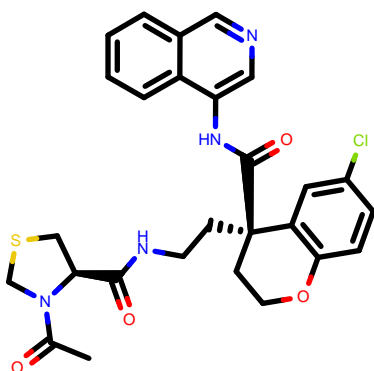
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5OCCc6

RUN: RUN4274

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.23

EN300-56202_3_2_1



CID: EN300-56202_3_2_1

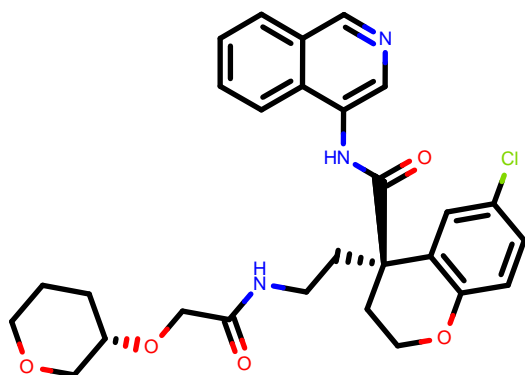
SMILES: CC(=O)N1CSC[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN3593

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.31

EN300-1627945_3_2_1



CID: EN300-1627945_3_2_1

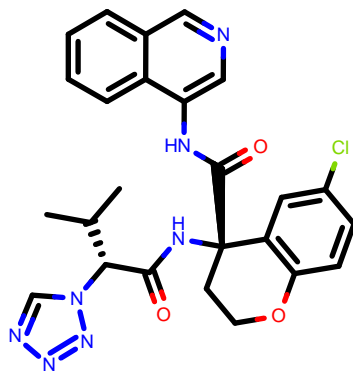
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@H]5CCOC5

RUN: RUN5777

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.23

EN300-297561_1_2_1



CID: EN300-297561_1_2_1

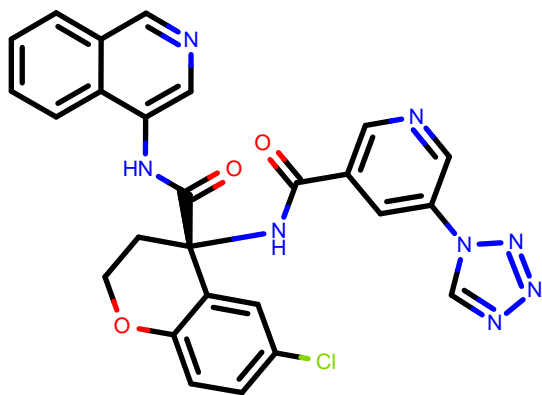
SMILES: CC(C)[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)n5cnn5

RUN: RUN2784

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.26

EN300-2690393_1_1_1



CID: EN300-2690393_1_1_1

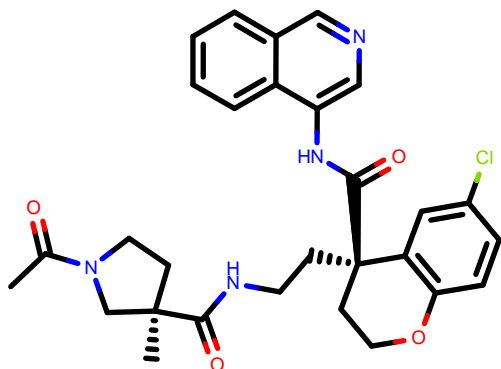
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(cnc5)n6cnm6

RUN: RUN3366

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.24

EN300-98018_3_1_1



CID: EN300-98018_3_1_1

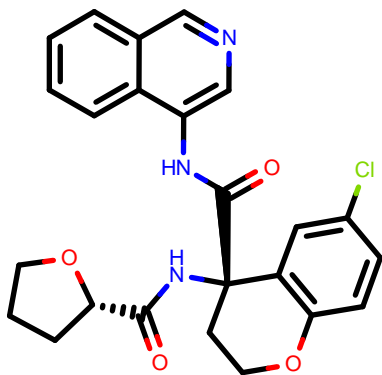
SMILES: CC(=O)N1CC[C@H](C1)C(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN3510

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.37

EN300-21009_1_1_1



CID: EN300-21009_1_1_1

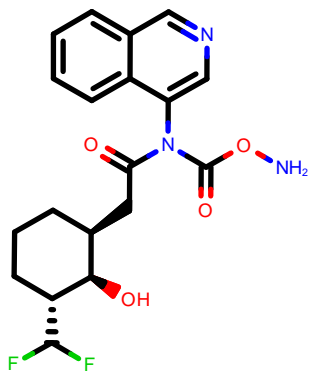
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCC5

RUN: RUN3225

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.24

MAK-UNK-c749d764-29_3



CID: MAK-UNK-c749d764-29_3

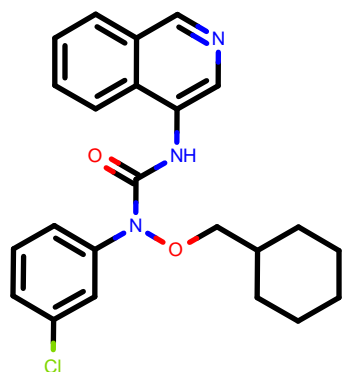
SMILES: c1ccc2c(c1)cnc2N(C(=O)C[C@@H]3CCCC[C@H](C3)[C@@H]3O)C(F)F(=O)ON

RUN: RUN1085

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.37

PET-UNK-a17c93d1-1_1



CID: PET-UNK-a17c93d1-1_1

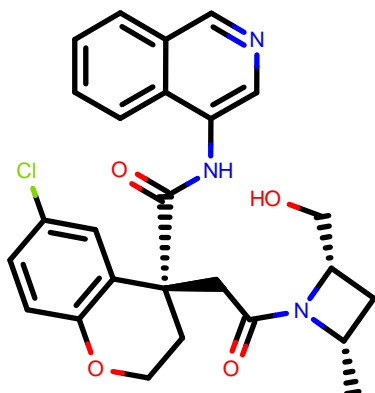
SMILES: c1ccc2c(c1)nc2NC(=O)N(c3cccc(c3)Cl)OCC4CCCCC4

RUN: RUN459

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.36

EN300-1709410_1_4_1



CID: EN300-1709410_1_4_1

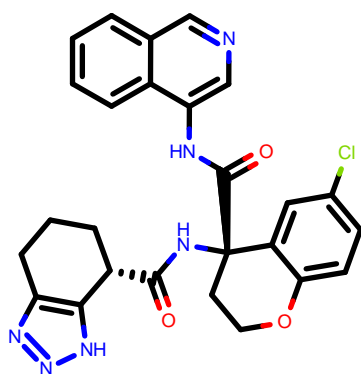
SMILES: C[C@H]1C[C@H](N1C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5)CO

RUN: RUN4112

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.28

EN300-208236_1_2_1



CID: EN300-208236_1_2_1

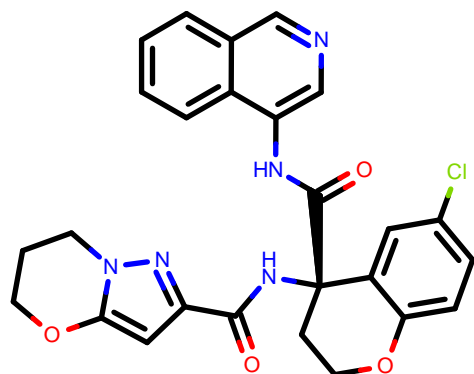
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCc6c5n[nH]6

RUN: RUN3416

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.26

EN300-103720_1_1_1



CID: EN300-103720_1_1_1

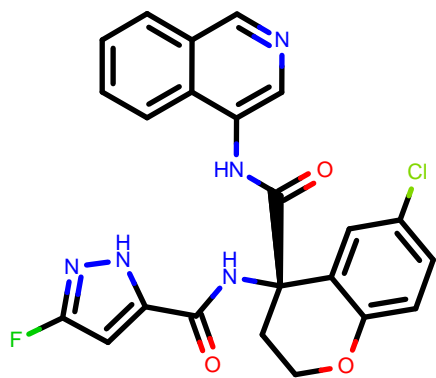
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCCO6

RUN: RUN4809

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.23

EDG-MED-90036822-72_1



CID: EDG-MED-90036822-72_1

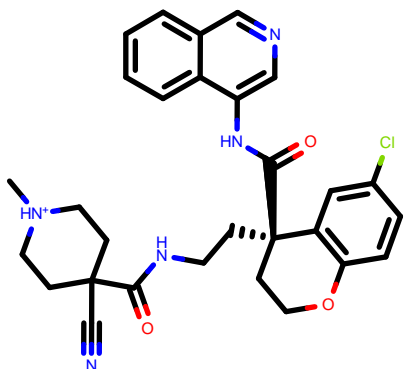
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[nH]n5F

RUN: RUN1618

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.18

EN300-7473378_3_1_1



CID: EN300-7473378_3_1_1

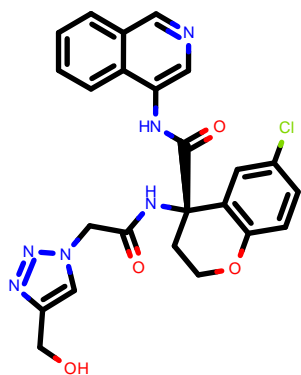
SMILES: C[NH+]1CCC(CC1)(C#N)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncsc5c4ccc5

RUN: RUN4066

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.41

EN300-108236_1_1_1



CID: EN300-108236_1_1_1

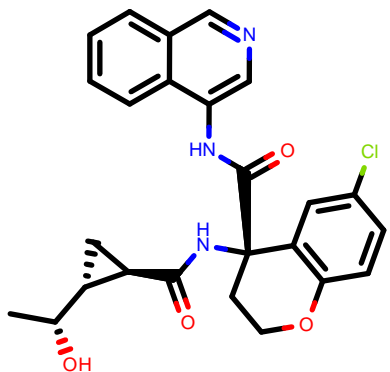
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5sc[nH]5CO

RUN: RUN3500

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.28

EN300-6729572_1_6_1



CID: EN300-6729572_1_6_1

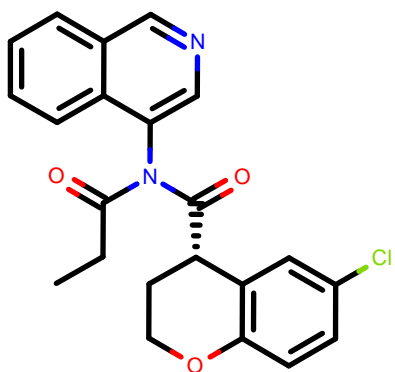
SMILES: C[C@H]([C@@H]1C[C@H]1C(=O)N)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncsc5c4ccc5O

RUN: RUN3177

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.24

MAT-POS-090737b9-1_2



CID: MAT-POS-090737b9-1_2

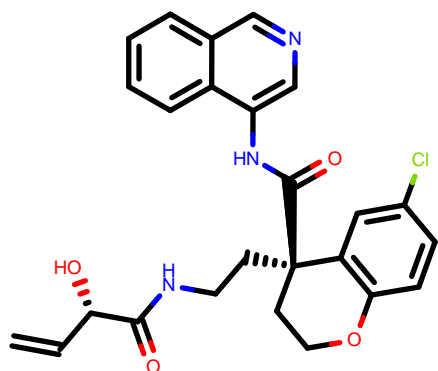
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN2002

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.37

EN300-181492_3_1_1



CID: EN300-181492_3_1_1

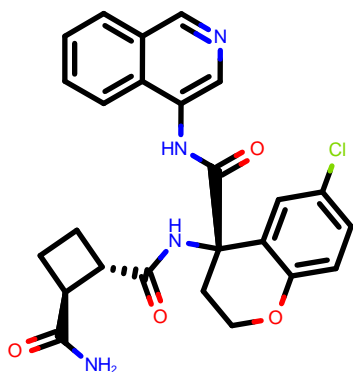
SMILES: C=C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3829

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.30

EN300-217107_1_2_1



CID: EN300-217107_1_2_1

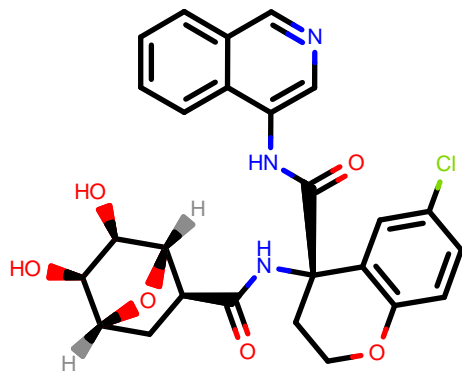
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@@H]5C(=O)N

RUN: RUN2806

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.26

EN300-6764836_1_8_1



CID: EN300-6764836_1_8_1

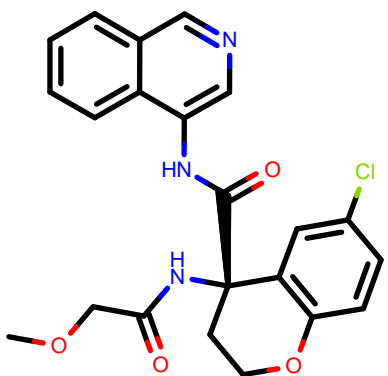
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H]6[C@H](C)[C@@H]5O6O

RUN: RUN3412

DDG (kcal/mol): -2.56

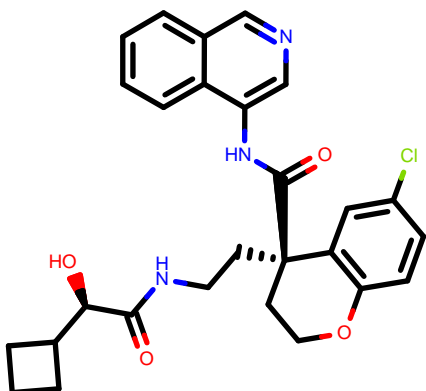
dDDG (kcal/mol): 0.27

EDG-MED-90036822-34_1



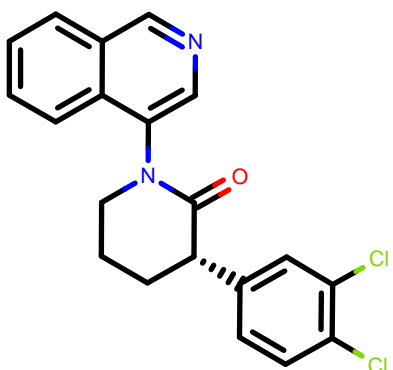
CID:	EDG-MED-90036822-34_1
SMILES:	<chem>COCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4</chem>
RUN:	RUN1534
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.18

EN300-249764_3_1_1



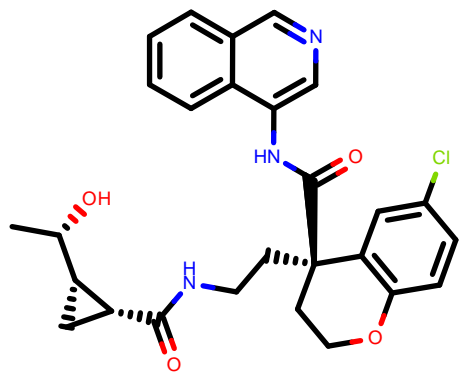
CID:	EN300-249764_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C5CC5)O</chem>
RUN:	RUN4223
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.23

ALP-POS-e0fe77e5-1_2



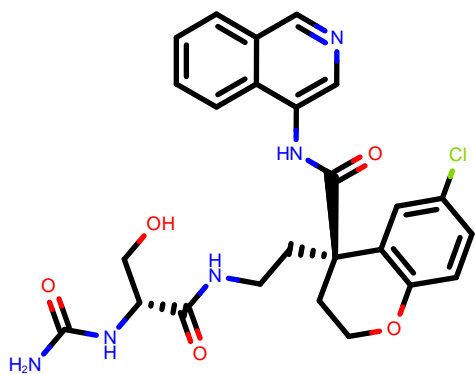
CID:	ALP-POS-e0fe77e5-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCCC[C@H](C3=O)c4ccc(c(c4)Cl)Cl</chem>
RUN:	RUN2140
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.31

EN300-6729572_3_7_1



CID:	EN300-6729572_3_7_1
SMILES:	<chem>C[C@@H](C@H)[C@H]1C[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5O</chem>
RUN:	RUN3648
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.28

EN300-10170_3_1_1



CID: EN300-10170_3_1_1

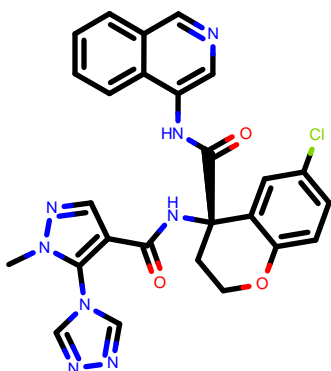
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](CO)NC(=O)N

RUN: RUN3818

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.28

EN300-157527_1_1_1



CID: EN300-157527_1_1_1

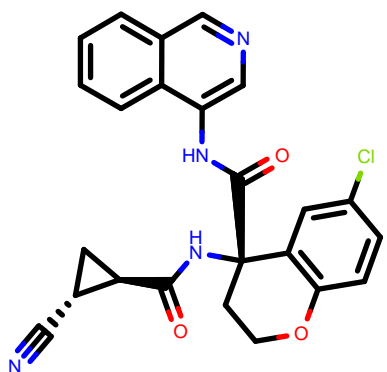
SMILES: Cn1c(c(en1)C(=O)N)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5)n6cnm6

RUN: RUN3227

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.30

EN300-1600363_1_1_1



CID: EN300-1600363_1_1_1

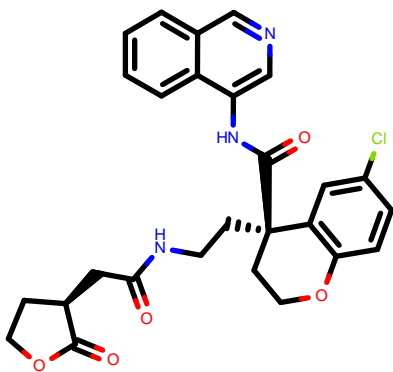
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@H]5C#N

RUN: RUN3654

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.20

EN300-1072972_3_1_1



CID: EN300-1072972_3_1_1

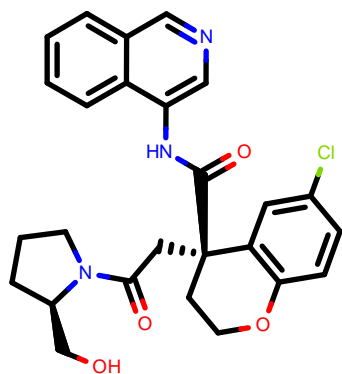
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCOC5=O

RUN: RUN4553

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.38

EN300-54891_1_1_1



CID: EN300-54891_1_1_1

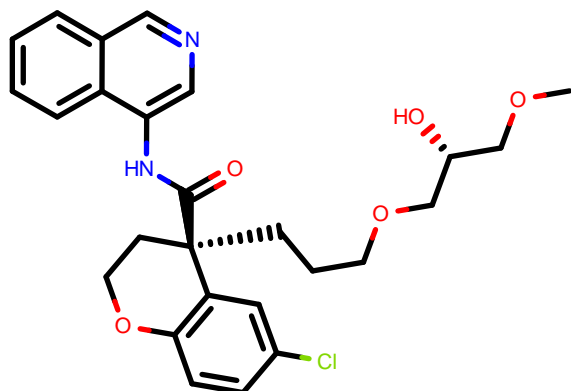
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5CCCC[C@@H]5CO

RUN: RUN3536

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.25

EN300-1915260_4_2_1



CID: EN300-1915260_4_2_1

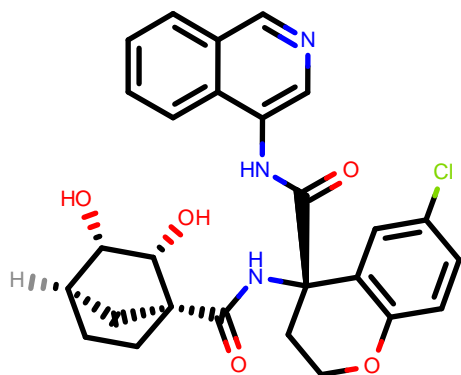
SMILES: COC[C@H](COCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6041

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.45

EN300-7432302_1_1_1



CID: EN300-7432302_1_1_1

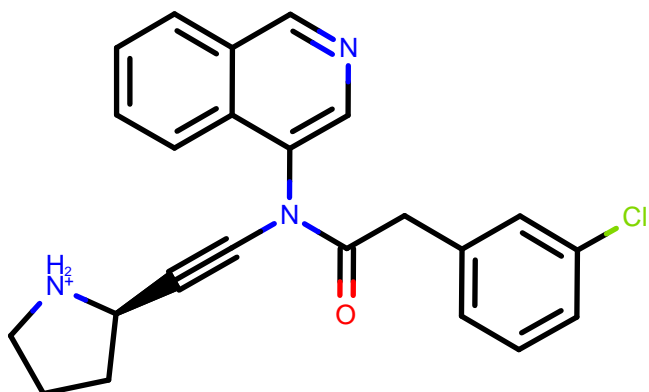
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)[C@@H]5[C@@H](C)C[C@@H]5O)O

RUN: RUN2759

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.34

DAR-DIA-076fb6ea-9_2



CID: DAR-DIA-076fb6ea-9_2

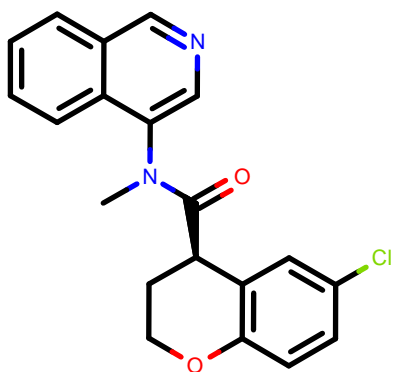
SMILES: c1ccc2c(c1)cnc2N(C#C[C@H]3CCCC[NH2+]3)C(=O)Cc4ccc(cc4)Cl

RUN: RUN1276

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.45

MAK-UNK-3875bbc8-2_1



CID: MAK-UNK-3875bbc8-2_1

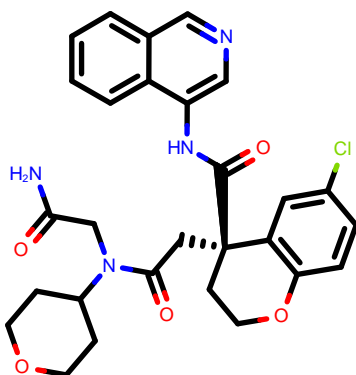
SMILES: CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN718

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.09

EDJ-MED-d203f206-31_1



CID: EDJ-MED-d203f206-31_1

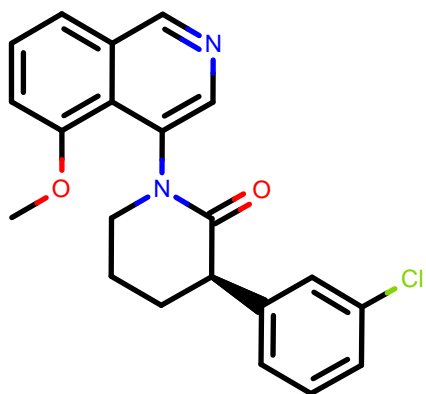
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)C5CCOC5

RUN: RUN2457

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.31

MIC-UNK-50cce87d-12_1



CID: MIC-UNK-50cce87d-12_1

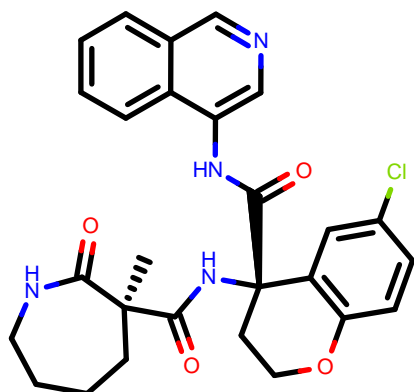
SMILES: COc1cccc2c1c(cnc2)N3CCCC[C@@H](C3=O)c4cccc(c4)Cl

RUN: RUN567

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.21

EN300-6745081_1_1_1



CID: EN300-6745081_1_1_1

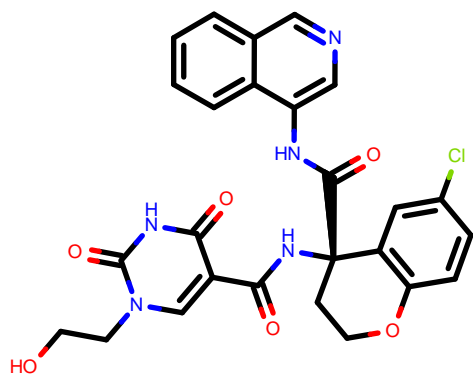
SMILES: C[C@@H]1(CCCNC1=O)C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3133

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.31

EN300-101291_1_1_1



CID: EN300-101291_1_1_1

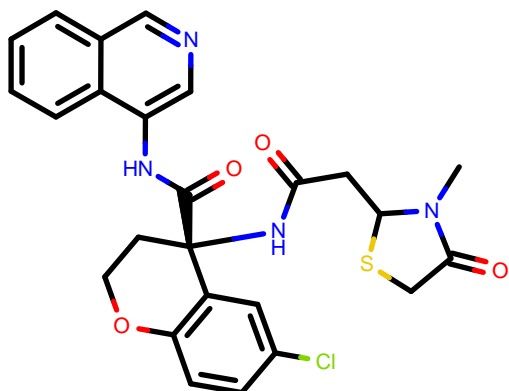
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3C(=O)C(=O)NC(=O)C5=O)[NH]5=O)CCO

RUN: RUN5631

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.39

EN300-143564_1_1_1



CID: EN300-143564_1_1_1

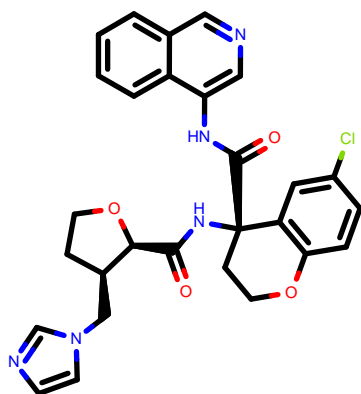
SMILES: CN1C(=O)CS/C1=C/C(=O)N[C@@]2[C@@](C(=O)O3C2C(=O)C(=O)C(=O)Nc4ncnc5c4ccc5

RUN: RUN4048

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.22

EN300-310173_1_1_1



CID: EN300-310173_1_1_1

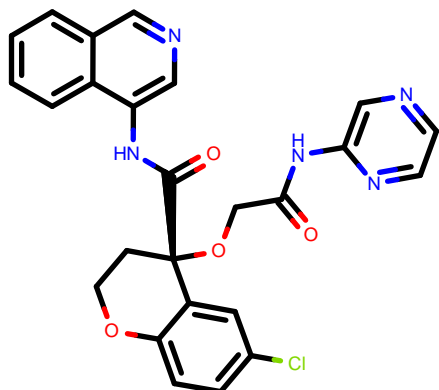
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3C(=O)C(=O)NC(=O)C(=O)Nc5cnc6c5

RUN: RUN3054

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.37

EN300-105267_1_1_1



CID: EN300-105267_1_1_1

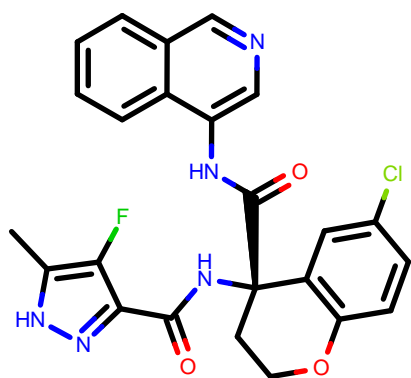
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3C(=O)C(=O)C(=O)Nc5cnc6c5

RUN: RUN4019

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.22

EDG-MED-90036822-79_1



CID: EDG-MED-90036822-79_1

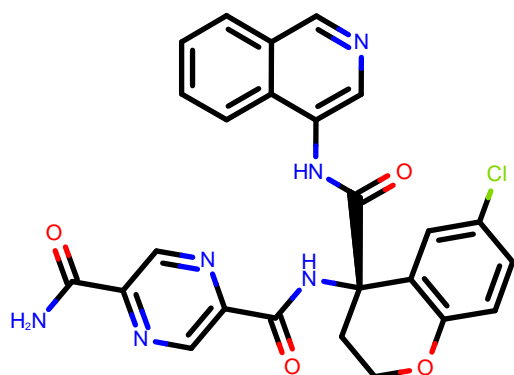
SMILES: Cc1c(c(n[nH]1)C(=O)N)C(=O)N[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5F

RUN: RUN1614

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.28

EN300-1273172_1_1_1



CID: EN300-1273172_1_1_1

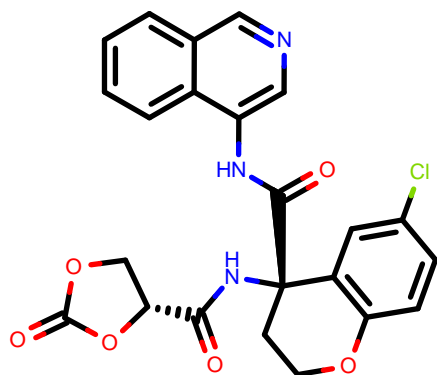
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)NC(=O)c5ncnc(en5)C(=O)N

RUN: RUN3820

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.26

EN300-5253939_1_2_1



CID: EN300-5253939_1_2_1

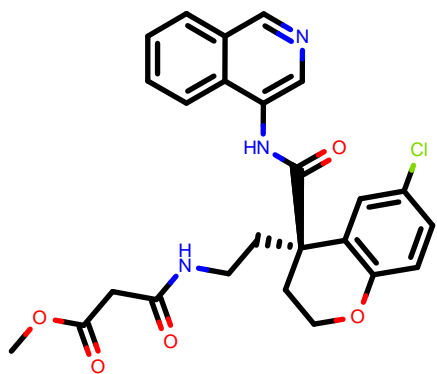
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)NC(=O)[C@@H]5COC(=O)O5

RUN: RUN3790

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.22

EN300-20668_3_1_1



CID: EN300-20668_3_1_1

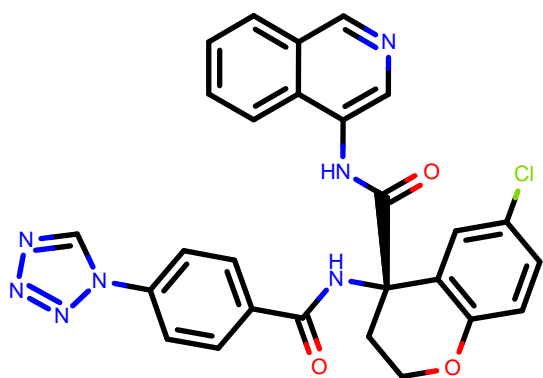
SMILES: COC(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5029

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.27

EN300-06030_1_1_1



CID: EN300-06030_1_1_1

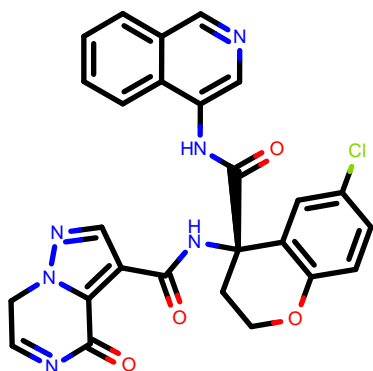
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)n6cnm6

RUN: RUN4992

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.30

EN300-6526669_1_1_1



CID: EN300-6526669_1_1_1

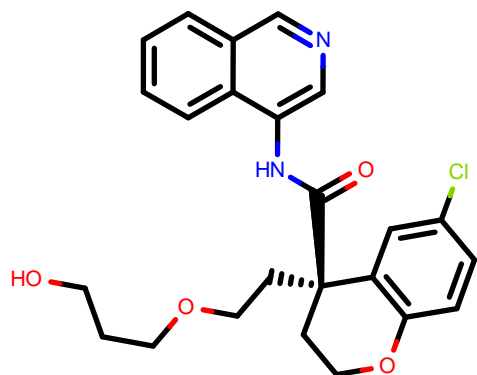
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5C(=O)NCC6

RUN: RUN2953

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.26

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

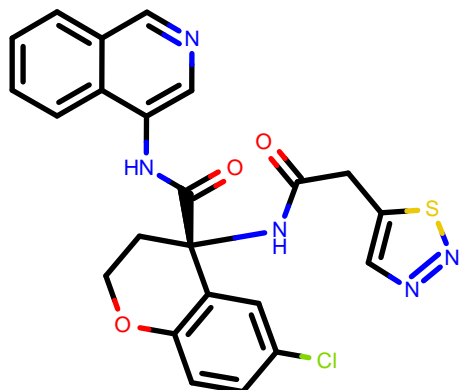
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN3784

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.25

EN300-260152_1_1_1



CID: EN300-260152_1_1_1

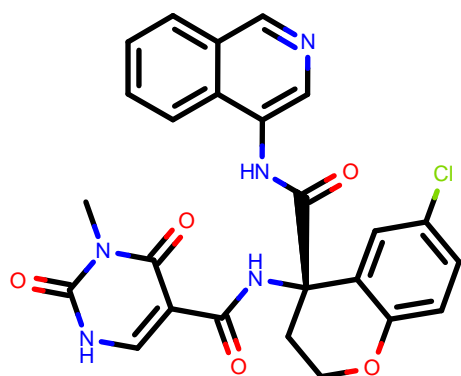
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnn5

RUN: RUN2892

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.23

EN300-102487_1_1_1



CID: EN300-102487_1_1_1

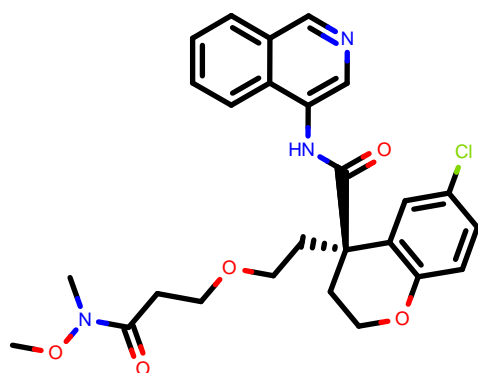
SMILES: Cn1c(=O)c[nH]c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3427

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.31

EN300-174603_3_1_1



CID: EN300-174603_3_1_1

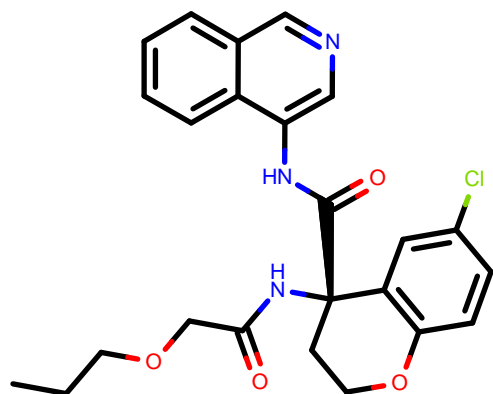
SMILES: CN(C(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN4409

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.31

EN300-44821_1_1_1



CID: EN300-44821_1_1_1

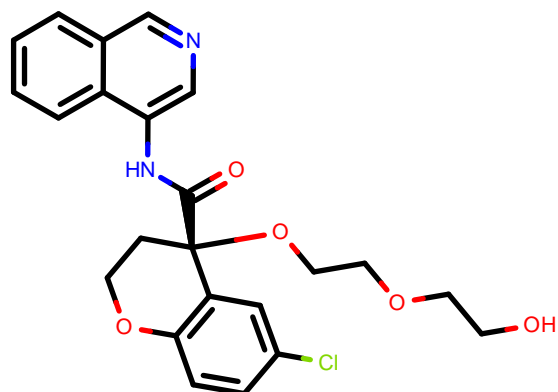
SMILES: C=CCOCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN3405

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.18

EN300-52467_1_1_1



CID: EN300-52467_1_1_1

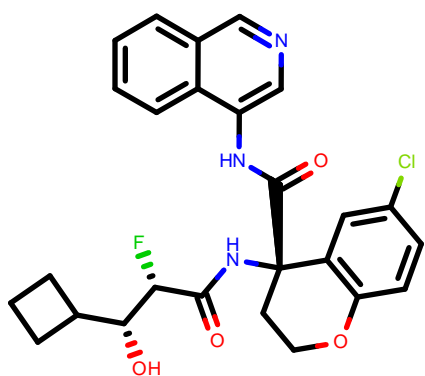
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN5004

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.25

EDG-MED-90036822-99_2



CID: EDG-MED-90036822-99_2

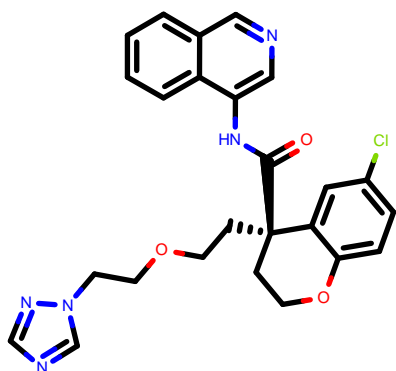
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C=O)[C@H]([C@@H](C5CC5)O)F

RUN: RUN1725

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.30

EN300-6255179_3_1_1



CID: EN300-6255179_3_1_1

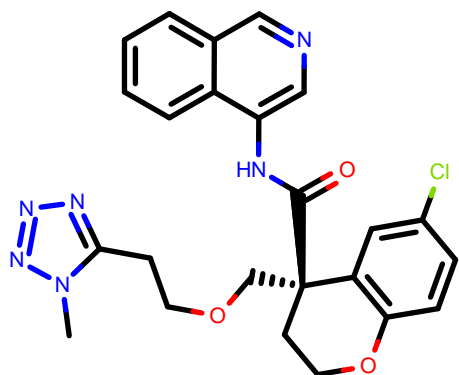
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCn5cncn5

RUN: RUN3705

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.25

EN300-365398_2_1_1



CID: EN300-365398_2_1_1

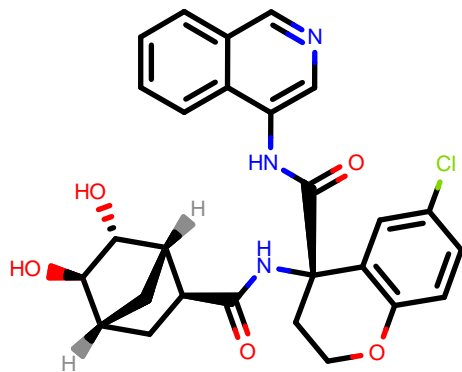
SMILES: Cn1c(nnn1)CCOC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3291

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.30

EN300-6744028_1_4_1



CID: EN300-6744028_1_4_1

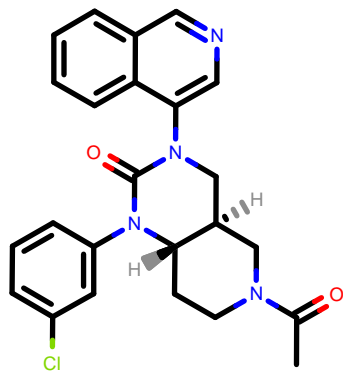
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C=O)[C@H]5[C@@H]6[C@@H]7[C@@H]8[C@@H]9[C@@H]10

RUN: RUN3548

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.29

MIC-UNK-9582b2c5-3_4



CID: MIC-UNK-9582b2c5-3_4

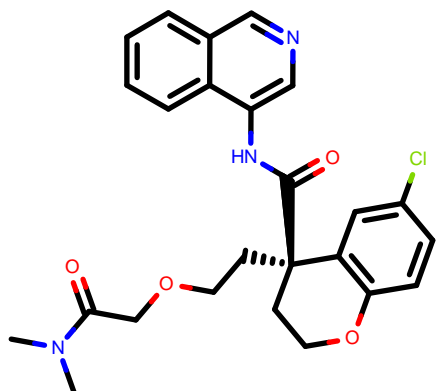
SMILES: CC(=O)N1CC[C@H]2[C@H](C1)CN(C(=O)N2c3cccc(c3)Cl)c4cccc5c4cccc5

RUN: RUN170

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.31

EN300-216063_3_1_1



CID: EN300-216063_3_1_1

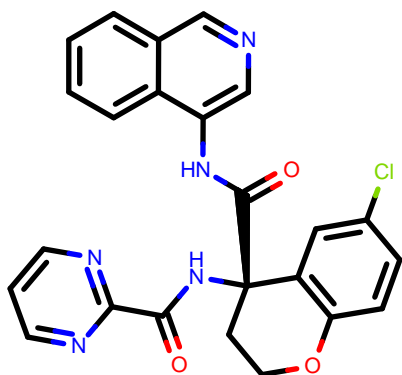
SMILES: CN(C)C(=O)COCC[C@]1(C)C(CO2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3954

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.20

EN300-80230_1_1_1



CID: EN300-80230_1_1_1

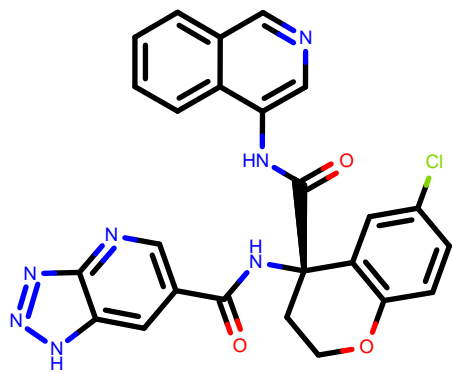
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO4c3cc(cc4)Cl)NC(=O)c5ncccc5

RUN: RUN3108

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.19

EDJ-MED-6864a934-7_1



CID: EDJ-MED-6864a934-7_1

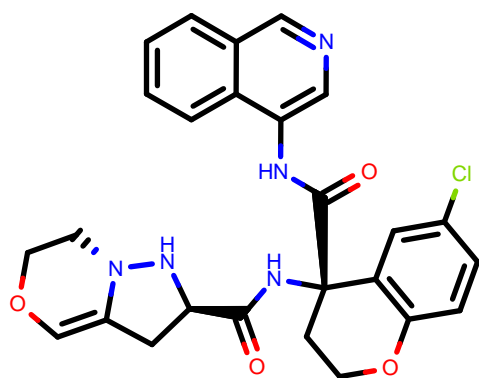
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO4c3cc(cc4)Cl)NC(=O)c5cc6c(nc5)n[nH]6

RUN: RUN2435

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.22

EN300-244278_1_1_2



CID: EN300-244278_1_1_2

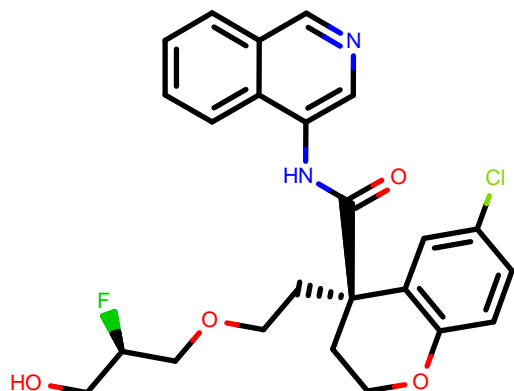
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C=C6COC[C@]6N5

RUN: RUN2939

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.28

EN300-1600517_3_1_1



CID: EN300-1600517_3_1_1

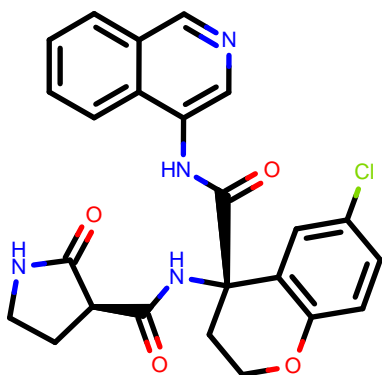
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@]3(F)CO

RUN: RUN3181

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.30

EN300-94945_1_2_1



CID: EN300-94945_1_2_1

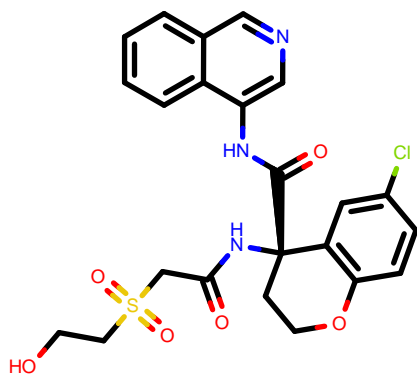
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCNC5=O

RUN: RUN3003

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.21

EN300-4293814_1_1_1



CID: EN300-4293814_1_1_1

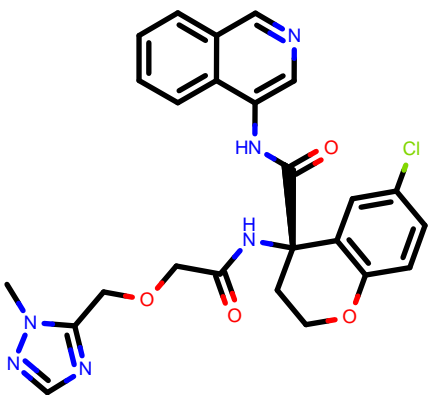
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS(=O)(=O)CCO

RUN: RUN3694

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.50

EN300-213358_1_1_1



CID: EN300-213358_1_1_1

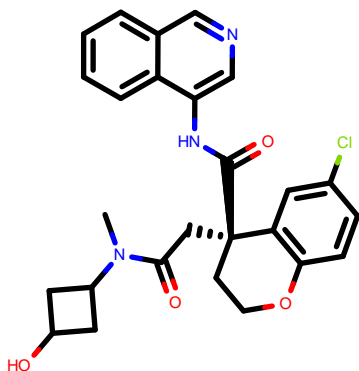
SMILES: Cn1c(ncn1)COCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5251

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.25

EN300-97697_1_1_1



CID: EN300-97697_1_1_1

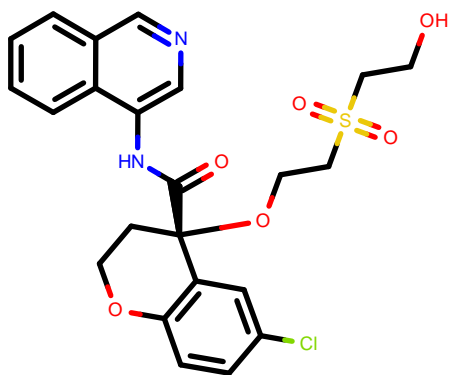
SMILES: CN(C)CC(C1O)C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3311

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.30

EN300-7463171_1_1_1



CID: EN300-7463171_1_1_1

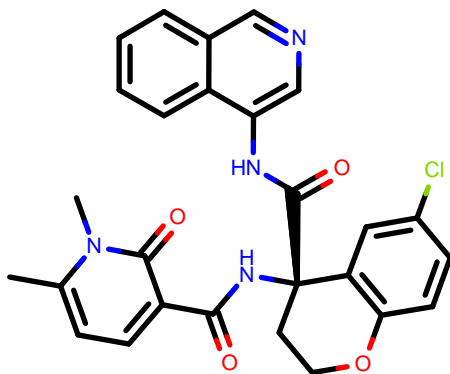
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCCS(=O)(=O)CO

RUN: RUN3826

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.44

EN300-41423_1_1_1



CID: EN300-41423_1_1_1

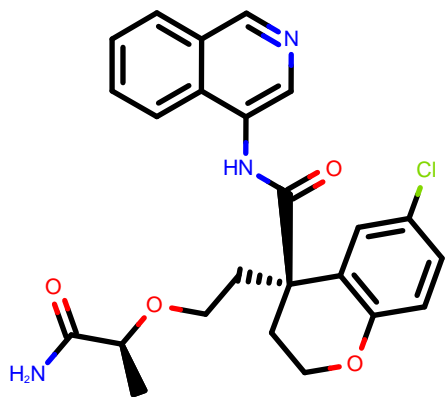
SMILES: Cc1ccc(c(=O)n1C)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3243

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.30

EN300-17381_3_1_1



CID: EN300-17381_3_1_1

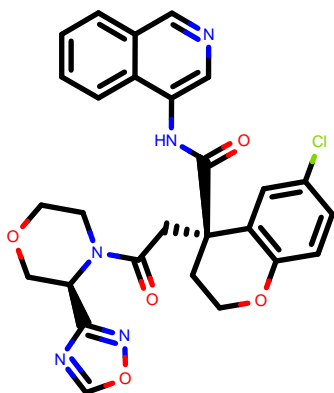
SMILES: C[C@@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4638

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-3_1



CID: EDJ-MED-d203f206-3_1

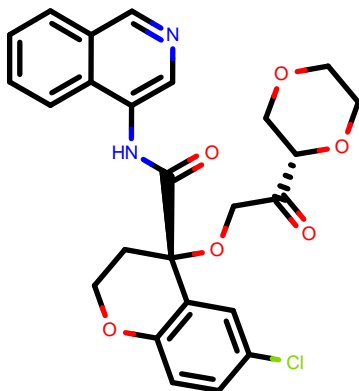
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5COCOC[C@@H]5c6ncon6

RUN: RUN2442

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.41

EN300-6238494_1_1_1



CID: EN300-6238494_1_1_1

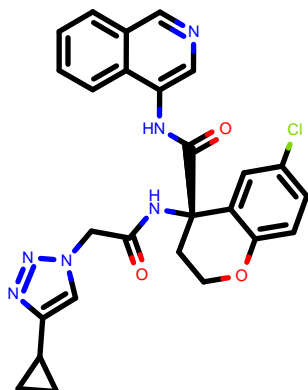
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COCOC5

RUN: RUN4186

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.28

EN300-107892_1_1_1



CID: EN300-107892_1_1_1

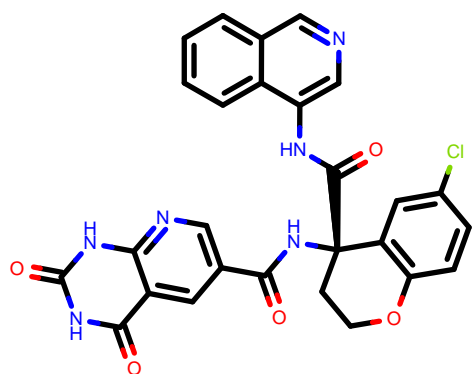
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cc(mn5)C6C6

RUN: RUN3322

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.30

EN300-42131_1_1_1



CID: EN300-42131_1_1_1

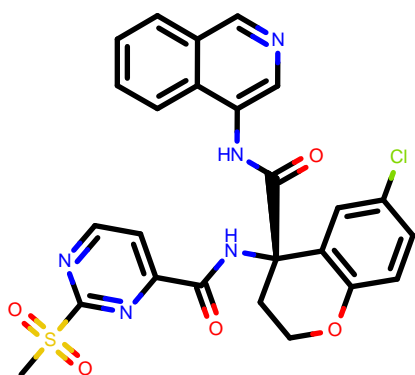
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c([nH]c(=O)[nH]c6=O)nc5

RUN: RUN2910

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.29

EN300-205622_1_1_1



CID: EN300-205622_1_1_1

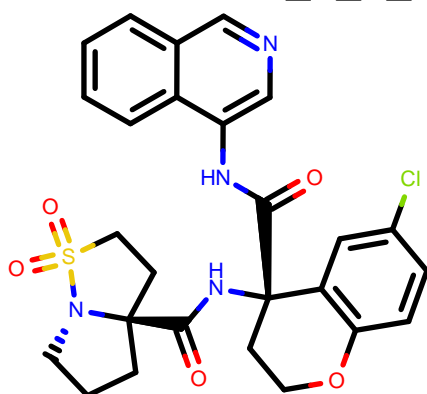
SMILES: CS(=O)(=O)c1nccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN3236

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.28

EN300-6733459_1_1_1



CID: EN300-6733459_1_1_1

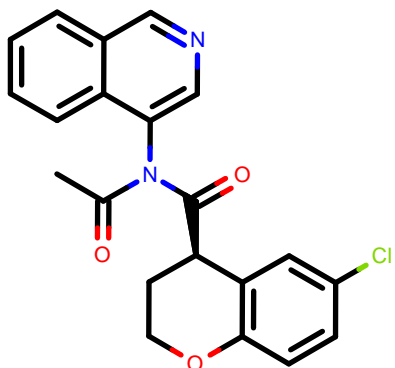
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(S(=O)(=O)O)CCN5

RUN: RUN3185

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.53

VLA-UCB-50c39ae8-1_1



CID: VLA-UCB-50c39ae8-1_1

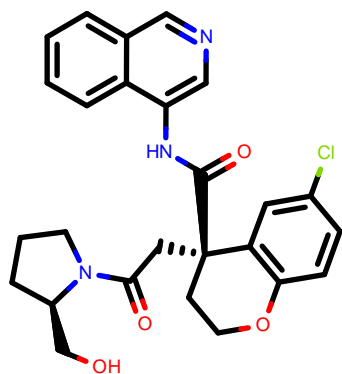
SMILES: CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)C)Cl

RUN: RUN326

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.14

EDJ-MED-d203f206-41_1



CID: EDJ-MED-d203f206-41_1

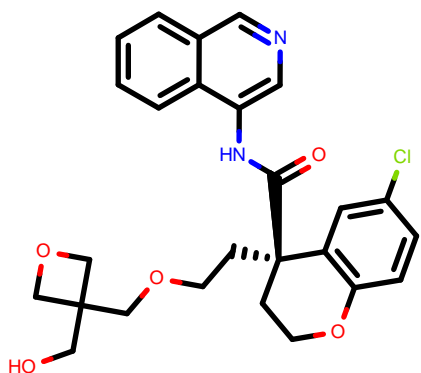
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)N5CC[C@@H]5CO

RUN: RUN2434

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.27

EN300-102347_3_1_1



CID: EN300-102347_3_1_1

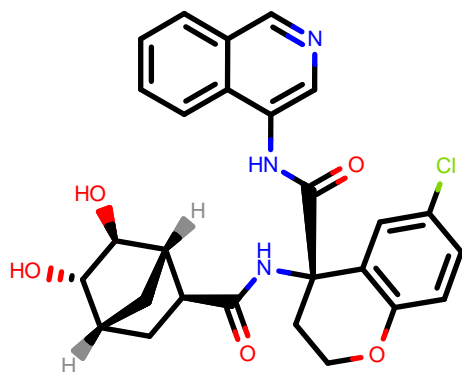
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCOCC5(COC5)CO

RUN: RUN2956

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.28

EN300-6744028_1_6_1



CID: EN300-6744028_1_6_1

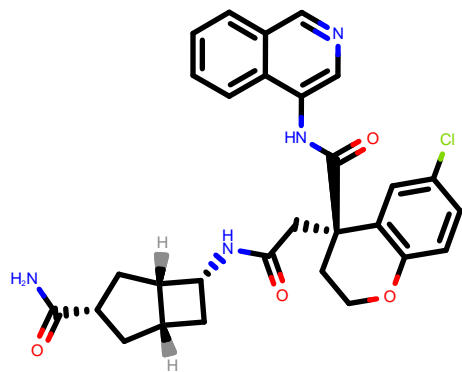
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)[C@@H]5C[C@@H]6[C@@H]7[C@@H]8O[C@H]8O

RUN: RUN2931

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.23

EN300-1268016_1_11_1



CID: EN300-1268016_1_11_1

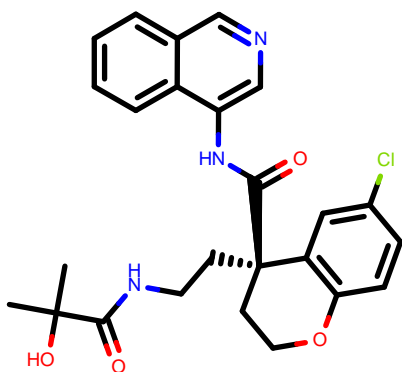
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)N[C@@]5(C)[C@@H]6[C@@H]7[C@@H]8Cl[C@H]8N

RUN: RUN4057

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.38

EN300-59285_3_1_1



CID: EN300-59285_3_1_1

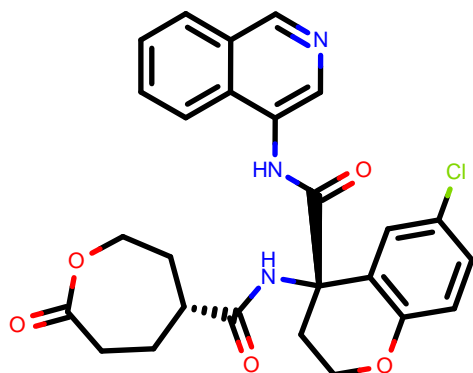
SMILES: CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN5564

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.27

EN300-2011083_1_1_1



CID: EN300-2011083_1_1_1

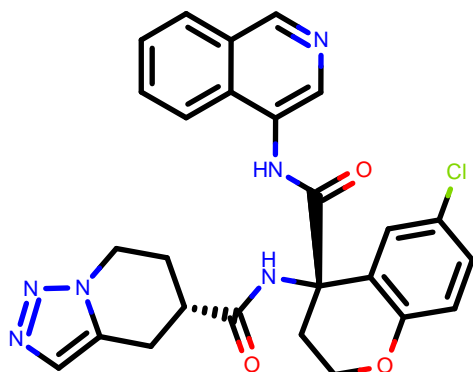
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)OCC5

RUN: RUN4483

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.29

EN300-7430501_1_2_1



CID: EN300-7430501_1_2_1

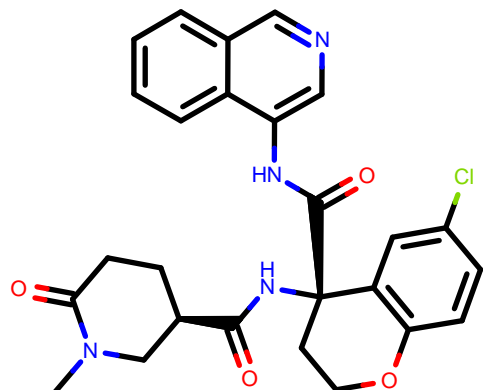
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5Cn6c(cnn6)C5

RUN: RUN2790

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.26

EN300-52983_1_1_1



CID: EN300-52983_1_1_1

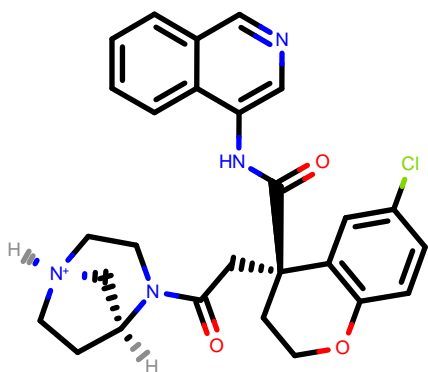
SMILES: CN1C[C@@H](CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4467

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.27

EN300-227218_1_1_1



CID: EN300-227218_1_1_1

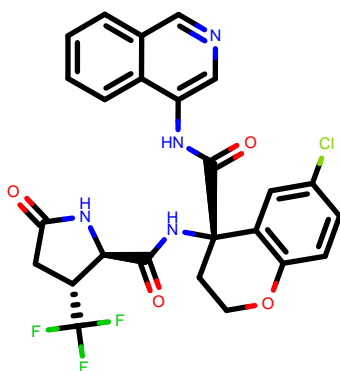
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[N+]@H6CC[C@H]5C6

RUN: RUN3946

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.31

EN300-169955_1_2_1



CID: EN300-169955_1_2_1

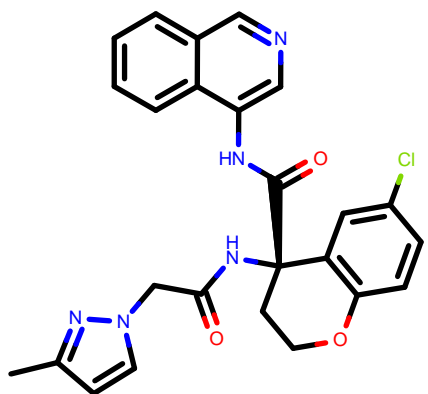
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@H]5C[C@H](C(F)(F)F)C5

RUN: RUN3100

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.25

EN300-226964_1_1_1



CID: EN300-226964_1_1_1

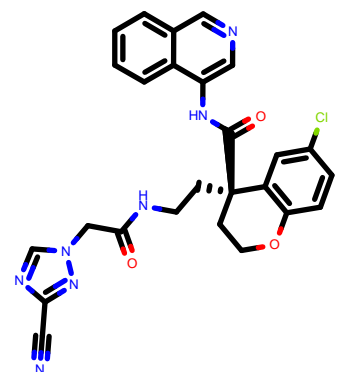
SMILES: Cc1ccn(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncnc5c4cccc5

RUN: RUN4851

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.21

EN300-111863_3_1_1



CID: EN300-111863_3_1_1

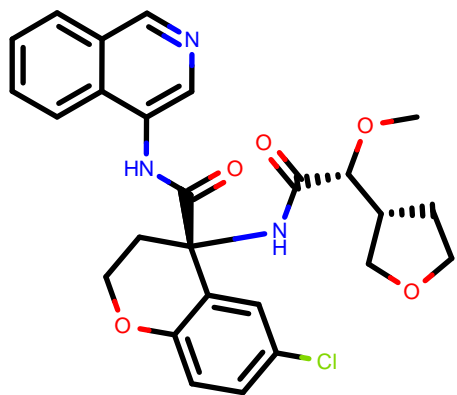
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc(n5)C#N

RUN: RUN3386

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.30

EN300-298552_1_2_1



CID: EN300-298552_1_2_1

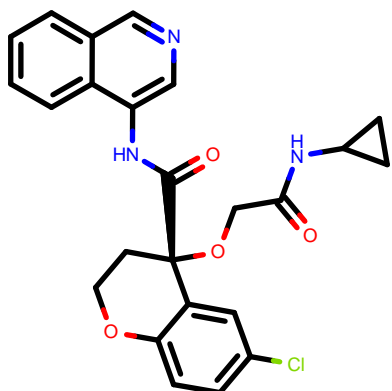
SMILES: CO[C@H]([C@@H]1CCOC1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3252

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.25

EN300-1253178_1_1_1



CID: EN300-1253178_1_1_1

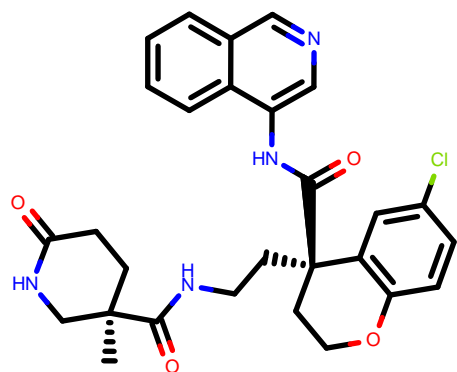
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN: RUN3063

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.17

EN300-195924_3_2_1



CID: EN300-195924_3_2_1

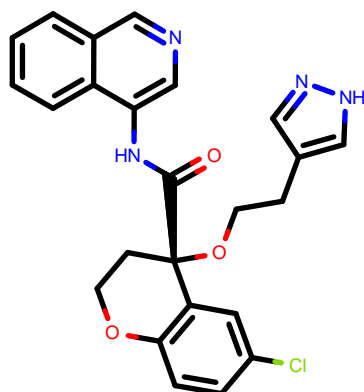
SMILES: C[C@@]1(CCC(=O)NC1)C(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4307

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.42

EDJ-MED-28ec730d-5_1_1



CID: EDJ-MED-28ec730d-5_1_1

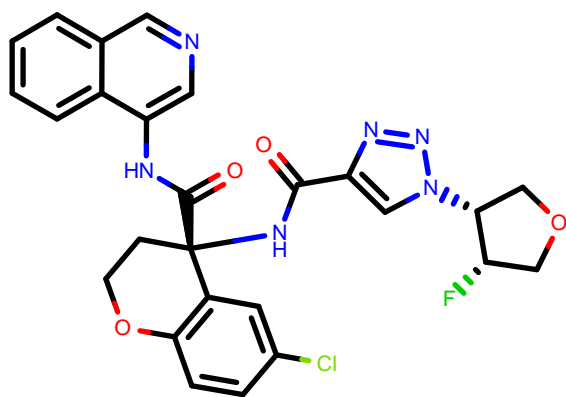
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCCc5c[nH]nc5

RUN: RUN3056

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.26

EN300-6759512_1_1_1



CID: EN300-6759512_1_1_1

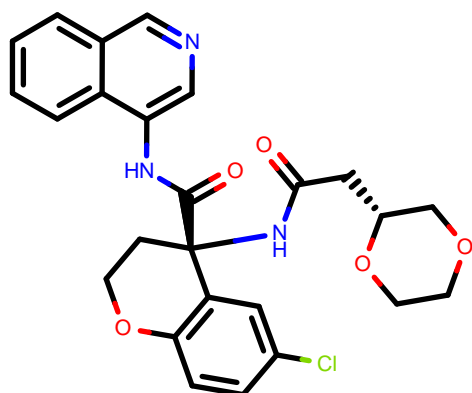
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6cnc5c6F

RUN: RUN5171

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.29

EN300-731622_1_1_1



CID: EN300-731622_1_1_1

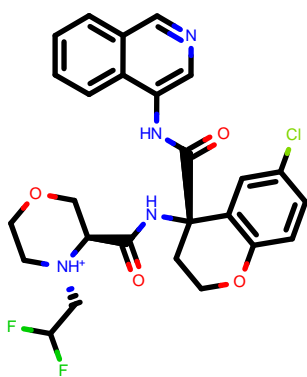
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5OCCO5

RUN: RUN3567

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.21

EN300-140582_1_1_1



CID: EN300-140582_1_1_1

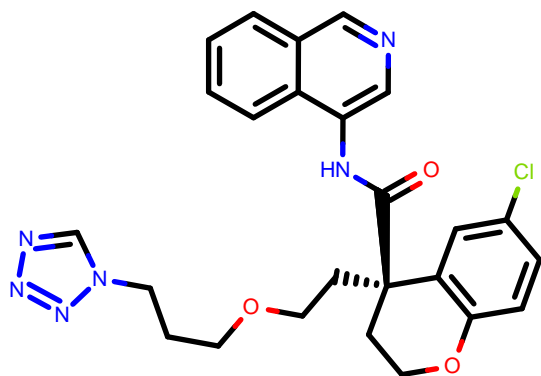
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5COC(F)F5

RUN: RUN2930

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.25

EN300-1696962_3_1_1



CID: EN300-1696962_3_1_1

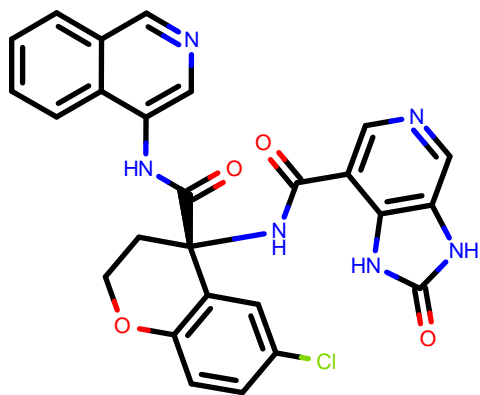
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCn5cnn5

RUN: RUN3034

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

EN300-7434209_1_1_1



CID: EN300-7434209_1_1_1

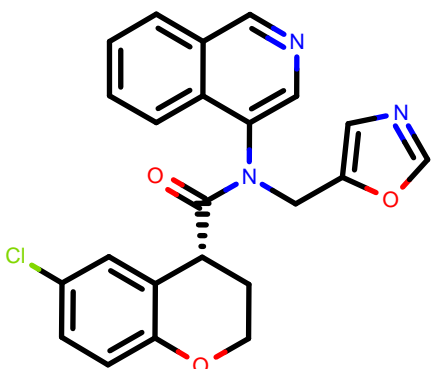
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncc6c5[nH]c(=O)[nH]6

RUN: RUN3439

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.26

ALP-UNI-44c99a80-3_1



CID: ALP-UNI-44c99a80-3_1

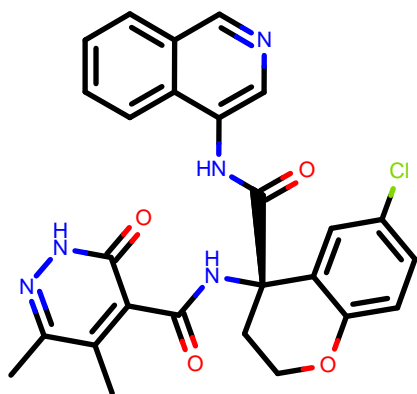
SMILES: c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@]4[H]4CCOc5c4cc(cc5)Cl

RUN: RUN446

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.19

EN300-29220_1_1_1



CID: EN300-29220_1_1_1

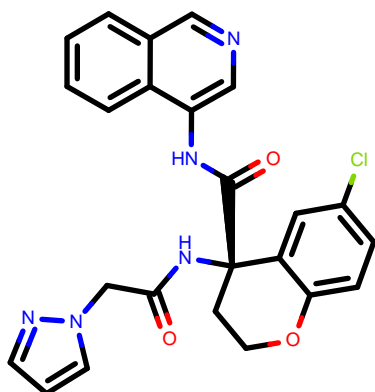
SMILES: Cc1c[nH]c(=O)c1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5C

RUN: RUN6549

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

EN300-23942_1_1_1



CID: EN300-23942_1_1_1

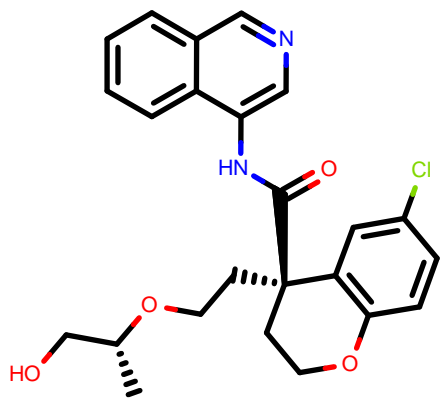
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cccn5

RUN: RUN3022

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.22

EN300-175186_3_2_1



CID: EN300-175186_3_2_1

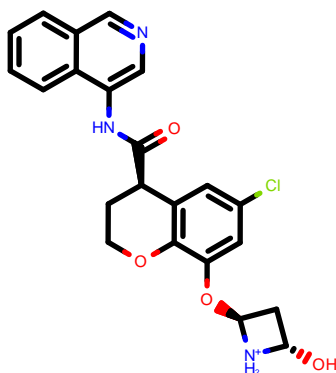
SMILES: C[C@H](CO)OCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2885

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.28

VLA-UCB-50c39ae8-8_2_1



CID: VLA-UCB-50c39ae8-8_2_1

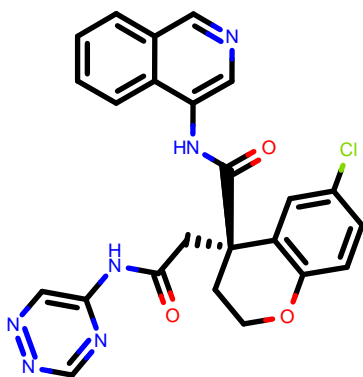
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4)C[C@H]5C[C@@H]([NH2+])O)Cl

RUN: RUN3384

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.33

EDJ-MED-d203f206-13_1



CID: EDJ-MED-d203f206-13_1

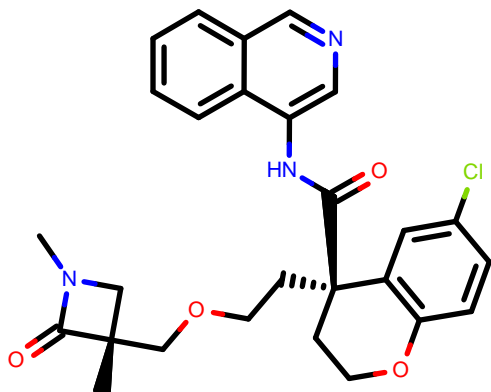
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)Nc5nncn5

RUN: RUN2371

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.25

EN300-1273362_3_1_1



CID: EN300-1273362_3_1_1

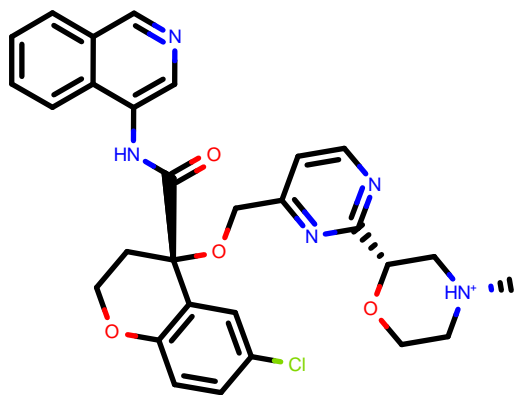
SMILES: C[C@@]1(CN(C1=O)C)OCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3365

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.33

ED_-GRI-5b13fbe2-74_1



CID: ED_-GRI-5b13fbe2-74_1

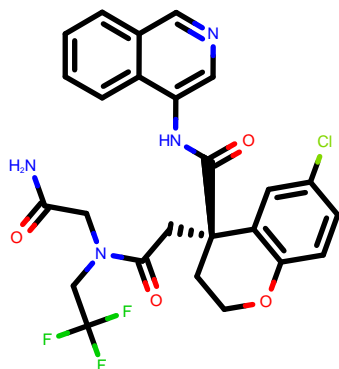
SMILES: CN@@H]CCO[C@@H](C1)2nccc2)C(C@@)3(CCOc4c3cc(cc4)C)C(=O)Nc5ncc6c5ccc6

RUN: RUN1538

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.33

EN300-138676_1_1_1



CID: EN300-138676_1_1_1

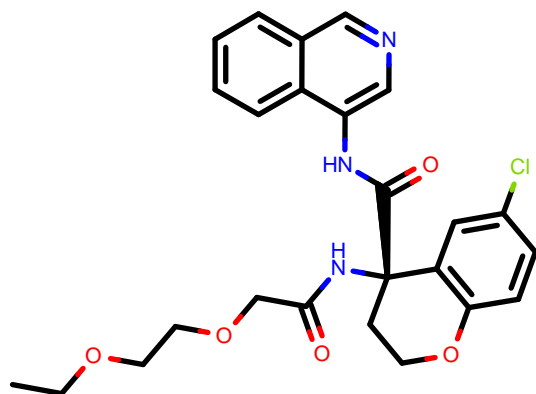
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(CC(=O)N)CC(F)(F)F

RUN: RUN3755

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.28

EN300-54304_1_1_1



CID: EN300-54304_1_1_1

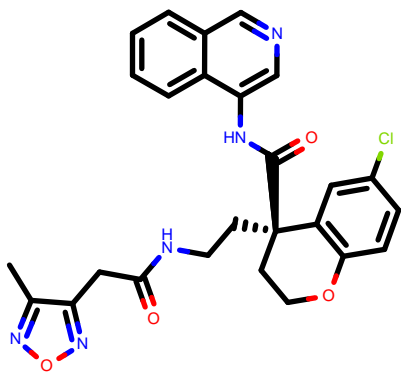
SMILES: CCOCCOCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN5032

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.24

EN300-254883_3_1_1



CID: EN300-254883_3_1_1

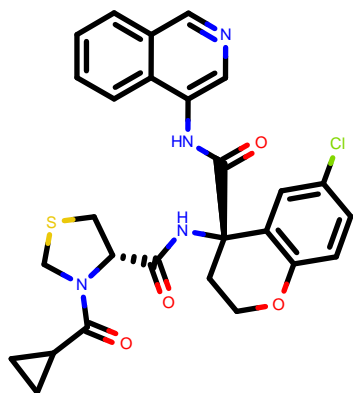
SMILES: Cc1c(non1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3642

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.26

EN300-18928_1_2_1



CID: EN300-18928_1_2_1

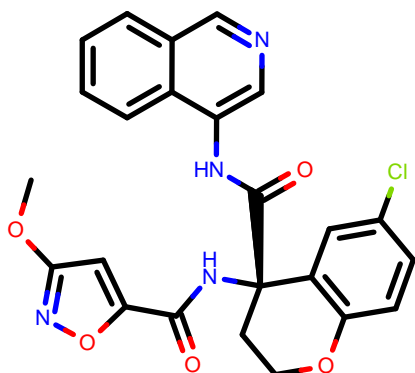
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CSCN5C(=O)C6CC6

RUN: RUN3392

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.35

EN300-131465_1_1_1



CID: EN300-131465_1_1_1

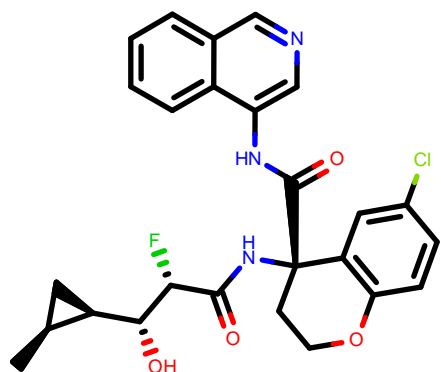
SMILES: COc1cc(on1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3350

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.22

EDG-MED-90036822-94_8



CID: EDG-MED-90036822-94_8

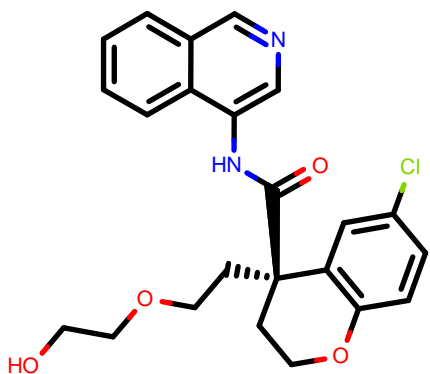
SMILES: C[C@@H]1[C@@H]2[C@@H]3[C@@H]4[C@@H]5C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5F1O

RUN: RUN1670

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.26

EN300-21258_3_1_1



CID: EN300-21258_3_1_1

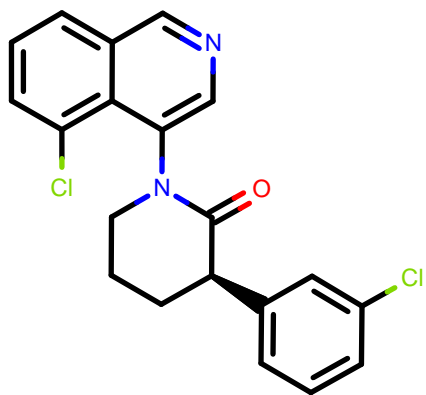
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN3090

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.22

MIC-UNK-50cce87d-10_2



CID: MIC-UNK-50cce87d-10_2

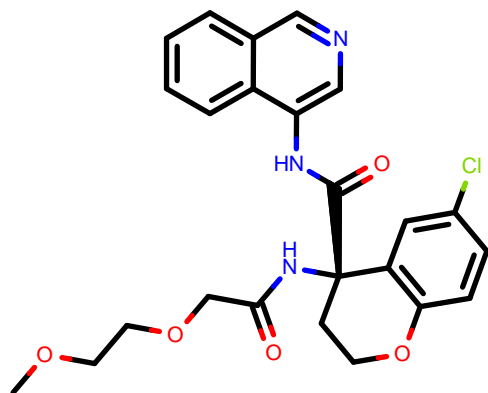
SMILES: c1cc(cc(c1)Cl)[C@H]2CCCN(C2=O)c3cncc4c3c(ccc4)Cl

RUN: RUN560

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.22

EN300-20375_1_1_1



CID: EN300-20375_1_1_1

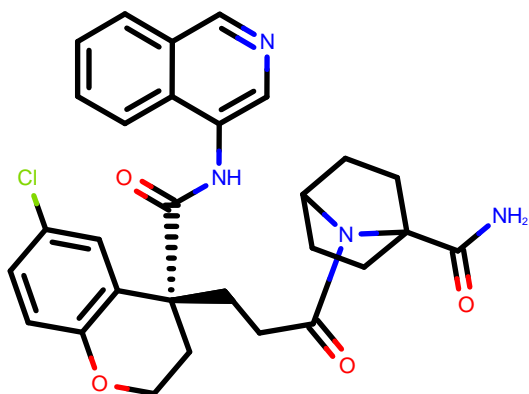
SMILES: COCOCOC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3224

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.23

EN300-637522_2_1_1



CID: EN300-637522_2_1_1

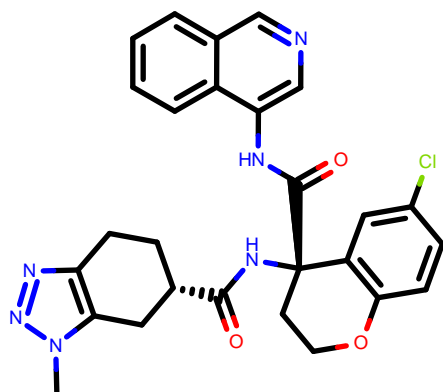
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C6CCCC5(CC6)C(=O)N

RUN: RUN7648

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.29

EN300-217343_1_1_1



CID: EN300-217343_1_1_1

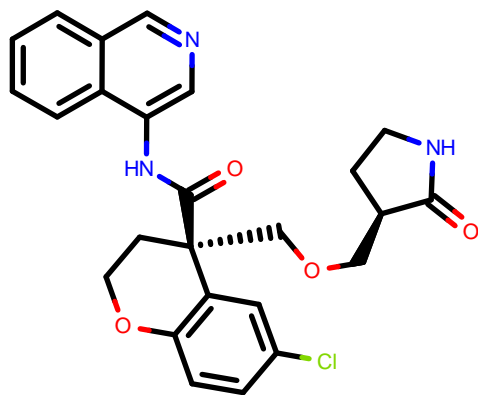
SMILES: Cn1c2c(n1)CC[C@@H](C2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN4594

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.31

EN300-246248_2_2_1



CID: EN300-246248_2_2_1

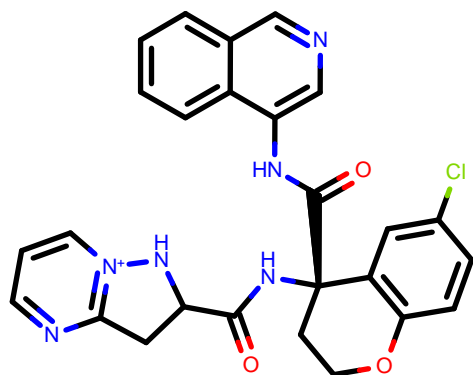
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)COC[C@H]5CCNC5=O

RUN: RUN3590

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.23

EN300-83527_1_1_1



CID: EN300-83527_1_1_1

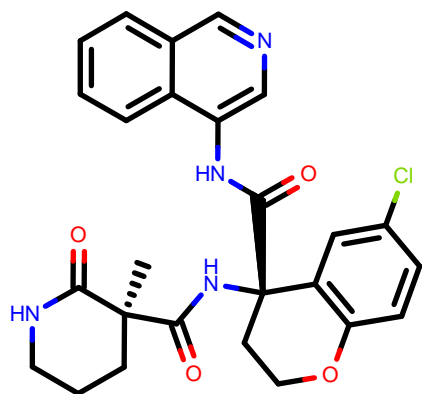
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5ccnccn6n5

RUN: RUN3283

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.23

EN300-178876_1_1_1



CID: EN300-178876_1_1_1

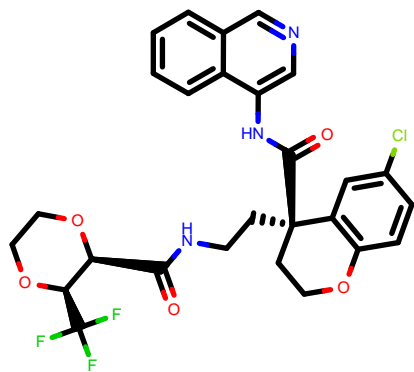
SMILES: C[C@@]1(CCCNC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN3015

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.40

EN300-322400_3_1_1



CID: EN300-322400_3_1_1

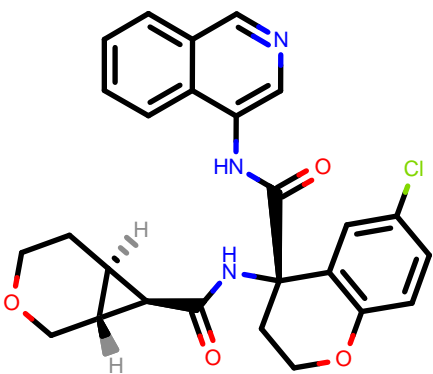
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)COCNC(=O)C(=O)C(F)(F)F

RUN: RUN3082

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.31

EN300-1644723_1_7_1



CID: EN300-1644723_1_7_1

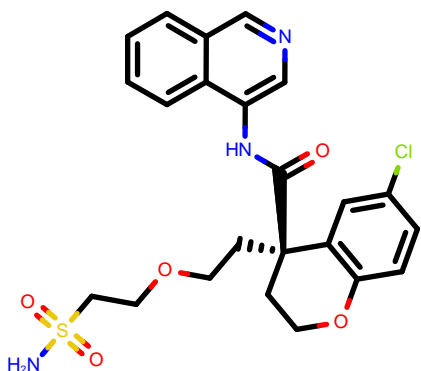
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C@H6C@H5COC65

RUN: RUN3595

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.21

EN300-270710_3_1_1



CID: EN300-270710_3_1_1

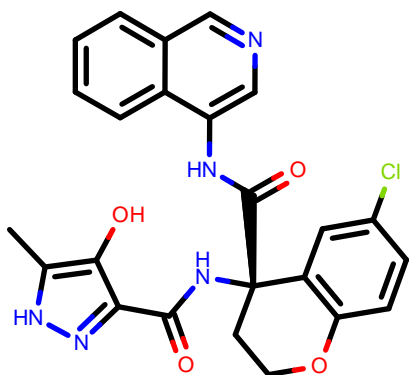
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NS

RUN: RUN3083

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.25

EN300-114526_1_1_1



CID: EN300-114526_1_1_1

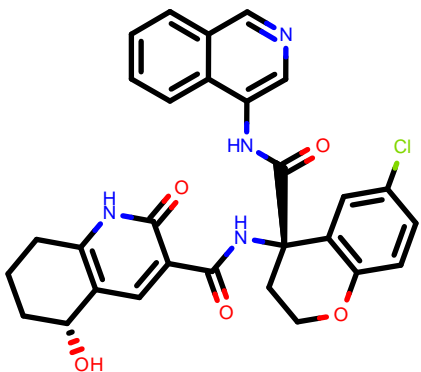
SMILES: Cc1c(c([nH]1)C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5O

RUN: RUN2707

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.23

EN300-238234_1_2_1



CID: EN300-238234_1_2_1

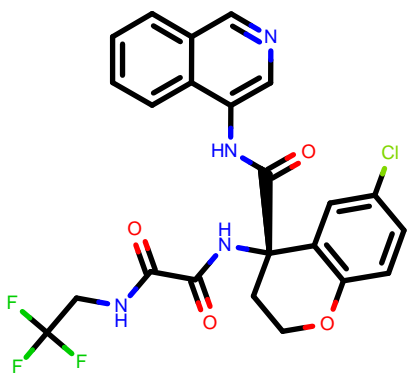
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[nH]5c6c[nH]5c6O

RUN: RUN5157

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.40

EN300-139268_1_1_1



CID: EN300-139268_1_1_1

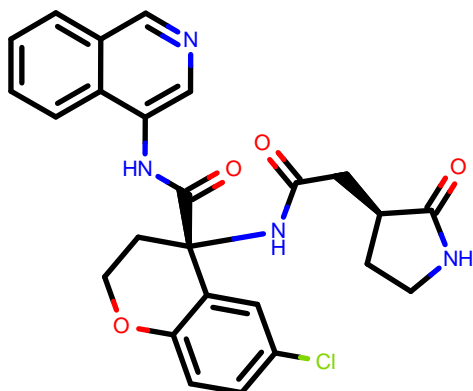
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NC(F)(F)F

RUN: RUN5050

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.22

EN300-343474_1_1_1



CID: EN300-343474_1_1_1

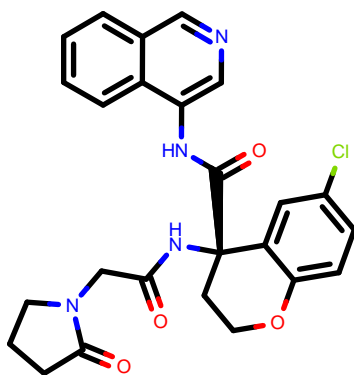
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCNC5=O

RUN: RUN3511

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.25

EN300-11934_1_1_1



CID: EN300-11934_1_1_1

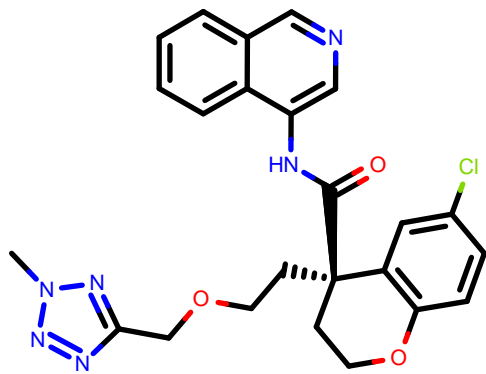
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5CCCC5=O

RUN: RUN4056

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.30

EN300-90225_3_1_1



CID: EN300-90225_3_1_1

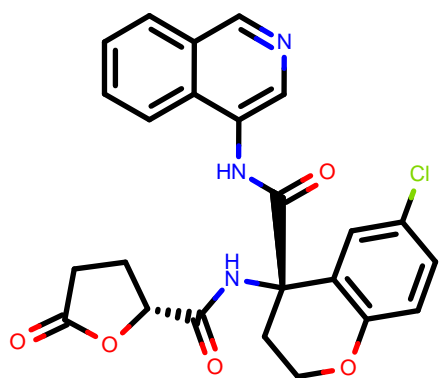
SMILES: Cn1nc(nn1)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2880

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.25

EN300-332606_1_1_1



CID: EN300-332606_1_1_1

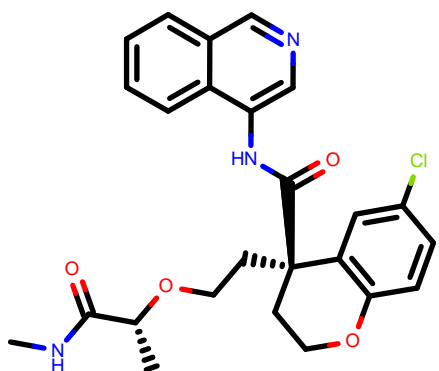
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC(=O)O5

RUN: RUN3320

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.22

EN300-211482_3_2_1



CID: EN300-211482_3_2_1

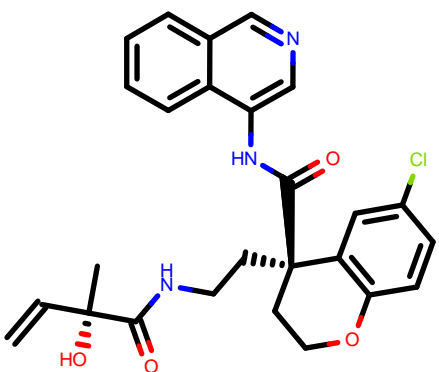
SMILES: C[C@H](C(=O)NC)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN2995

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.33

EN300-248888_3_2_1



CID: EN300-248888_3_2_1

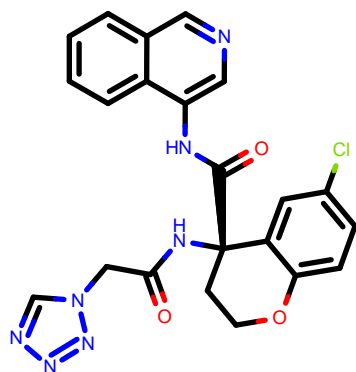
SMILES: C[C@](C=C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O

RUN: RUN6389

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.35

EN300-20980_1_1_1



CID: EN300-20980_1_1_1

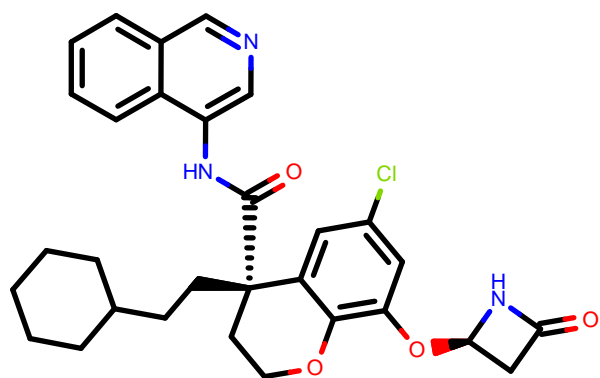
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnnn5

RUN: RUN3116

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.24

VLA-UCB-05e51b3f-12_1_1



CID: VLA-UCB-05e51b3f-12_1_1

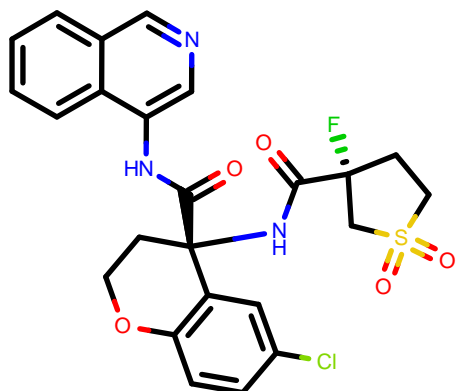
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)C1CCC6CCCC6

RUN: RUN5205

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.49

EN300-311920_1_2_1



CID: EN300-311920_1_2_1

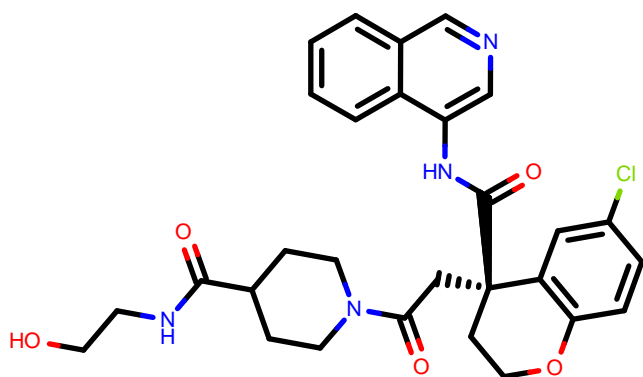
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCS(=O)(=O)C5)F

RUN: RUN2915

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.27

EN300-344753_1_1_1



CID: EN300-344753_1_1_1

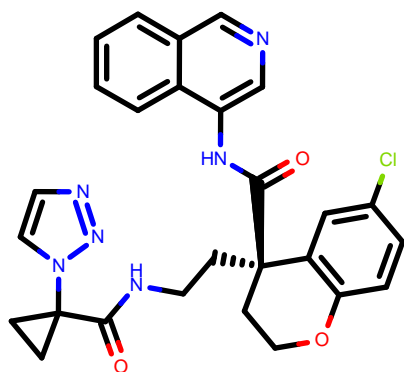
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(C5)NCCO

RUN: RUN3993

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.48

EN300-658559_3_1_1



CID: EN300-658559_3_1_1

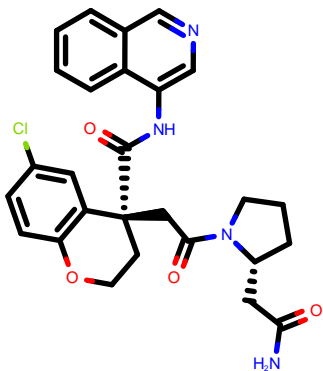
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCS(=O)n6ccn6

RUN: RUN4391

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.35

EDJ-MED-d203f206-8_1



CID: EDJ-MED-d203f206-8_1

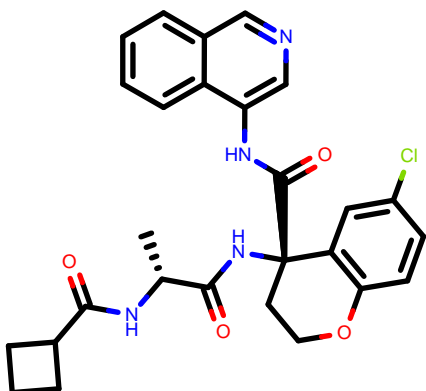
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CC(=O)N

RUN: RUN2413

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.28

ALP-UNI-dbbfd3db-15_2



CID: ALP-UNI-dbbfd3db-15_2

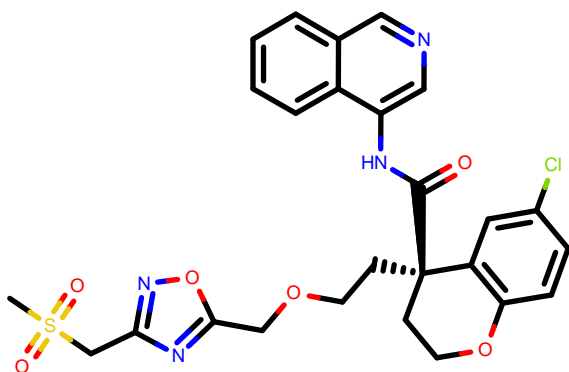
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)C5CC5

RUN: RUN2652

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.32

EN300-94900_3_1_1



CID: EN300-94900_3_1_1

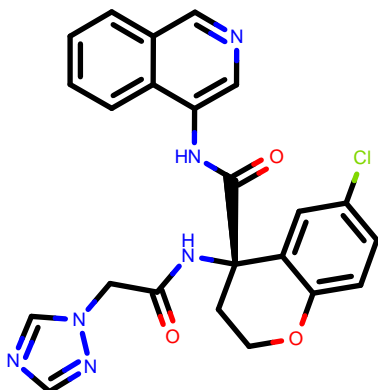
SMILES: CS(=O)(=O)C1=NC(=O)N1COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3217

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.41

EN300-06654_1_1_1



CID: EN300-06654_1_1_1

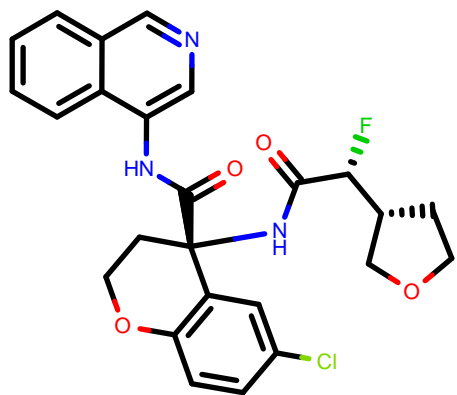
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncn5

RUN: RUN3582

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.22

EN300-783124_1_1_1



CID: EN300-783124_1_1_1

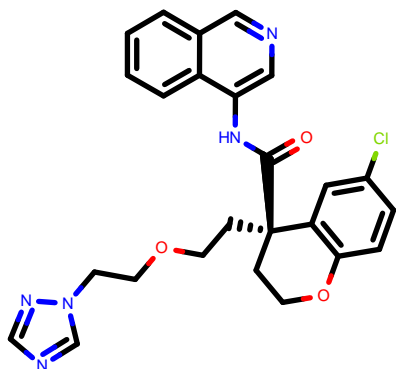
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@@H]5CCOC5)F

RUN: RUN3667

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.19

EN300-6255179_3_1_1



CID: EN300-6255179_3_1_1

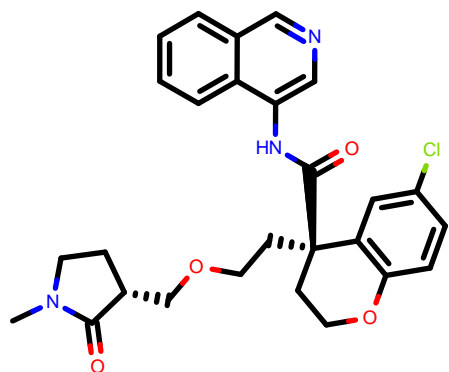
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCn5ncn5

RUN: RUN3624

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.31

EN300-260816_3_1_1



CID: EN300-260816_3_1_1

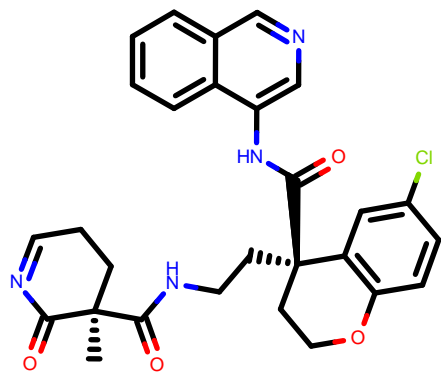
SMILES: CN1CC[C@@H](C1=O)COCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3704

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.31

EN300-178876_3_2_1



CID: EN300-178876_3_2_1

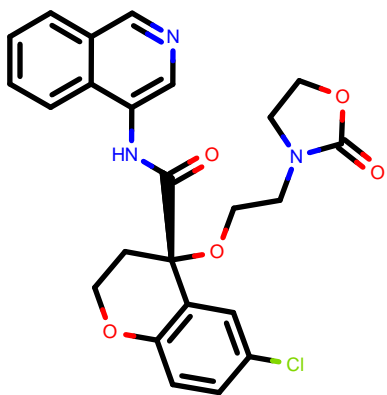
SMILES: C[C@]1(CCCNC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3787

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.47

EN300-370967_1_1_1



CID: EN300-370967_1_1_1

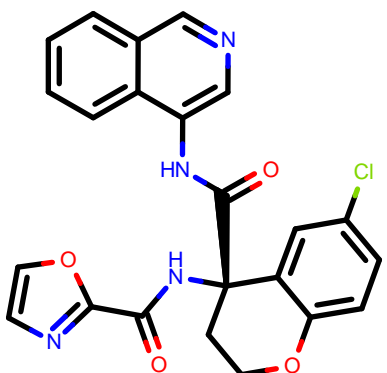
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O

RUN: RUN3627

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.24

EN300-318344_1_1_1



CID: EN300-318344_1_1_1

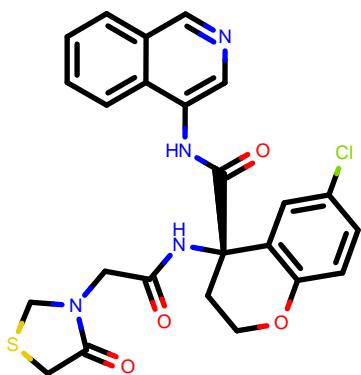
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nccn5

RUN: RUN3316

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.21

EN300-10747_1_1_1



CID: EN300-10747_1_1_1

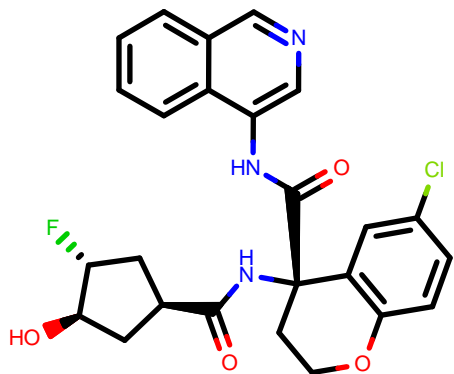
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CSCC5=O

RUN: RUN3193

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.27

EN300-7461217_1_2_1



CID: EN300-7461217_1_2_1

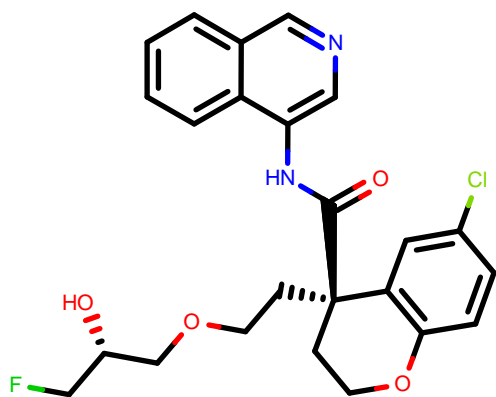
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H](C(F)O)[C@@H](C5)F5O

RUN: RUN5176

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.25

EN300-1968342_3_2_1



CID: EN300-1968342_3_2_1

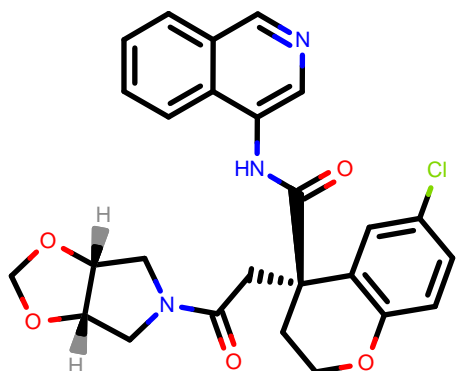
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN3610

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.33

EN300-1717795_1_1_1



CID: EN300-1717795_1_1_1

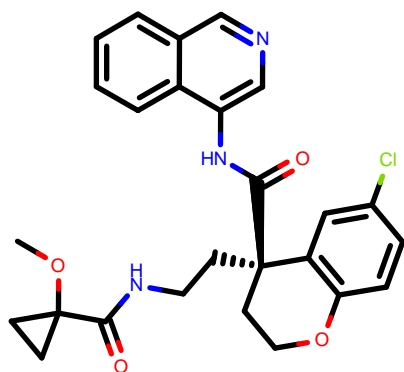
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5[C@@H](C)[C@H](C5)OCC6

RUN: RUN3928

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.30

EN300-182124_3_1_1



CID: EN300-182124_3_1_1

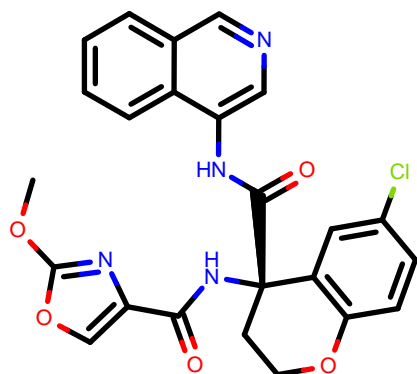
SMILES: COC1(CC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3485

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.25

EN300-245205_1_1_1



CID: EN300-245205_1_1_1

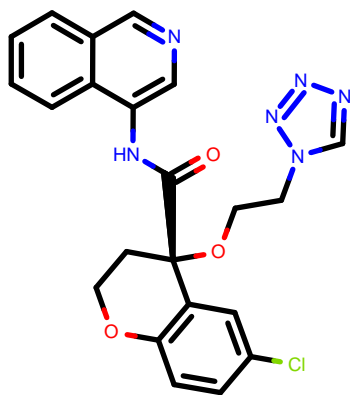
SMILES: COc1nc(cc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4283

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.21

EN300-364679_1_1_1



CID: EN300-364679_1_1_1

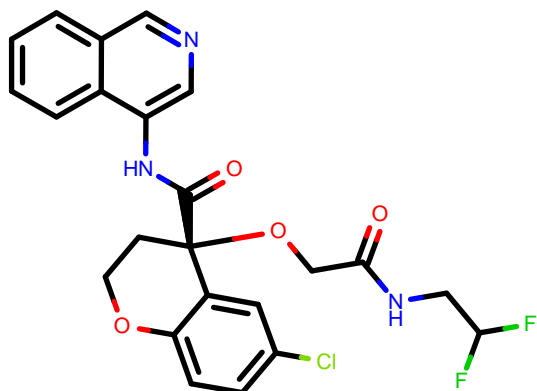
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnn5

RUN: RUN4548

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.22

EN300-120586_1_1_1



CID: EN300-120586_1_1_1

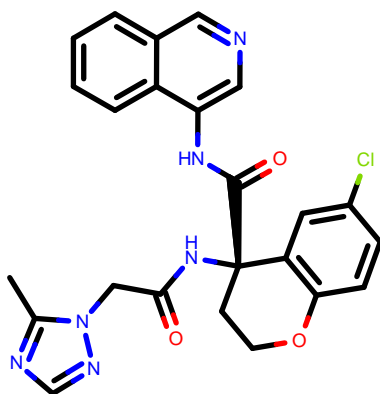
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCC(F)F

RUN: RUN4360

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.24

EN300-7536177_1_1_1



CID: EN300-7536177_1_1_1

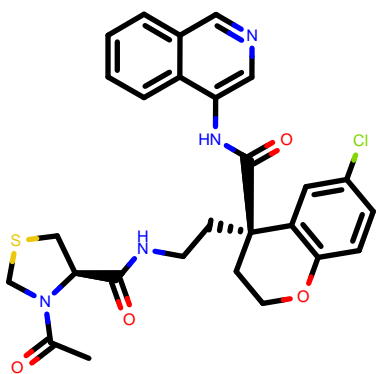
SMILES: Cc1nccn1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4299

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.24

EN300-736749_3_1_1



CID: EN300-736749_3_1_1

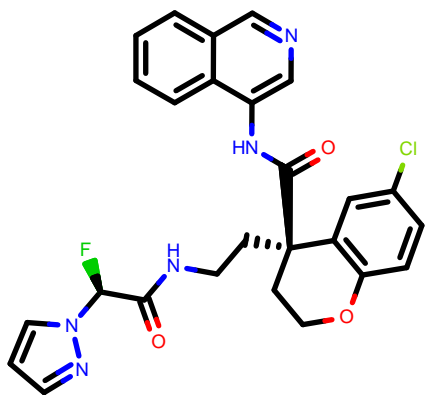
SMILES: CC(=O)N1CSC[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3321

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.32

EN300-1726277_3_1_1



CID: EN300-1726277_3_1_1

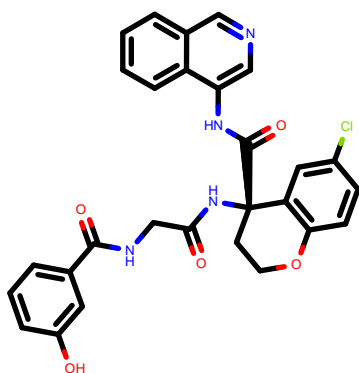
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](n5cccn5)F

RUN: RUN3330

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.27

EN300-54417_1_1_1



CID: EN300-54417_1_1_1

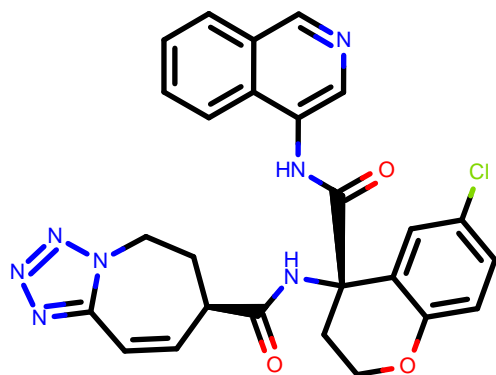
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)CNC(=O)c5ccc(O)c5

RUN: RUN3551

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.26

EN300-253571_1_2_1



CID: EN300-253571_1_2_1

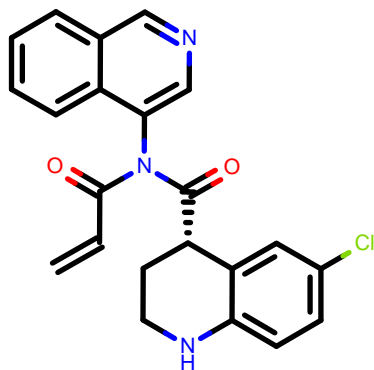
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5COC6N=NN=C65

RUN: RUN2976

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.31

MAT-POS-e69ad64a-1_2



CID: MAT-POS-e69ad64a-1_2

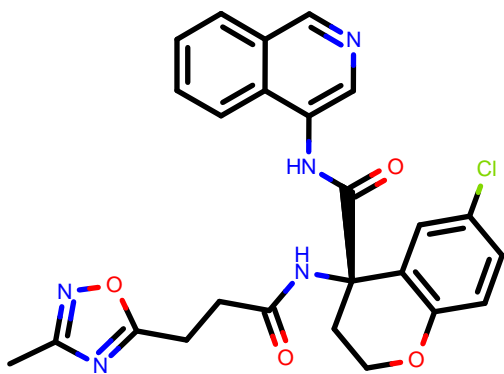
SMILES: C=CC(=O)N(c1nc(=O)c2ccccc2)C(=O)[C@@H]3CCNC4C3C(Cc4)C1

RUN: RUN2194

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.36

EN300-27268_1_1_1



CID: EN300-27268_1_1_1

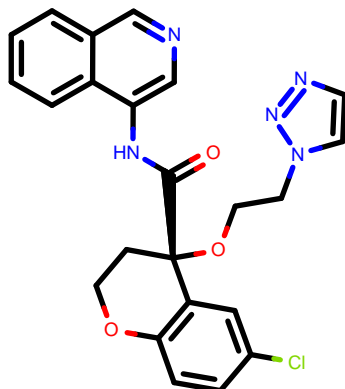
SMILES: Cc1nc(on1)CCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3761

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.22

EN300-1715993_1_1_1



CID: EN300-1715993_1_1_1

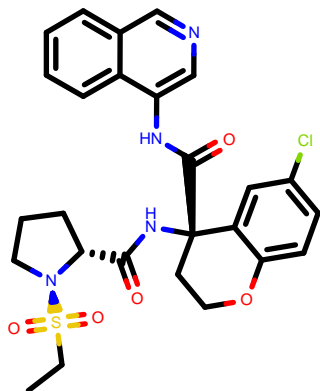
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCCn5cnn5

RUN: RUN3726

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.20

EN300-16091_1_1_1



CID: EN300-16091_1_1_1

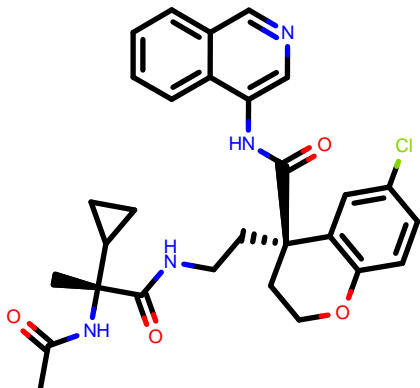
SMILES: CCS(=O)(=O)N@[1]CCC[C@@]H[C@@]1C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5163

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.56

EN300-67073_3_2_1



CID: EN300-67073_3_2_1

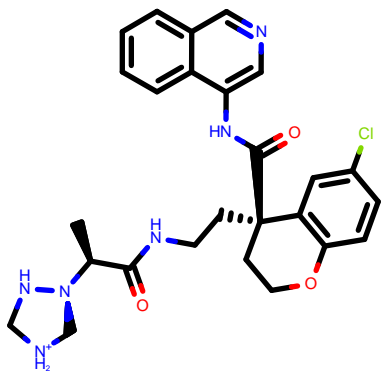
SMILES: CC(=O)N[C@@](C)(C1CC1)C(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6116

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.31

EN300-30397_3_1_1



CID: EN300-30397_3_1_1

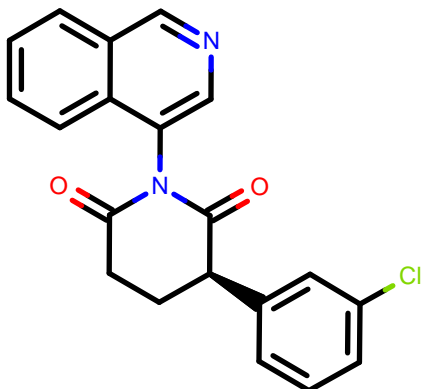
SMILES: C[C@@H](C(=O)NC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)n5cncn5

RUN: RUN4267

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.26

VLA-UCB-1dbca3b4-10_1



CID: VLA-UCB-1dbca3b4-10_1

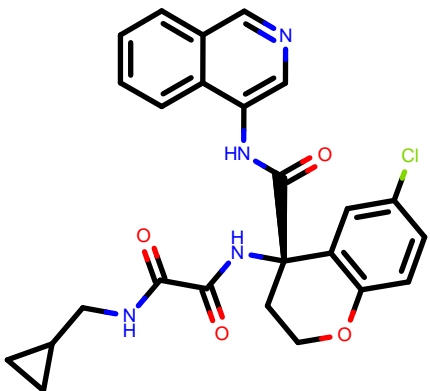
SMILES: c1ccc2c(c1)cncc2N3C(=O)CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN60

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.22

EN300-173216_1_1_1



CID: EN300-173216_1_1_1

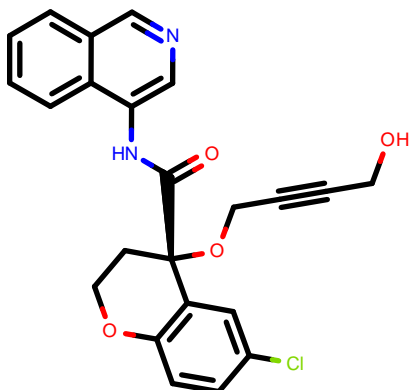
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NCC5CC5

RUN: RUN3258

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.24

EN300-83766_1_1_1



CID: EN300-83766_1_1_1

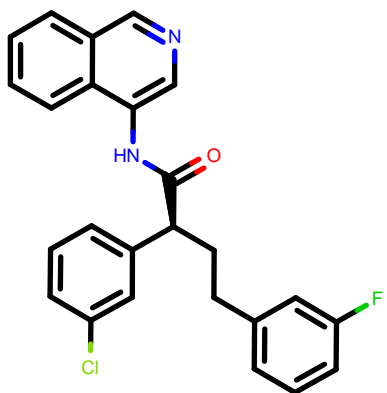
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC#CCO

RUN: RUN3976

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.20

MIC-UNK-c66144cb-1_1



CID: MIC-UNK-c66144cb-1_1

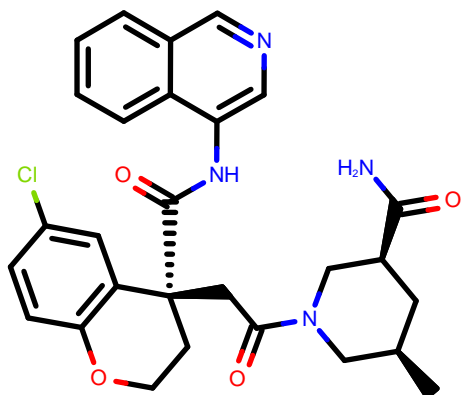
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(Cc3ccccc(c3)F)c4ccccc(c4)Cl

RUN: RUN155

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.26

EN300-1724086_1_1_1



CID: EN300-1724086_1_1_1

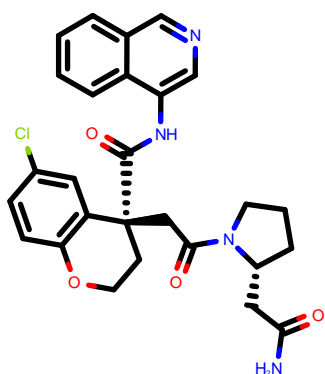
SMILES: C[C@@H]1C[C@@H](CN(C1)C(=O)C[C@@H]2(C)COC3=CC(=O)C(C1=O)N4=CC=CC=C4C(=O)N

RUN: RUN3812

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.32

EN300-124652_1_1_1



CID: EN300-124652_1_1_1

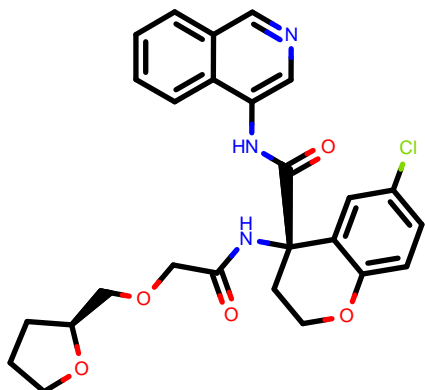
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(C)C(=O)N5CC[C@H]5C(=O)N

RUN: RUN2800

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.22

EN300-60033_1_1_1



CID: EN300-60033_1_1_1

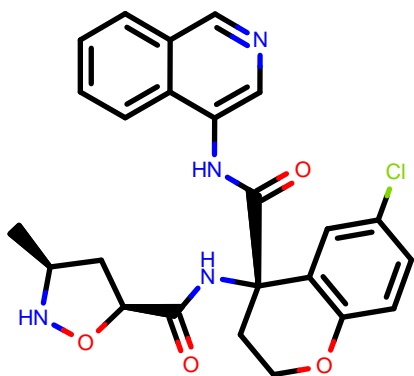
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(C)C(=O)N(C)C(=O)COC[C@H]5CCCO5

RUN: RUN3445

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.31

EN300-92447_1_1_2



CID: EN300-92447_1_1_2

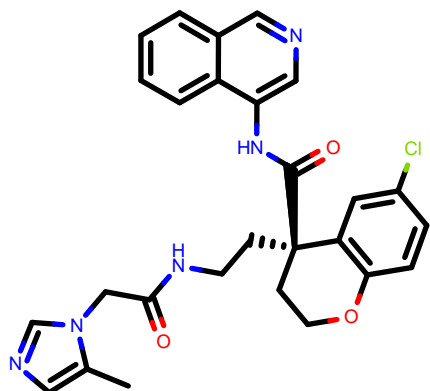
SMILES: C[C@H]1C[C@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3437

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.30

EN300-315453_3_1_1



CID: EN300-315453_3_1_1

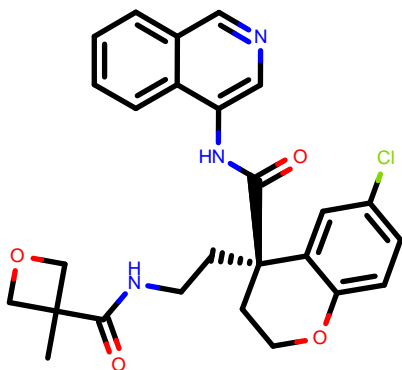
SMILES: Cc1cn[nH]1CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN4754

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.31

EN300-78753_3_1_1



CID: EN300-78753_3_1_1

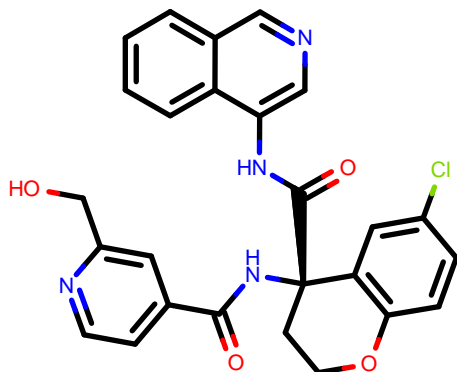
SMILES: CC1(COC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3158

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.30

EN300-396748_1_1_1



CID: EN300-396748_1_1_1

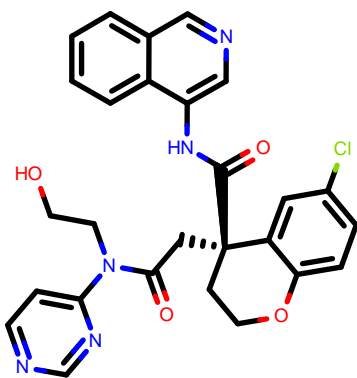
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)c5cccnc5)CO

RUN: RUN3776

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.23

EN300-256174_1_1_1



CID: EN300-256174_1_1_1

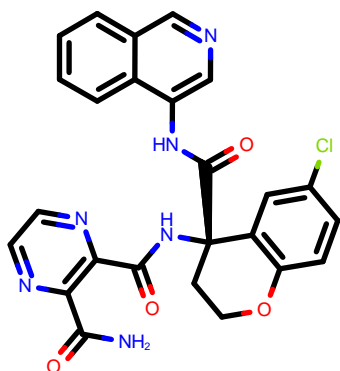
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5ccnnc5

RUN: RUN4593

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.40

EN300-21200_1_1_1



CID: EN300-21200_1_1_1

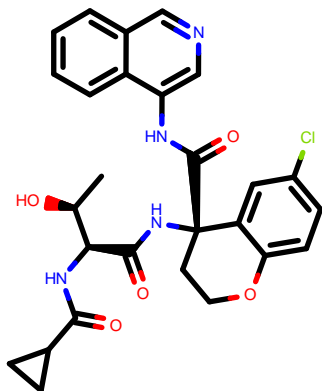
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ncnc5)C(=O)N

RUN: RUN7136

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.25

EN300-96362_1_1_1



CID: EN300-96362_1_1_1

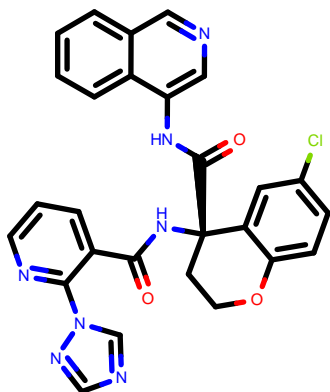
SMILES: C[C@@H](C[C@@H](C)[C@@H](C)N)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc4c3ccccc4N(C(=O)C5C)O

RUN: RUN4645

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.28

EN300-28571_1_1_1



CID: EN300-28571_1_1_1

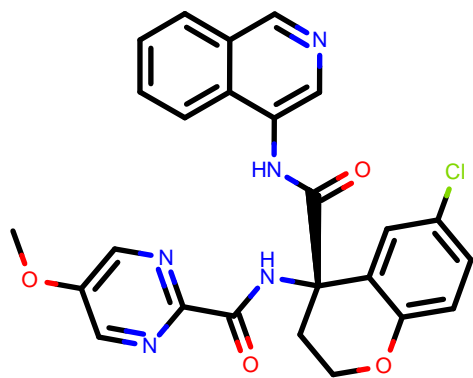
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5n6cnc6

RUN: RUN3653

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.22

EN300-225053_1_1_1



CID: EN300-225053_1_1_1

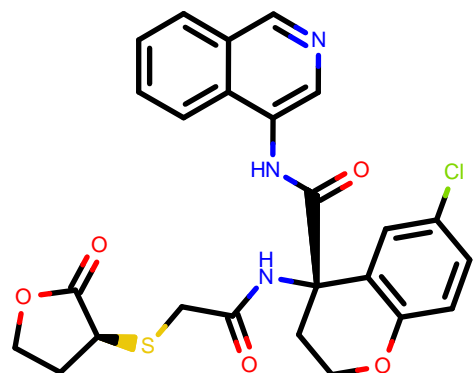
SMILES: COc1cnc(nc1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3641

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.19

EN300-113218_1_2_1



CID: EN300-113218_1_2_1

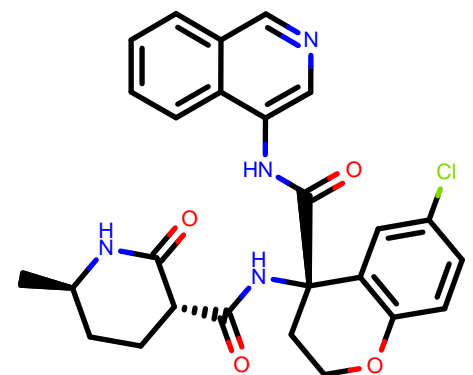
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)CS[C@@H]5CCOC5=O

RUN: RUN4106

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.30

EN300-6505003_1_3_1



CID: EN300-6505003_1_3_1

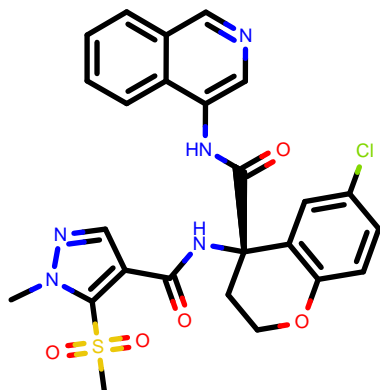
SMILES: C[C@@]1CC[C@@H](C(=O)N)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3440

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.24

EN300-180069_1_1_1



CID: EN300-180069_1_1_1

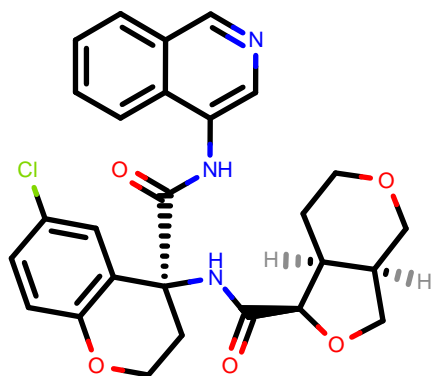
SMILES: Cn1c(c(en1)C(=O)N)[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5S(=O)(=O)C

RUN: RUN3136

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.27

EN300-746830_1_1_1



CID: EN300-746830_1_1_1

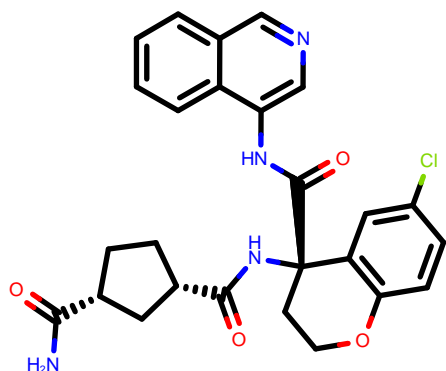
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)N(C=O)[C@H]5[C@@H](C)CC[C@@H]5C6=CC=CC=C6

RUN: RUN2781

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.22

EN300-370753_1_1_1



CID: EN300-370753_1_1_1

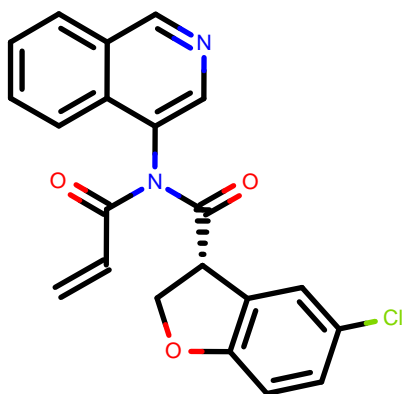
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)N(C=O)[C@H]5[C@@H](C)CC[C@@H]5C6=CC=CC=C6

RUN: RUN3296

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.30

MAT-POS-e69ad64a-2_2



CID: MAT-POS-e69ad64a-2_2

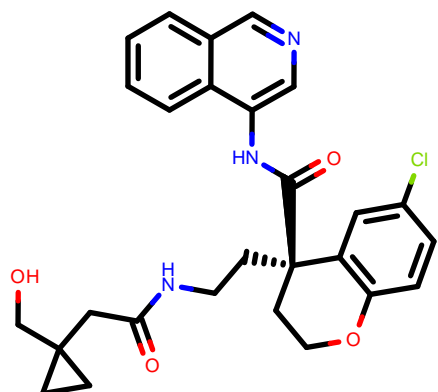
SMILES: C=CC(=O)N(c1cnc2c1cccc2)C(=O)[C@H]3COC4=CC=CC=C4

RUN: RUN2150

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.28

EN300-107048_3_1_1



CID: EN300-107048_3_1_1

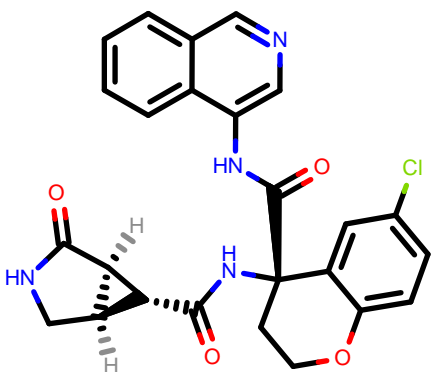
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)CCN(C=O)CC5(C)C=CC5

RUN: RUN4779

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.31

EN300-7501017_1_1_1



CID: EN300-7501017_1_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C)NC(=O)[C@@H]5C[C@@H]6[C@@H]5C[C@@H]6

RUN:

RUN3107

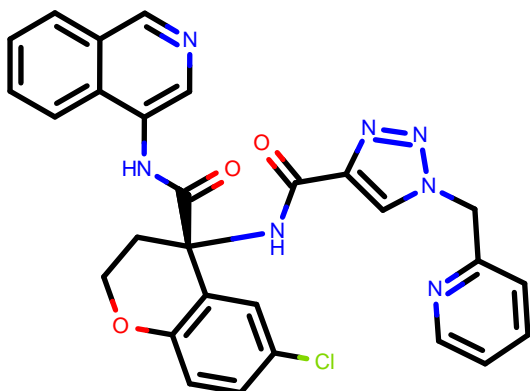
DDG (kcal/mol):

-2.33

dDDG (kcal/mol):

0.26

EN300-91315_1_1_1



CID: EN300-91315_1_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C)NC(=O)c5cn(nn5)Cc6ccccc6

RUN:

RUN4837

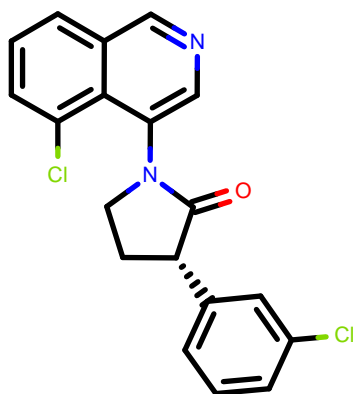
DDG (kcal/mol):

-2.32

dDDG (kcal/mol):

0.31

MIC-UNK-50cce87d-6_1



CID: MIC-UNK-50cce87d-6_1

SMILES:

c1cc(cc(c1)Cl)[C@@H]2CCN(C2=O)c3cnc4c3c(ccc4)Cl

RUN:

RUN536

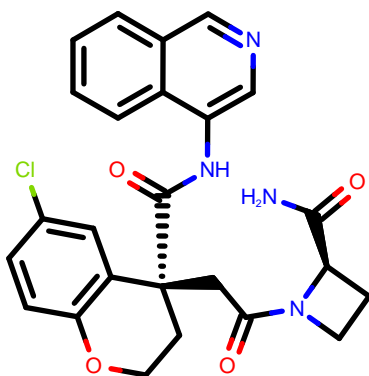
DDG (kcal/mol):

-2.32

dDDG (kcal/mol):

0.26

EDG-MED-ba1ac7b9-1_1



CID: EDG-MED-ba1ac7b9-1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C)CC(=O)N5CC[C@@H]5C(=O)N

RUN:

RUN2438

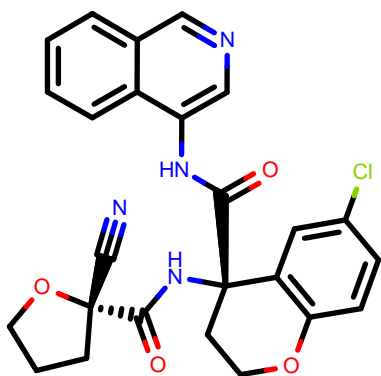
DDG (kcal/mol):

-2.32

dDDG (kcal/mol):

0.26

EN300-3710141_1_1_1



CID: EN300-3710141_1_1_1

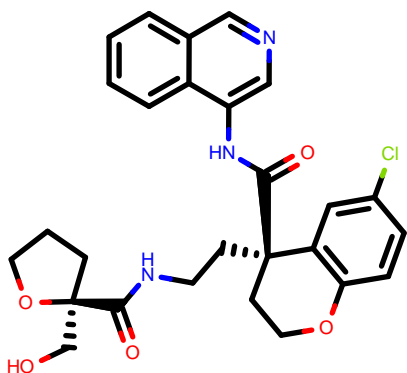
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCO5)C#N

RUN: RUN3287

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.29

EN300-1425677_3_1_1



CID: EN300-1425677_3_1_1

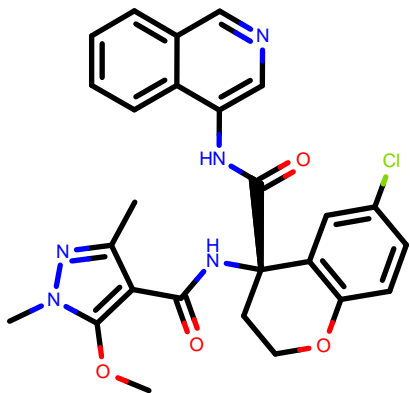
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCO5)CO

RUN: RUN4214

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.31

EN300-75482_1_1_1



CID: EN300-75482_1_1_1

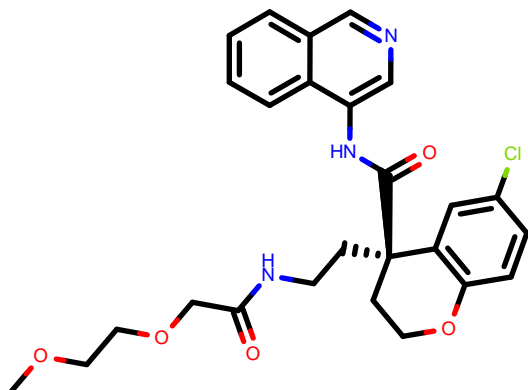
SMILES: Cc1c(c(n1)C)OC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3072

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.32

EN300-20375_3_1_1



CID: EN300-20375_3_1_1

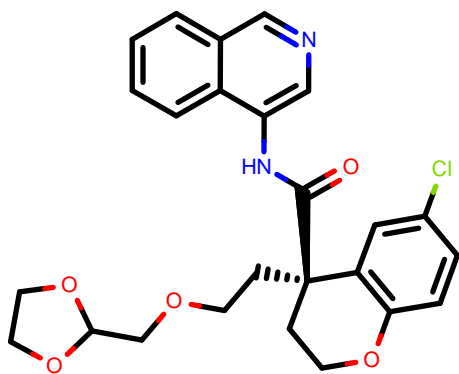
SMILES: COCCOCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccc4

RUN: RUN4126

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.32

EN300-77092_3_1_1



CID: EN300-77092_3_1_1

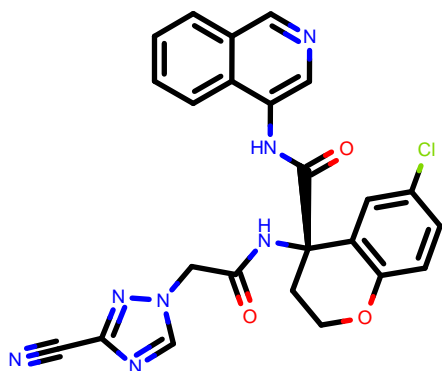
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5

RUN: RUN3213

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.33

EN300-111863_1_1_1



CID: EN300-111863_1_1_1

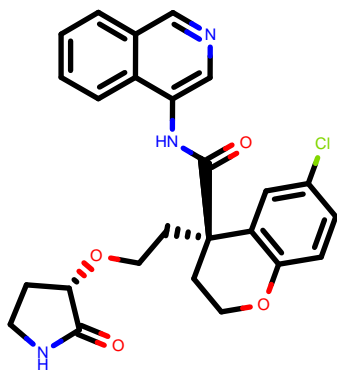
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc(n5)C#N

RUN: RUN3017

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.24

EN300-6736413_3_2_1



CID: EN300-6736413_3_2_1

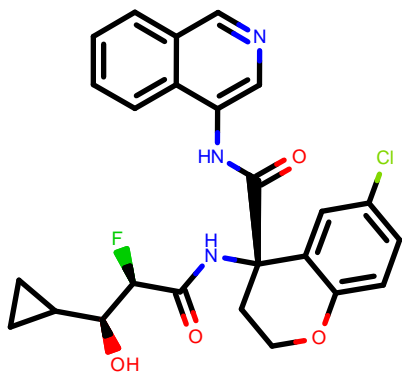
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CNC5=O

RUN: RUN3530

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.27

EDG-MED-90036822-78_3



CID: EDG-MED-90036822-78_3

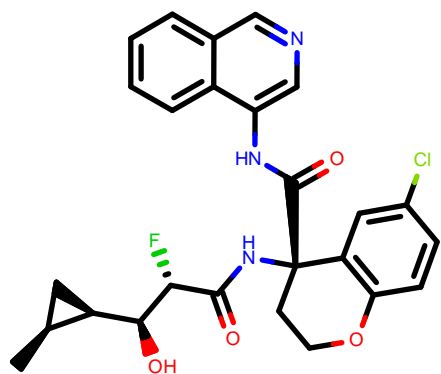
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]3(CO)C[C@H](C5CC5)O

RUN: RUN1657

DDG (kcal/mol): -2.31

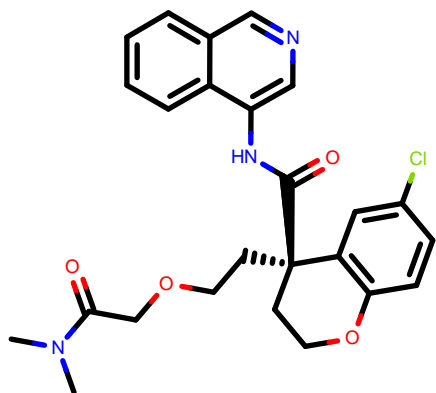
dDDG (kcal/mol): 0.21

EDG-MED-90036822-94_4



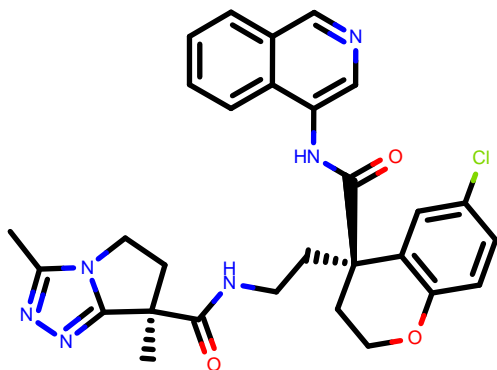
CID:	EDG-MED-90036822-94_4
SMILES:	<chem>C1C=NC2=CC=CC=C2NC1NC(=O)C[C@@H](C(F)O)C(=O)N[C@@H]3CCOC3</chem>
RUN:	RUN1691
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.25

EN300-216063_3_1_1



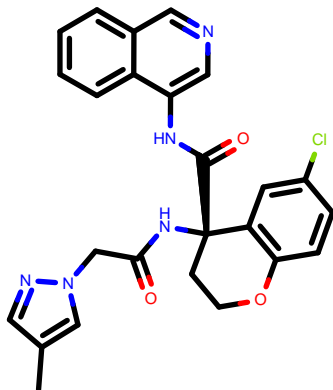
CID:	EN300-216063_3_1_1
SMILES:	<chem>CN(C)C(=O)COCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN4086
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.22

EN300-7431629_3_1_1



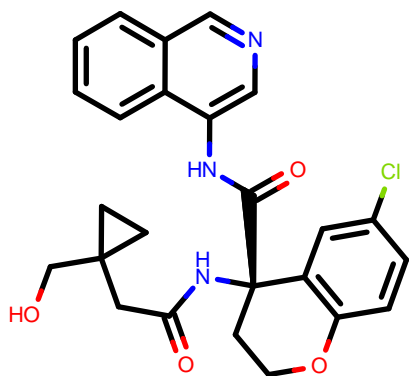
CID:	EN300-7431629_3_1_1
SMILES:	<chem>Cc1nc2n1CC[C@@]2(C)C(=O)NCC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6</chem>
RUN:	RUN2926
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.37

EN300-51832_1_1_1



CID:	EN300-51832_1_1_1
SMILES:	<chem>Cc1cnn(c1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN3324
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.23

EN300-107048_1_1_1



CID: EN300-107048_1_1_1

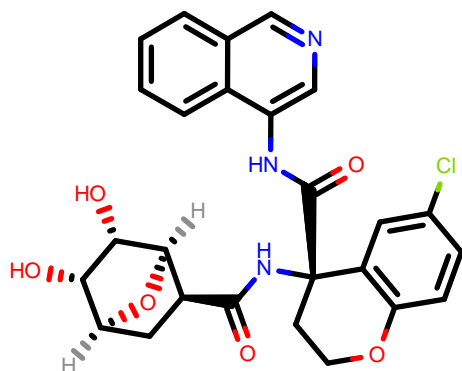
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5(CC5)CO

RUN: RUN3730

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.25

EN300-6764836_1_2_1



CID: EN300-6764836_1_2_1

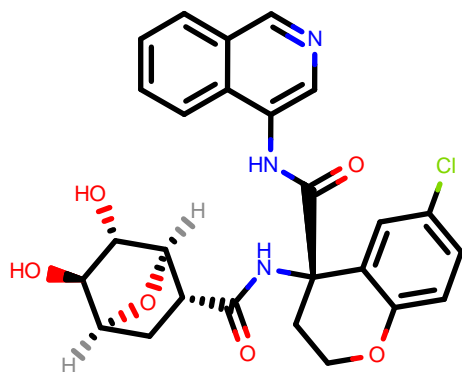
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]5[C@@H]5[C@@H]5[C@@H]5CO

RUN: RUN2821

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.28

EN300-6764836_1_3_1



CID: EN300-6764836_1_3_1

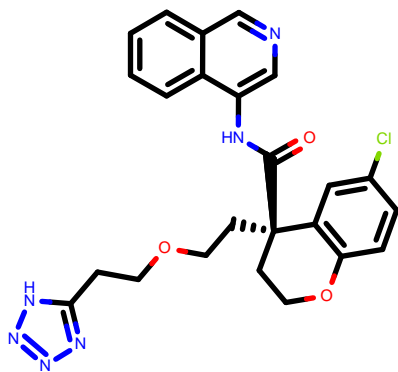
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]5[C@@H]5[C@@H]5[C@@H]5CO

RUN: RUN3159

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.25

EN300-183231_3_1_1



CID: EN300-183231_3_1_1

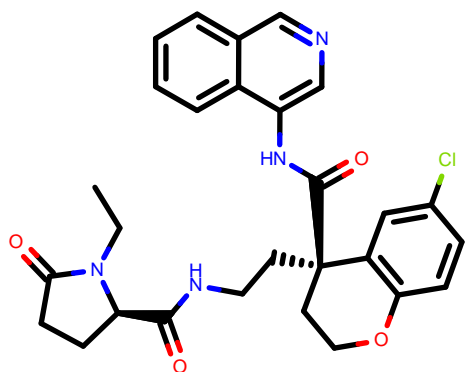
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOCC5n[n-]nn5

RUN: RUN5369

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.39

EN300-718785_3_2_1



CID: EN300-718785_3_2_1

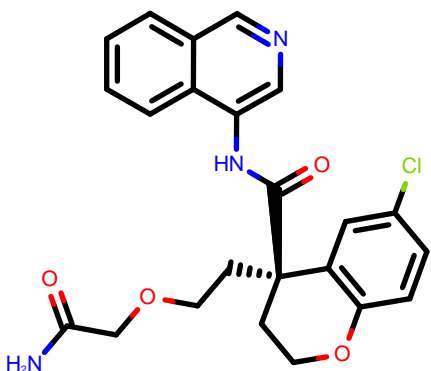
SMILES: CCN1C@H](CC(=O)N)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5531

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.36

EN300-18249_3_1_1



CID: EN300-18249_3_1_1

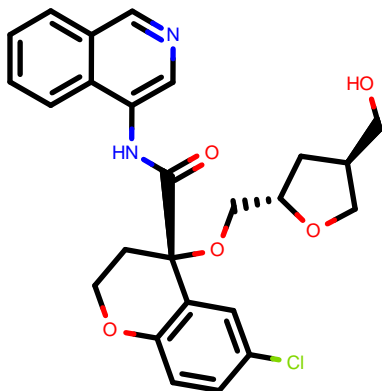
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N

RUN: RUN3071

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.20

EN300-6494158_1_3_1



CID: EN300-6494158_1_3_1

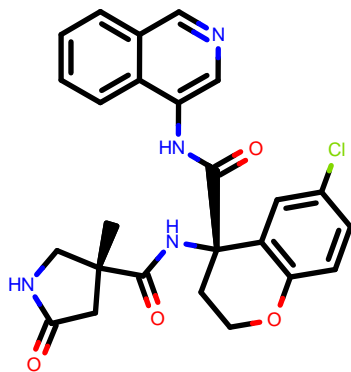
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5(C)C@H](CO)COC5

RUN: RUN4903

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.29

EN300-132157_1_2_1



CID: EN300-132157_1_2_1

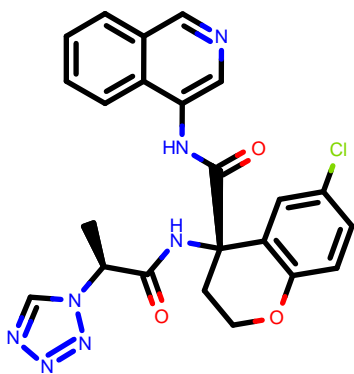
SMILES: C[C@]1(C(=O)N)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3237

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.27

EN300-191915_1_1_1



CID: EN300-191915_1_1_1

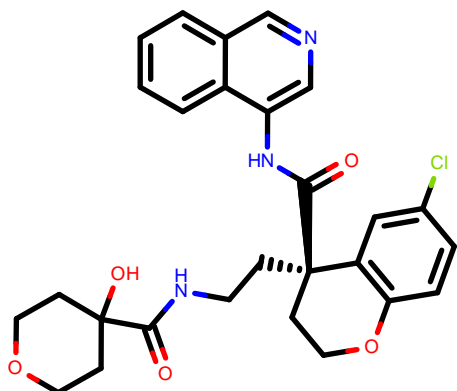
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)n5ennn5

RUN: RUN2875

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.27

EN300-69368_3_1_1



CID: EN300-69368_3_1_1

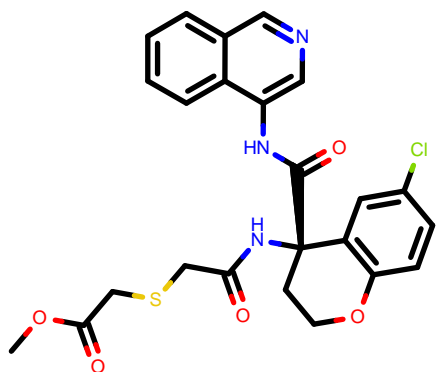
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COCCOC5)O

RUN: RUN6910

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.34

EN300-135060_1_1_1



CID: EN300-135060_1_1_1

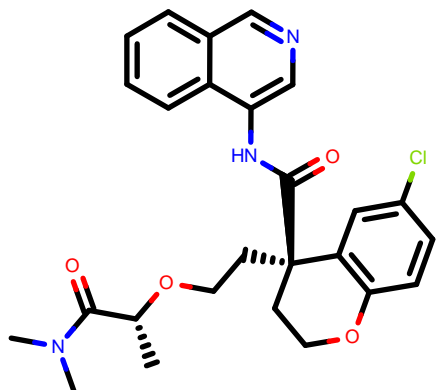
SMILES: COC(=O)CSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN3885

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.25

EN300-14458_3_2_1



CID: EN300-14458_3_2_1

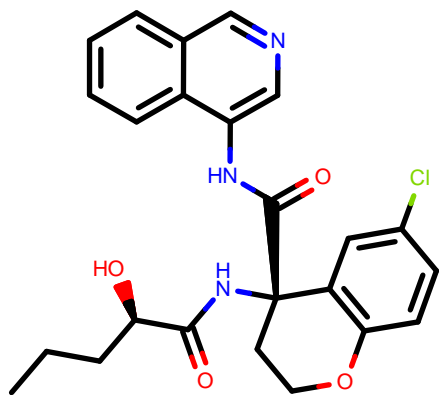
SMILES: C[C@@H](C(=O)N(C)C)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN3200

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.26

EN300-300217_1_4_1



CID: EN300-300217_1_4_1

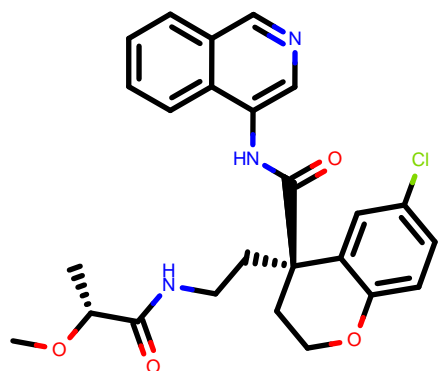
SMILES: C/C=C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN3168

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.22

EN300-247951_3_1_1



CID: EN300-247951_3_1_1

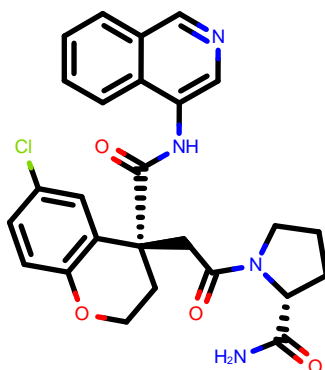
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)OC

RUN: RUN3398

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-22_1



CID: EDJ-MED-d203f206-22_1

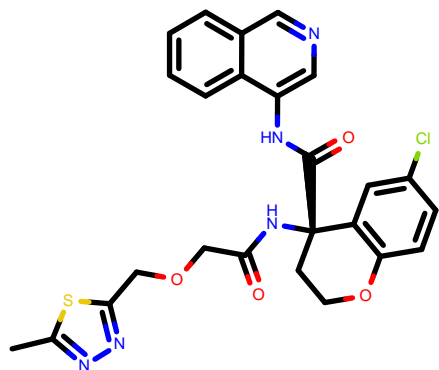
SMILES: c1ccc2c(c1)ncnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@]3H)5C(=O)N

RUN: RUN2423

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.31

EN300-206870_1_1_1



CID: EN300-206870_1_1_1

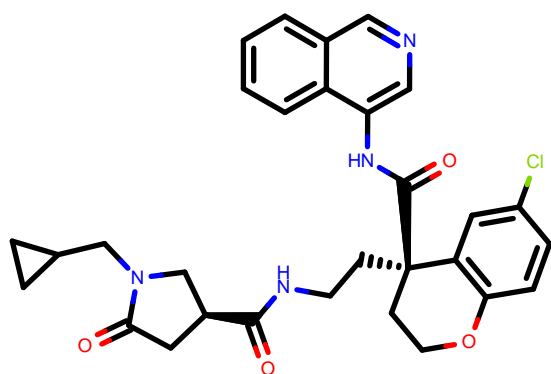
SMILES: Cc1nnc(s1)COCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3974

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.34

EN300-31969_3_2_1



CID: EN300-31969_3_2_1

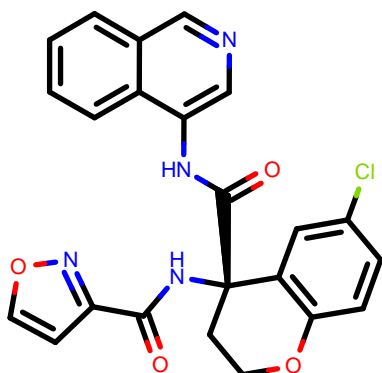
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H5CC(O)COC6C6

RUN: RUN6906

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.38

EN300-22245_1_1_1



CID: EN300-22245_1_1_1

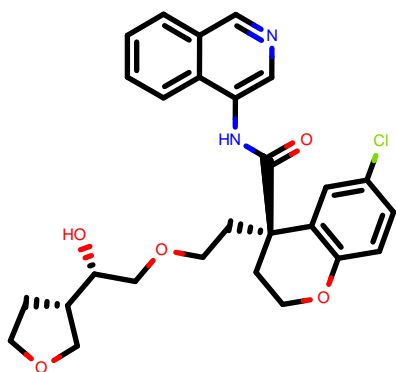
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccoc5

RUN: RUN3190

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.19

EN300-1911992_3_4_1



CID: EN300-1911992_3_4_1

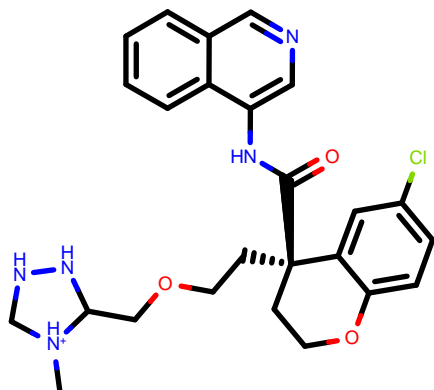
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C(O)COC5O

RUN: RUN4858

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.45

EN300-113112_3_1_1



CID: EN300-113112_3_1_1

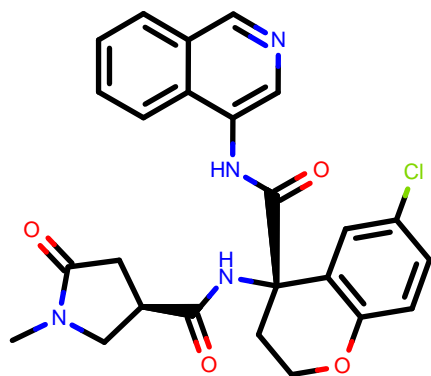
SMILES: Cn1nnc1COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3821

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-33601_1_1_1



CID: EN300-33601_1_1_1

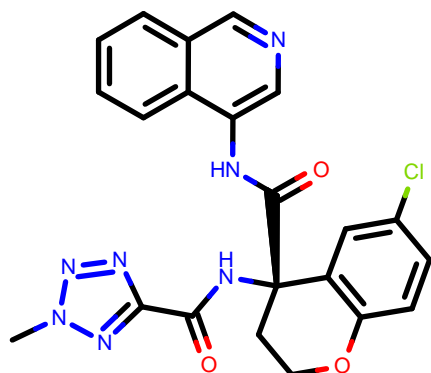
SMILES: CN1C[C@@H](CC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3899

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-216978_1_1_1



CID: EN300-216978_1_1_1

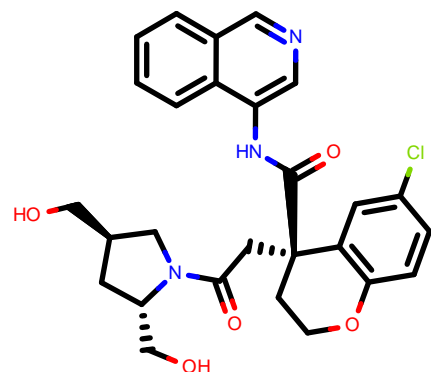
SMILES: Cn1nc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3004

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.18

EN300-1212400_1_3_1



CID: EN300-1212400_1_3_1

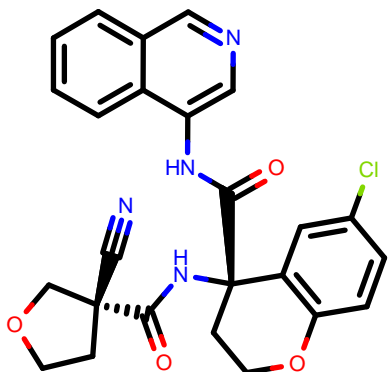
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@H]5O)CO

RUN: RUN4005

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.39

EN300-261210_1_1_1



CID: EN300-261210_1_1_1

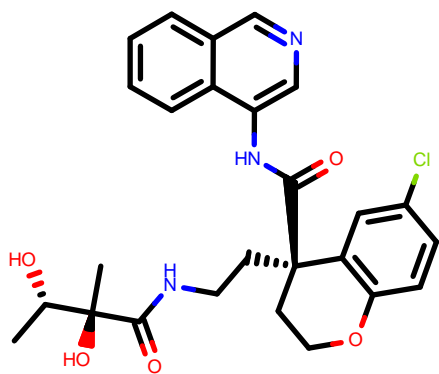
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOc5)C#N

RUN: RUN3323

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-202922_3_3_1



CID: EN300-202922_3_3_1

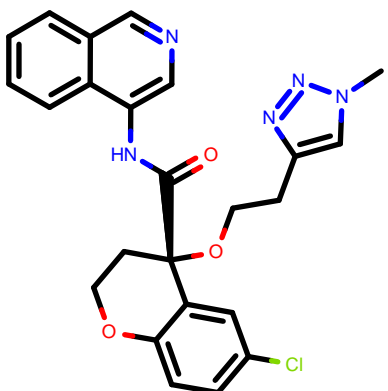
SMILES: C[C@@H]([C@](C)(C=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5064

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.30

EN300-1600786_1_1_1



CID: EN300-1600786_1_1_1

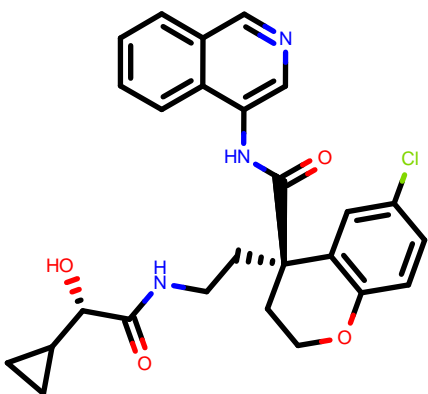
SMILES: Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4970

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.22

EN300-72211_3_2_1



CID: EN300-72211_3_2_1

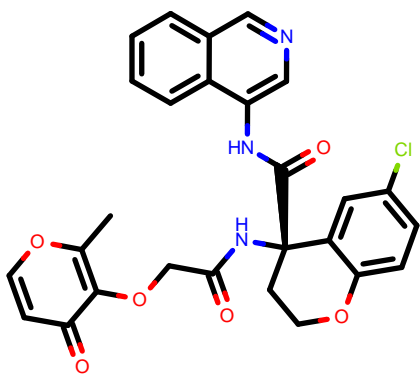
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CC5)O

RUN: RUN5141

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.30

EN300-702714_1_1_1



CID: EN300-702714_1_1_1

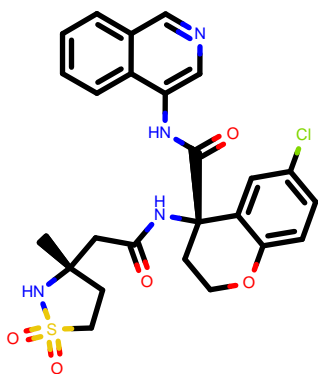
SMILES: Cc1c(c(=O)ccc1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3513

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.31

EN300-385235_1_2_1



CID: EN300-385235_1_2_1

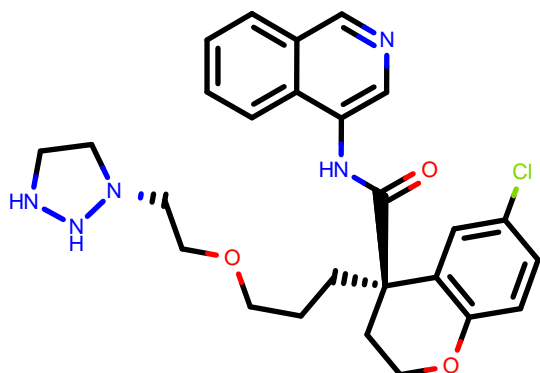
SMILES: C[C@]1(CCS(=O)(=O)N1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3368

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.33

EN300-1715993_4_1_1



CID: EN300-1715993_4_1_1

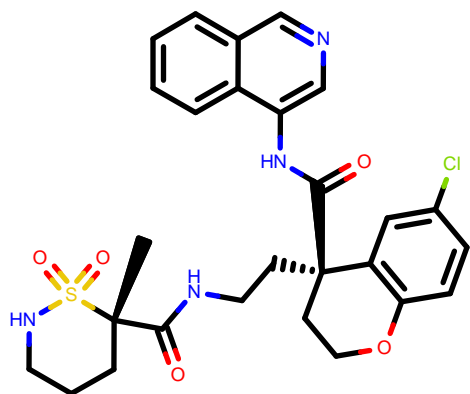
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCN5c5cnn5

RUN: RUN5039

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.30

EN300-1709315_3_2_1



CID: EN300-1709315_3_2_1

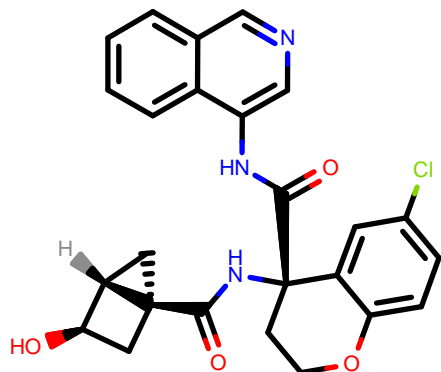
SMILES: C[C@]1(CCCNS1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN7699

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.49

EN300-6493972_1_1_1



CID: EN300-6493972_1_1_1

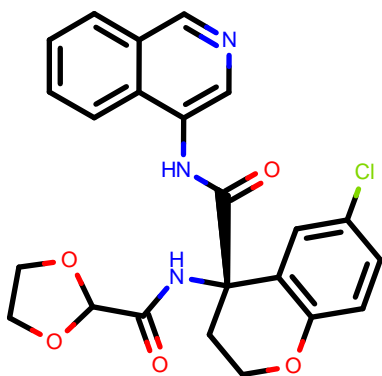
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5(C)C(O)C@H5[C@@]6(C)O

RUN: RUN3955

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.20

EN300-154942_1_1_1



CID: EN300-154942_1_1_1

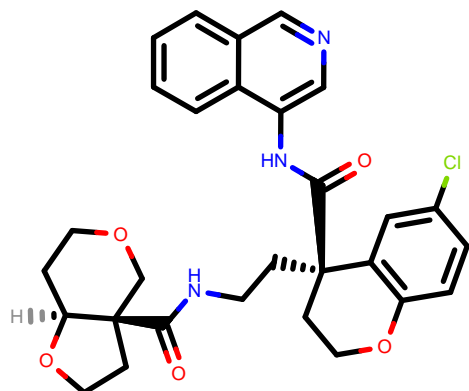
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCO5

RUN: RUN3394

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.19

EN300-341337_3_3_1



CID: EN300-341337_3_3_1

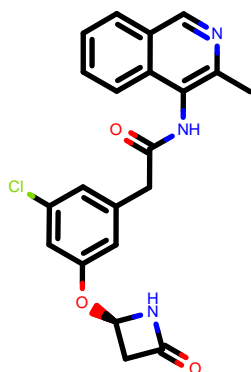
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]56CCO[C@H]5COC6

RUN: RUN3182

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.46

RAL-THA-065e0743-2_1



CID: RAL-THA-065e0743-2_1

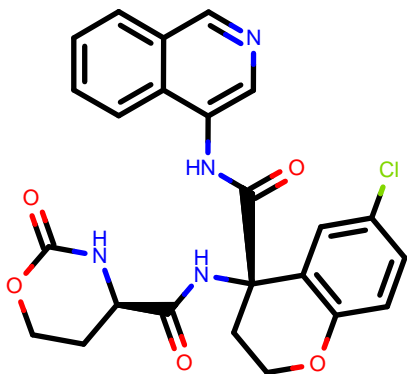
SMILES: Cc1c(c2ccccc2n1)NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN369

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.35

EN300-249804_1_2_1



CID: EN300-249804_1_2_1

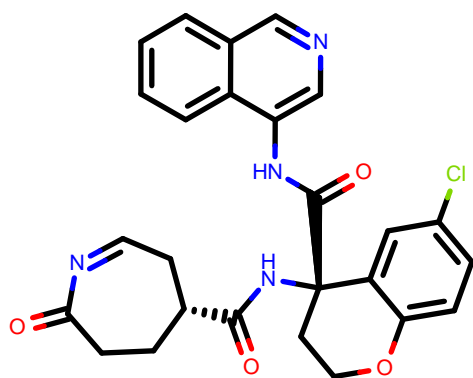
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC(=O)N5

RUN: RUN3385

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.27

EN300-152337_1_1_1



CID: EN300-152337_1_1_1

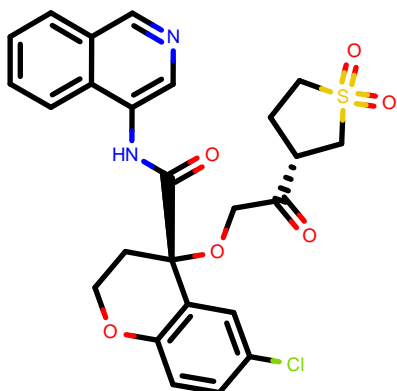
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)NC55

RUN: RUN3288

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.30

EN300-226314_1_1_1



CID: EN300-226314_1_1_1

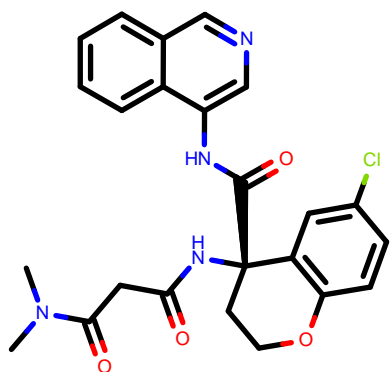
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5CCS(=O)(=O)C5

RUN: RUN5418

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.29

EN300-93573_1_1_1



CID: EN300-93573_1_1_1

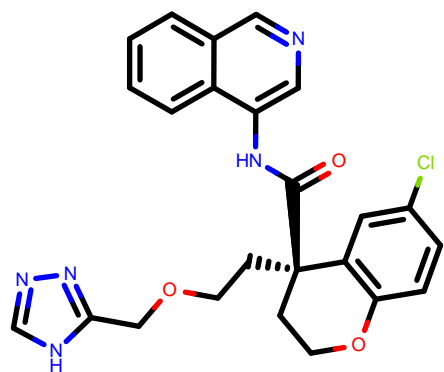
SMILES: CN(C)C(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN3120

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.27

EN300-306316_3_1_1



CID: EN300-306316_3_1_1

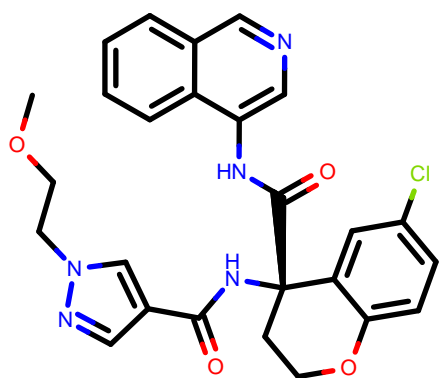
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]nnc5

RUN: RUN3105

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.22

EN300-194199_1_1_1



CID: EN300-194199_1_1_1

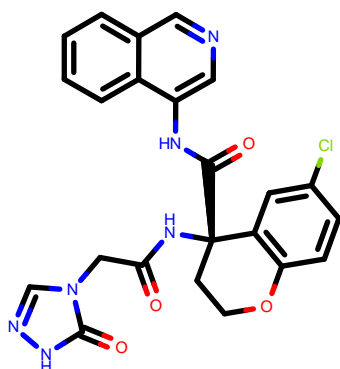
SMILES: COCc1cc(cn1)C(=O)N[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3921

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.32

EN300-120820_1_1_1



CID: EN300-120820_1_1_1

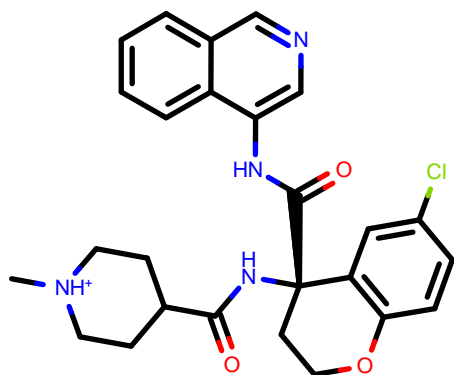
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)NC(=O)Cn5cn[nH]5=O

RUN: RUN3152

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.24

EN300-51886_1_1_1



CID: EN300-51886_1_1_1

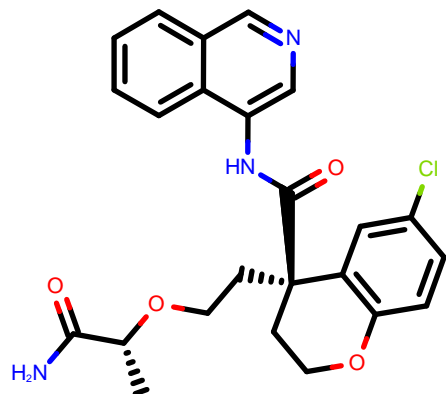
SMILES: C[NH+]1CCC(CC1)C(=O)N[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4905

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.36

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

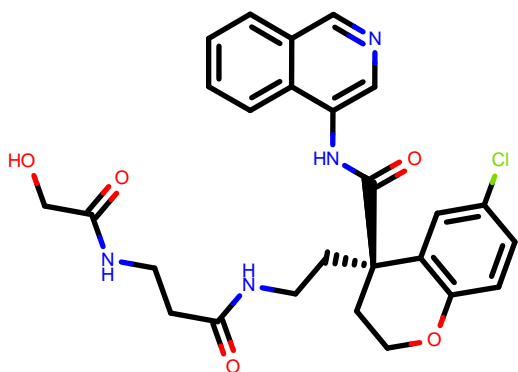
SMILES: C[C@H](C(=O)N)OCC[C@@1](CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2986

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.24

EN300-383904_3_1_1



CID: EN300-383904_3_1_1

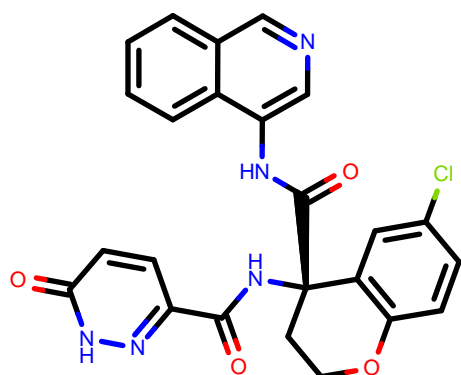
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCO

RUN: RUN5068

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.31

EN300-04614_1_1_1



CID: EN300-04614_1_1_1

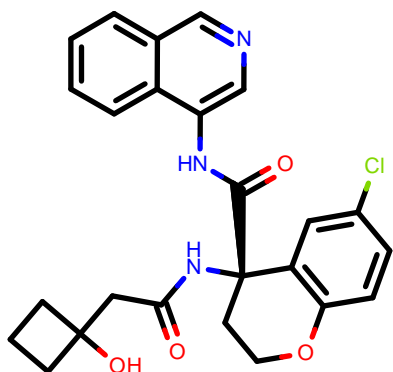
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc([nH])n5

RUN: RUN4428

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.19

EN300-246423_1_1_1



CID: EN300-246423_1_1_1

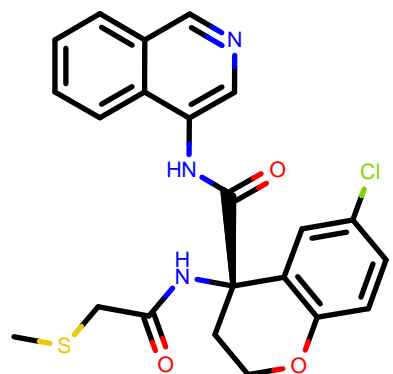
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5(CCC5)O

RUN: RUN3326

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.24

EN300-07879_1_1_1



CID: EN300-07879_1_1_1

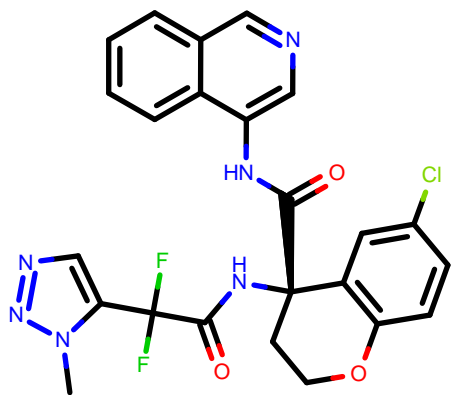
SMILES: CSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN2978

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.20

EN300-1726073_1_1_1



CID: EN300-1726073_1_1_1

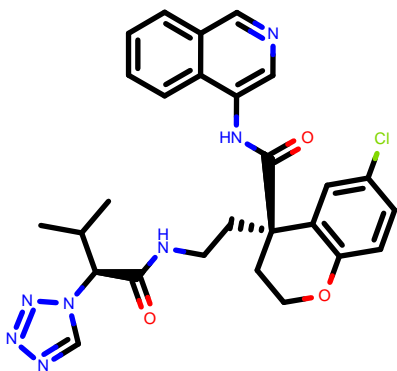
SMILES: Cn1c(cnn1)C(C(=O)N)C@2(CCOCc3c2cc(cc3)Cl)C(=O)Nc4cncnc5c4cccc5(F)F

RUN: RUN3101

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.26

EN300-297561_3_1_1



CID: EN300-297561_3_1_1

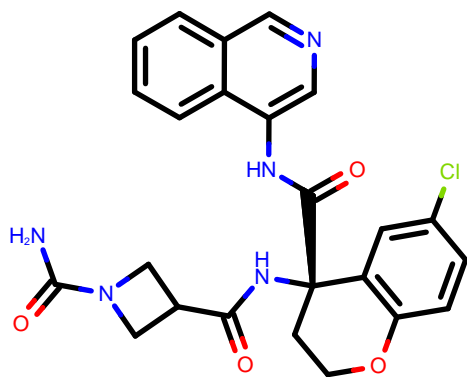
SMILES: CC(C)[C@@H](C(=O)N)CC[C@1](CCOCc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)n5cnm5

RUN: RUN2773

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.38

EN300-1248250_1_1_1



CID: EN300-1248250_1_1_1

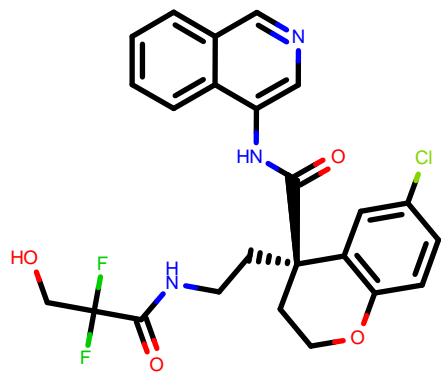
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@3](CCOCc4c3cc(cc4)Cl)NC(=O)C5CN(C5)C(=O)N

RUN: RUN2839

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.28

EN300-123489_3_1_1



CID: EN300-123489_3_1_1

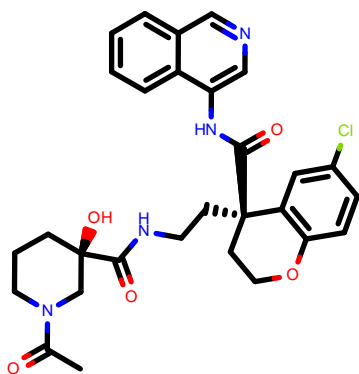
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@3](CCOCc4c3cc(cc4)Cl)CCNC(=O)C(CO)(F)F

RUN: RUN3533

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.21

EN300-210552_3_1_1



CID: EN300-210552_3_1_1

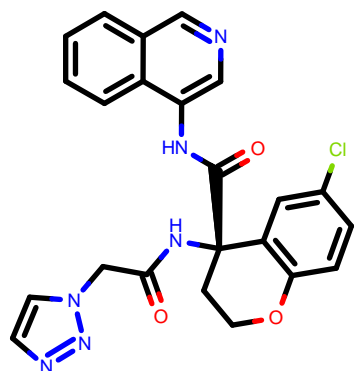
SMILES: CC(=O)N1CCC[C@@](C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5O

RUN: RUN3745

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.49

EN300-100467_1_1_1



CID: EN300-100467_1_1_1

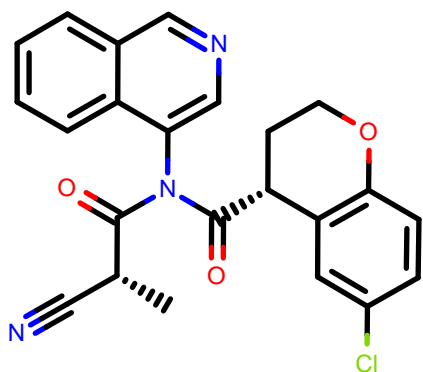
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnn5

RUN: RUN2886

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.24

VLA-UCB-34f3ed0c-1_1_2



CID: VLA-UCB-34f3ed0c-1_1_2

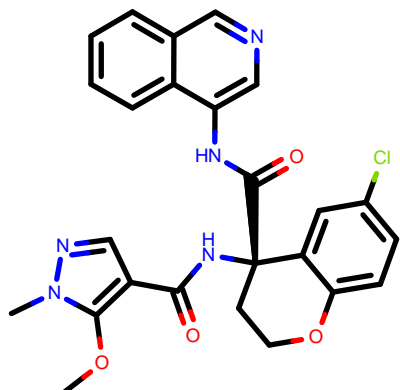
SMILES: C[C@H](C#N)C(=O)N(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C

RUN: RUN3436

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.19

EN300-227310_1_1_1



CID: EN300-227310_1_1_1

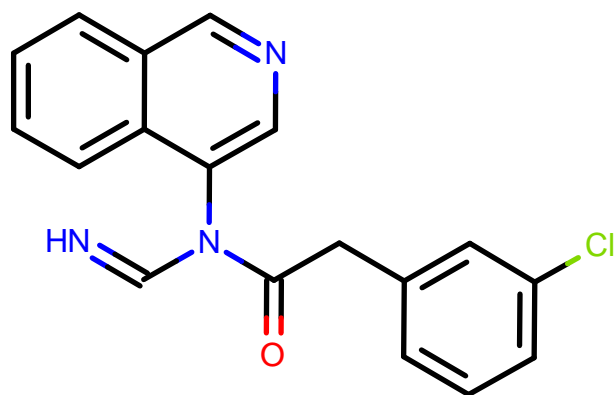
SMILES: Cn1c(c(en1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)OC

RUN: RUN3240

DDG (kcal/mol): -2.23

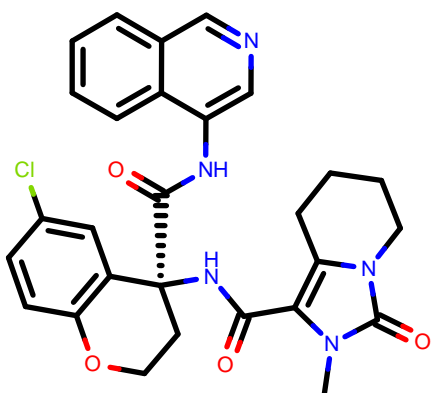
dDDG (kcal/mol): 0.28

PET-UNK-5ecb6237-1_1



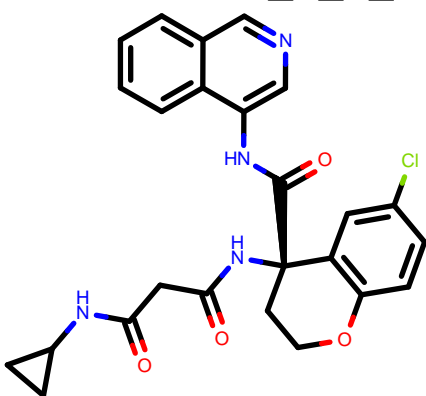
CID:	PET-UNK-5ecb6237-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN443
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.31

EN300-221156_1_1_1



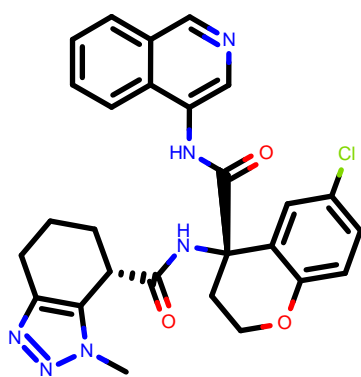
CID:	EN300-221156_1_1_1
SMILES:	<chem>Cn1c(c2n(c1=O)CCCC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6</chem>
RUN:	RUN3847
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.29

EN300-128464_1_1_1



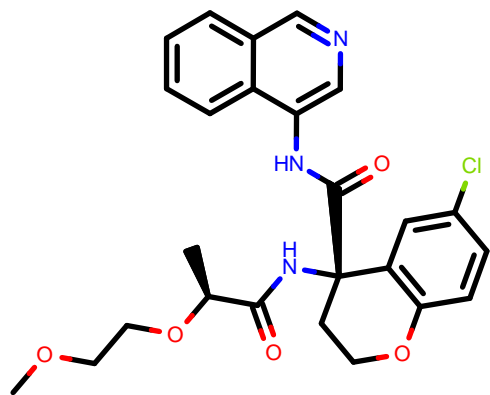
CID:	EN300-128464_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC(=O)Nc5ccc5</chem>
RUN:	RUN5263
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.28

EN300-1664865_1_1_1



CID:	EN300-1664865_1_1_1
SMILES:	<chem>Cn1c2c(nn1)CCC[C@@]H2C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6</chem>
RUN:	RUN3239
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.24

EN300-77359_1_1_1



CID: EN300-77359_1_1_1

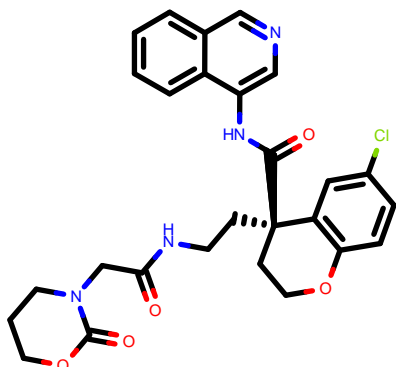
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OCCOC

RUN: RUN3862

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.27

EN300-103638_3_1_1



CID: EN300-103638_3_1_1

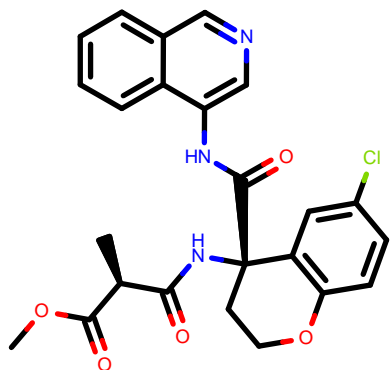
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCOC5=O

RUN: RUN3683

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.30

EN300-1239522_1_1_1



CID: EN300-1239522_1_1_1

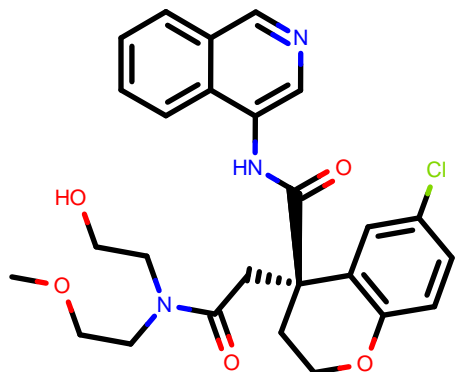
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)C(=O)OC

RUN: RUN3482

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.23

EN300-66849_1_1_1



CID: EN300-66849_1_1_1

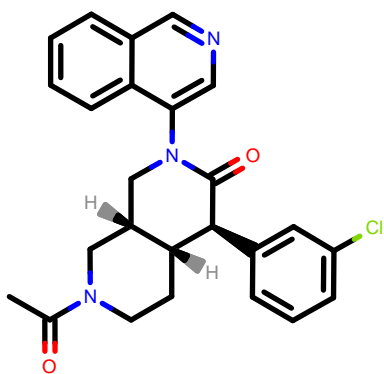
SMILES: COCCN(CCO)C(=O)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4321

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.45

MIC-UNK-9582b2c5-1_7



CID: MIC-UNK-9582b2c5-1_7

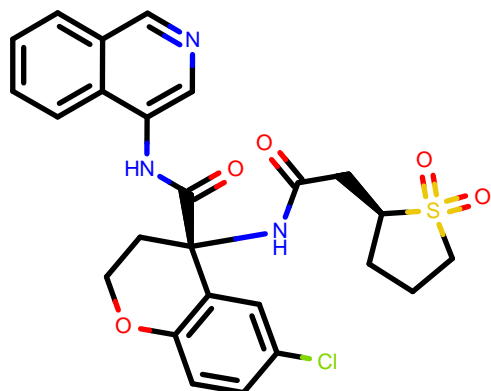
SMILES: CC(=O)N1CC[C@@H]2[C@H](C1)CN(C(=O)[C@H]2c3cccc(c3)Cl)c4nccc5c4cccc5

RUN: RUN172

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.34

EN300-155176_1_1_1



CID: EN300-155176_1_1_1

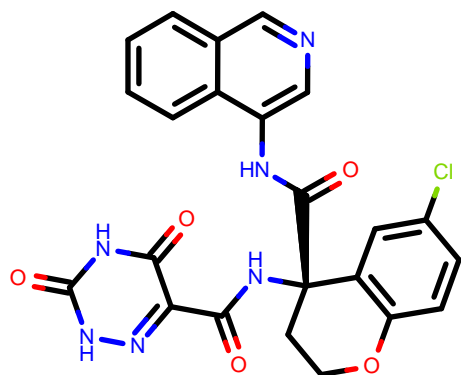
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC5(=O)=O

RUN: RUN4124

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.34

EN300-122319_1_1_1



CID: EN300-122319_1_1_1

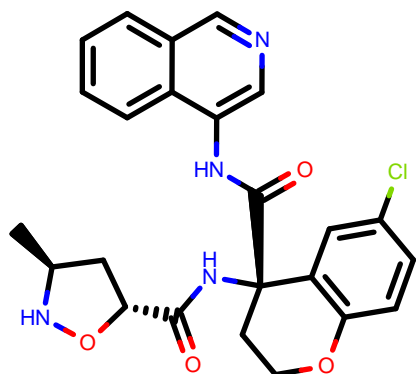
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)c5c(=O)[nH]c(=O)[nH]n5

RUN: RUN3356

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EN300-92447_1_2_2



CID: EN300-92447_1_2_2

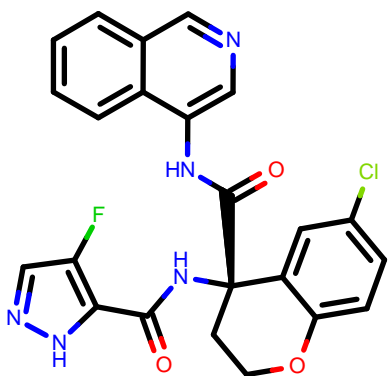
SMILES: C[C@H]1C[C@@H](ON1)C(=O)N[C@@]2(CCCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN3494

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.28

EN300-98143_1_1_1



CID: EN300-98143_1_1_1

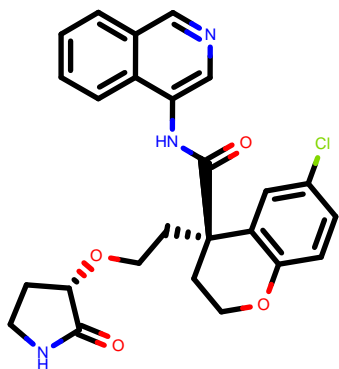
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(en[nH]5)F

RUN: RUN3605

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EN300-6736413_3_2_1



CID: EN300-6736413_3_2_1

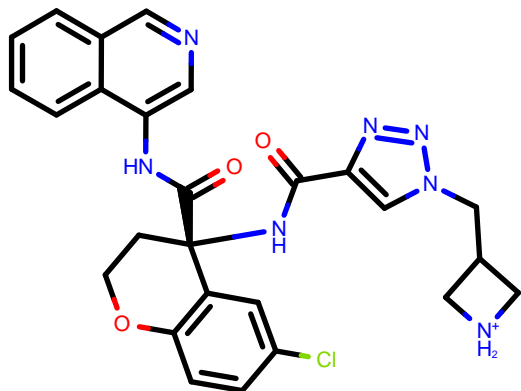
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCNC5=O

RUN: RUN3285

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.25

EDG-MED-90036822-6_1



CID: EDG-MED-90036822-6_1

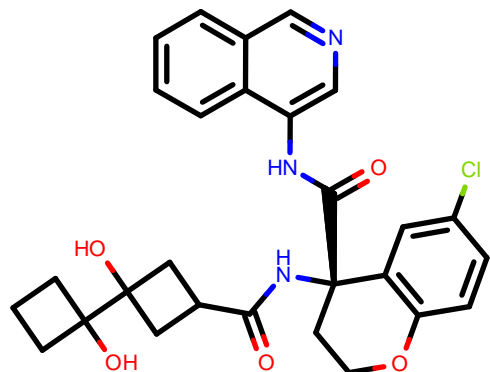
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(n5)C6C[NH2+]C6

RUN: RUN1525

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.31

EN300-7459768_1_1_1



CID: EN300-7459768_1_1_1

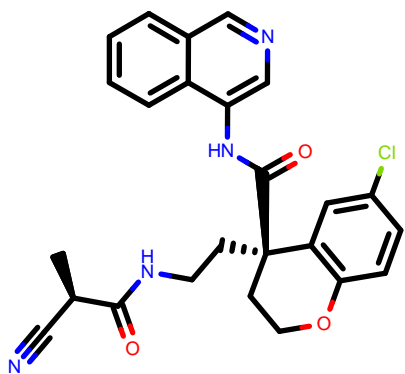
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(C5)(C6(CC6)O)O

RUN: RUN3238

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.29

EN300-72730_3_2_1



CID: EN300-72730_3_2_1

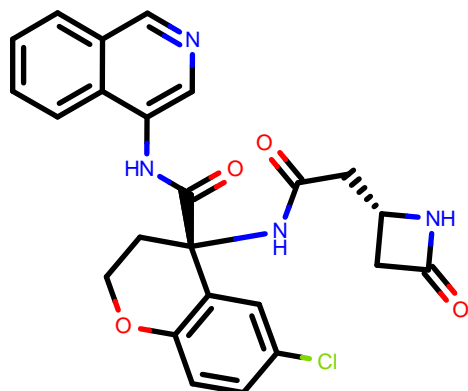
SMILES: C[C@H](C#N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5726

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.23

EN300-250593_1_2_1



CID: EN300-250593_1_2_1

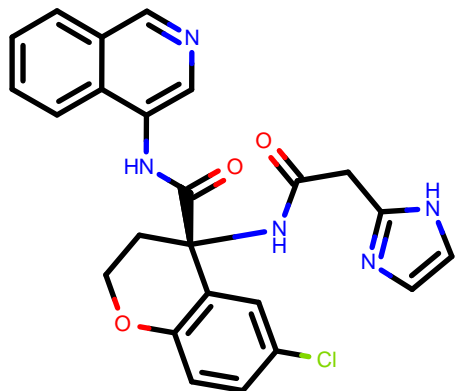
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@H]5CC(=O)N5

RUN: RUN5544

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.23

EN300-220527_1_1_1



CID: EN300-220527_1_1_1

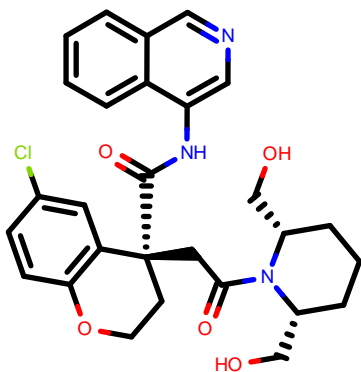
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@H]5[nH]cnc5

RUN: RUN3912

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EDJ-MED-d203f206-19_1



CID: EDJ-MED-d203f206-19_1

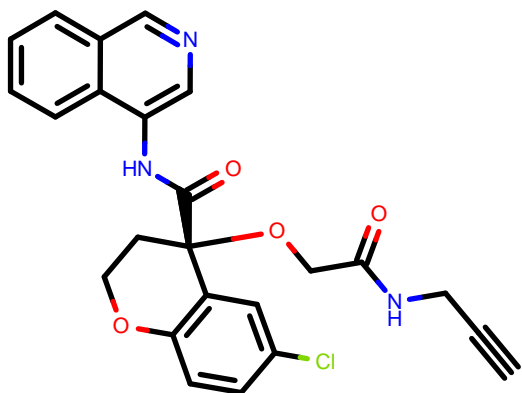
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5[C@H](CCC[C@H]5CO)CO

RUN: RUN2420

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.49

EN300-1659582_1_1_1



CID: EN300-1659582_1_1_1

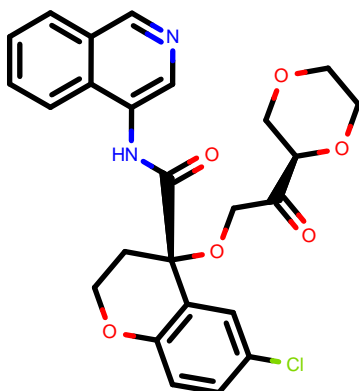
SMILES: C#CCNC(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4104

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.21

CHO-MSK-5891c1ff-2_1



CID: CHO-MSK-5891c1ff-2_1

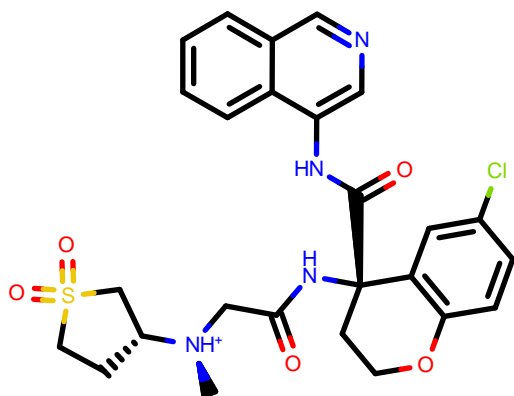
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COCCO5

RUN: RUN1774

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.29

EN300-14628_1_1_1



CID: EN300-14628_1_1_1

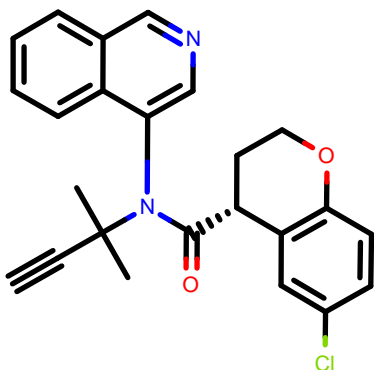
SMILES: CN(C)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5046

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.40

DAR-DIA-5ff57136-14_1



CID: DAR-DIA-5ff57136-14_1

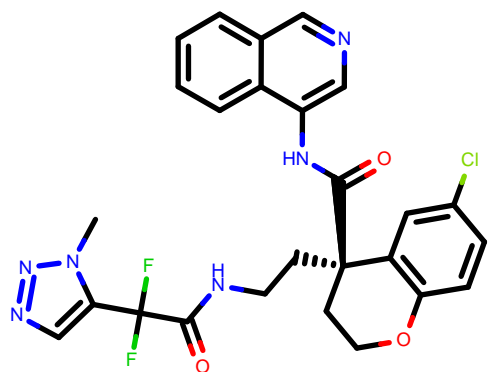
SMILES: CC(C)(C#C)N(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN1258

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.18

EN300-1726073_3_1_1



CID: EN300-1726073_3_1_1

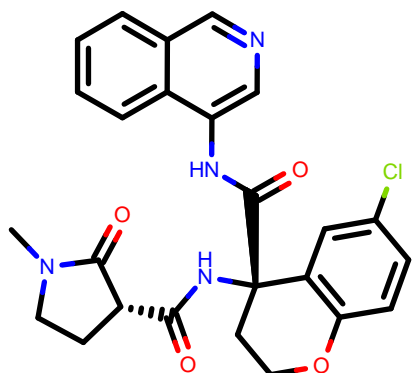
SMILES: Cn1c(cnn1)C(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)F)F

RUN: RUN5929

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.41

EN300-141695_1_2_1



CID: EN300-141695_1_2_1

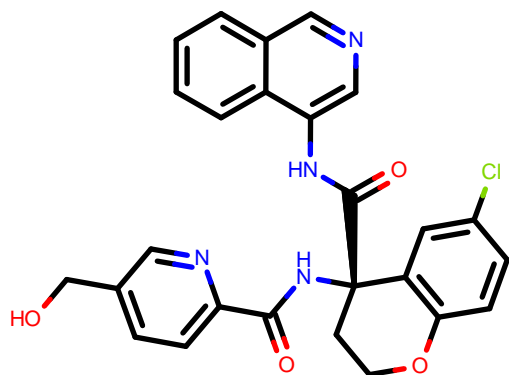
SMILES: CN1CC[C@H](C1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN3581

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.26

EN300-1270299_1_1_1



CID: EN300-1270299_1_1_1

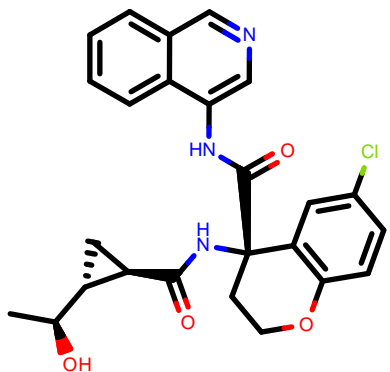
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccocn5)CO

RUN: RUN5813

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.24

EN300-6729572_1_5_1



CID: EN300-6729572_1_5_1

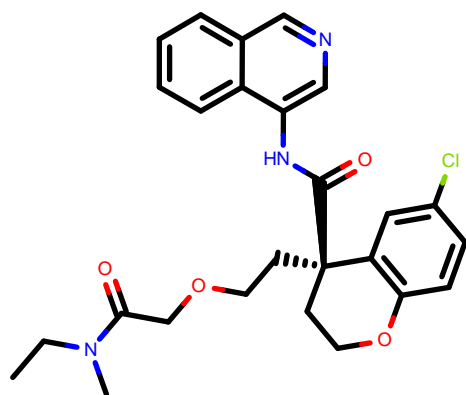
SMILES: C[C@@H](C@H)[C@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)O

RUN: RUN3466

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.27

EN300-1253122_3_1_1



CID: EN300-1253122_3_1_1

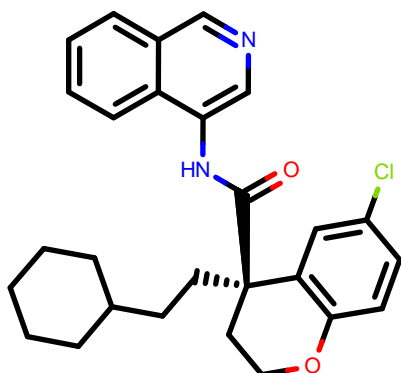
SMILES: CCN(C)C(=O)COCC[C@@]1(C)C(CO)C2c1cc(cc2)C(C(=O)Nc3ccc4c3cccc4

RUN: RUN4000

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.22

DAR-DIA-6a508060-9_1



CID: DAR-DIA-6a508060-9_1

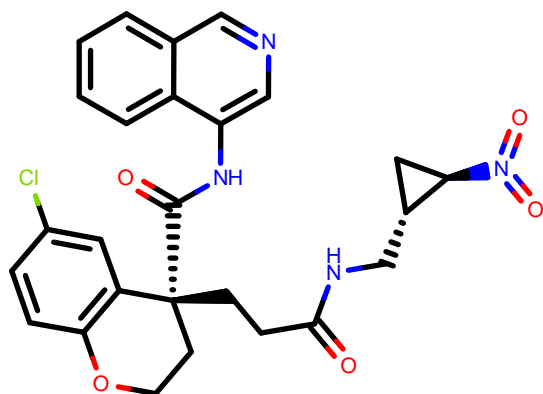
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C1CCCCC5

RUN: RUN316

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.24

EN300-7465222_2_1_1



CID: EN300-7465222_2_1_1

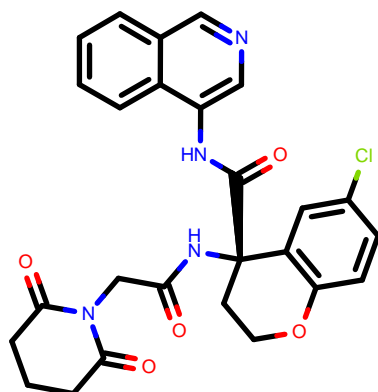
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(C(=O)N[C@@]5(C)C5)N(=O)=O

RUN: RUN5114

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.24

EN300-54837_1_1_1



CID: EN300-54837_1_1_1

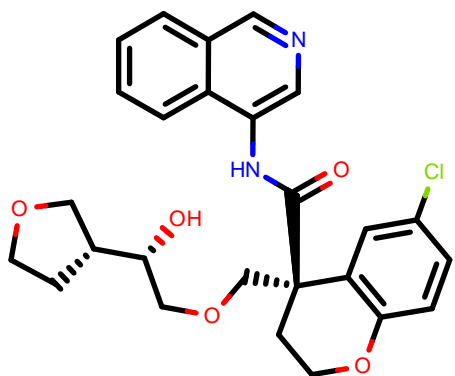
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(C(=O)N5C(=O)CCCC5=O

RUN: RUN7331

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.27

EN300-1911992_2_2_1



CID: EN300-1911992_2_2_1

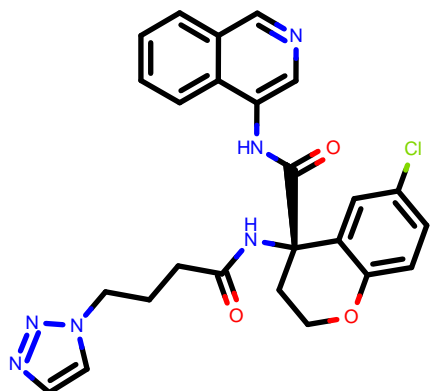
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@H](C@@H)5CCOC5O

RUN: RUN4208

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.34

EN300-124301_1_1_1



CID: EN300-124301_1_1_1

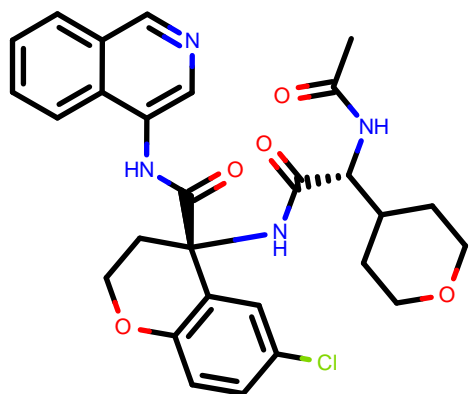
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCN5ccnn5

RUN: RUN3457

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.27

EN300-158292_1_2_1



CID: EN300-158292_1_2_1

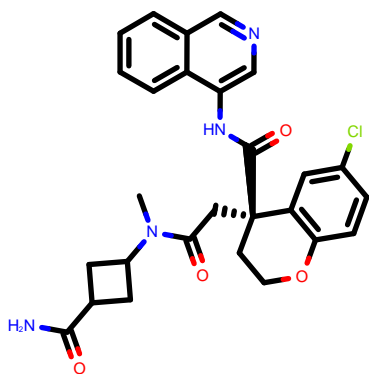
SMILES: CC(=O)N[C@H](C1CCOC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccoc5

RUN: RUN3767

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.27

EN300-321459_1_1_1



CID: EN300-321459_1_1_1

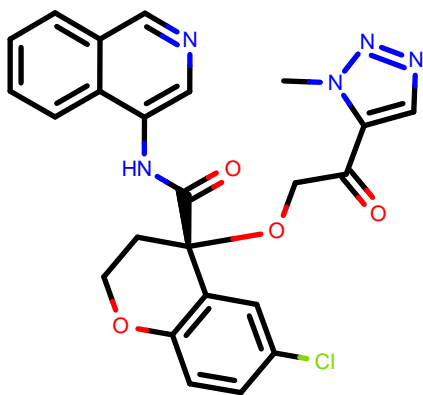
SMILES: CN(C1CC(C1)C(=O)N)C(=O)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccoc5

RUN: RUN5309

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.23

EN300-204936_1_1_1



CID: EN300-204936_1_1_1

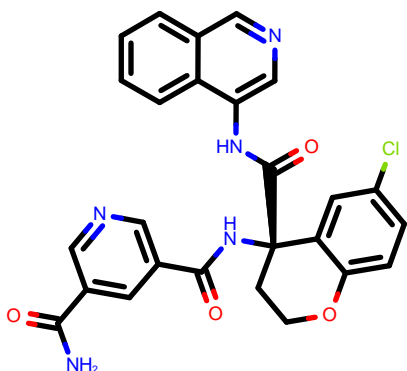
SMILES: Cn1c(cnn1)C(=O)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4084

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.20

EN300-44993_1_1_1



CID: EN300-44993_1_1_1

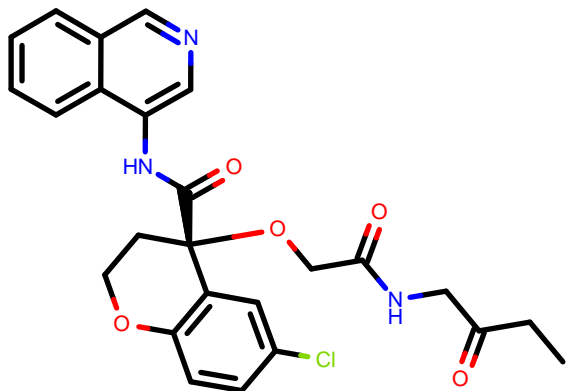
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cnc5)Cl(=O)N

RUN: RUN6010

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.23

EN300-132624_1_1_1



CID: EN300-132624_1_1_1

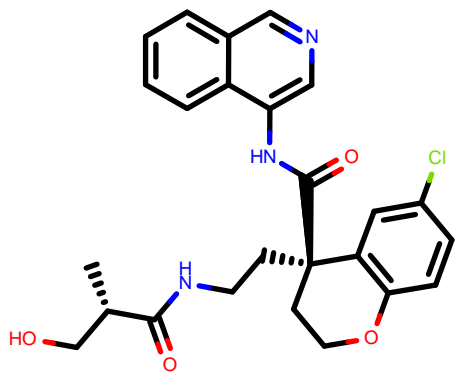
SMILES: CCC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6878

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.28

EN300-55072_3_1_1



CID: EN300-55072_3_1_1

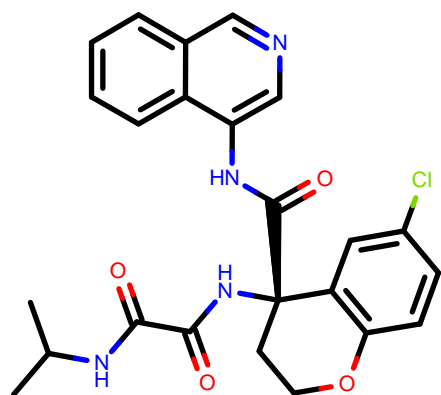
SMILES: C[C@@H](CO)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4250

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.26

EN300-1262640_1_1_1



CID: EN300-1262640_1_1_1

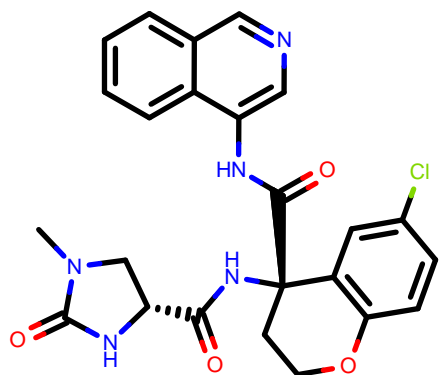
SMILES: CC(C)NC(=O)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3299

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.25

EN300-255795_1_1_1



CID: EN300-255795_1_1_1

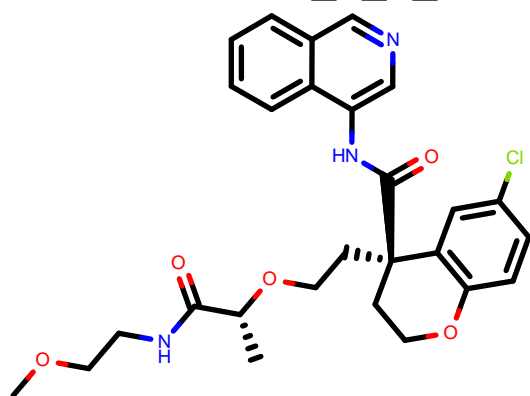
SMILES: CN1C[C@@H](NC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3057

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.22

EN300-23317_3_2_1



CID: EN300-23317_3_2_1

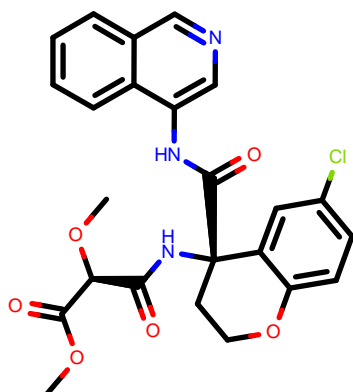
SMILES: C[C@@H](C(=O)NCCOC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4675

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.34

EN300-1718194_1_1_1



CID: EN300-1718194_1_1_1

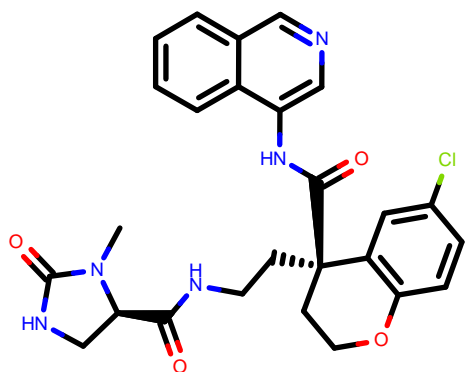
SMILES: CO[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)C(=O)NCC

RUN: RUN3732

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.28

EN300-307008_3_2_1



CID: EN300-307008_3_2_1

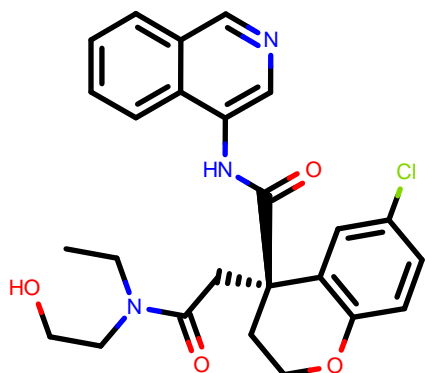
SMILES: CN1[C@H](CNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5895

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.32

EN300-74448_1_1_1



CID: EN300-74448_1_1_1

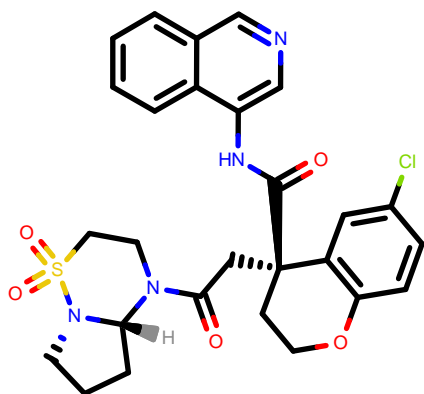
SMILES: CCN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3779

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.32

EN300-1688983_1_2_1



CID: EN300-1688983_1_2_1

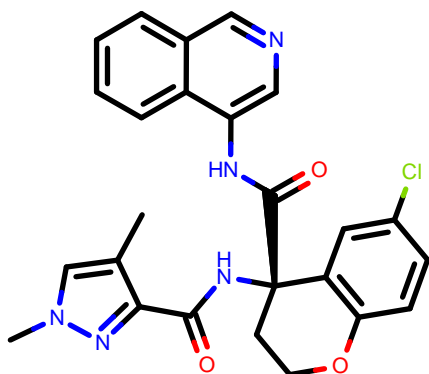
SMILES: c1ccc2c(e1)ncnc2N[C@@]3(C)[C@@H](C(=O)NCC[C@]4(CCOc5c3ccccc5)CC(=O)N5CCS(=O)(=O)N5)N3

RUN: RUN7377

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.38

EN300-255422_1_1_1



CID: EN300-255422_1_1_1

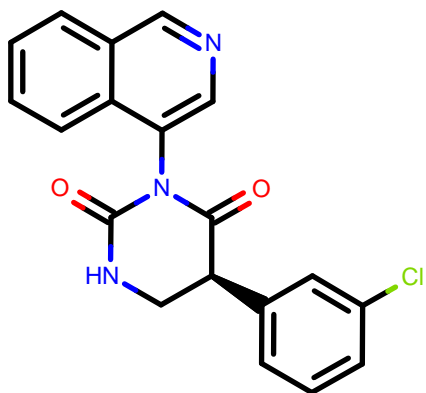
SMILES: Cc1cn(nc1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN3471

DDG (kcal/mol): -2.17

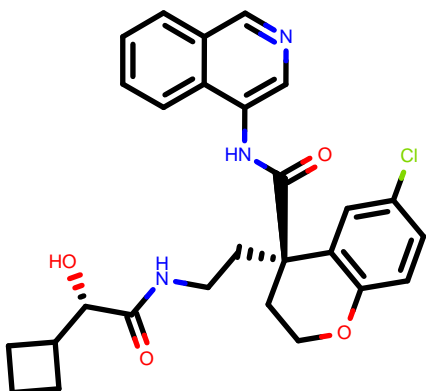
dDDG (kcal/mol): 0.25

VLA-UCB-1dbca3b4-18_2



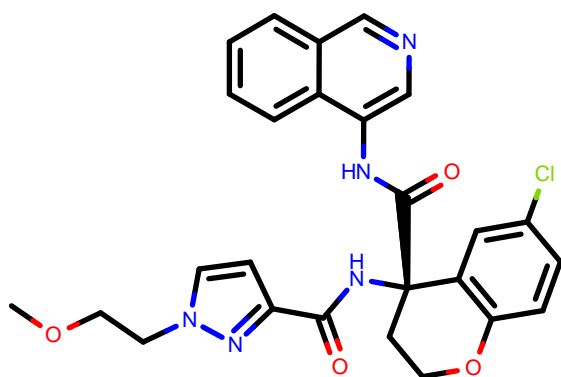
CID:	VLA-UCB-1dbca3b4-18_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@H](CNC3=O)c4cccc(c4)Cl</chem>
RUN:	RUN111
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.21

EN300-249764_3_2_1



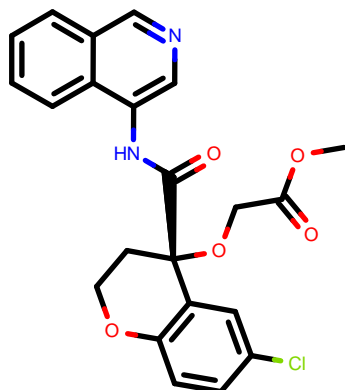
CID:	EN300-249764_3_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CCO5)O</chem>
RUN:	RUN3619
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.35

EN300-160277_1_1_1



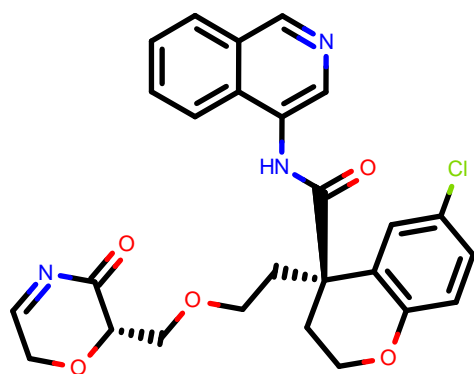
CID:	EN300-160277_1_1_1
SMILES:	<chem>COCc1ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN2867
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.29

EN300-19700_1_1_1



CID:	EN300-19700_1_1_1
SMILES:	<chem>COC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN4154
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.18

EN300-1706036_3_2_1



CID: EN300-1706036_3_2_1

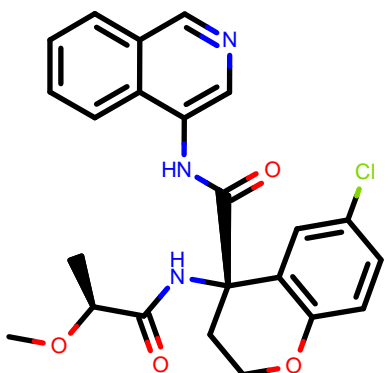
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C(=O)NCCO5

RUN: RUN6796

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.33

EN300-258477_1_1_1



CID: EN300-258477_1_1_1

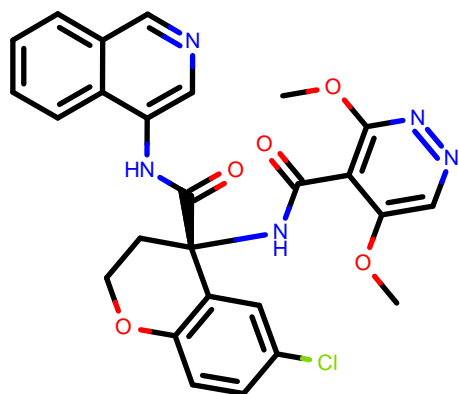
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN3932

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.25

EN300-366931_1_1_1



CID: EN300-366931_1_1_1

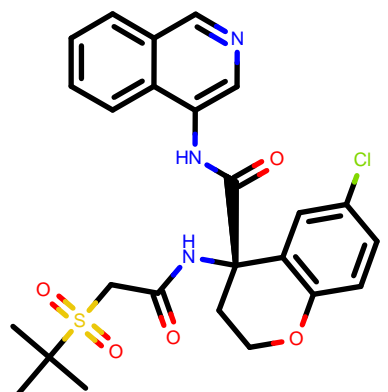
SMILES: COc1nnc(c1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5)OC

RUN: RUN3475

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.31

EN300-123589_1_1_1



CID: EN300-123589_1_1_1

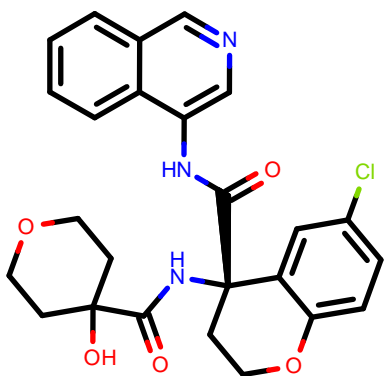
SMILES: CC(C)(C)S(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN3161

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.32

EN300-69368_1_1_1



CID: EN300-69368_1_1_1

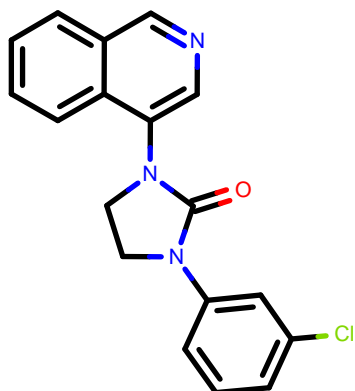
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)O

RUN: RUN3244

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.27

PET-UNK-7be94445-2_1



CID: PET-UNK-7be94445-2_1

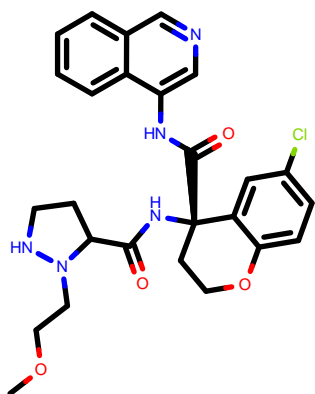
SMILES: c1ccc2c(c1)cncc2N3CCN(C3=O)c4cccc(c4)Cl

RUN: RUN42

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.35

EN300-92664_1_1_1



CID: EN300-92664_1_1_1

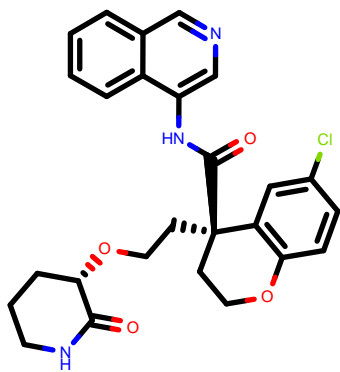
SMILES: COCc1c(ccn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3081

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.28

EN300-107267_3_2_1



CID: EN300-107267_3_2_1

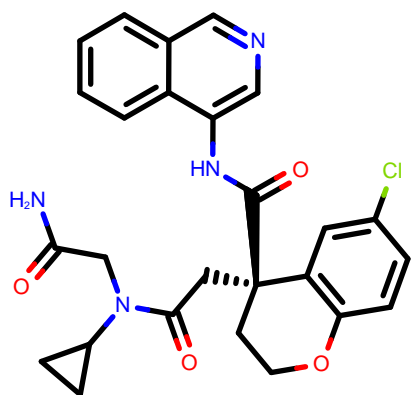
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCNCC5=O

RUN: RUN4293

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.26

EN300-112500_1_1_1



CID: EN300-112500_1_1_1

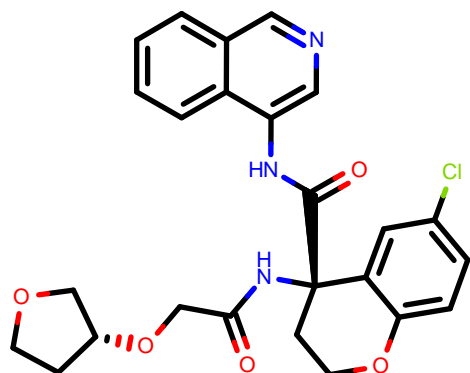
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)C5CC5

RUN: RUN2972

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.26

EN300-99391_1_1_1



CID: EN300-99391_1_1_1

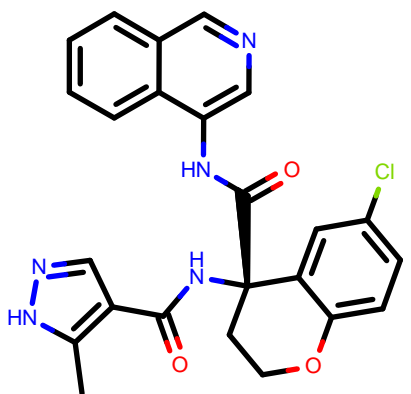
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@]4HJ5CCOC5

RUN: RUN2890

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.26

EN300-27672_1_1_1



CID: EN300-27672_1_1_1

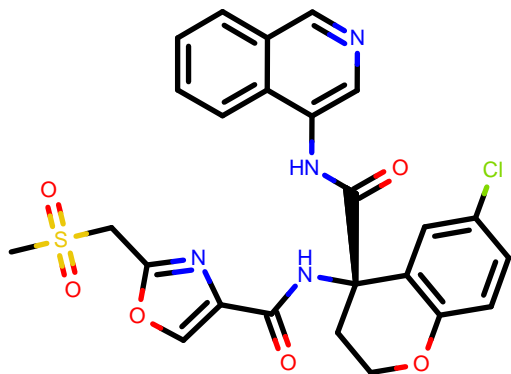
SMILES: Cc1c(c[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5718

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.23

EN300-263392_1_1_1



CID: EN300-263392_1_1_1

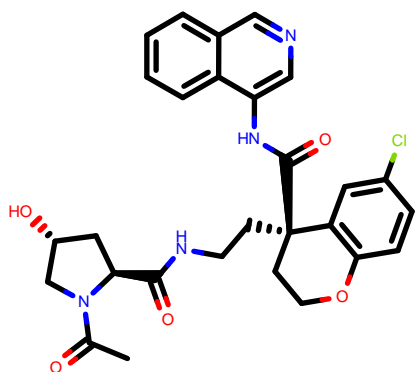
SMILES: CS(=O)(=O)Cc1nc(cc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN7193

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.33

EN300-1703718_3_1_1



CID: EN300-1703718_3_1_1

SMILES:

CC(=O)N1C[C@H](C[C@@H]1C(=O)NC[C@@]2(CCOc3cc2cc3)C1C(=O)Nc4nc5c4ccc5)O

RUN:

RUN5037

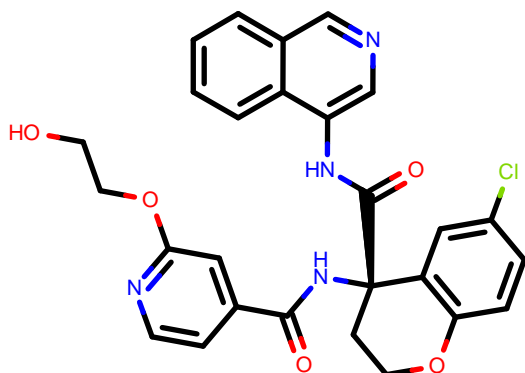
DDG (kcal/mol):

-2.16

dDDG (kcal/mol):

0.39

EN300-101796_1_1_1



CID: EN300-101796_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)OCCO

RUN:

RUN4410

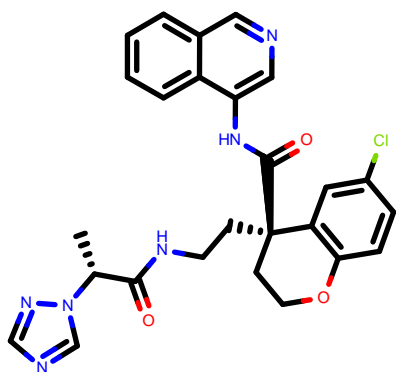
DDG (kcal/mol):

-2.16

dDDG (kcal/mol):

0.34

EN300-30397_3_2_1



CID: EN300-30397_3_2_1

SMILES:

C[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)n5cn[nH]5

RUN:

RUN3303

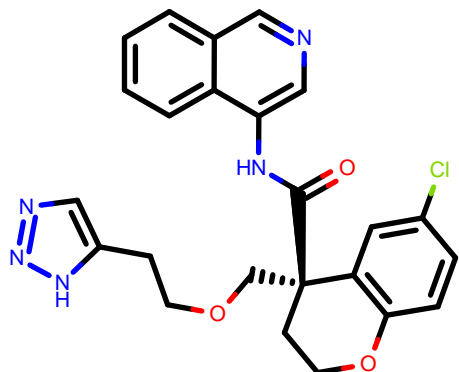
DDG (kcal/mol):

-2.16

dDDG (kcal/mol):

0.32

EN300-222357_2_1_1



CID: EN300-222357_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCc5cn[nH]n5

RUN:

RUN3313

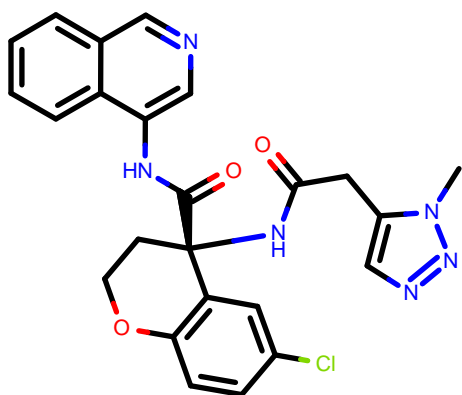
DDG (kcal/mol):

-2.16

dDDG (kcal/mol):

0.31

EN300-6486855_1_1_1



CID: EN300-6486855_1_1_1

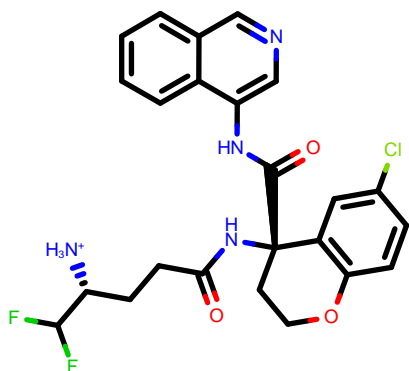
SMILES: Cn1c(cnn1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2984

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.23

EDG-MED-90036822-57_2



CID: EDG-MED-90036822-57_2

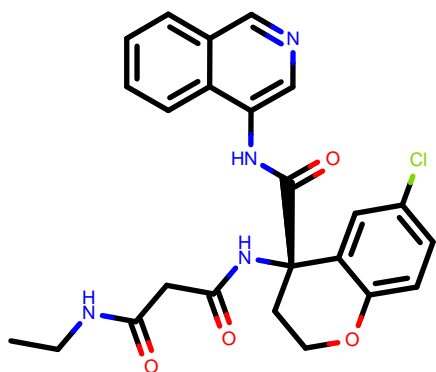
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H](C(F)F)N

RUN: RUN1654

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.43

EN300-129455_1_1_1



CID: EN300-129455_1_1_1

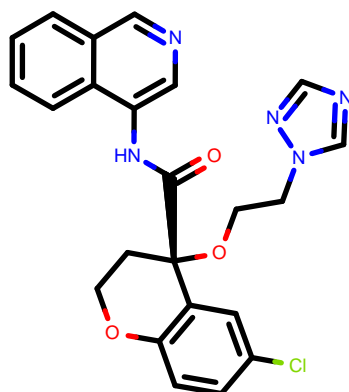
SMILES: CCNC(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3996

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.26

EN300-6255179_1_1_1



CID: EN300-6255179_1_1_1

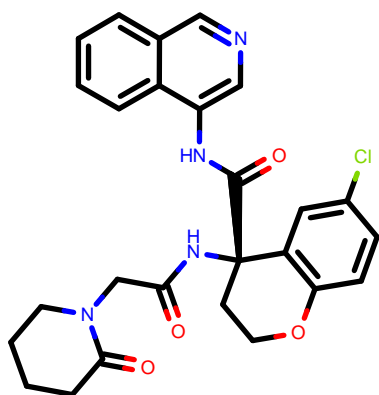
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnc5

RUN: RUN4412

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.25

EN300-36111_1_1_1



CID: EN300-36111_1_1_1

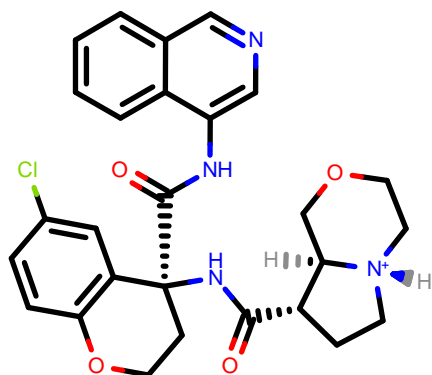
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)C)NC(=O)CN5CCCCC5=O

RUN: RUN4096

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.31

EN300-1588613_1_2_1



CID: EN300-1588613_1_2_1

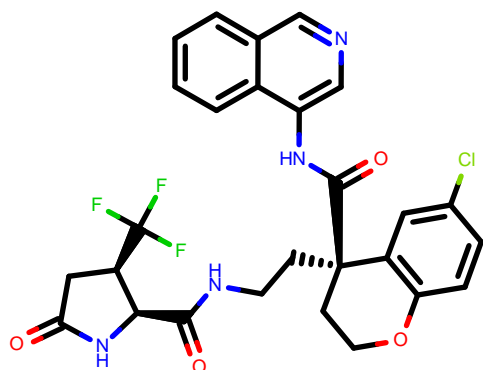
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)C)NC(=O)C@H5CCN@H+R[C@@H]5COCC6

RUN: RUN3760

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.26

EN300-169955_3_1_1



CID: EN300-169955_3_1_1

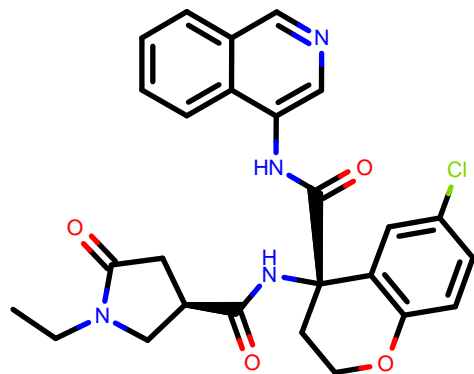
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)C)NC(=O)C@H5C@H(C)CC(=O)N5C(F)F(F)F

RUN: RUN3516

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.29

EN300-33478_1_1_1



CID: EN300-33478_1_1_1

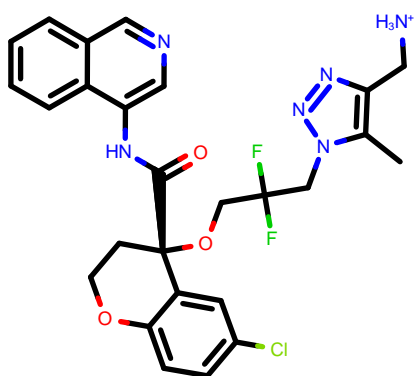
SMILES: CCN1C[C@@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3C)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3770

DDG (kcal/mol): -2.14

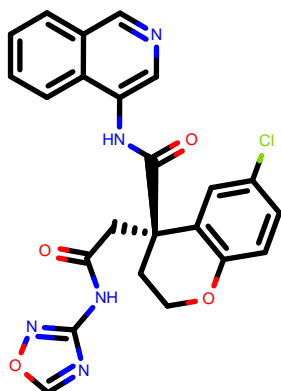
dDDG (kcal/mol): 0.26

ED_-GRI-5b13fbe2-44_1



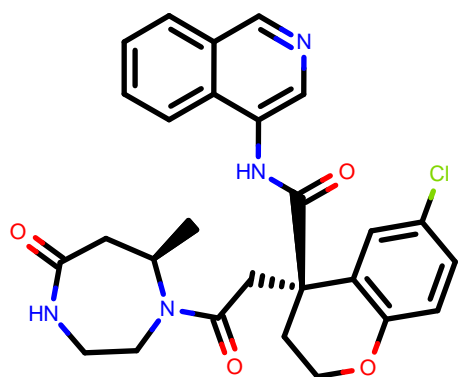
CID:	ED_-GRI-5b13fbe2-44_1
SMILES:	<chem>Cc1c(nnn1CC(CO)[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)(F)F)C[NH3+]</chem>
RUN:	RUN1484
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.33

EDJ-MED-d203f206-2_1



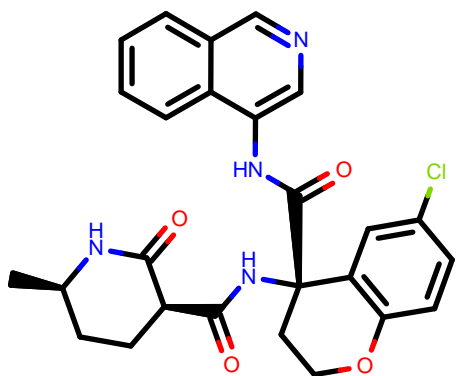
CID:	EDJ-MED-d203f206-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncon5</chem>
RUN:	RUN2354
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.23

EN300-74029_1_1_1



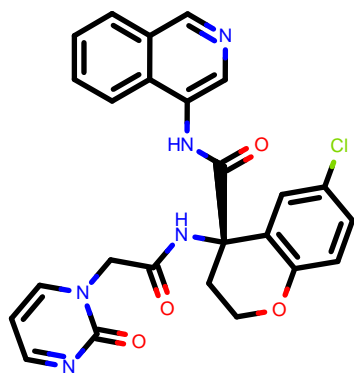
CID:	EN300-74029_1_1_1
SMILES:	<chem>C[C@@H]1CC(=O)NCCN1C(=O)C[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN3575
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.29

EN300-6505003_1_1_1



CID:	EN300-6505003_1_1_1
SMILES:	<chem>C[C@@H]1CC[C@@H](C(=O)N1)C(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN2861
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.43

EN300-35789_1_1_1



CID: EN300-35789_1_1_1

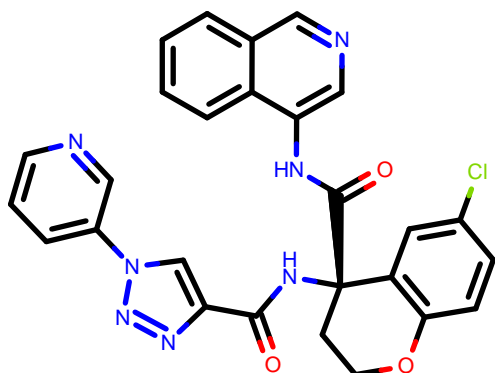
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccoc5=O

RUN: RUN3892

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.28

EN300-151330_1_1_1



CID: EN300-151330_1_1_1

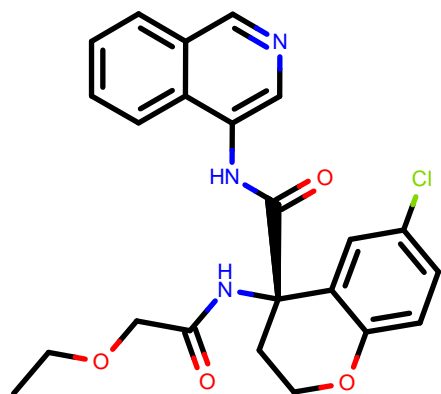
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nh5)c6ccoc6

RUN: RUN3312

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.20

EN300-21303_1_1_1



CID: EN300-21303_1_1_1

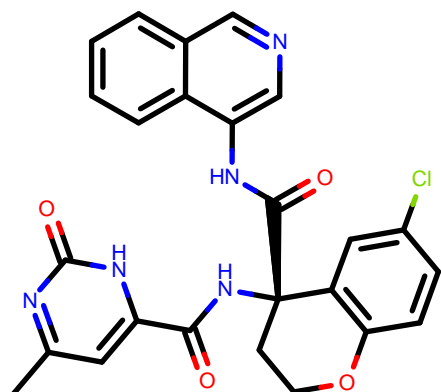
SMILES: CCOCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN5019

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.20

EN300-42536_1_1_1



CID: EN300-42536_1_1_1

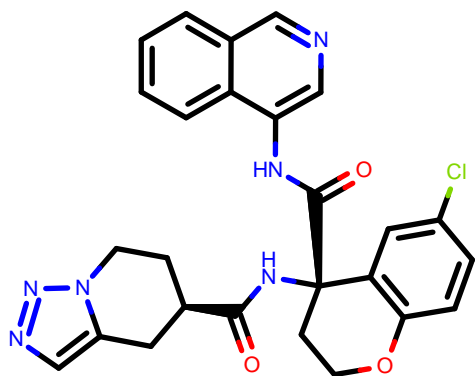
SMILES: Cc1cc(nc(=O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN4731

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.21

EN300-7430501_1_1_1



CID: EN300-7430501_1_1_1

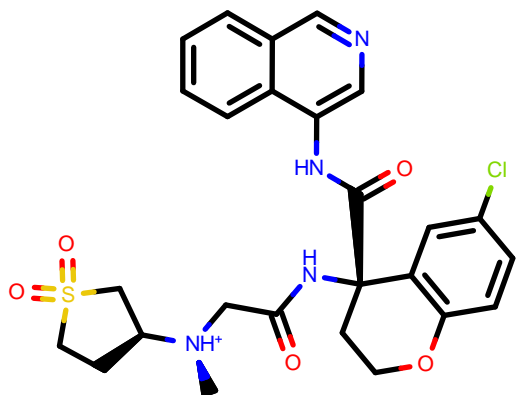
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5C5Cn6c(cnn6)C5

RUN: RUN2942

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.25

EN300-14628_1_2_1



CID: EN300-14628_1_2_1

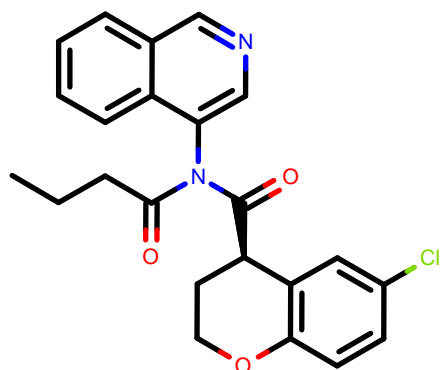
SMILES: CN[C@@H]3CC(=O)N[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4[C@@H]5C5S(=O)(=O)C5

RUN: RUN3682

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.43

DAR-DIA-5ff57136-11_1_1



CID: DAR-DIA-5ff57136-11_1_1

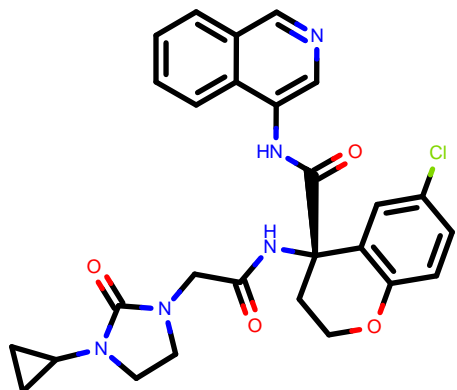
SMILES: C/C=C/C(=O)N(c1ncc2c1ccccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)C)C

RUN: RUN2770

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.23

ALP-UNI-dbbfd3db-3_1



CID: ALP-UNI-dbbfd3db-3_1

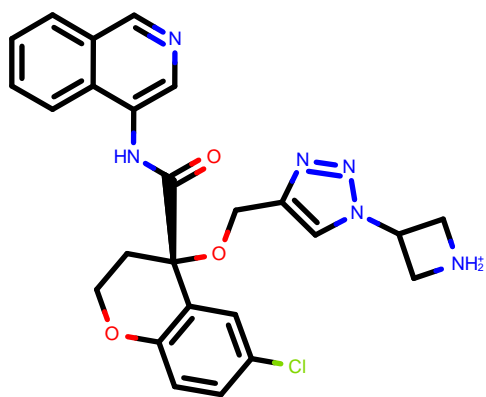
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5CCN(C5=O)C6CC6

RUN: RUN2638

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.31

ED_-GRI-5b13fbe2-32_1



CID: ED_-GRI-5b13fbe2-32_1

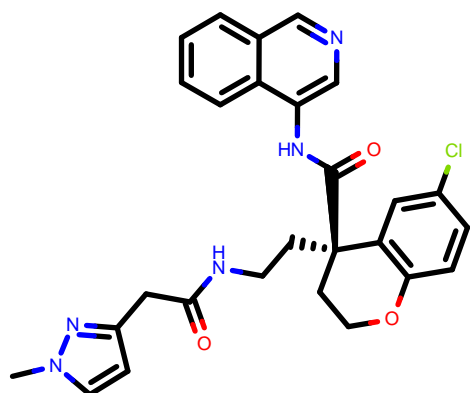
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(n5)C6C[NH2+]C6

RUN: RUN1442

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.33

EN300-258702_3_1_1



CID: EN300-258702_3_1_1

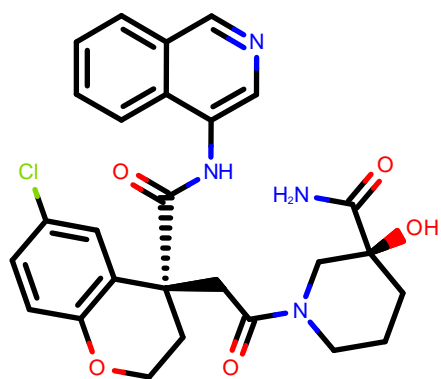
SMILES: Cn1ccc(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4728

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-39_1



CID: EDJ-MED-d203f206-39_1

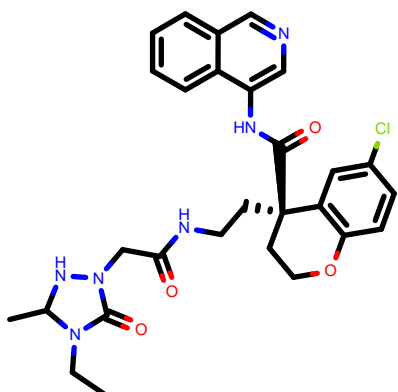
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@]5(C)C(=O)NO

RUN: RUN2468

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.38

EN300-6478433_3_1_1



CID: EN300-6478433_3_1_1

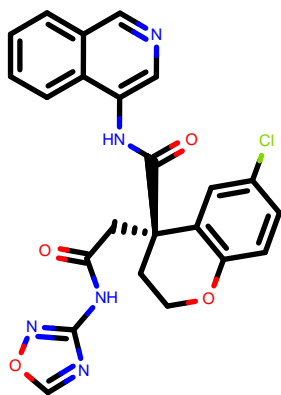
SMILES: CCn1c(nn(c1=O)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN7558

DDG (kcal/mol): -2.13

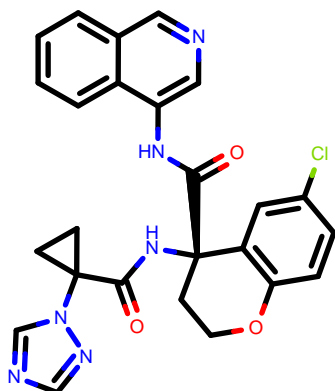
dDDG (kcal/mol): 0.38

CHO-MSK-a31cca77-4_1



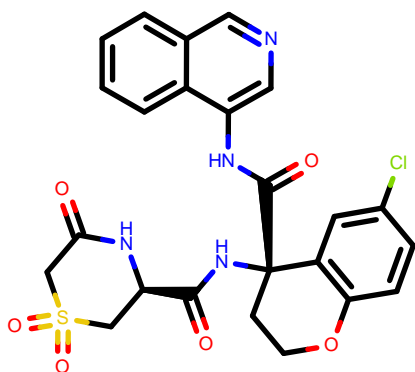
CID:	CHO-MSK-a31cca77-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncon5</chem>
RUN:	RUN2050
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.22

EN300-246440_1_1_1



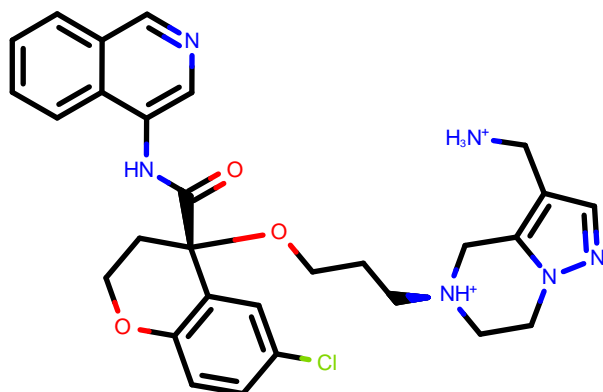
CID:	EN300-246440_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(C)C5n6enon6</chem>
RUN:	RUN3088
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.28

EN300-702756_1_2_1



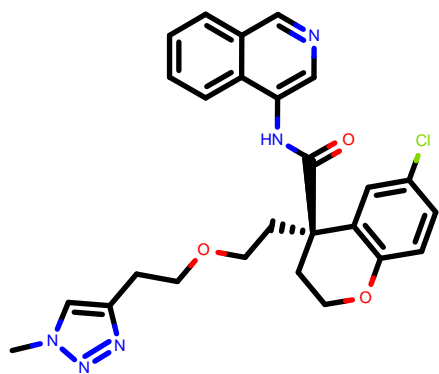
CID:	EN300-702756_1_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CS(=O)(=O)CC(=O)N5</chem>
RUN:	RUN2703
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.22

ED_-GRI-5b13fbe2-38_1



CID:	ED_-GRI-5b13fbe2-38_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N+]([H])5COC6c7c(en6)C[NH+]7C5</chem>
RUN:	RUN1456
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.46

EN300-1600786_3_1_1



CID: EN300-1600786_3_1_1

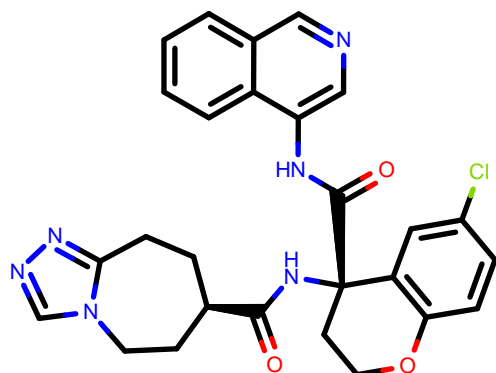
SMILES: Cn1cc(nn1)CCOCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2811

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.25

EN300-366687_1_1_1



CID: EN300-366687_1_1_1

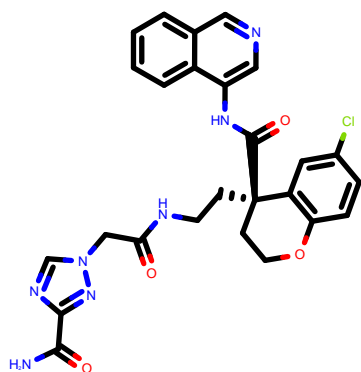
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5[H]5CCc6nncn6CC5

RUN: RUN5235

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.24

EN300-262604_3_1_1



CID: EN300-262604_3_1_1

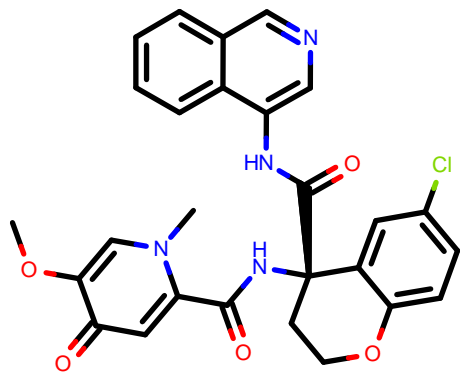
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ncn(n5)C(=O)N

RUN: RUN4815

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.28

EN300-236175_1_1_1



CID: EN300-236175_1_1_1

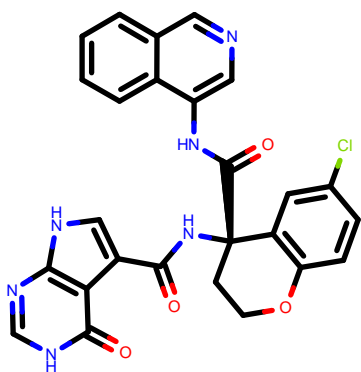
SMILES: Cn1cc(c(=O)cc1C(=O)N)[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC

RUN: RUN7381

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.31

EN300-746311_1_1_1



CID: EN300-746311_1_1_1

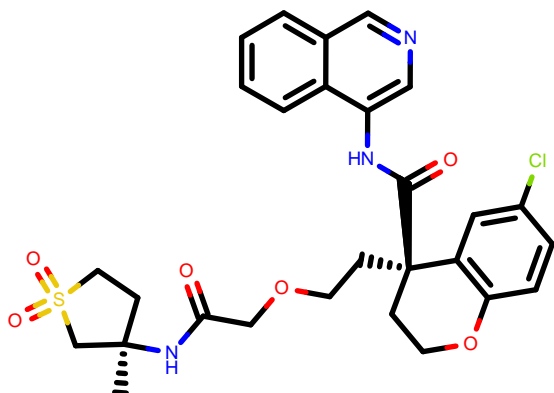
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]c6c5c(=O)[nH]c6n6

RUN: RUN3424

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.24

EN300-10414_3_2_1



CID: EN300-10414_3_2_1

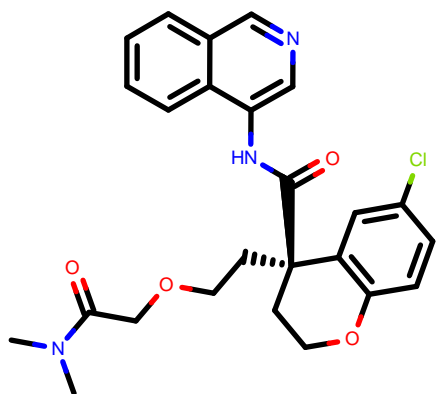
SMILES: C[C@]1(CC(=O)C(=O)C1)NC(=O)COCC[C@]2(CCOc3c2cc(cc3)O)C(=O)Nc4cnc5c4ccccc5

RUN: RUN6404

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.42

EN300-216063_3_1_1



CID: EN300-216063_3_1_1

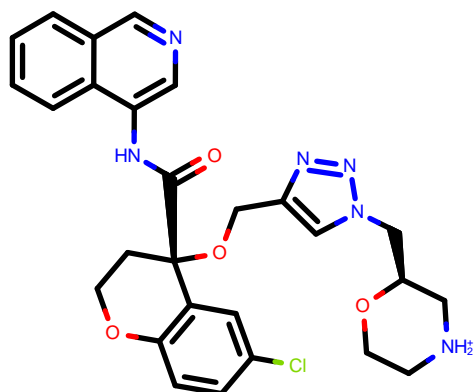
SMILES: CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccccc4

RUN: RUN4149

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.23

ED_-GRI-5b13fbe2-7_2



CID: ED_-GRI-5b13fbe2-7_2

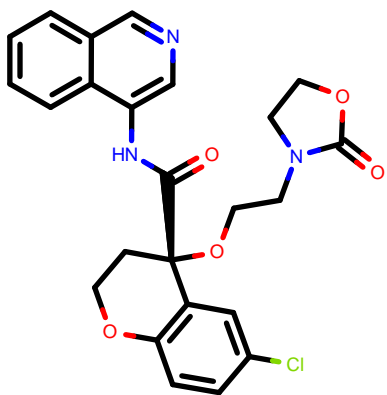
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5n(nn5)C[C@]6C[NH2+]CCO6

RUN: RUN1402

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.34

EN300-370967_1_1_1



CID: EN300-370967_1_1_1

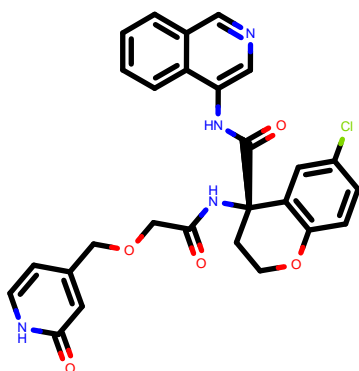
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O

RUN: RUN3449

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.27

EN300-316258_1_1_1



CID: EN300-316258_1_1_1

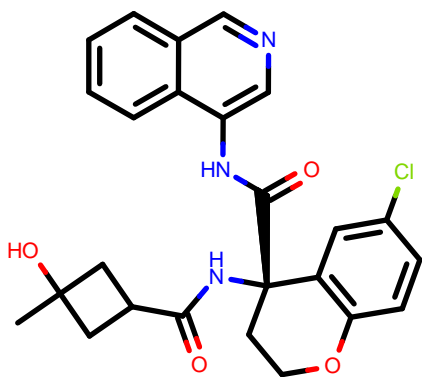
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COCc5cc[nH]c(=O)c5

RUN: RUN3524

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.25

EN300-247343_1_1_1



CID: EN300-247343_1_1_1

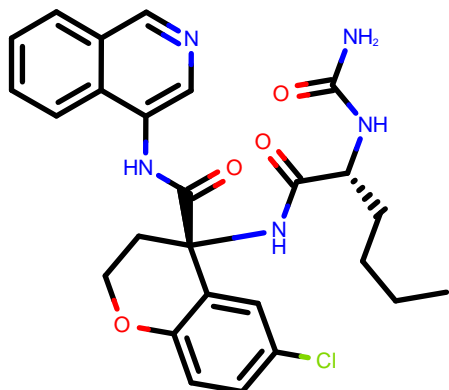
SMILES: CC1(CC(C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)O

RUN: RUN4948

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.22

EN300-55744_1_2_1



CID: EN300-55744_1_2_1

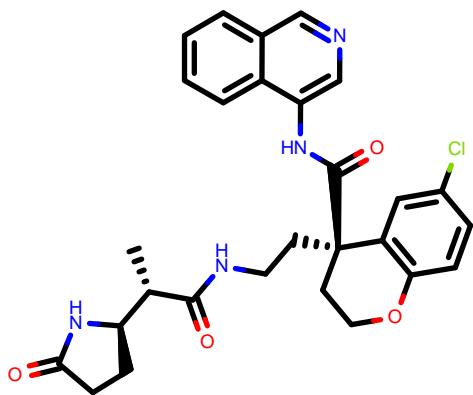
SMILES: CCCC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)NC(=O)N

RUN: RUN6563

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.38

EN300-249421_3_3_1



CID: EN300-249421_3_3_1

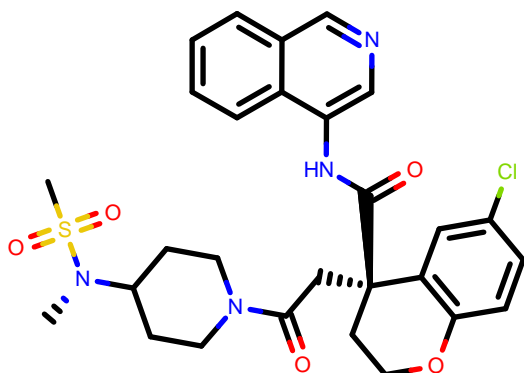
SMILES: C[C@@H]([C@H]1CCC(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3458

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.33

KAD-UNI-8a629cb0-17_2



CID: KAD-UNI-8a629cb0-17_2

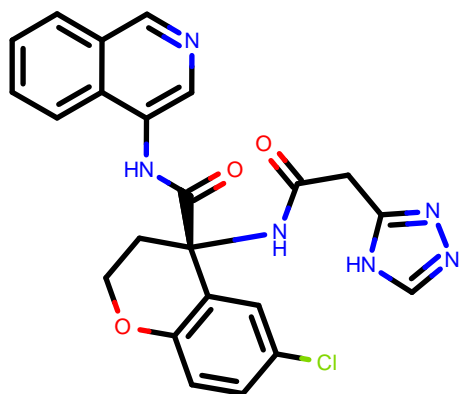
SMILES: CN([C]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C

RUN: RUN2012

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.27

EN300-96159_1_1_1



CID: EN300-96159_1_1_1

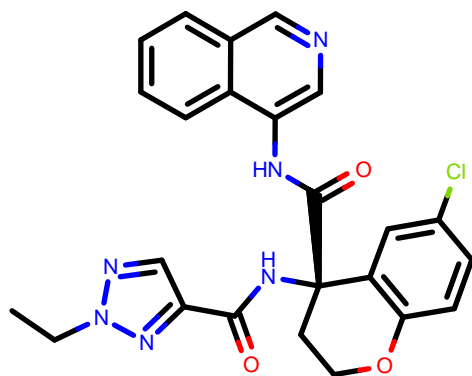
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]nnc5

RUN: RUN4067

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.18

EN300-215465_1_1_1



CID: EN300-215465_1_1_1

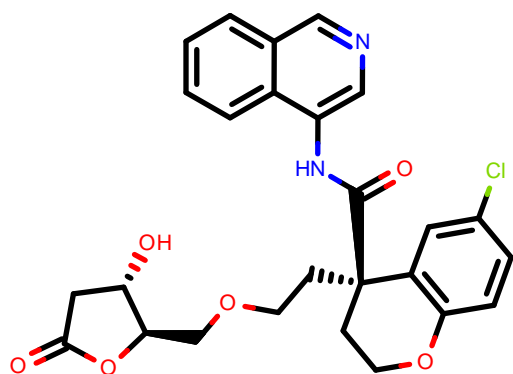
SMILES: CCn1ncc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3382

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.19

EN300-6487407_3_1_1



CID: EN300-6487407_3_1_1

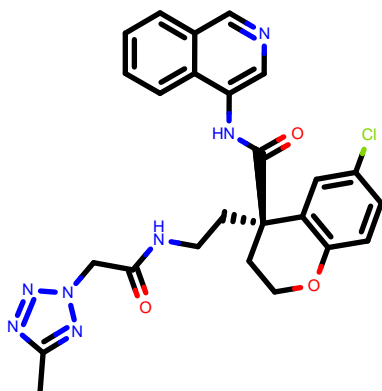
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H]5[C@H](CC(=O)O)O5)O

RUN: RUN3603

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.33

EN300-6487680_3_1_1



CID: EN300-6487680_3_1_1

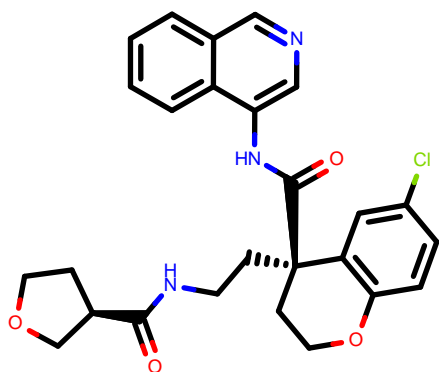
SMILES: Cc1nnn(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3729

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.34

EN300-697519_3_1_1



CID: EN300-697519_3_1_1

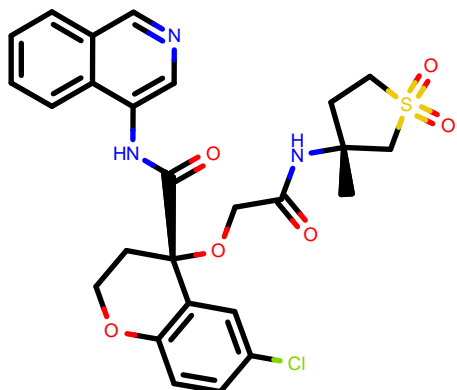
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@H]5CCOC5

RUN: RUN5930

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.33

EN300-10414_1_2_1



CID: EN300-10414_1_2_1

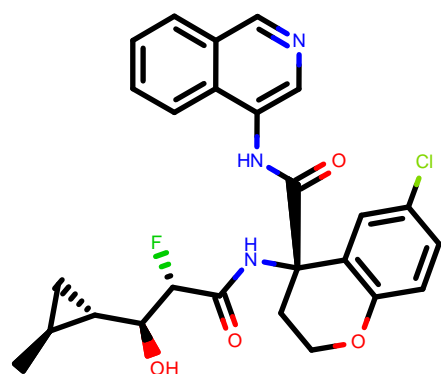
SMILES: C[C@@]1(CCS(=O)(=O)C1)NC(=O)CO[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4472

DDG (kcal/mol): -2.10

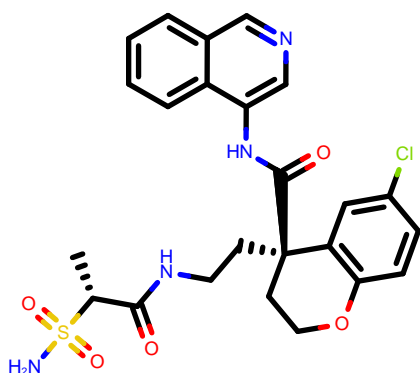
dDDG (kcal/mol): 0.43

EDG-MED-90036822-94_2



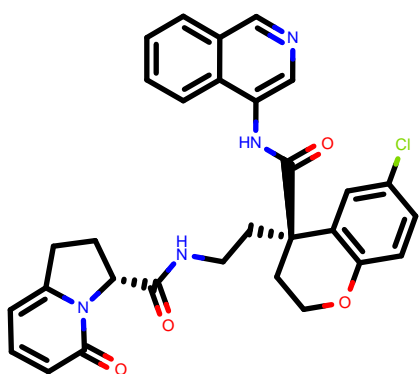
CID:	EDG-MED-90036822-94_2
SMILES:	<chem>C[C@H](C)C[C@@H](C)C[C@@H](C)C(=O)N[C@@H](COC(=O)C1C[C@@H](O)N4C[C@@H](C)O4)F</chem>
RUN:	RUN1666
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.23

EN300-132615_3_2_1



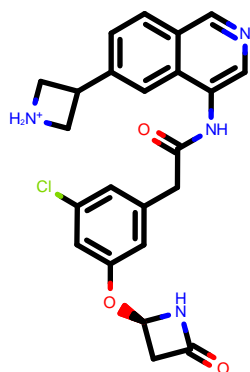
CID:	EN300-132615_3_2_1
SMILES:	<chem>C[C@H](C)C(=O)NCC[C@H]1(COC(=O)C1)C(=O)Nc3ccc(Cl)cc3S(=O)(=O)N</chem>
RUN:	RUN3260
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.34

EN300-332002_3_2_1



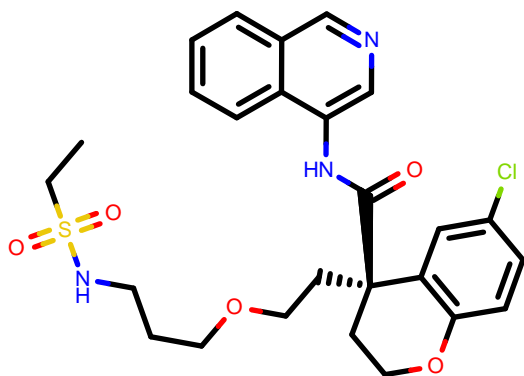
CID:	EN300-332002_3_2_1
SMILES:	<chem>C1CC2C(C1)NCC(=O)N[C@@H](C)C(=O)Nc3ccc(Cl)cc3C4CCNC(=O)N4C5C(=O)NCC5=O</chem>
RUN:	RUN6927
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.35

ALF-EVA-0b412456-8_1



CID:	ALF-EVA-0b412456-8_1
SMILES:	<chem>C1CC2C(C1)NCC(=O)N[C@@H](C)C(=O)Nc3ccc(Cl)cc3C4CCNC(=O)N4C5C(=O)NCC5=O</chem>
RUN:	RUN2603
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.36

EN300-116092_3_1_1



CID: EN300-116092_3_1_1

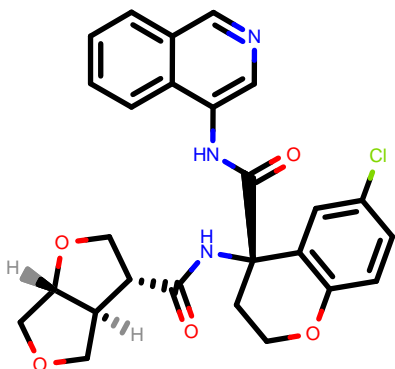
SMILES: CCS(=O)(=O)NCCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4

RUN: RUN7489

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.42

EN300-6482296_1_2_1



CID: EN300-6482296_1_2_1

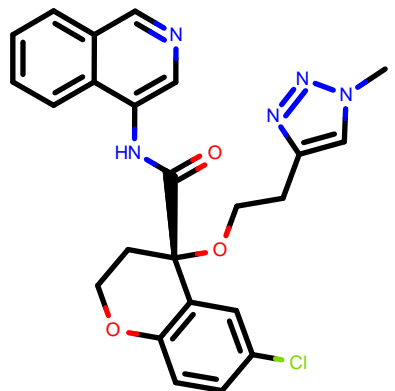
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cc6c5ccoc6

RUN: RUN3417

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.26

EN300-1600786_1_1_1



CID: EN300-1600786_1_1_1

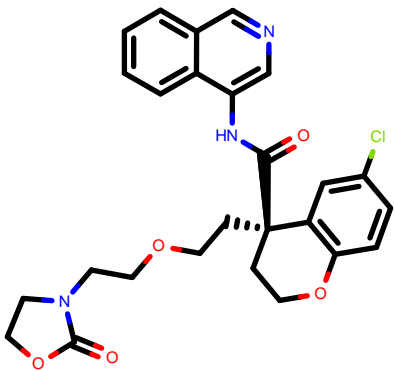
SMILES: Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5540

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.23

EN300-370967_3_1_1



CID: EN300-370967_3_1_1

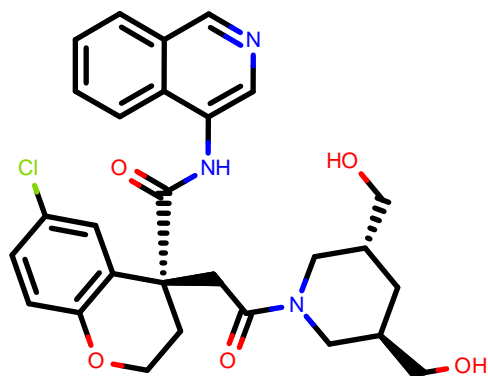
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5COC(=O)5

RUN: RUN3831

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.30

EN300-2007627_1_3_1



CID: EN300-2007627_1_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc3cc(Cl)cc1=O)N5C[C@@H](C[C@@H](C5)CO)CO

RUN:

RUN4888

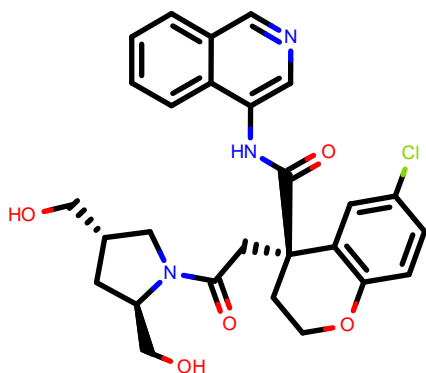
DDG (kcal/mol):

-2.09

dDDG (kcal/mol):

0.36

EN300-1212400_1_2_1



CID: EN300-1212400_1_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc3cc(Cl)cc1=O)N5C[C@@H](C[C@@H](C5)CO)CO

RUN:

RUN3678

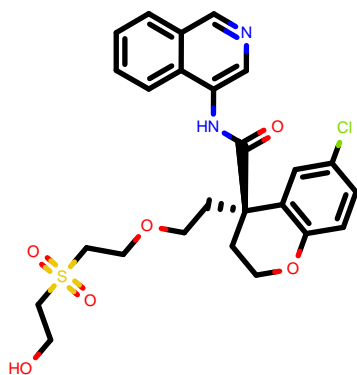
DDG (kcal/mol):

-2.09

dDDG (kcal/mol):

0.31

EN300-7463171_3_1_1



CID: EN300-7463171_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc3cc(Cl)cc1=O)CCOCCS(=O)(=O)CO

RUN:

RUN3231

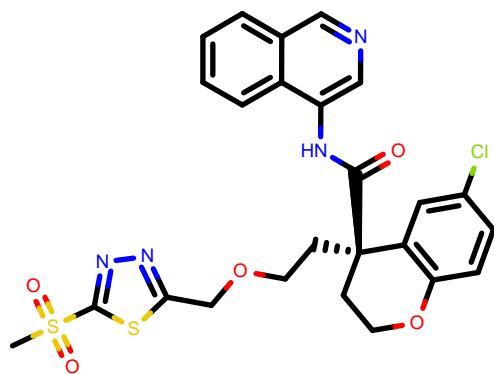
DDG (kcal/mol):

-2.09

dDDG (kcal/mol):

0.55

EN300-160080_3_1_1



CID: EN300-160080_3_1_1

SMILES:

CS(=O)(=O)c1nnc(s1)COC[C@@H](C)COCc3cc(Cl)cc1=O)Nc4ncnc5c4ccc5

RUN:

RUN4442

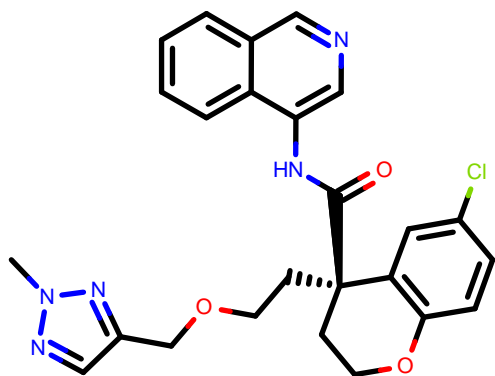
DDG (kcal/mol):

-2.08

dDDG (kcal/mol):

0.32

EN300-219020_3_1_1



CID: EN300-219020_3_1_1

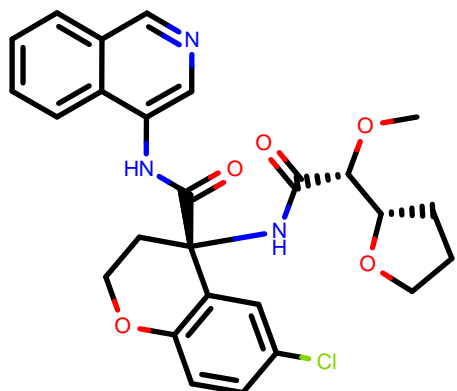
SMILES: Cn1ncc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3431

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.27

EN300-6277108_1_2_1



CID: EN300-6277108_1_2_1

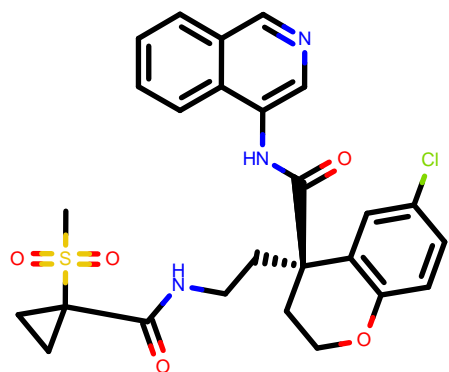
SMILES: CO[C@H]([C@@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3370

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-191495_3_1_1



CID: EN300-191495_3_1_1

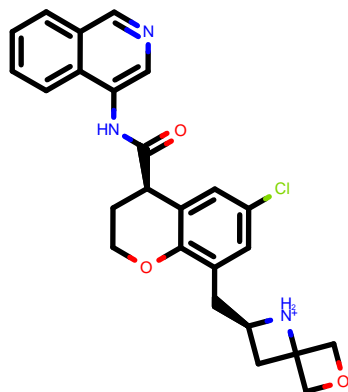
SMILES: CS(=O)(=O)C1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4199

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.41

DAR-DIA-23e5a6a0-8_1



CID: DAR-DIA-23e5a6a0-8_1

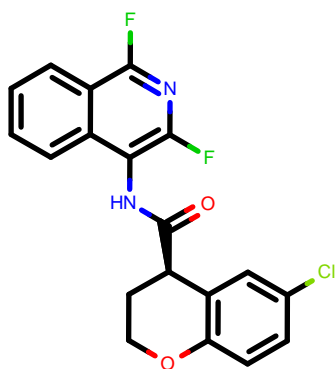
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]([C@@H]3CCOC4c3cc(cc4)C)[C@@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN347

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.28

JOH-SUS-a69c159d-6_1



CID: JOH-SUS-a69c159d-6_1

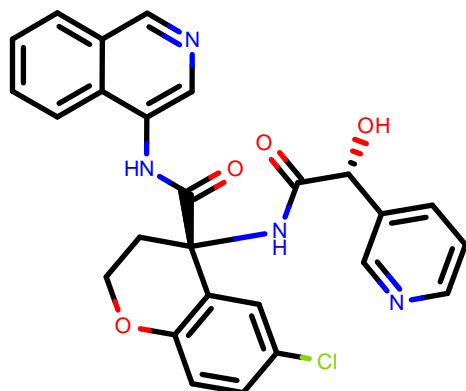
SMILES: c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1060

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.06

EN300-134855_1_1_1



CID: EN300-134855_1_1_1

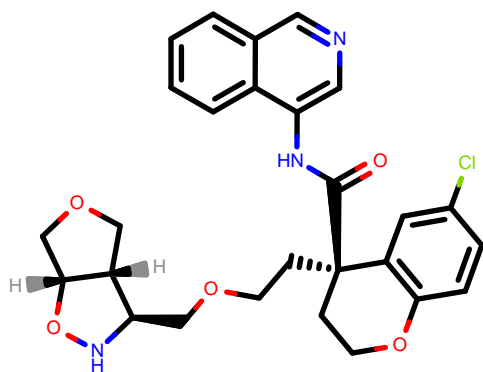
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4c3cc(cc4)Cl)NC(=O)[C@@H](c5ccncc5)O

RUN: RUN3806

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.24

EN300-7436306_3_1_1



CID: EN300-7436306_3_1_1

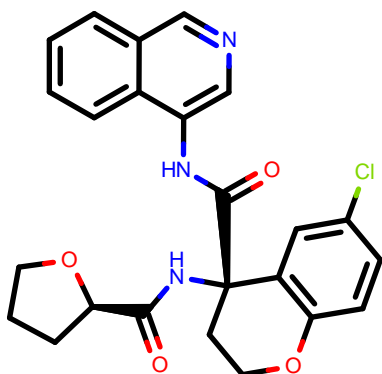
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4c3cc(cc4)Cl)COC[C@@H]5[C@@H](COC6c5ccncc6)O

RUN: RUN3073

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.28

EN300-116234_1_1_1



CID: EN300-116234_1_1_1

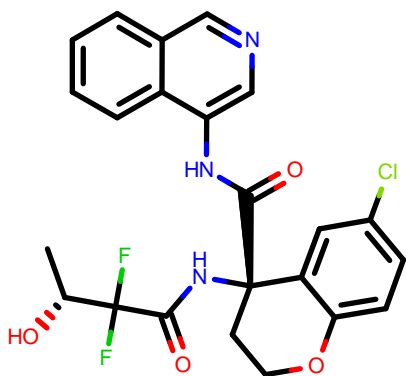
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4c3cc(cc4)Cl)NC(=O)[C@@H]5COCOC5

RUN: RUN2816

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-185398_1_2_1



CID: EN300-185398_1_2_1

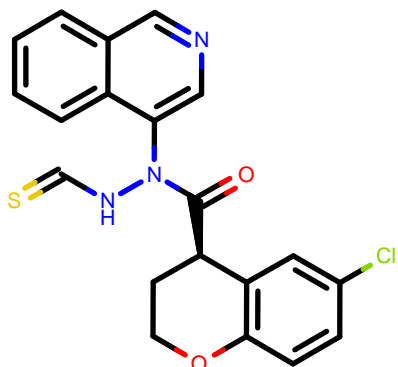
SMILES: C[C@H](C(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4(F)F)O

RUN: RUN3487

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.20

DAR-DIA-5ff57136-18_1



CID: DAR-DIA-5ff57136-18_1

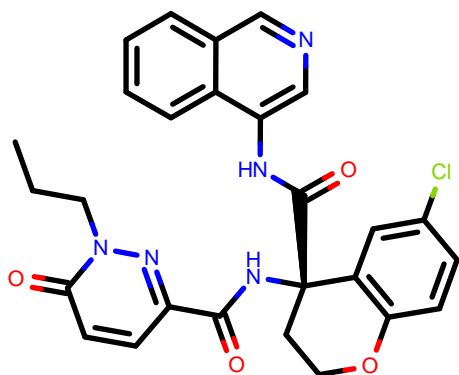
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOC4c3cc(cc4)Cl)N=C=S

RUN: RUN1269

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.14

EN300-09334_1_1_1



CID: EN300-09334_1_1_1

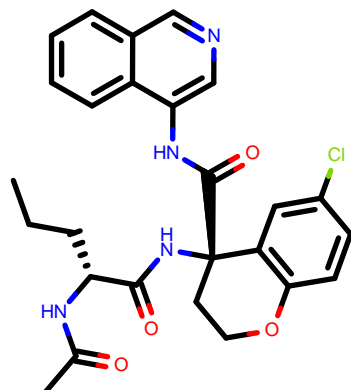
SMILES: CCCn1c(=O)ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN2747

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.26

EN300-51801_1_2_1



CID: EN300-51801_1_2_1

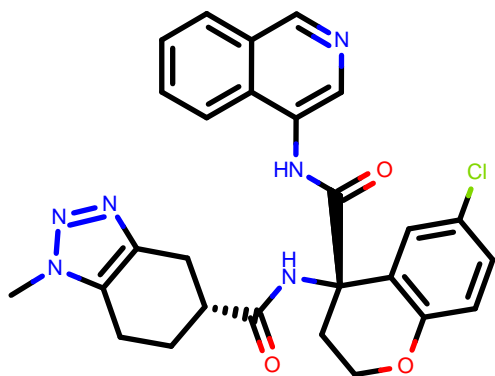
SMILES: CCC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)C

RUN: RUN3307

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.32

EN300-185727_1_1_1



CID: EN300-185727_1_1_1

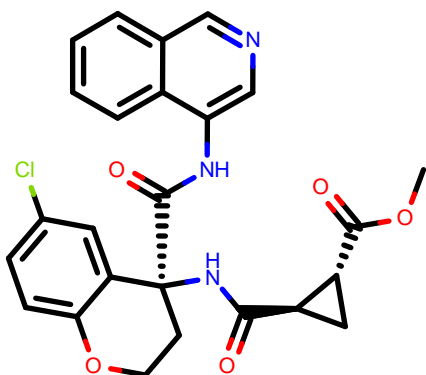
SMILES: Cn1c2c(n1)C[C@@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4348

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.30

EN300-66764_1_3_1



CID: EN300-66764_1_3_1

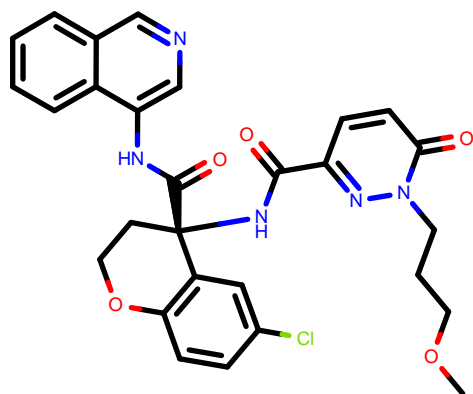
SMILES: COC(=O)C[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3768

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-297872_1_1_1



CID: EN300-297872_1_1_1

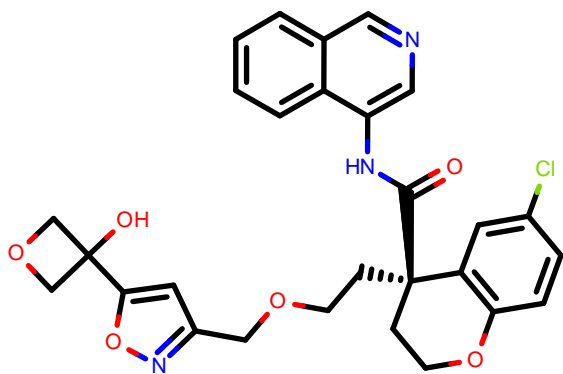
SMILES: COCCN1c(=O)ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN2817

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.28

EN300-7457159_3_1_1



CID: EN300-7457159_3_1_1

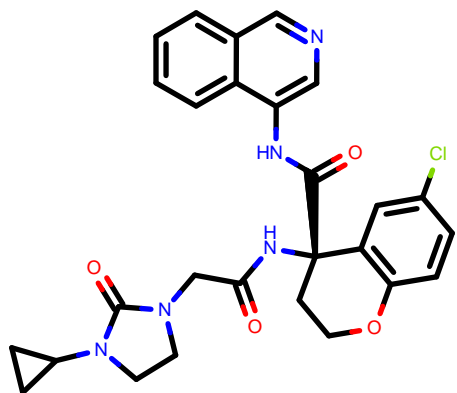
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5cc(on5)C6(COC6)O

RUN: RUN3962

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.35

KAD-UNI-8a629cb0-13_1



CID: KAD-UNI-8a629cb0-13_1

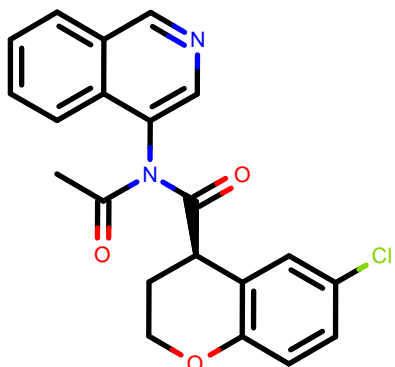
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5CCN(C5=O)C6CC6

RUN: RUN2010

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.33

VLA-UCB-50c39ae8-1_1_1



CID: VLA-UCB-50c39ae8-1_1_1

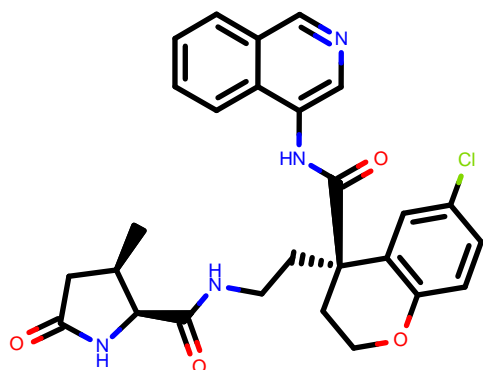
SMILES: CC(=O)N(c1cnc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN4306

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.13

EN300-155362_3_1_1



CID: EN300-155362_3_1_1

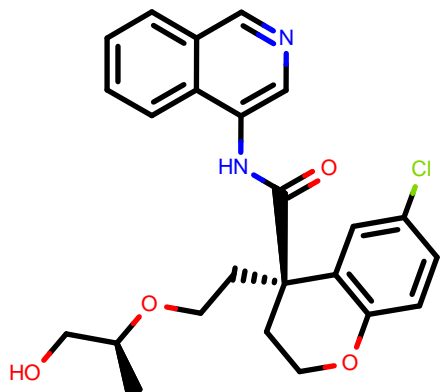
SMILES: C[C@@H]1CC(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)O)C(=O)Nc4cnc5c4cccc5

RUN: RUN4232

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.29

EN300-175186_3_1_1



CID: EN300-175186_3_1_1

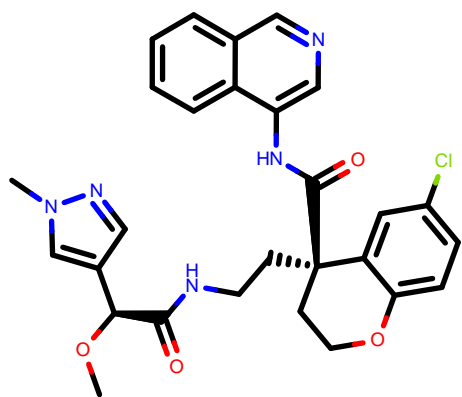
SMILES: C[C@@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3970

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.31

EN300-198240_3_1_1



CID: EN300-198240_3_1_1

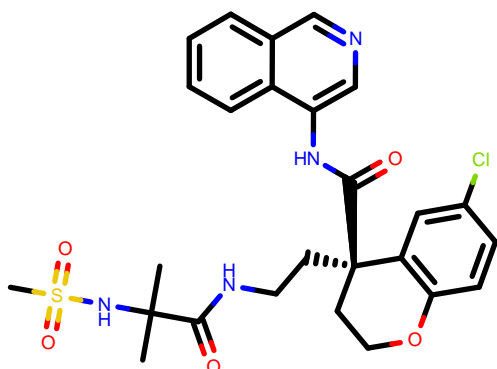
SMILES: Cn1cc(n1)[C@@H](C(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC

RUN: RUN4492

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.37

EN300-85849_3_1_1



CID: EN300-85849_3_1_1

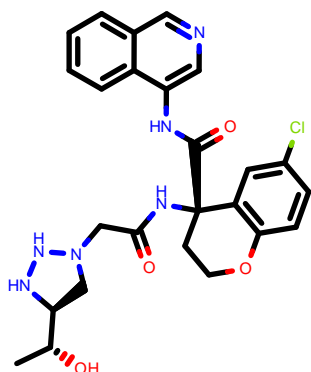
SMILES: CC(C)(C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C

RUN: RUN6557

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.32

EN300-109540_1_2_1



CID: EN300-109540_1_2_1

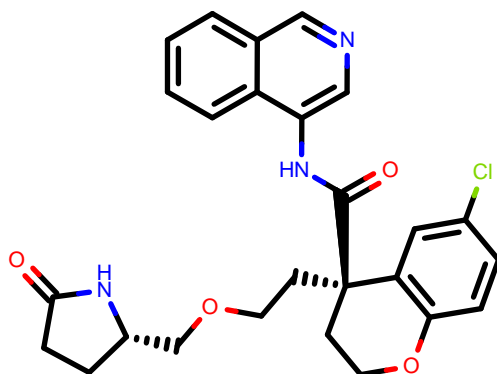
SMILES: C[C@H](c1cn(n1)CC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN5391

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.35

EN300-195756_3_1_1



CID: EN300-195756_3_1_1

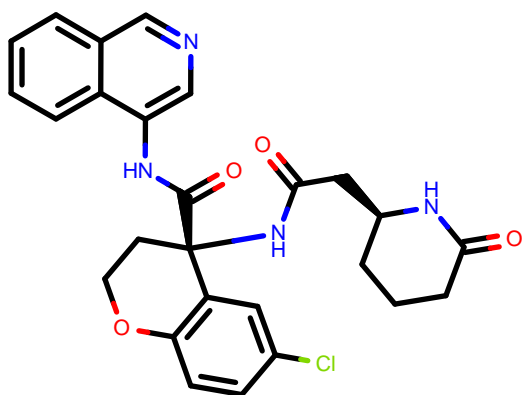
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5H5CCCC(=O)NS

RUN: RUN3332

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.26

EN300-210084_1_1_1



CID: EN300-210084_1_1_1

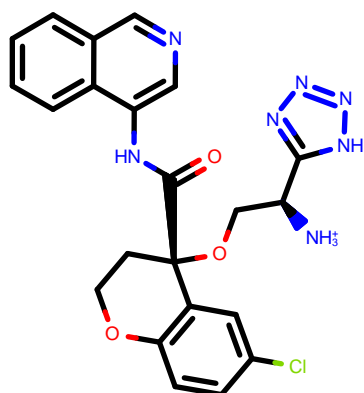
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCC(=O)N5

RUN: RUN3247

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.20

ED_-GRI-5b13fbe2-5_1



CID: ED_-GRI-5b13fbe2-5_1

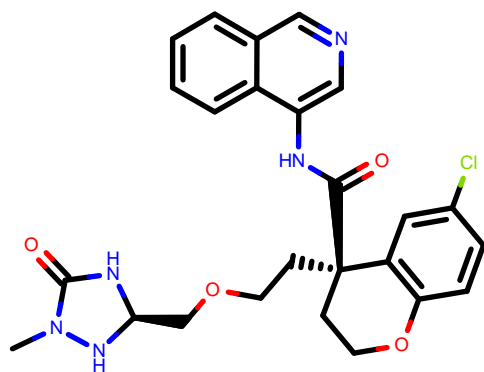
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5C([n-][n-])[nH5]

RUN: RUN1401

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.31

EN300-124918_3_1_2



CID: EN300-124918_3_1_2

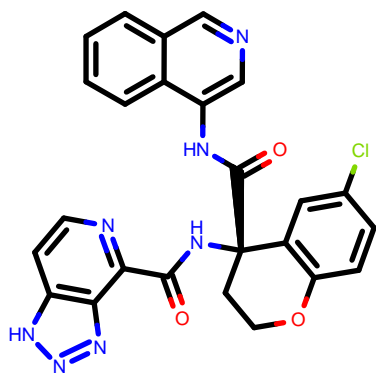
SMILES: CN1C(=O)N[C@@H]([NH2+])C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4443

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.36

EN300-7426383_1_1_1



CID: EN300-7426383_1_1_1

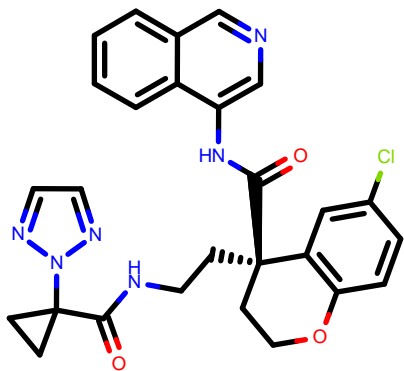
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6c(ccn5)n[nH]6

RUN: RUN4118

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.24

EN300-1722017_3_1_1



CID: EN300-1722017_3_1_1

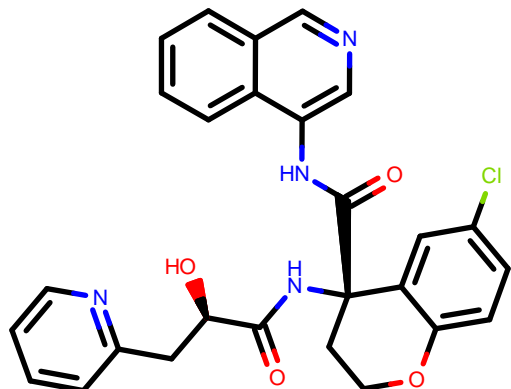
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5n6ncn6

RUN: RUN2965

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.30

EN300-6762327_1_1_1



CID: EN300-6762327_1_1_1

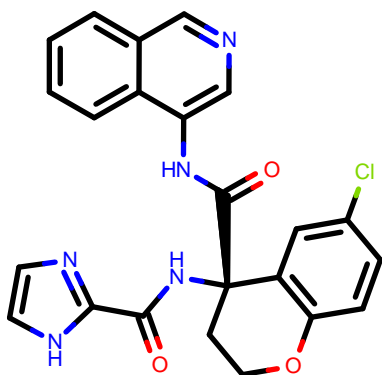
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)[C@@]5[H](C5c6cccn6)O

RUN: RUN4997

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.29

EN300-315836_1_1_1



CID: EN300-315836_1_1_1

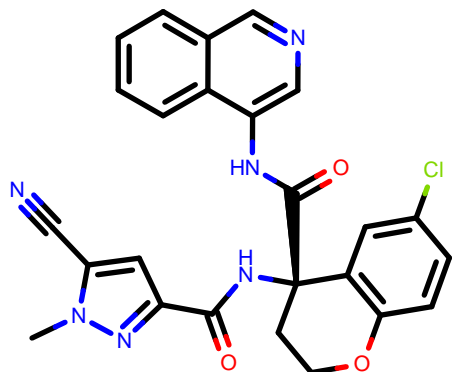
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)c5[nH]cnc5

RUN: RUN2838

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.22

EN300-248982_1_1_1



CID: EN300-248982_1_1_1

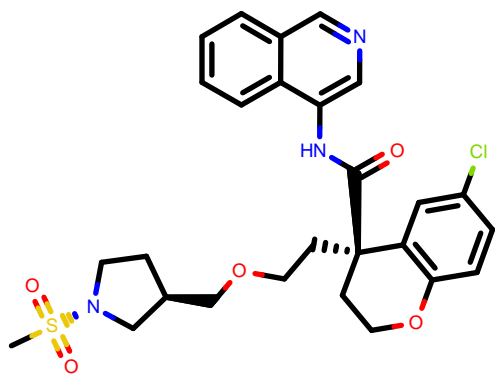
SMILES: Cn1c(ccn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5C#N

RUN: RUN2702

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.22

EN300-261986_3_2_1



CID: EN300-261986_3_2_1

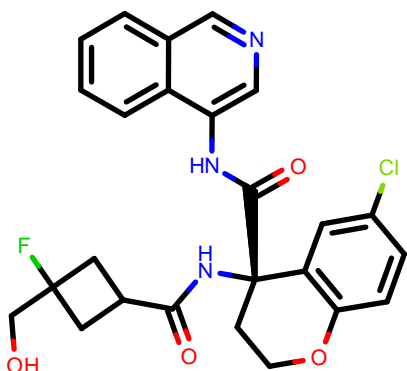
SMILES: CS(=O)(=O)N@@1CC[C@H](C1)C(=O)C[C@2](CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4715

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.44

EN300-6746918_1_1_1



CID: EN300-6746918_1_1_1

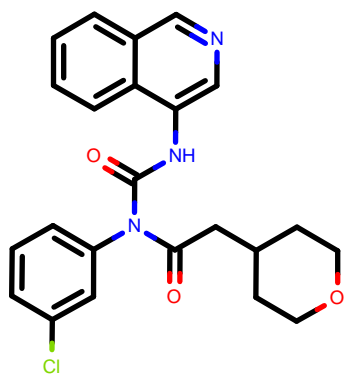
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@3](CCOC4c3cc(cc4)C)NC(=O)C5CC(C5)(CO)F

RUN: RUN4537

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.26

ADA-UCB-dc2b944c-18_1



CID: ADA-UCB-dc2b944c-18_1

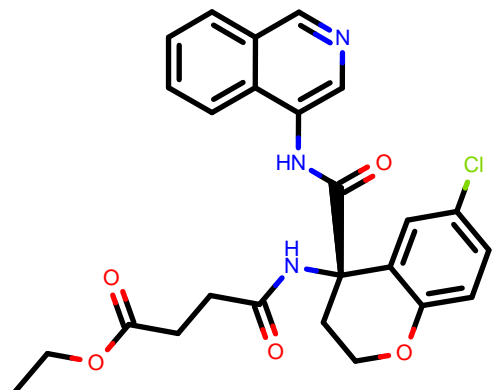
SMILES: c1ccc2c(c1)cnc2NC(=O)N(c3cccc(c3)Cl)C(=O)CC4CCOCC4

RUN: RUN596

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.34

EN300-17161_1_1_1



CID: EN300-17161_1_1_1

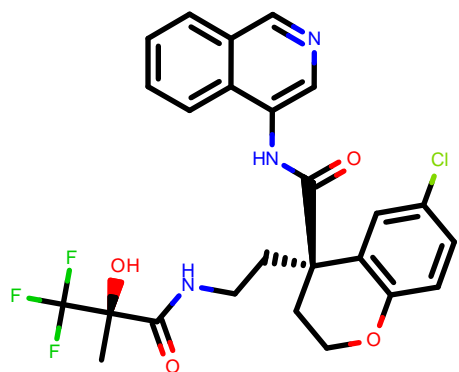
SMILES: CCOC(=O)CCC(=O)N[C@@1](CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3338

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.25

EN300-159633_3_1_1



CID: EN300-159633_3_1_1

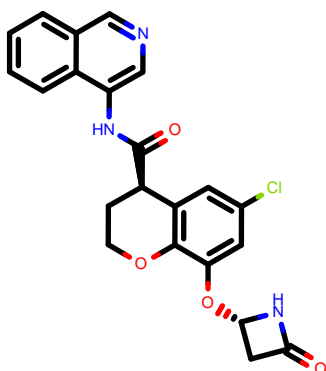
SMILES: C[C@@](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)(C(F)(F)F)O

RUN: RUN4425

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.34

VLA-UCB-50c39ae8-8_2



CID: VLA-UCB-50c39ae8-8_2

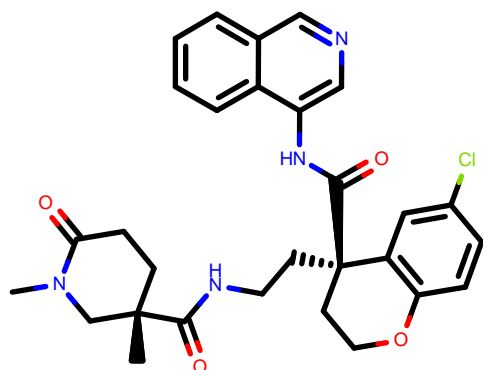
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4O[C@@H]5C(=O)N5)Cl

RUN: RUN320

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.20

EN300-6734171_3_1_1



CID: EN300-6734171_3_1_1

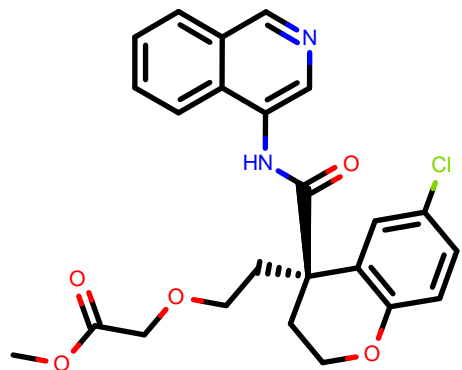
SMILES: C[C@@]1(CCC(=O)N(C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7175

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.37

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

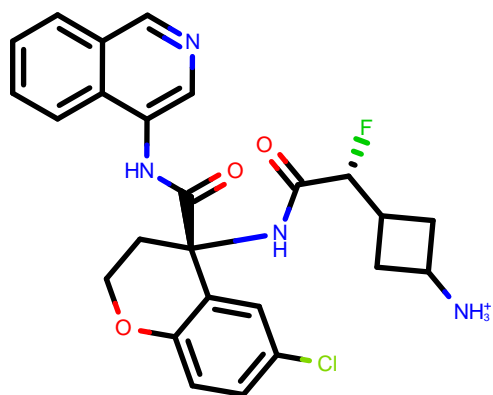
SMILES: COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3638

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.22

EDG-MED-90036822-35_2



CID: EDG-MED-90036822-35_2

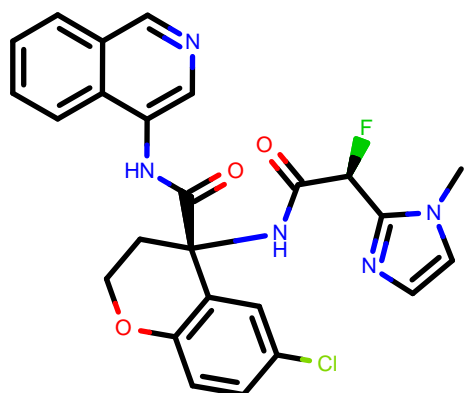
SMILES: c1cc2c(cnc2)NC(=O)[C@]3(c4c(ccc4)OC)C3NC(=O)[C@H](F)[C@H]5C[C@H](C5)N[+]3c1

RUN: RUN1559

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.33

EDG-MED-90036822-19_1



CID: EDG-MED-90036822-19_1

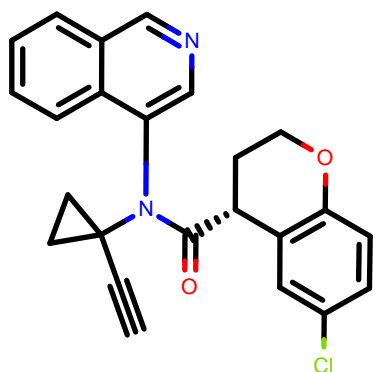
SMILES: Cn1cnc1[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)F

RUN: RUN1531

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.28

DAR-DIA-5ff57136-15_1_1



CID: DAR-DIA-5ff57136-15_1_1

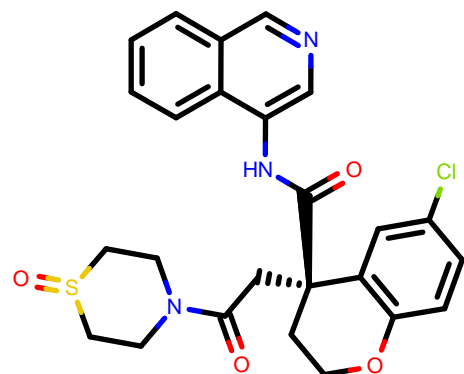
SMILES: C#CC1(CC1)N(c2ncc3c2ccc3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN4458

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.16

EN300-69588_1_1_1



CID: EN300-69588_1_1_1

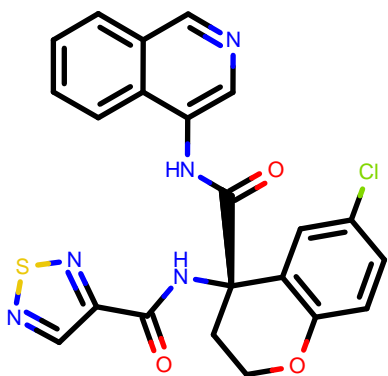
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(c4c(ccc4)OC)C3C(=O)N5CCS(=O)CC5

RUN: RUN5297

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.34

EN300-42270_1_1_1



CID: EN300-42270_1_1_1

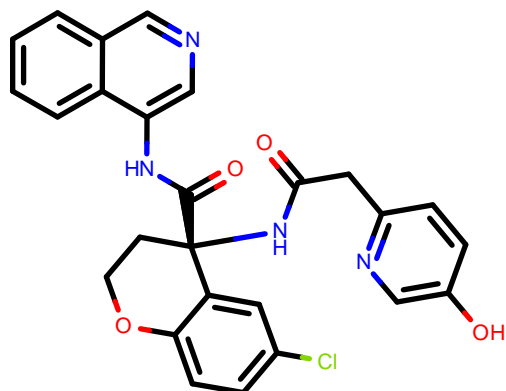
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnsn5

RUN: RUN2830

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.17

EN300-188341_1_1_1



CID: EN300-188341_1_1_1

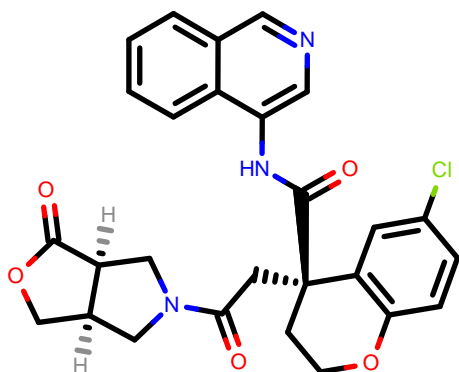
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(O)cc5

RUN: RUN3637

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.21

EN300-316193_1_1_1



CID: EN300-316193_1_1_1

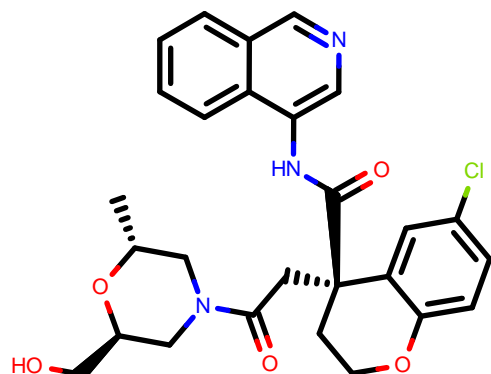
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@@H]6COC(=O)C[C@H]65

RUN: RUN4365

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.34

EN300-157776_1_3_1



CID: EN300-157776_1_3_1

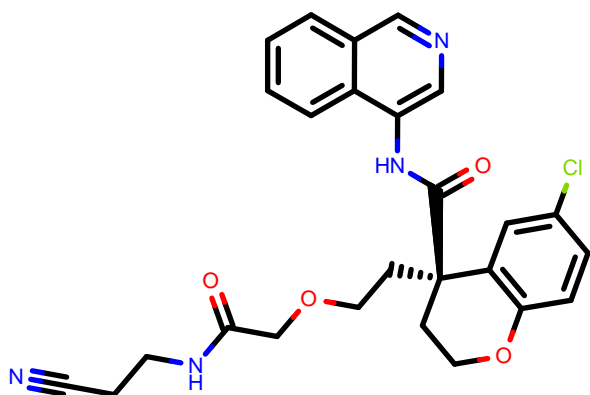
SMILES: C[C@@H]1CN(C[C@@H](O1)CO)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN3555

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.38

EN300-10895_3_1_1



CID: EN300-10895_3_1_1

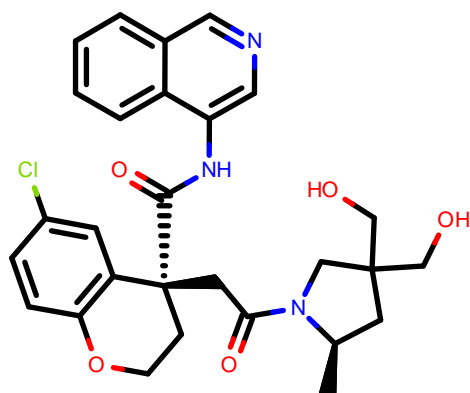
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)COC(=O)NCCC#N

RUN: RUN3623

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.26

EN300-6495717_1_1_1



CID: EN300-6495717_1_1_1

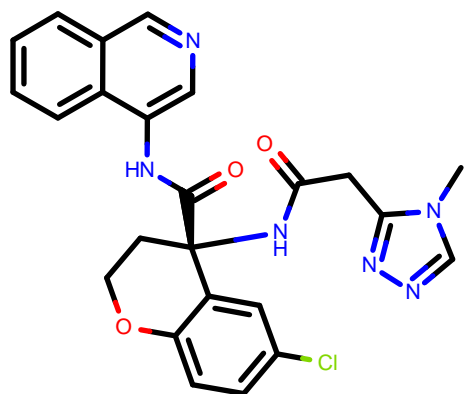
SMILES: C[C@@]1(C)C(CN1C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)C(O)CO

RUN: RUN4001

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.32

EN300-6494474_1_1_1



CID: EN300-6494474_1_1_1

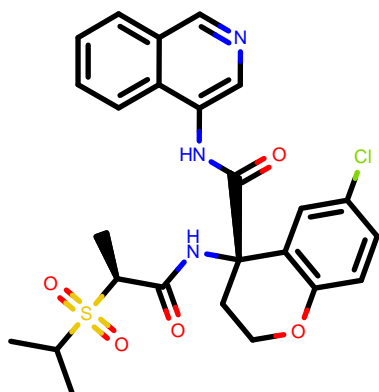
SMILES: Cn1cnc1CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3198

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.25

EN300-40947_1_1_1



CID: EN300-40947_1_1_1

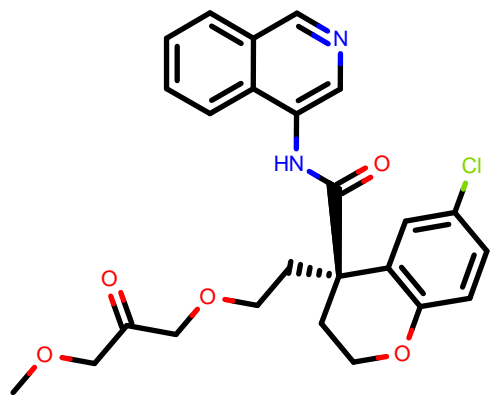
SMILES: C[C@@]1(C)C(CN1C(=O)N[C@@]2(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)S(=O)(=O)C(C)C

RUN: RUN3491

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.35

EN300-125140_3_1_1



CID: EN300-125140_3_1_1

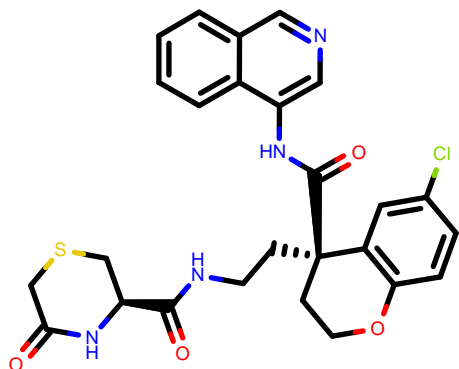
SMILES: COCC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3333

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.28

EN300-657320_3_1_1



CID: EN300-657320_3_1_1

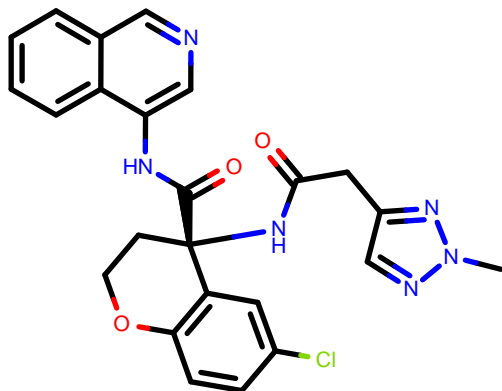
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5CS(=O)N5

RUN: RUN3040

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.25

EN300-755161_1_1_1



CID: EN300-755161_1_1_1

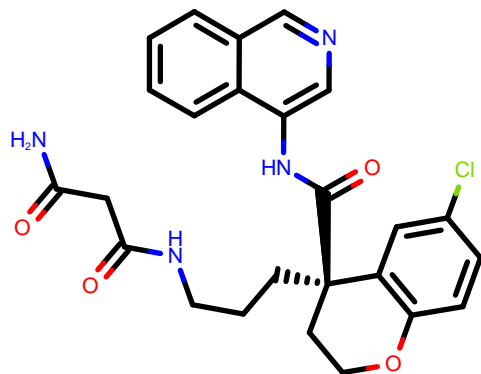
SMILES: Cn1ncc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3665

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.24

EN300-82179_4_1_1



CID: EN300-82179_4_1_1

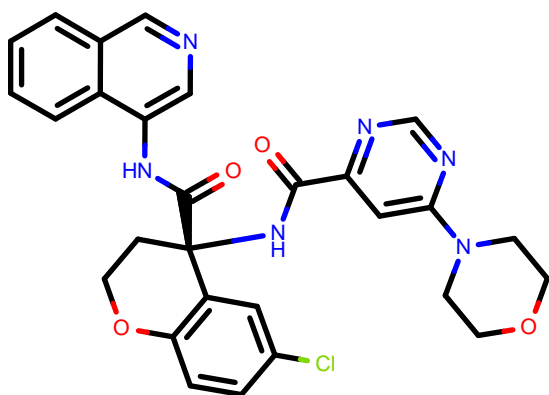
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)N

RUN: RUN4980

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.29

EN300-313410_1_1_1



CID: EN300-313410_1_1_1

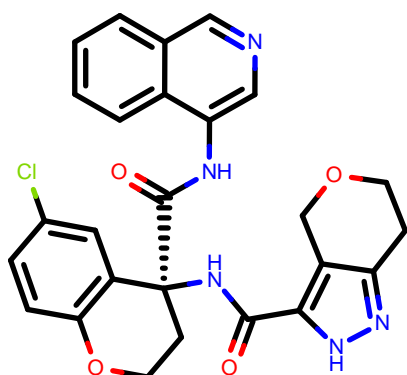
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(n[nH]5)N6CCOCC6

RUN: RUN4689

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.26

EN300-103031_1_1_1



CID: EN300-103031_1_1_1

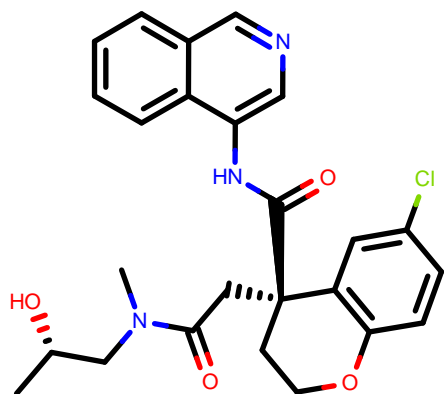
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c[nH]n5)CCOCC6

RUN: RUN3662

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.23

EN300-210254_1_1_1



CID: EN300-210254_1_1_1

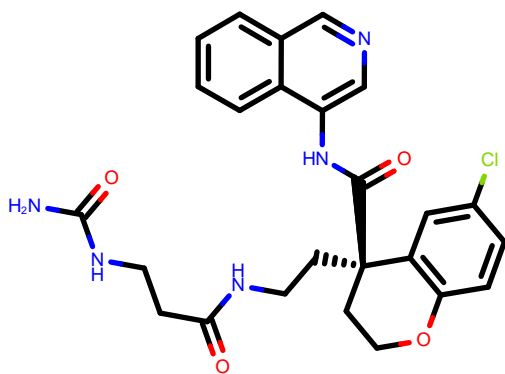
SMILES: C[C@@H](CN(C)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)O

RUN: RUN4479

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.37

EN300-10729_3_1_1



CID: EN300-10729_3_1_1

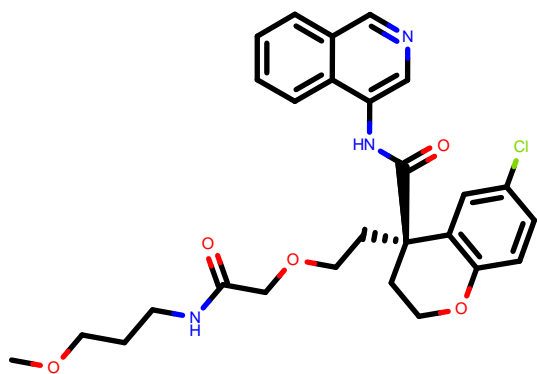
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCNC(=O)N

RUN: RUN6928

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.30

EN300-04492_3_1_1



CID: EN300-04492_3_1_1

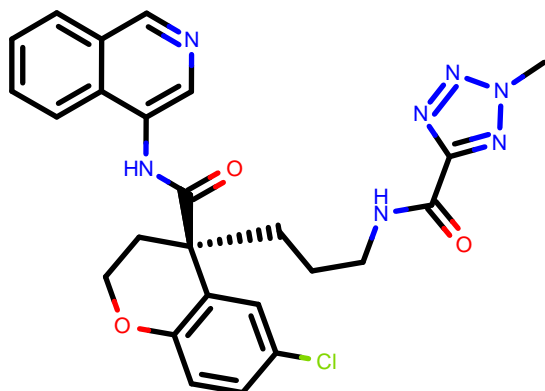
SMILES: COCCNC(=O)COCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7758

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.28

EN300-216978_4_1_1



CID: EN300-216978_4_1_1

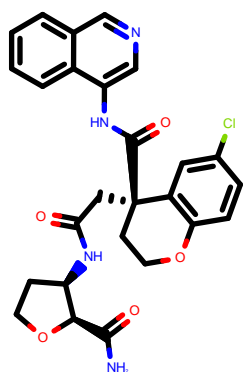
SMILES: Cn1nc(nn1)C(=O)NCCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3290

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.29

EN300-7435545_1_1_1



CID: EN300-7435545_1_1_1

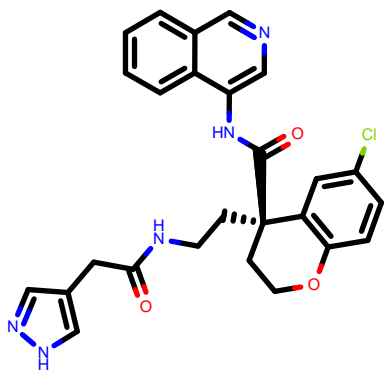
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cnc6c5cnc6O

RUN: RUN3695

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.32

EN300-1589101_3_1_1



CID: EN300-1589101_3_1_1

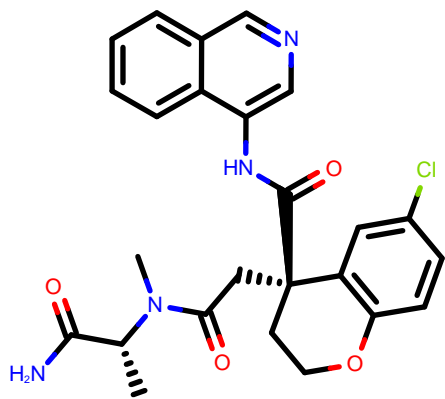
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5c[nH]je5

RUN: RUN3992

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.26

EN300-125409_1_2_1



CID: EN300-125409_1_2_1

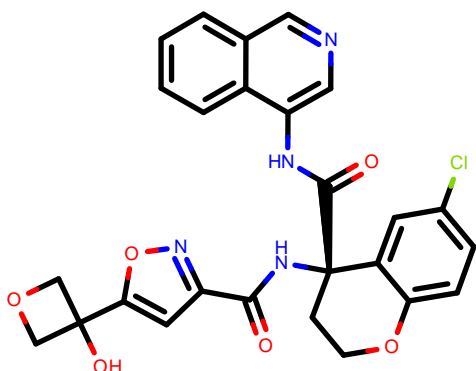
SMILES: C[C@H](C(=O)N)N(C)C(=O)C[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccoc4

RUN: RUN3794

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.33

EN300-365017_1_1_1



CID: EN300-365017_1_1_1

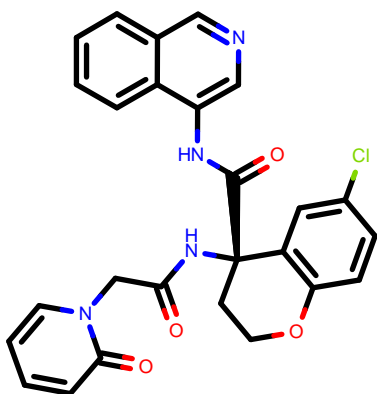
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(oc5)C6(COC6)O

RUN: RUN3738

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.28

EN300-11714_1_1_1



CID: EN300-11714_1_1_1

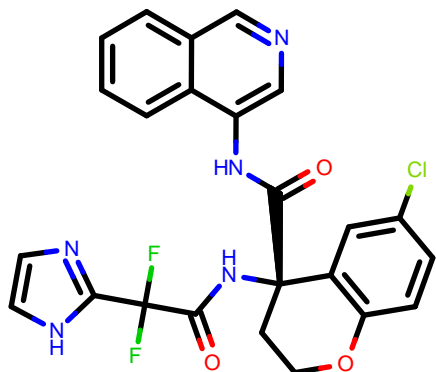
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ccccc5=O

RUN: RUN3041

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.29

EDG-MED-90036822-45_1



CID: EDG-MED-90036822-45_1

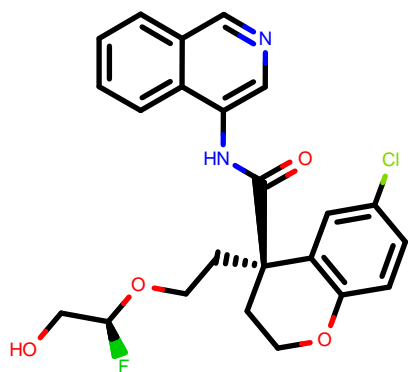
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]cn5(F)F

RUN: RUN1579

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.22

EN300-861925_3_2_1



CID: EN300-861925_3_2_1

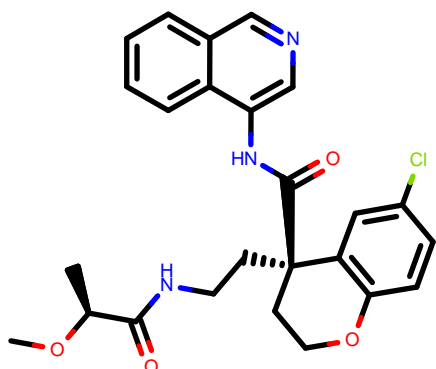
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@H](CO)F

RUN: RUN3270

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.28

EN300-51257_3_1_1



CID: EN300-51257_3_1_1

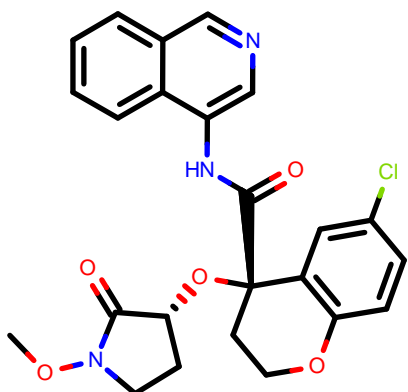
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)OC

RUN: RUN4424

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.24

EN300-302058_1_2_1



CID: EN300-302058_1_2_1

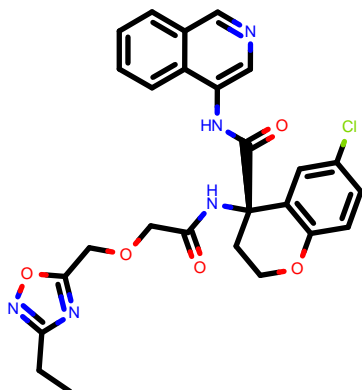
SMILES: CON1CC[C@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN7115

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.24

EN300-702615_1_1_1



CID: EN300-702615_1_1_1

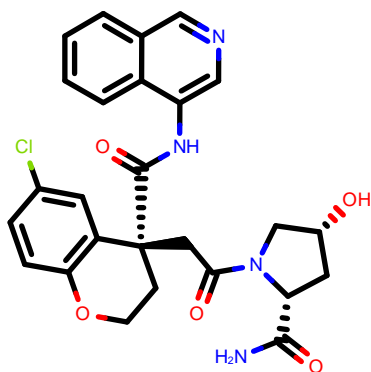
SMILES: CCc1nc(n1)COC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN3433

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-33_1



CID: EDJ-MED-d203f206-33_1

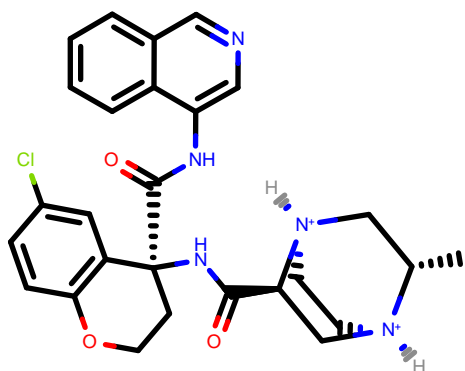
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H](C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN2432

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.28

EN300-120414_1_4_1



CID: EN300-120414_1_4_1

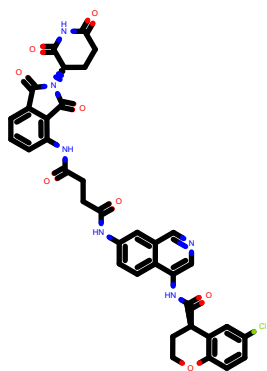
SMILES: C[C@@H](C)N[C@@H](C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN5420

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.37

DAR-DIA-9e4459de-15_8



CID: DAR-DIA-9e4459de-15_8

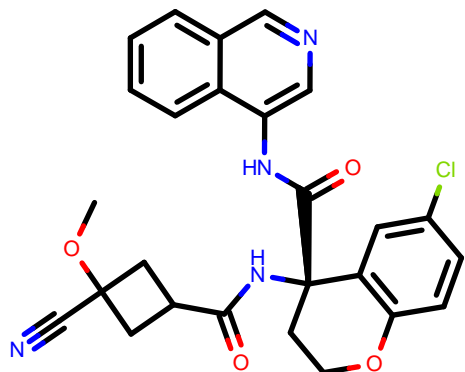
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H](C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN1380

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.25

EN300-1073533_1_1_1



CID: EN300-1073533_1_1_1

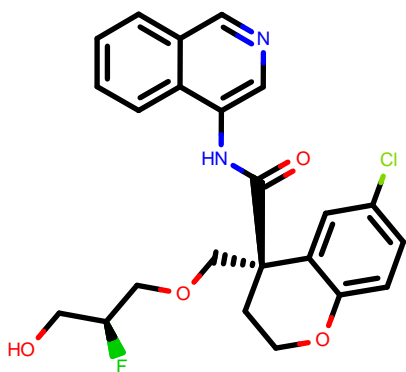
SMILES: COc1c(C)cc(O)nc1C(=O)N[C@@H](C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN3747

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.23

EN300-1600517_2_2_1



CID: EN300-1600517_2_2_1

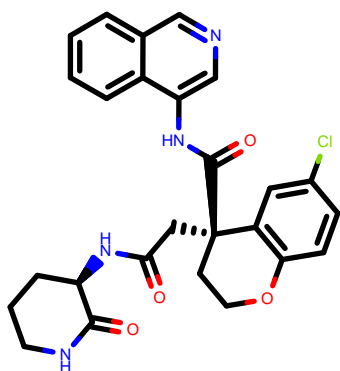
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F

RUN: RUN3797

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.29

EDJ-MED-d203f206-23_1



CID: EDJ-MED-d203f206-23_1

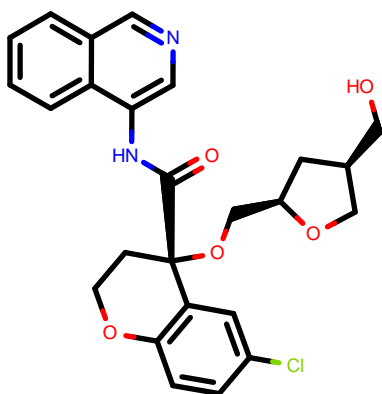
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5CCNC5=O

RUN: RUN2418

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.25

EN300-6494158_1_4_1



CID: EN300-6494158_1_4_1

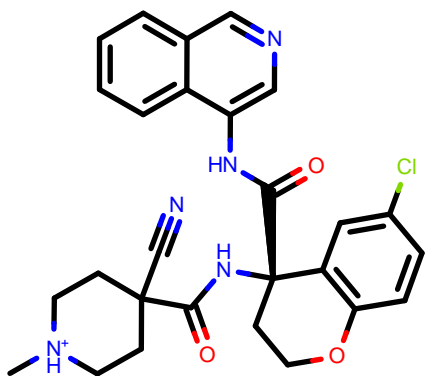
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@H](CO)CO

RUN: RUN3175

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.32

EN300-7473378_1_1_1



CID: EN300-7473378_1_1_1

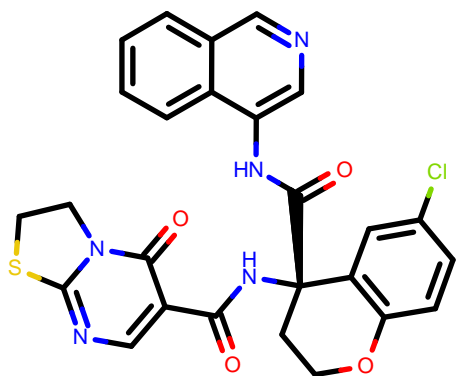
SMILES: C[NH+]1CCC(CC1)(C#N)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN3024

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.32

EN300-14405_1_1_1



CID: EN300-14405_1_1_1

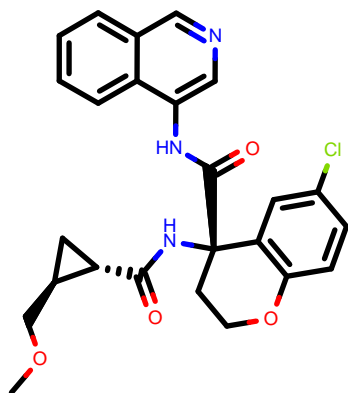
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6n(c5=O)CCS6

RUN: RUN4229

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.31

EN300-7352438_1_1_1



CID: EN300-7352438_1_1_1

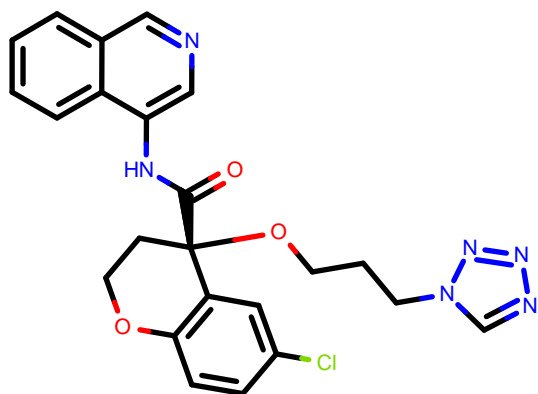
SMILES: COC[C@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN3272

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.28

EN300-1696962_1_1_1



CID: EN300-1696962_1_1_1

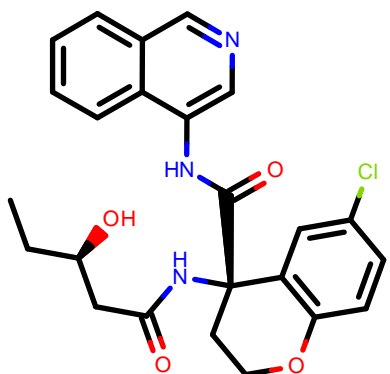
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cnn5

RUN: RUN4198

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.28

EN300-224741_1_2_1



CID: EN300-224741_1_2_1

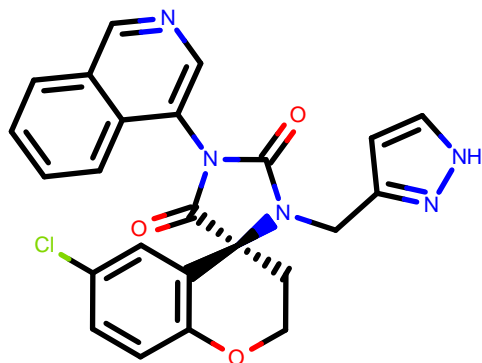
SMILES: CC[C@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)O

RUN: RUN5030

DDG (kcal/mol): -2.01

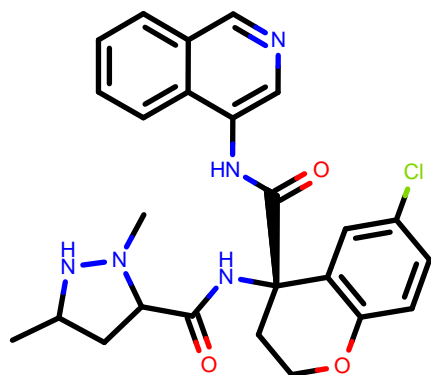
dDDG (kcal/mol): 0.22

VLA-UNK-f702bf1c-2_1



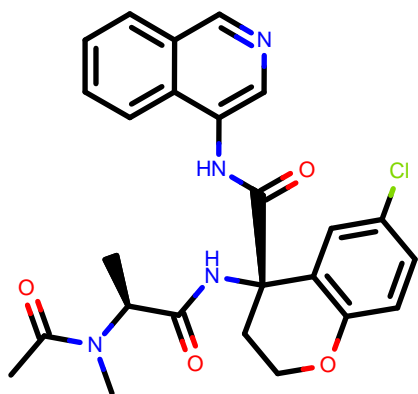
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCCOc5c4cc(cc5)C)N(C3=O)C6ccn[nH]6</chem>
RUN:	RUN2113
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.29

EN300-51244_1_1_1



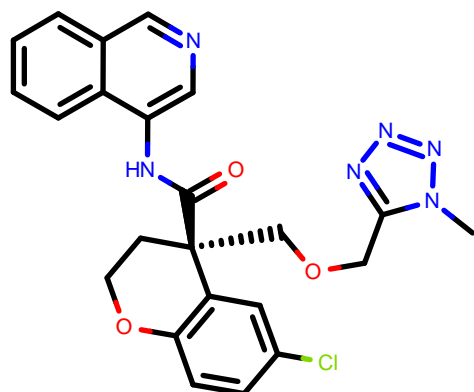
CID:	EN300-51244_1_1_1
SMILES:	<chem>Cc1cc(n(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN3824
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.18

EN300-863933_1_1_1



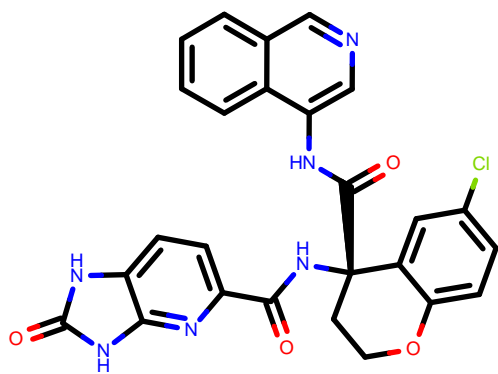
CID:	EN300-863933_1_1_1
SMILES:	<chem>C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)N(C)C(=O)C</chem>
RUN:	RUN4121
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.28

EN300-62574_2_1_1



CID:	EN300-62574_2_1_1
SMILES:	<chem>Cn1c(nnn1)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN3119
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.25

EN300-203402_1_1_1



CID: EN300-203402_1_1_1

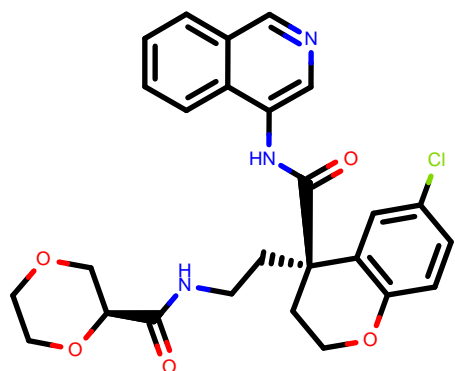
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)[nH]c(=O)[nH]6

RUN: RUN3503

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.26

EN300-36158_3_1_1



CID: EN300-36158_3_1_1

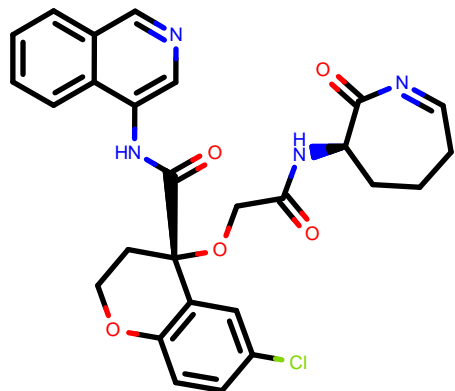
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5COCOC5

RUN: RUN5247

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.23

EN300-37195_1_1_1



CID: EN300-37195_1_1_1

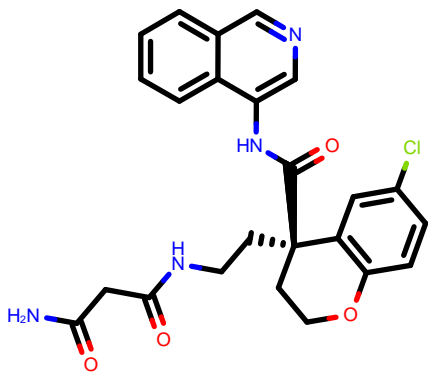
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@]5CCCCNC5=O

RUN: RUN7710

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.29

EN300-82179_3_1_1



CID: EN300-82179_3_1_1

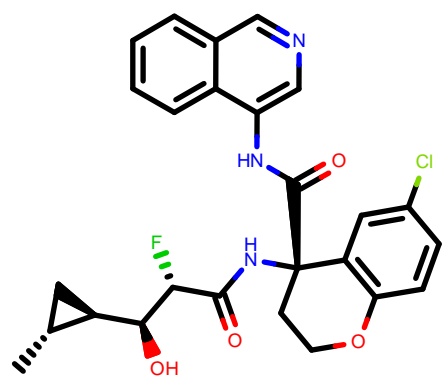
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)N

RUN: RUN5431

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.22

EDG-MED-90036822-94_3



CID: EDG-MED-90036822-94_3

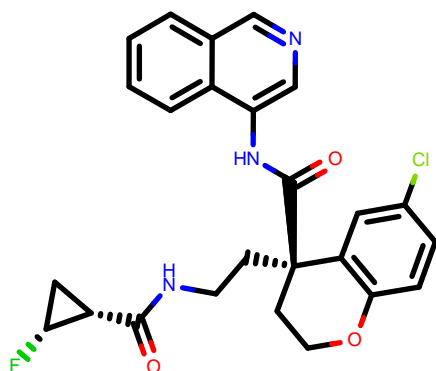
SMILES: C1C=CC=C2C(=O)N(C1)C(=O)N(C2)C(=O)N(C3)C(=O)N4C=CC=C(C3)C(=O)N4

RUN: RUN1719

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.24

EN300-97300_3_4_1



CID: EN300-97300_3_4_1

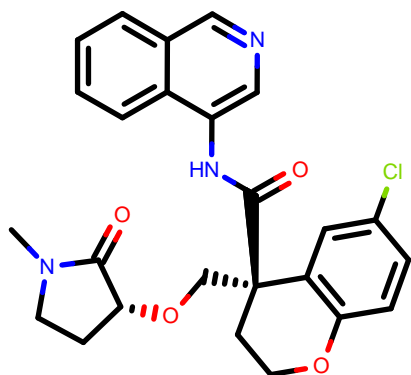
SMILES: C1C=CC=C2C(=O)N(C1)C(=O)N(C2)C(=O)N(C3)C(=O)N4C=CC=C(C3)C(=O)N4

RUN: RUN3221

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.21

EN300-98648_2_2_1



CID: EN300-98648_2_2_1

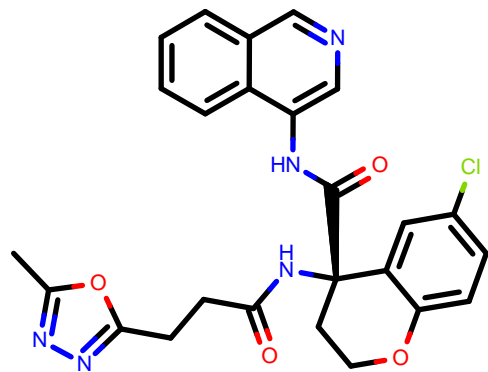
SMILES: CN1CC[C@H](C1=O)OC[C@]2(CCOc3c2cc(cc3)C)C(=O)N4Ncnc5c4ccccc5

RUN: RUN4012

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.25

EN300-304662_1_1_1



CID: EN300-304662_1_1_1

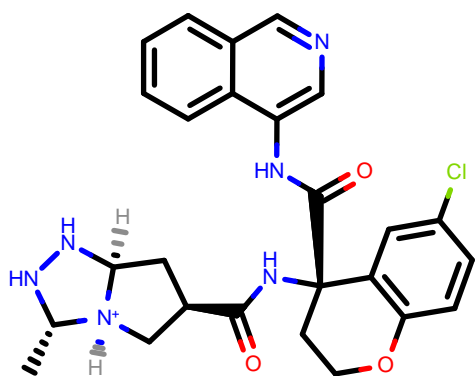
SMILES: Cc1nnc(o1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)N4Ncnc5c4ccccc5

RUN: RUN4811

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.28

EN300-6729747_1_1_1



CID: EN300-6729747_1_1_1

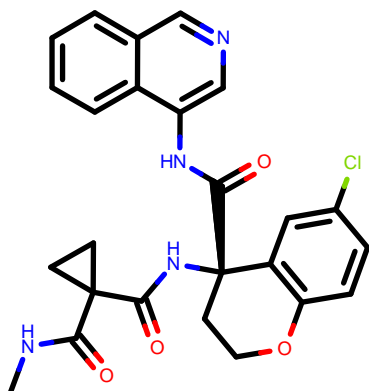
SMILES: C[C@@H]1N[C@@H]2[N@@H]1C[C@@H](C2)C(=O)N[C@@]3(CCOc4cc3cc(c4)Cl)C(=O)Nc5nc6c5ccc6

RUN: RUN3155

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.47

EN300-66770_1_1_1



CID: EN300-66770_1_1_1

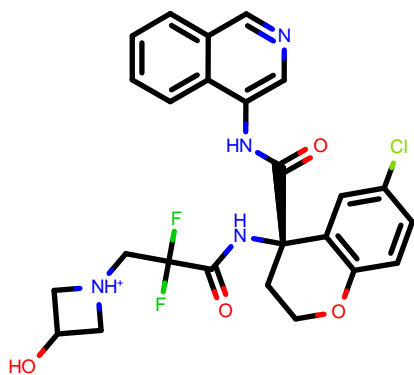
SMILES: CNC(=O)C1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN4261

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.24

EDG-MED-90036822-40_1



CID: EDG-MED-90036822-40_1

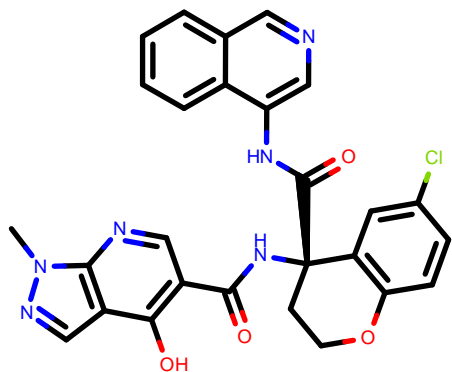
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5N5CC(C5)O(F)F

RUN: RUN1639

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.28

EN300-124384_1_1_1



CID: EN300-124384_1_1_1

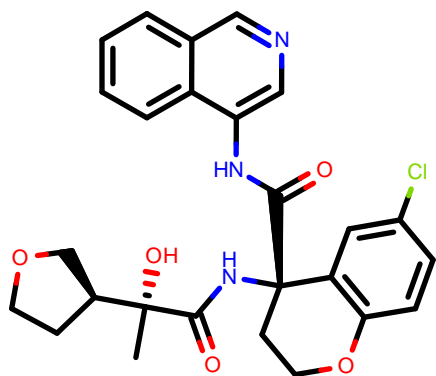
SMILES: Cn1c2c(n1)c(=O)c(c[nH]2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccc6

RUN: RUN3476

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.31

EN300-217494_1_3_1



CID: EN300-217494_1_3_1

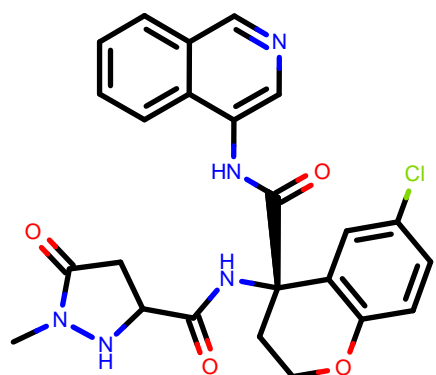
SMILES: C[C@@H](C@H)CCOC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5O

RUN: RUN6883

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-150749_1_1_1



CID: EN300-150749_1_1_1

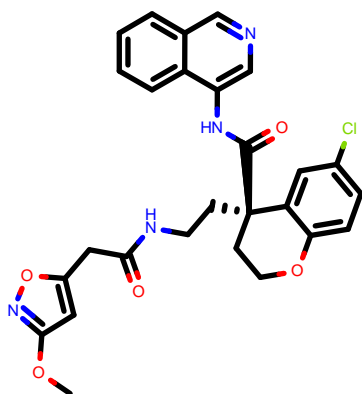
SMILES: Cn1c(=O)cc[nH]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4747

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.24

EN300-127197_3_1_1



CID: EN300-127197_3_1_1

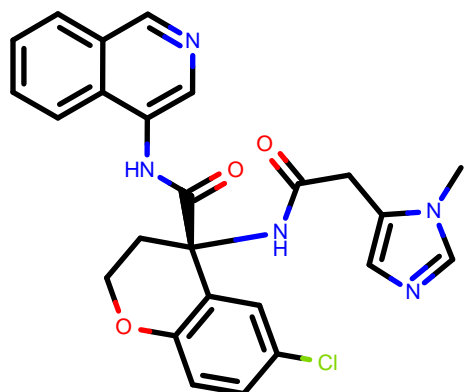
SMILES: COc1cc(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3220

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-152418_1_1_1



CID: EN300-152418_1_1_1

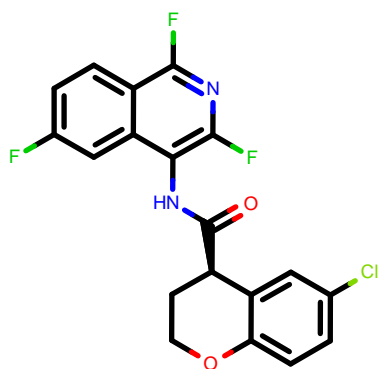
SMILES: Cn1ncc1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3558

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.25

JOH-SUS-a69c159d-7_1



CID: JOH-SUS-a69c159d-7_1

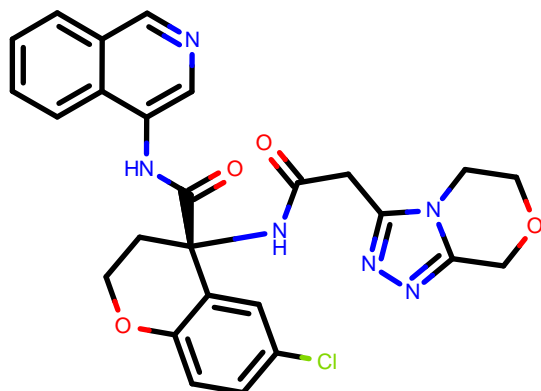
SMILES: c1cc2c(cc1F)c(nc2F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1045

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.06

EN300-1718836_1_1_1



CID: EN300-1718836_1_1_1

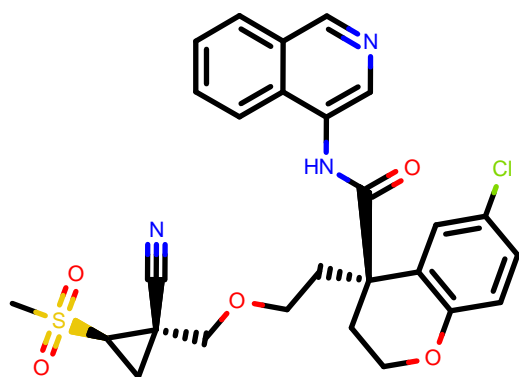
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4c3cc(cc4)Cl)NC(=O)C5nnc6n5CCOC6

RUN: RUN3109

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.28

EN300-633533_3_1_1



CID: EN300-633533_3_1_1

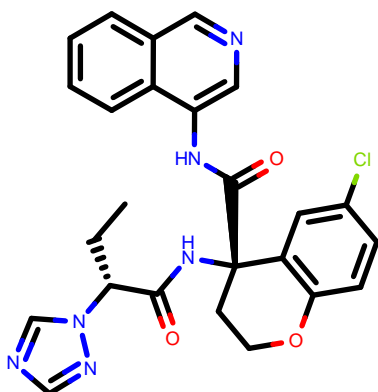
SMILES: CS(=O)(=O)[C@@H]1C[C@@H]2(COCC[C@@H]3(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)C#N

RUN: RUN3849

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-651307_1_2_1



CID: EN300-651307_1_2_1

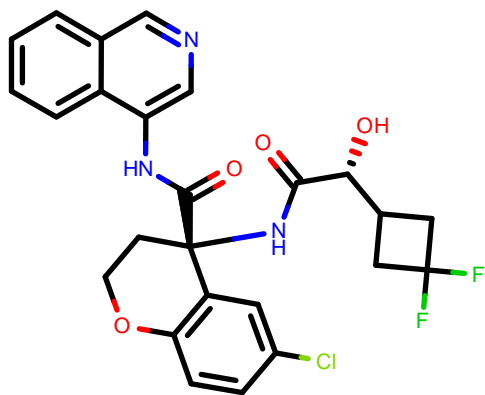
SMILES: CC[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)n5nncn5

RUN: RUN4833

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.26

EDG-MED-90036822-101_1



CID: EDG-MED-90036822-101_1

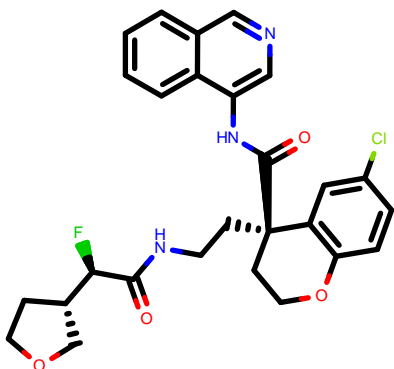
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5CC(C5)(F)F)O

RUN: RUN1709

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.31

EN300-783124_3_3_1



CID: EN300-783124_3_3_1

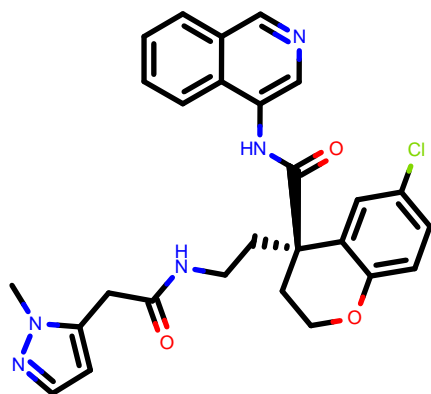
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C5COCOC5)F

RUN: RUN5208

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.27

EN300-114805_3_1_1



CID: EN300-114805_3_1_1

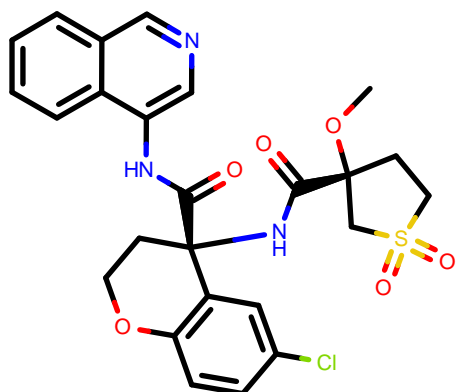
SMILES: Cn1c(ccn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5179

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.32

EN300-385267_1_1_1



CID: EN300-385267_1_1_1

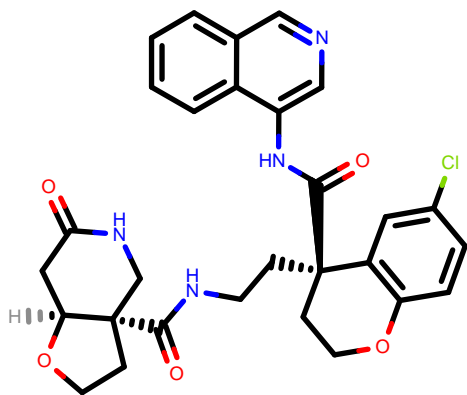
SMILES: CO[C@@]1(CCS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7409

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.39

EN300-6731226_3_1_1



CID: EN300-6731226_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(c4)C)CCNC(=O)[C@@]56CC[C@@H]5C[C@]1=O)N6

RUN:

RUN7251

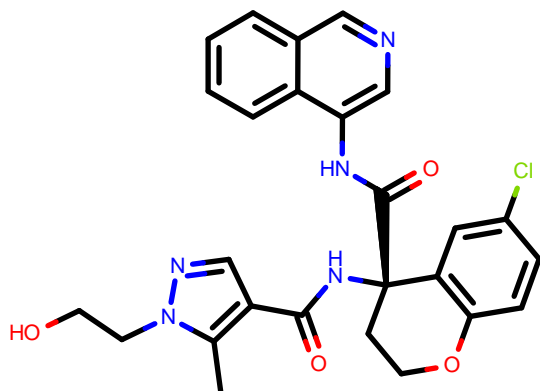
DDG (kcal/mol):

-1.98

dDDG (kcal/mol):

0.41

EN300-40225_1_1_1



CID: EN300-40225_1_1_1

SMILES:

Cc1c(cnn1CCO)C(=O)N[C@@]2(C)CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN:

RUN3578

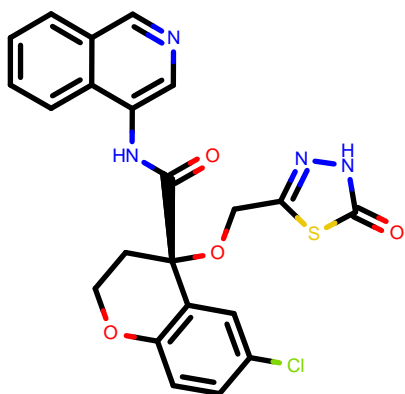
DDG (kcal/mol):

-1.98

dDDG (kcal/mol):

0.26

CHO-MSK-5891c1ff-7_1



CID: CHO-MSK-5891c1ff-7_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)OCc5n[nH]c(=O)s5

RUN:

RUN1722

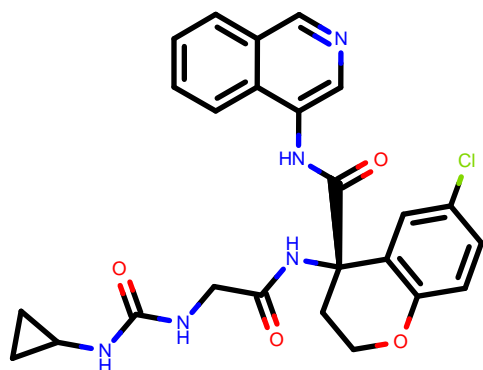
DDG (kcal/mol):

-1.98

dDDG (kcal/mol):

0.20

EN300-42591_1_1_1



CID: EN300-42591_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)CNC(=O)NC5CC5

RUN:

RUN7178

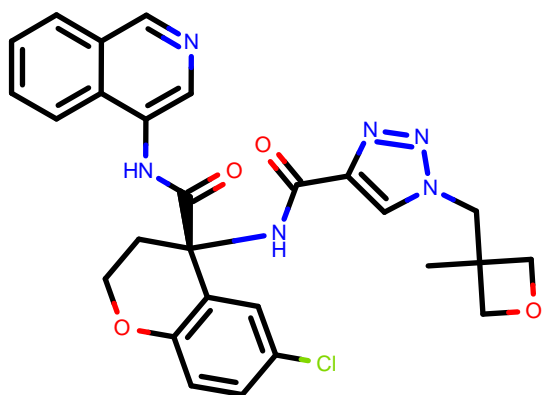
DDG (kcal/mol):

-1.98

dDDG (kcal/mol):

0.26

EN300-135660_1_1_1



CID: EN300-135660_1_1_1

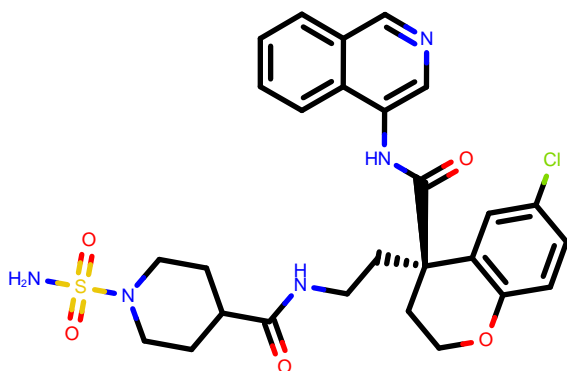
SMILES: CC1(COC1)Cn2cc(m2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccoc6

RUN: RUN4073

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.25

EN300-31102_3_1_1



CID: EN300-31102_3_1_1

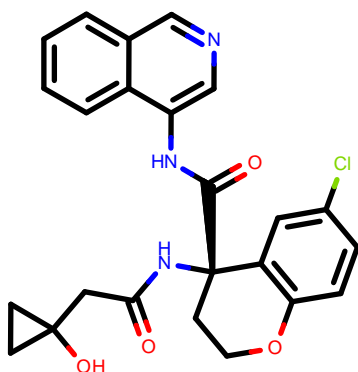
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CCN(C5)S(=O)(=O)N

RUN: RUN7349

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.24

EN300-207873_1_1_1



CID: EN300-207873_1_1_1

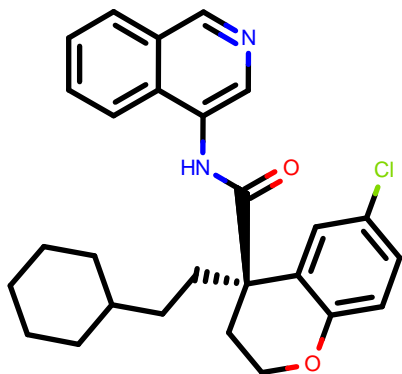
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CC5)O

RUN: RUN4332

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.21

VLA-UCB-50c39ae8-10_1_1



CID: VLA-UCB-50c39ae8-10_1_1

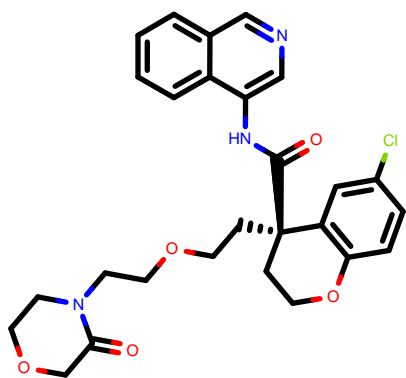
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCC5

RUN: RUN3517

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.26

EN300-219330_3_1_1



CID: EN300-219330_3_1_1

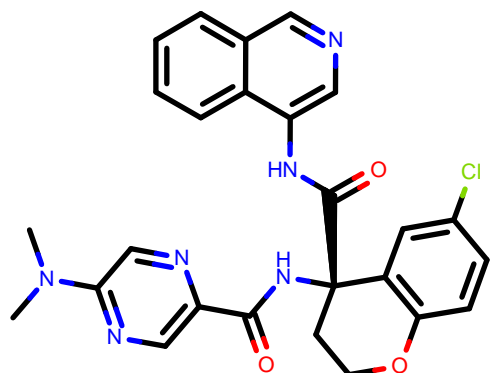
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOCC5=O

RUN: RUN3869

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.30

EN300-123916_1_1_1



CID: EN300-123916_1_1_1

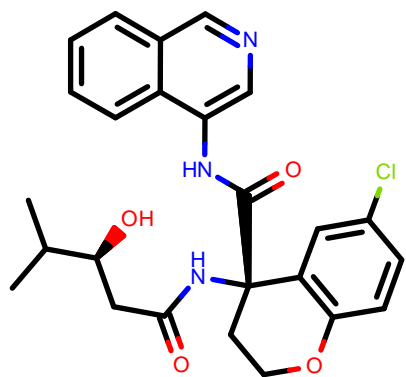
SMILES: CN(C)c1cnc(cn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4739

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.25

EN300-155498_1_1_2



CID: EN300-155498_1_1_2

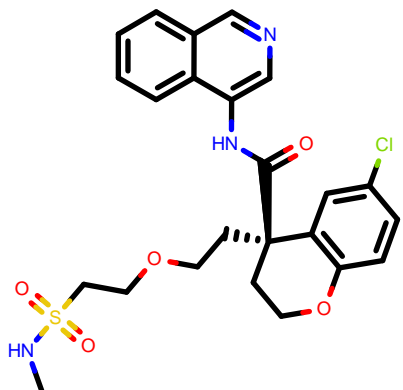
SMILES: CC(C)[C@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN6531

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.30

EN300-6482967_3_1_1



CID: EN300-6482967_3_1_1

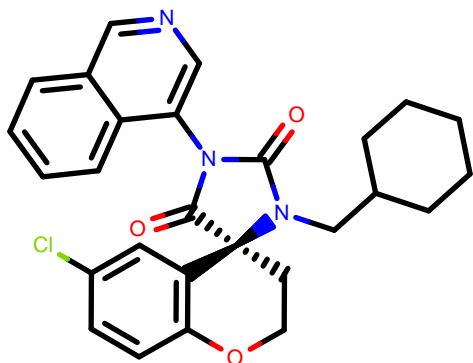
SMILES: CNS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN3883

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.33

VLA-UNK-f702bf1c-6_1



CID: VLA-UNK-f702bf1c-6_1

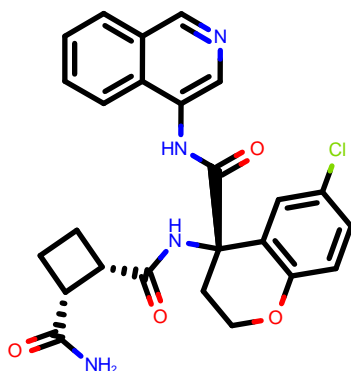
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c5)C)N(C3=O)CC6CCCC6

RUN: RUN2134

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.31

EN300-217107_1_4_1



CID: EN300-217107_1_4_1

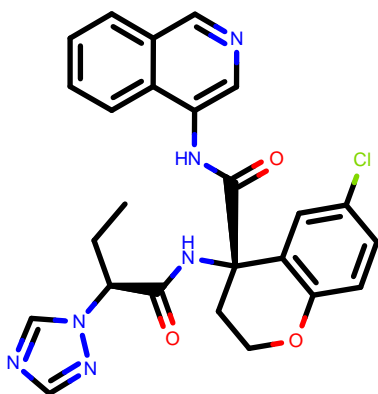
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC[C@H]5C(=O)N

RUN: RUN3032

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.23

EN300-651307_1_1_1



CID: EN300-651307_1_1_1

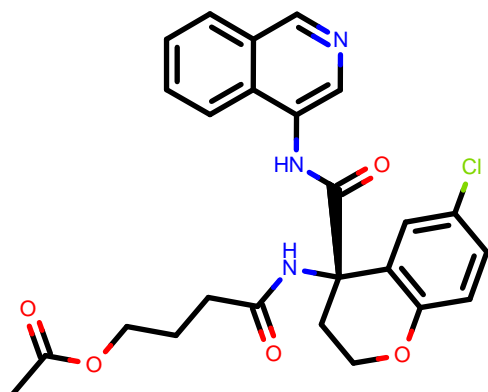
SMILES: CC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)n5cncn5

RUN: RUN2858

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.27

EN300-1696058_1_1_1



CID: EN300-1696058_1_1_1

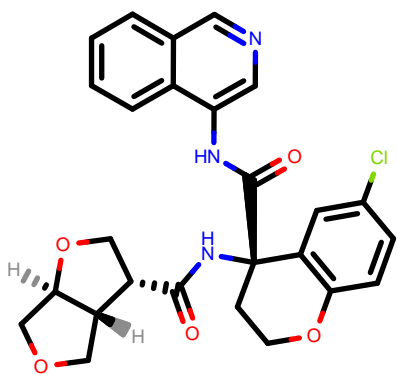
SMILES: CC(=O)OCCCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN6436

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.29

EN300-6482296_1_8_1



CID: EN300-6482296_1_8_1

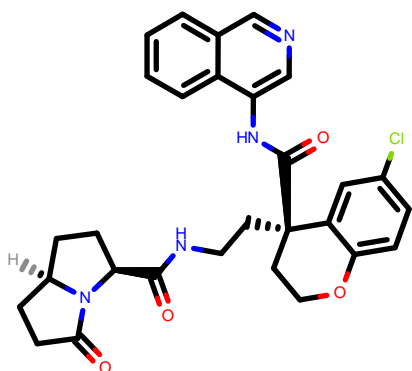
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)C(=O)C[C@@H]5C[C@@H]6C=C[C@H]5COC6

RUN: RUN3139

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.22

EN300-6479181_3_3_1



CID: EN300-6479181_3_3_1

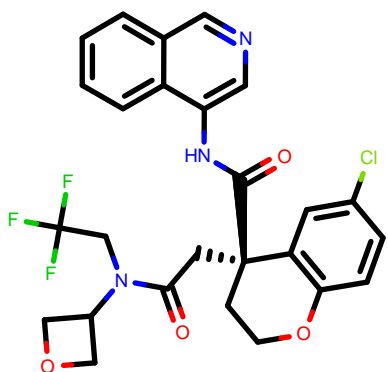
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)C(=O)C[C@@H]5C[C@@H]6C=C[C@H]5COC6

RUN: RUN4248

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.34

EDG-MED-ba1ac7b9-24_1



CID: EDG-MED-ba1ac7b9-24_1

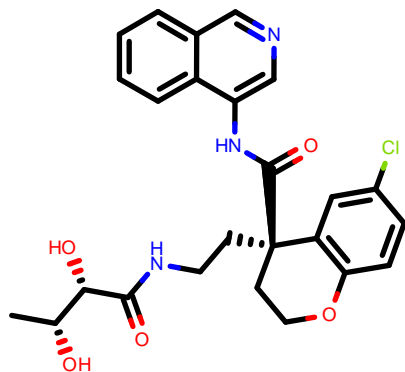
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)C(=O)N(CC(F)F)C5COC5

RUN: RUN2583

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.29

EN300-6974806_3_1_1



CID: EN300-6974806_3_1_1

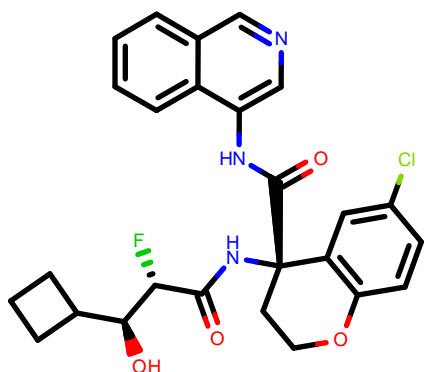
SMILES: C[C@@H](C)[C@@H](C(=O)NCC[C@@H]1(COC2c1cc(=O)C)C(=O)Nc3ncnc4c3ccccc4O)O

RUN: RUN4292

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.35

EDG-MED-90036822-99_4



CID: EDG-MED-90036822-99_4

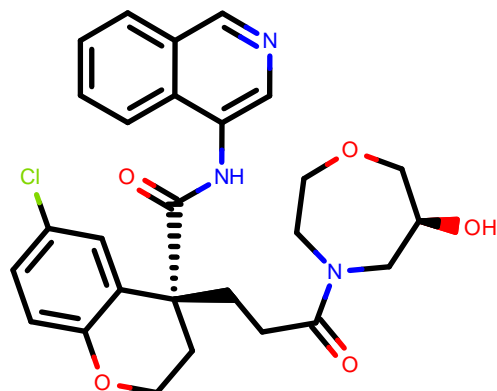
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc4)C)NC(=O)[C@H]([C@H](C5CC5)O)F

RUN: RUN1746

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.30

EN300-233951_2_2_1



CID: EN300-233951_2_2_1

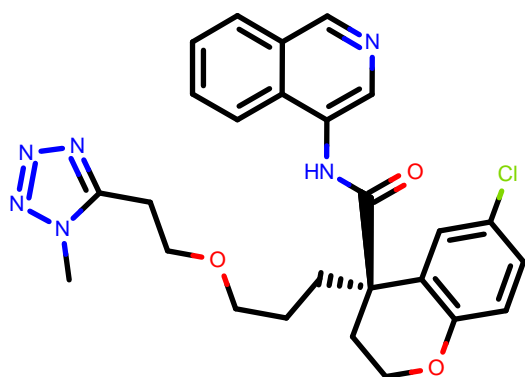
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc4)C)CCC(=O)N5CCOC[C@H](C5)O

RUN: RUN7730

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.29

EN300-365398_4_1_1



CID: EN300-365398_4_1_1

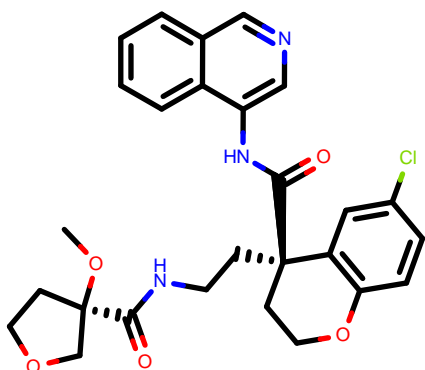
SMILES: Cn1c(nnn1)CCOCC[C@@]2(CCOc3cc2cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3352

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.37

EN300-174668_3_1_1



CID: EN300-174668_3_1_1

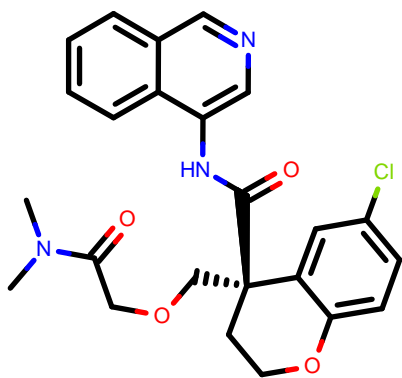
SMILES: COC[C@@]1(COC1)C(=O)NCC[C@@]2(CCOc3cc2cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4060

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.32

EN300-216063_2_1_1



CID: EN300-216063_2_1_1

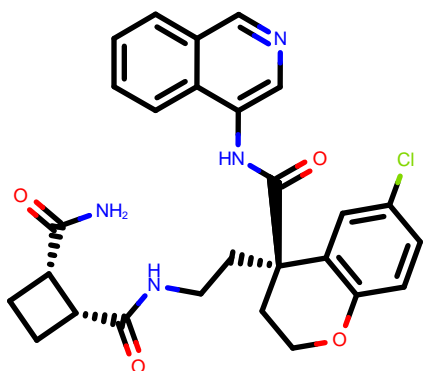
SMILES: CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5100

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.21

EN300-217107_3_1_1



CID: EN300-217107_3_1_1

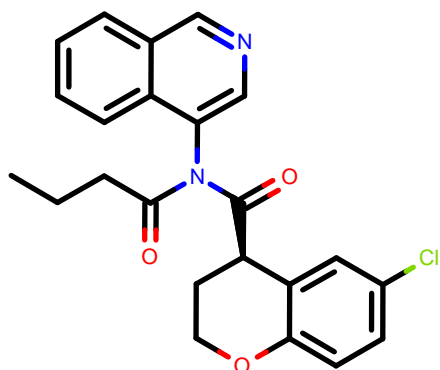
SMILES: c1ccc2c(c1)nccc2N[C@@]1(C)C(=O)Nc3nccc4c3cccc4N[C@@]1(C)C(=O)Nc5nccc6c5cccc6

RUN: RUN4239

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.33

DAR-DIA-5ff57136-11_1



CID: DAR-DIA-5ff57136-11_1

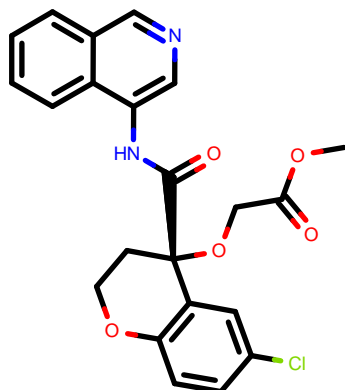
SMILES: C=CC(=O)N(c1nccc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN1277

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.21

EN300-19700_1_1_1



CID: EN300-19700_1_1_1

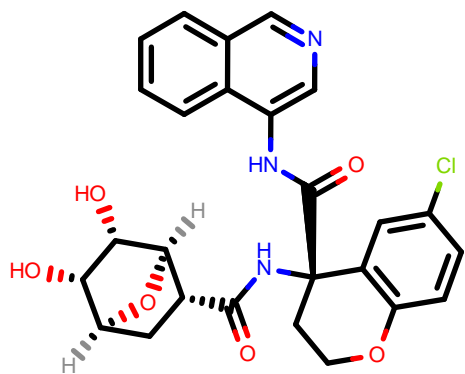
SMILES: COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN3360

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.18

EN300-6764836_1_1_1



CID: EN300-6764836_1_1_1

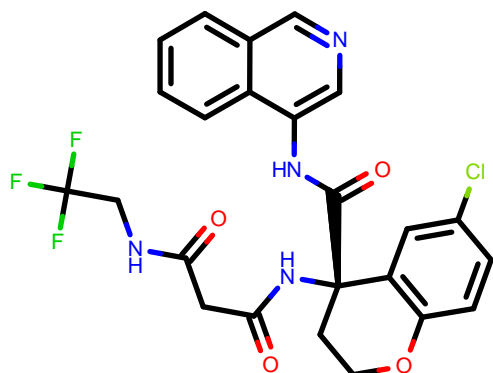
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc(cc4)NC(=O)[C@@H]5C[C@@H]6[C@@H]7[C@@H]5O6

RUN: RUN4599

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.25

EN300-128715_1_1_1



CID: EN300-128715_1_1_1

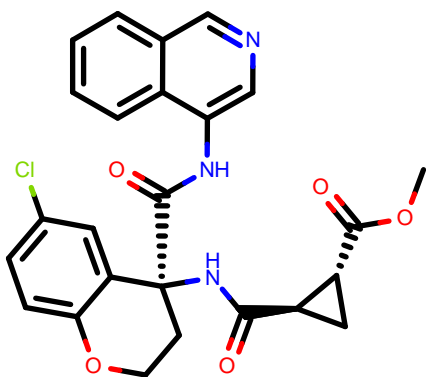
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc(cc4)NC(=O)CC(=O)NC(F)F

RUN: RUN3736

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.24

EN300-765003_1_1_1



CID: EN300-765003_1_1_1

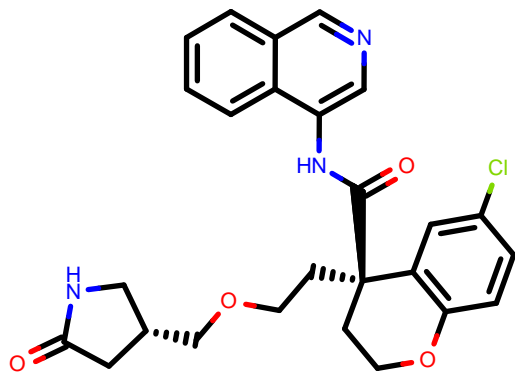
SMILES: COC(=O)[C@@]3(C)COCc4cc(cc4)NC(=O)[C@@H]5C[C@@H]6[C@@H]5O6

RUN: RUN4227

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.25

EN300-246747_3_1_1



CID: EN300-246747_3_1_1

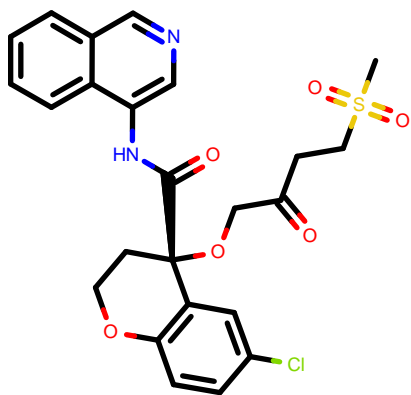
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C)COC[C@@]5(C)COC(=O)NC5

RUN: RUN3753

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.28

EN300-1988306_1_1_1



CID: EN300-1988306_1_1_1

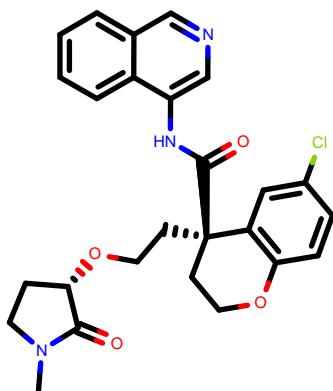
SMILES: CS(=O)(=O)CCC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN7032

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.33

EN300-98648_3_1_1



CID: EN300-98648_3_1_1

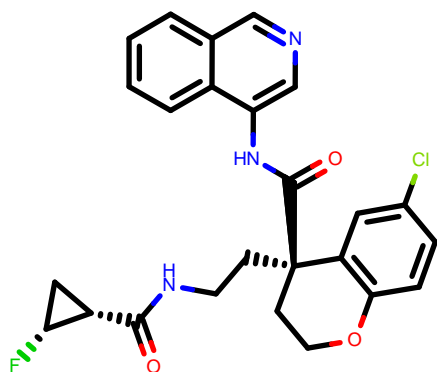
SMILES: CN1CC[C@@H](C1=O)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN4906

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.24

EN300-6953121_3_1_1



CID: EN300-6953121_3_1_1

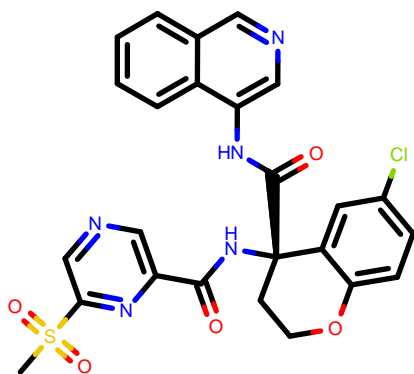
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@H]5F

RUN: RUN5746

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.23

EN300-206646_1_1_1



CID: EN300-206646_1_1_1

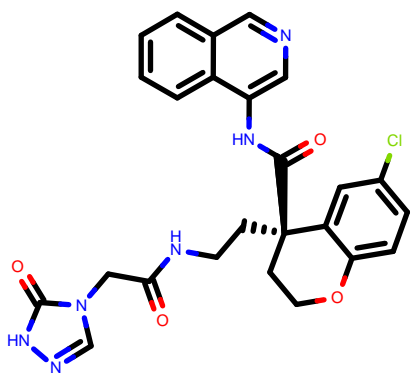
SMILES: CS(=O)(=O)c1nccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN3673

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.31

EN300-120820_3_1_1



CID: EN300-120820_3_1_1

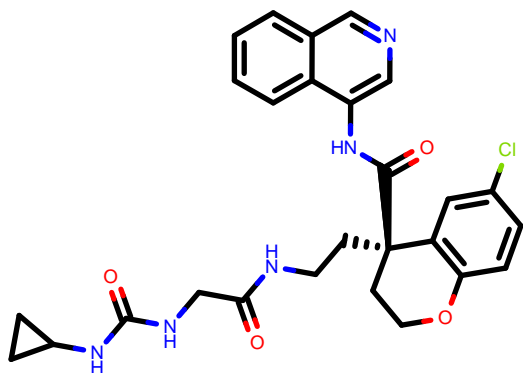
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cn[nH]5=O

RUN: RUN4576

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.31

EN300-42591_3_1_1



CID: EN300-42591_3_1_1

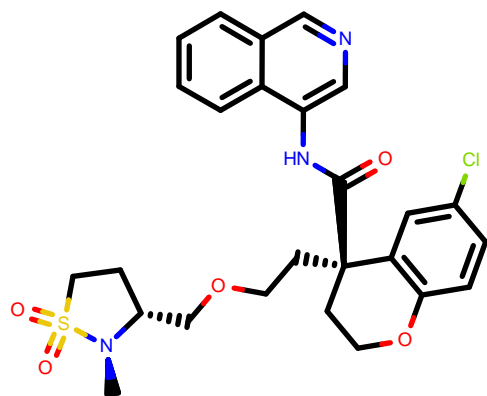
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CNC5=O)NC5CC5

RUN: RUN5195

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.32

EN300-393148_3_2_1



CID: EN300-393148_3_2_1

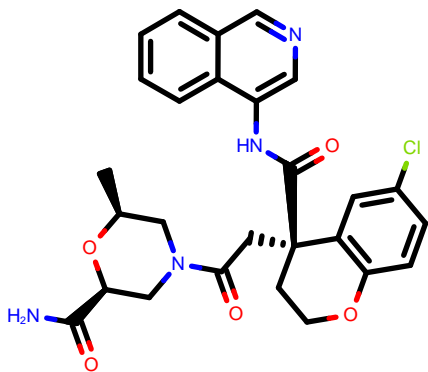
SMILES: C[N@@]1[C@H](CCS1(=O)=O)COCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5825

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.31

EN300-295905_1_4_1



CID: EN300-295905_1_4_1

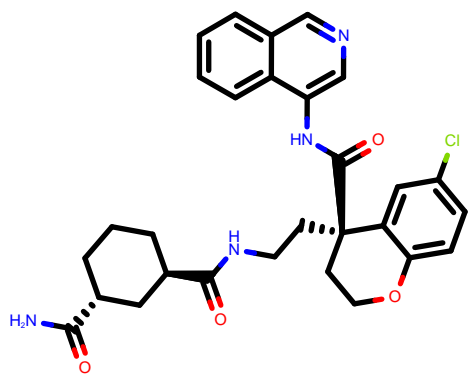
SMILES: C[C@H]1CN(C[C@H](O1)C(=O)N)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5325

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.32

EN300-90142_3_3_1



CID: EN300-90142_3_3_1

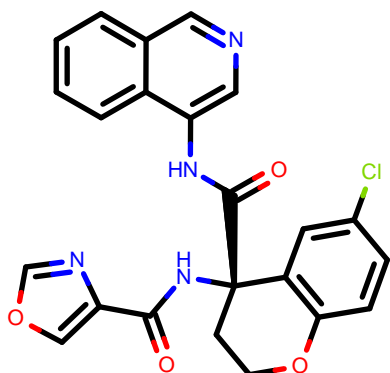
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@H5SCC[C@@H](C5)Cl=O

RUN: RUN4684

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.29

EN300-68618_1_1_1



CID: EN300-68618_1_1_1

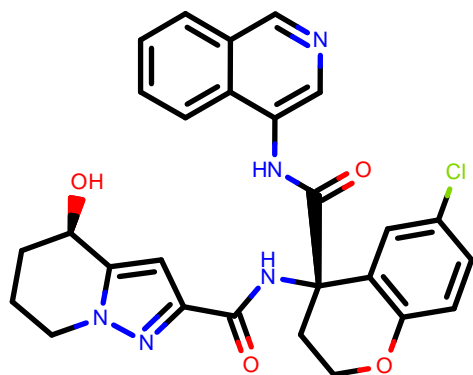
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5occn5

RUN: RUN3520

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.18

EN300-399606_1_2_1



CID: EN300-399606_1_2_1

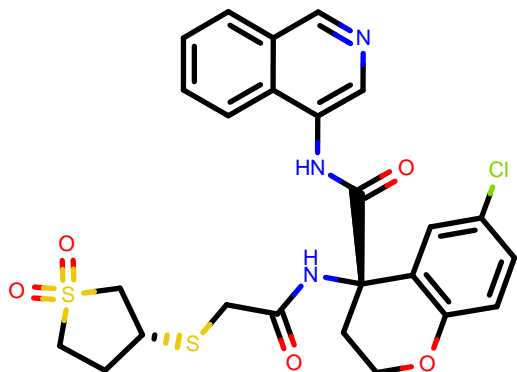
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6n(n5)CCC[C@@H]6O

RUN: RUN4832

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.33

EN300-13890_1_1_1



CID: EN300-13890_1_1_1

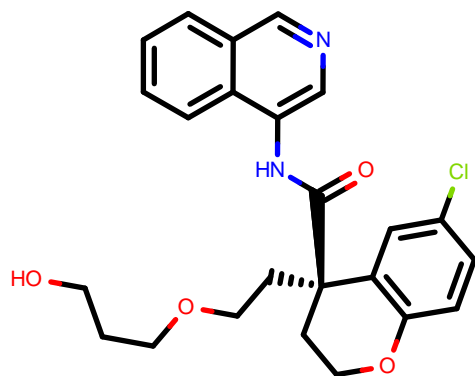
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@@H]5SCCS(=O)(=O)C5

RUN: RUN2835

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.31

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

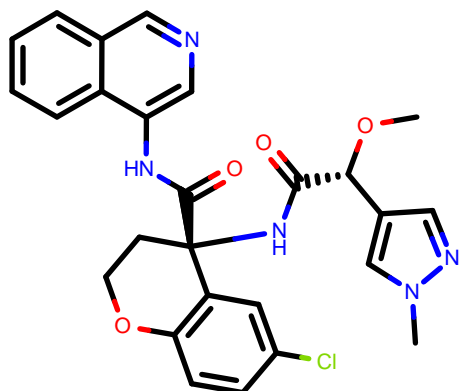
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN3959

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.21

EN300-198240_1_2_1



CID: EN300-198240_1_2_1

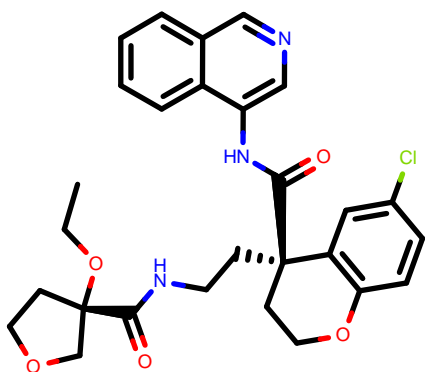
SMILES: Cn1cc(en1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC

RUN: RUN3314

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.28

EN300-259694_3_2_1



CID: EN300-259694_3_2_1

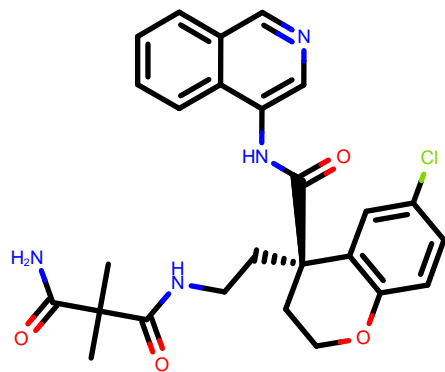
SMILES: CCO[C@@]1(CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4682

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.45

EN300-182913_3_1_1



CID: EN300-182913_3_1_1

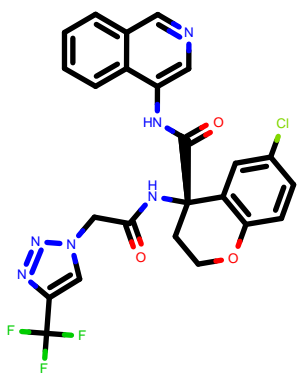
SMILES: CC(C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6176

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.27

EN300-2910941_1_1_1



CID: EN300-2910941_1_1_1

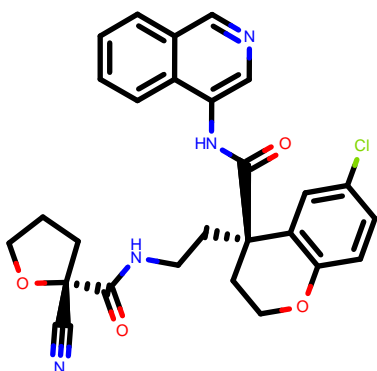
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(nn5)C(F)(F)F

RUN: RUN3013

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.23

EN300-3710141_3_2_1



CID: EN300-3710141_3_2_1

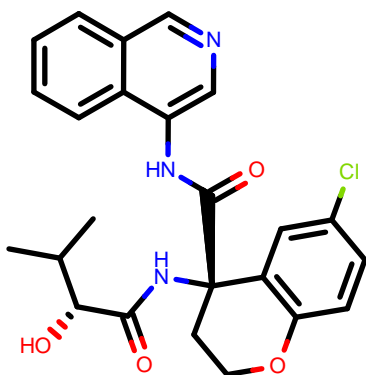
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@5(CCCO5)C#N

RUN: RUN3733

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.25

EN300-115017_1_1_1



CID: EN300-115017_1_1_1

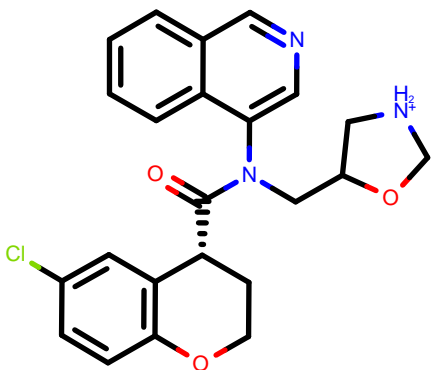
SMILES: CC(C)[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN2954

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.23

ALP-UNI-44c99a80-3_1_1



CID: ALP-UNI-44c99a80-3_1_1

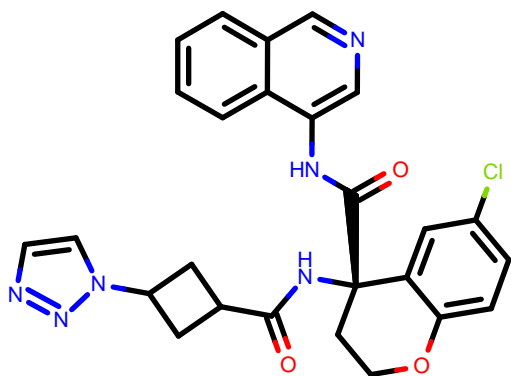
SMILES: c1ccc2c(c1)ncnc2N(Cc3ccc3)C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N

RUN: RUN4050

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.17

EN300-2008240_1_1_1



CID: EN300-2008240_1_1_1

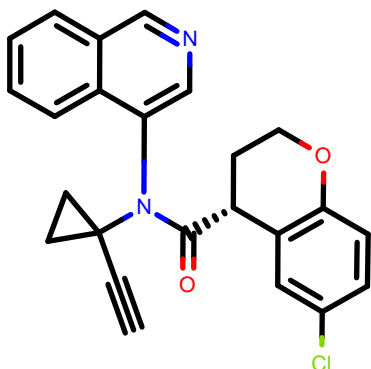
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC(C5)n6cnm6

RUN: RUN5388

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.30

DAR-DIA-5ff57136-15_1



CID: DAR-DIA-5ff57136-15_1

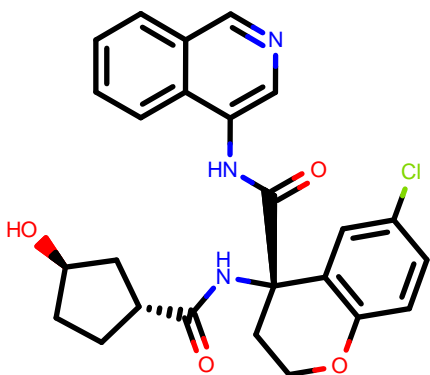
SMILES: C#CC1(CC1)N(c2ncnc3c2cccc3)C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN: RUN1263

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.18

EN300-321597_1_1_1



CID: EN300-321597_1_1_1

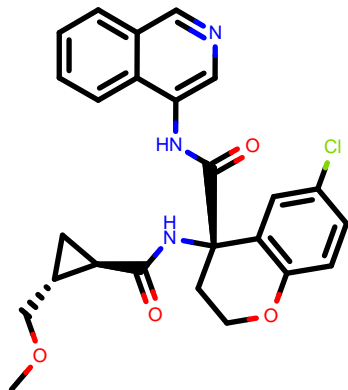
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC[C@H](C5)O

RUN: RUN3346

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.25

EN300-705386_1_1_1



CID: EN300-705386_1_1_1

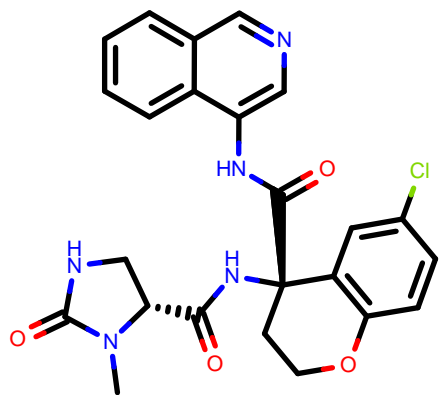
SMILES: COC[C@@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc54cccc5

RUN: RUN3344

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.22

EN300-307008_1_2_1



CID: EN300-307008_1_2_1

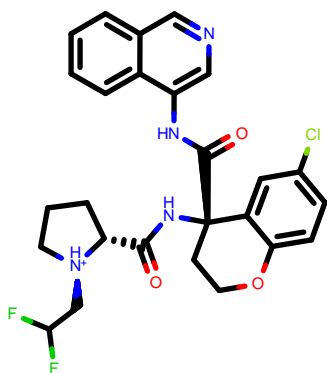
SMILES: CN1C[C@H](CNC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2983

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.24

EDG-MED-90036822-98_4



CID: EDG-MED-90036822-98_4

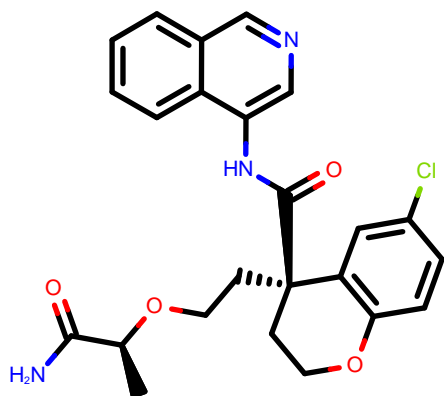
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5C[C@H](F)C(F)F

RUN: RUN1684

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.25

EN300-17381_3_1_1



CID: EN300-17381_3_1_1

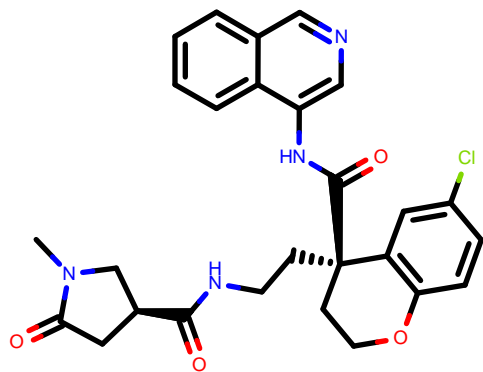
SMILES: C[C@@]3(C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3121

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.24

EN300-33601_3_2_1



CID: EN300-33601_3_2_1

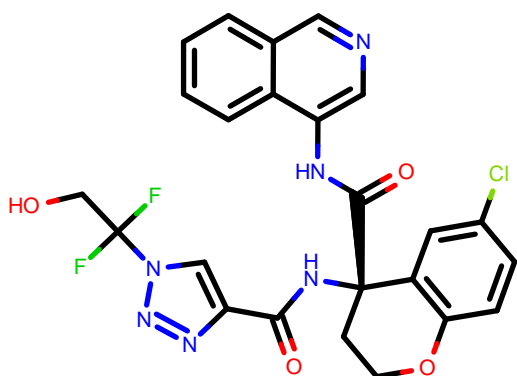
SMILES: CN1C[C@H](CC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4316

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.29

EN300-716207_1_1_1



CID: EN300-716207_1_1_1

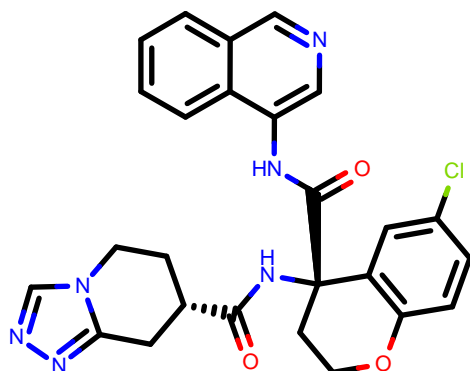
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[n](nn5)C(CO)F

RUN: RUN6475

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.26

EN300-6474341_1_2_1



CID: EN300-6474341_1_2_1

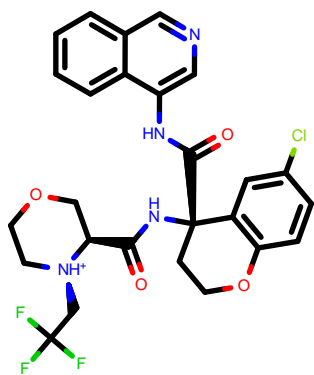
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCN6cnc6C5

RUN: RUN2822

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.24

EN300-201551_1_1_1



CID: EN300-201551_1_1_1

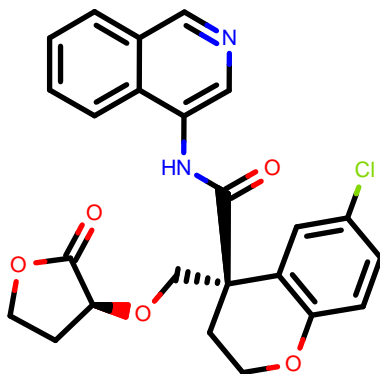
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5COCN6J5CC(F)F

RUN: RUN3522

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.32

EN300-20496_2_2_1



CID: EN300-20496_2_2_1

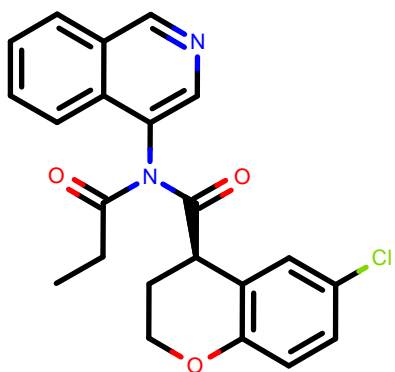
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CO[C@@H]5COCOS=O

RUN: RUN3830

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.21

VLA-UCB-50c39ae8-7_1_1



CID: VLA-UCB-50c39ae8-7_1_1

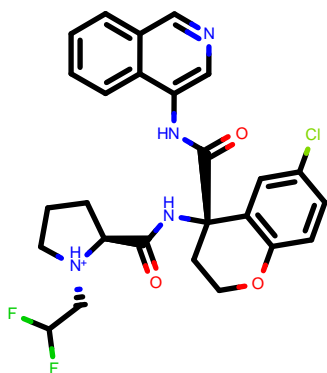
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN5545

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.17

EDG-MED-90036822-98_3



CID: EDG-MED-90036822-98_3

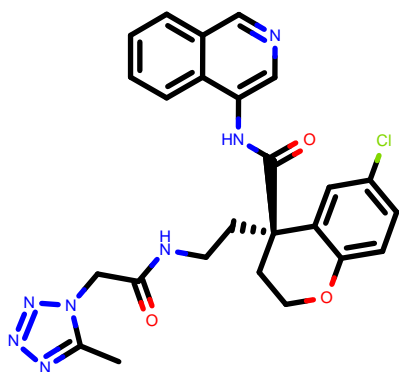
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCN@J5C(F)F

RUN: RUN1698

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.35

EN300-1244816_3_1_1



CID: EN300-1244816_3_1_1

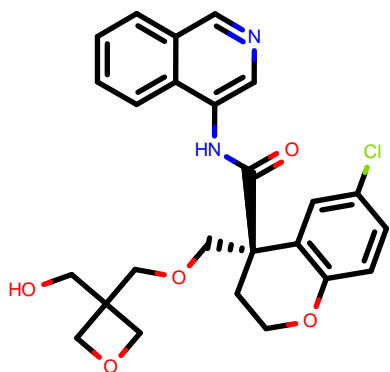
SMILES: Cc1nnnn1CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2901

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-2_1



CID: EDJ-MED-fcba3f31-2_1

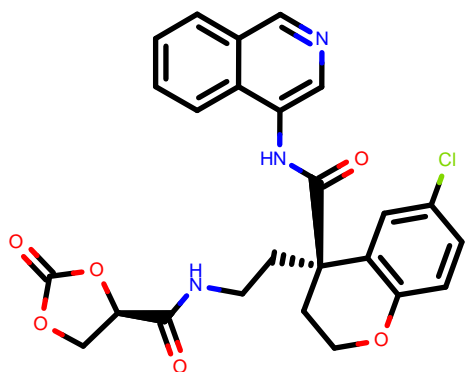
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(C)CO

RUN: RUN2403

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.25

EN300-5253939_3_2_1



CID: EN300-5253939_3_2_1

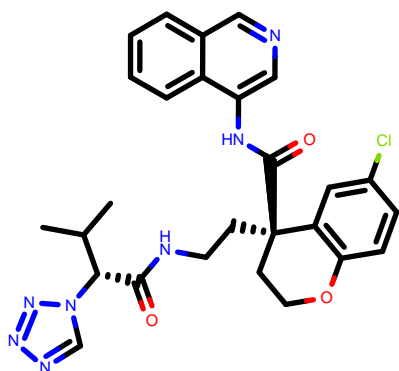
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CCNC(=O)C@H5COC(=O)O5

RUN: RUN5154

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.26

EN300-297561_3_2_1



CID: EN300-297561_3_2_1

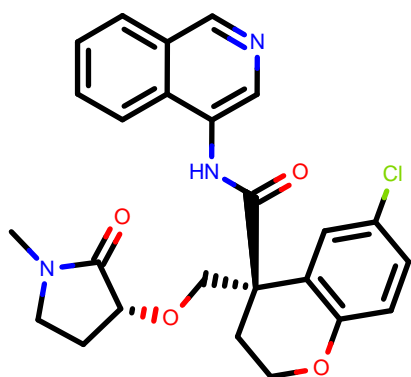
SMILES: CC(C)[C@H](C(=O)NCC[C@@1](CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)n5nnn5

RUN: RUN5374

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.29

EN300-98648_2_2_1



CID: EN300-98648_2_2_1

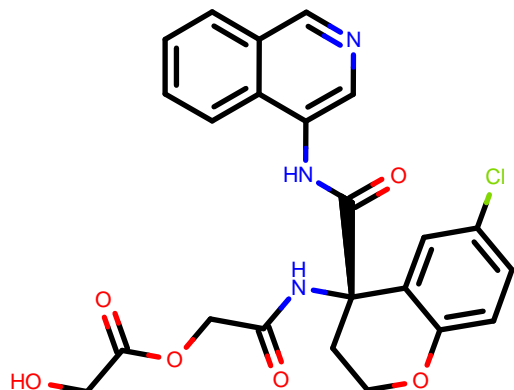
SMILES: CN1CC[C@H](C1=O)OC[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4355

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.26

EN300-7459916_1_1_1



CID: EN300-7459916_1_1_1

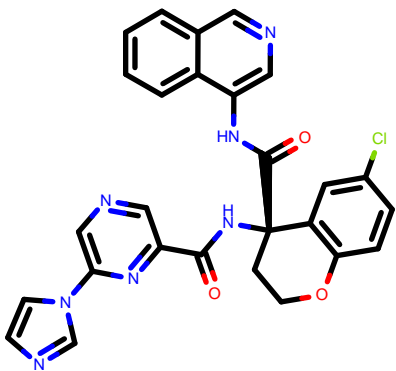
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)COC(=O)CO

RUN: RUN4031

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.23

EN300-2666482_1_1_1



CID: EN300-2666482_1_1_1

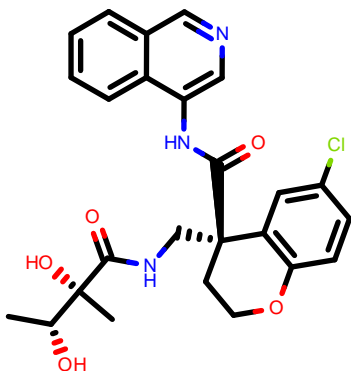
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncnc(n5)n6ccnc6

RUN: RUN6118

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.22

EN300-202922_2_4_1



CID: EN300-202922_2_4_1

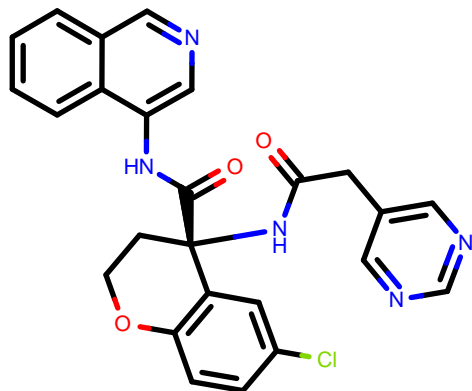
SMILES: C[C@H]([C@](C)(C)=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncnc4c3ccccc4O

RUN: RUN5336

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.30

EN300-185751_1_1_1



CID: EN300-185751_1_1_1

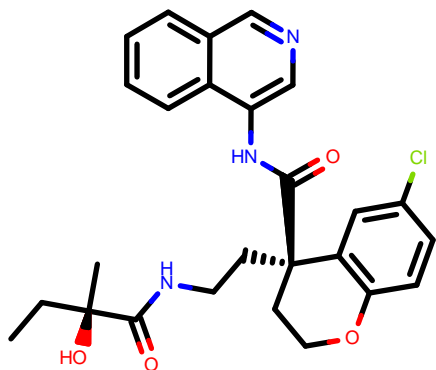
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cncnc5

RUN: RUN3923

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-104746_3_2_1



CID: EN300-104746_3_2_1

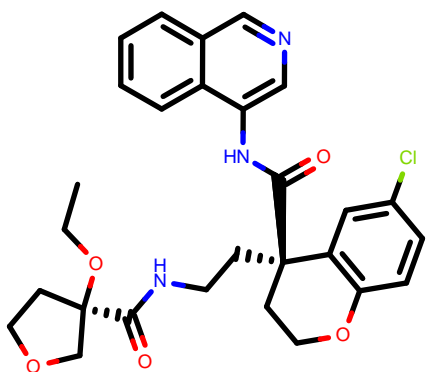
SMILES: CC[C@](C)(C)(C=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncnc4c3ccccc4O

RUN: RUN4518

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-259694_3_1_1



CID: EN300-259694_3_1_1

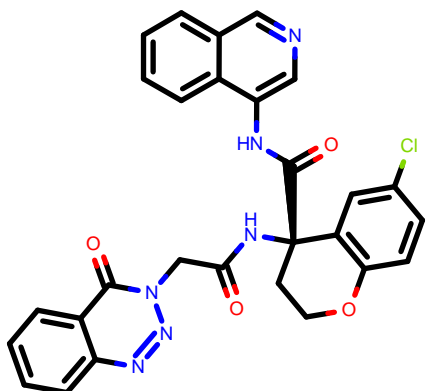
SMILES: CCO[C@@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5262

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.36

EN300-21813_1_1_1



CID: EN300-21813_1_1_1

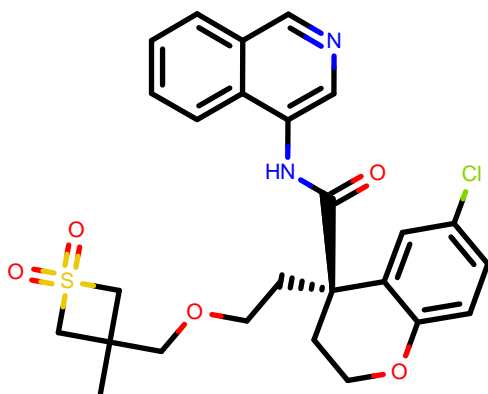
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c(=O)c6cccc6nn5

RUN: RUN6071

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.40

EN300-1705754_3_1_1



CID: EN300-1705754_3_1_1

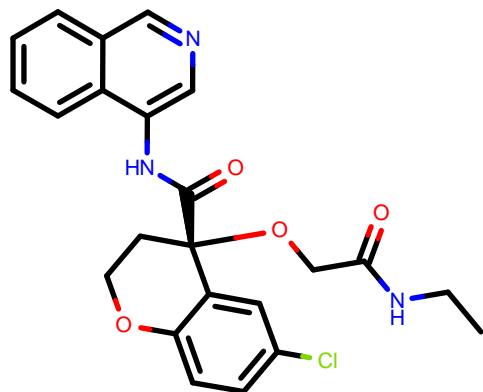
SMILES: CC1(CS(=O)(=O)C1)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3723

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.27

EN300-7003350_1_1_1



CID: EN300-7003350_1_1_1

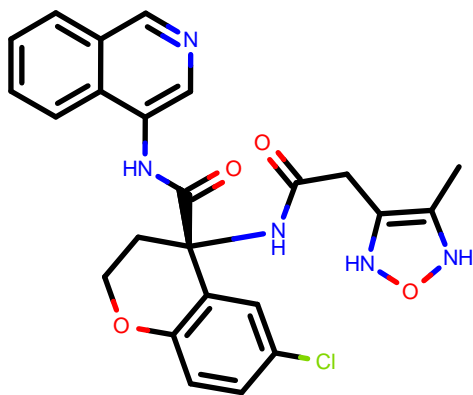
SMILES: CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN3518

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.19

EN300-254883_1_1_1



CID: EN300-254883_1_1_1

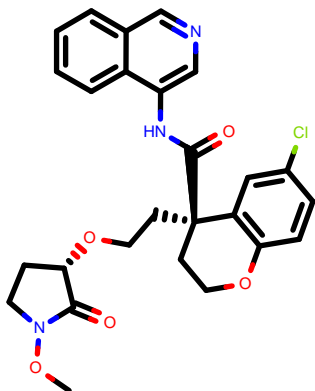
SMILES: Cc1c(non1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2993

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.25

EN300-302058_3_1_1



CID: EN300-302058_3_1_1

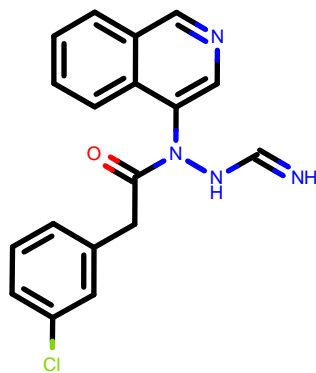
SMILES: CON1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6295

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.26

PET-UNK-a692de38-1_1



CID: PET-UNK-a692de38-1_1

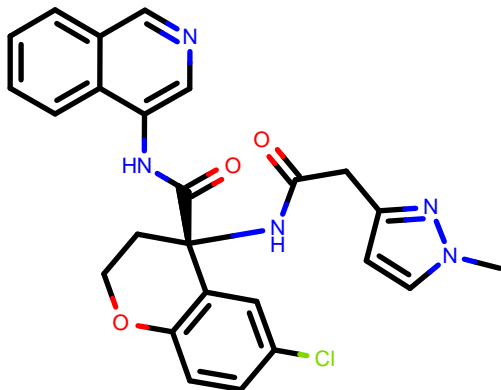
SMILES: c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)NC#N

RUN: RUN533

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.26

EN300-258702_1_1_1



CID: EN300-258702_1_1_1

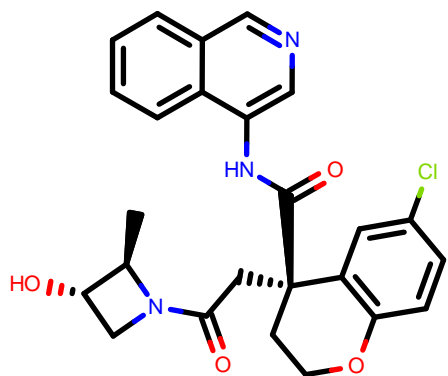
SMILES: Cn1ccc(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3354

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-7471076_1_3_1



CID: EN300-7471076_1_3_1

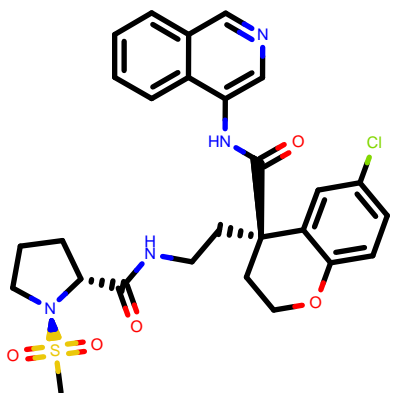
SMILES: C[C@@H]1[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN5102

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.27

EN300-10402_3_1_1



CID: EN300-10402_3_1_1

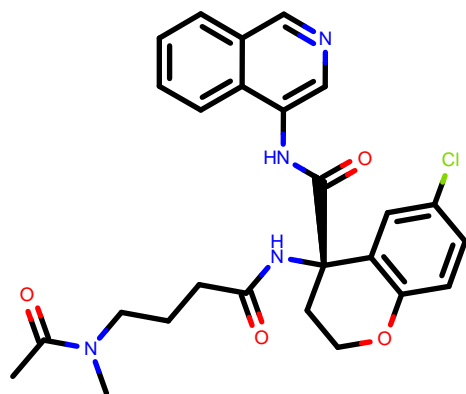
SMILES: CS(=O)(=O)N1CC[C@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4295

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-128750_1_1_1



CID: EN300-128750_1_1_1

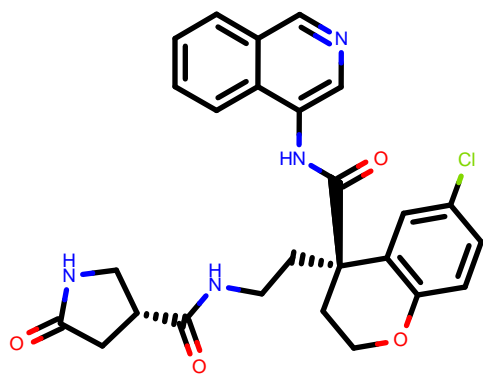
SMILES: CC(=O)N(C)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN3913

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.25

EN300-59487_3_1_1



CID: EN300-59487_3_1_1

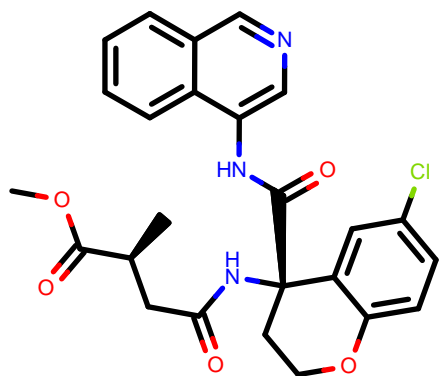
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CC(=O)NCS

RUN: RUN3658

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.29

EN300-108413_1_1_1



CID: EN300-108413_1_1_1

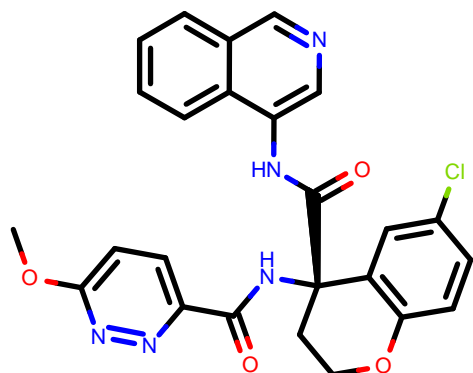
SMILES: C[C@@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)C(=O)OC

RUN: RUN5185

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.27

EN300-82553_1_1_1



CID: EN300-82553_1_1_1

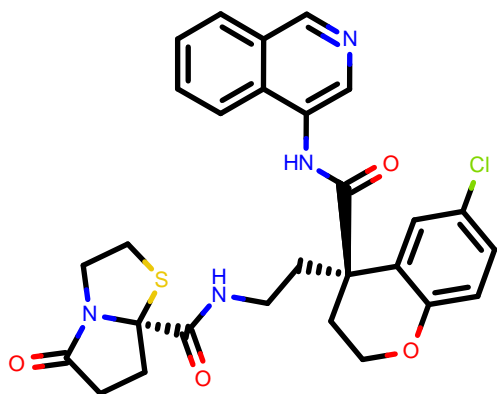
SMILES: COc1ccc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4173

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-10334_3_2_1



CID: EN300-10334_3_2_1

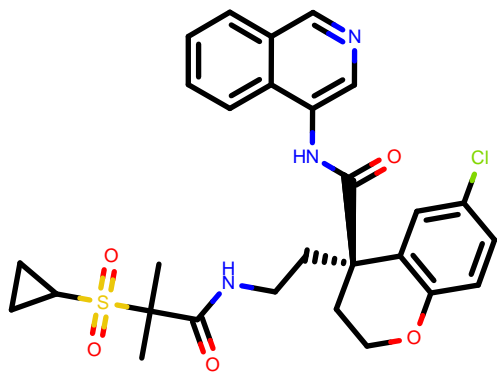
SMILES: c1ccc2c(c1)ncnc2N[C@@]C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5C6CCC(=O)N5C6S6

RUN: RUN5880

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-193399_3_1_1



CID: EN300-193399_3_1_1

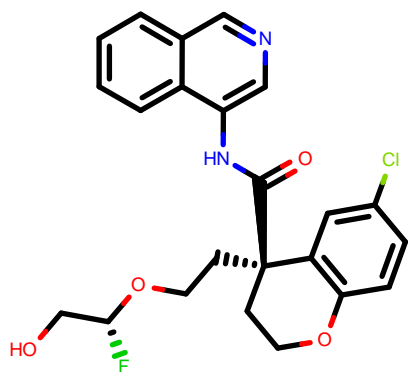
SMILES: CC(C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)S(=O)(=O)C5CC5

RUN: RUN4419

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.35

EN300-861925_3_1_1



CID: EN300-861925_3_1_1

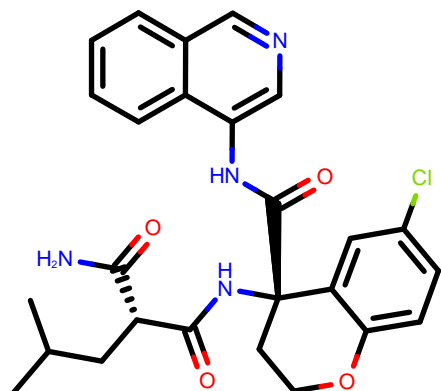
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H](CO)F

RUN: RUN4555

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.26

EN300-250126_1_2_1



CID: EN300-250126_1_2_1

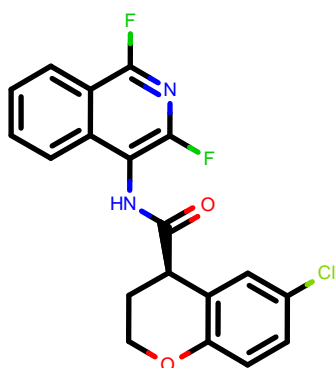
SMILES: CC(C)C[C@H](C(=O)N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5140

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.25

JOH-SUS-a69c159d-6_1_1



CID: JOH-SUS-a69c159d-6_1_1

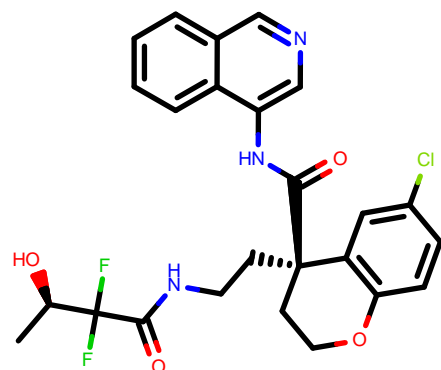
SMILES: c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN3441

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.05

EN300-185398_3_2_1



CID: EN300-185398_3_2_1

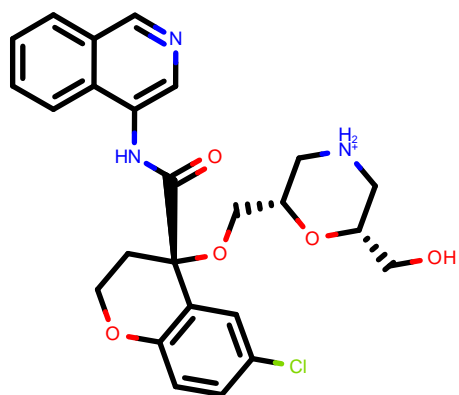
SMILES: C[C@H](C(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)(F)F)O

RUN: RUN4618

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-21_1



CID: ED_-GRI-5b13fbe2-21_1

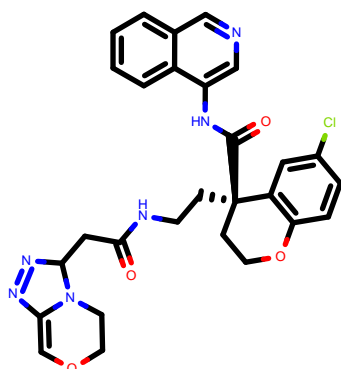
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc4)C1OC[C@@H]5C[NH2+][C@@H]5O5CO

RUN: RUN1432

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.35

EN300-1718836_3_1_1



CID: EN300-1718836_3_1_1

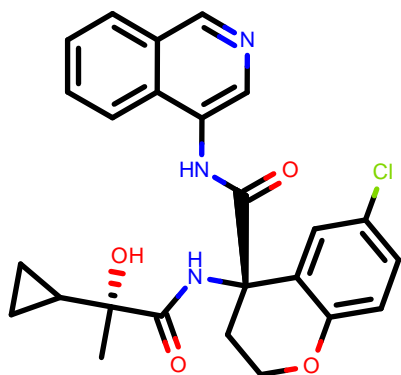
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc4)C1OCNC(=O)Cc5nnc6n5CCOC6

RUN: RUN4688

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.31

EN300-118760_1_1_1



CID: EN300-118760_1_1_1

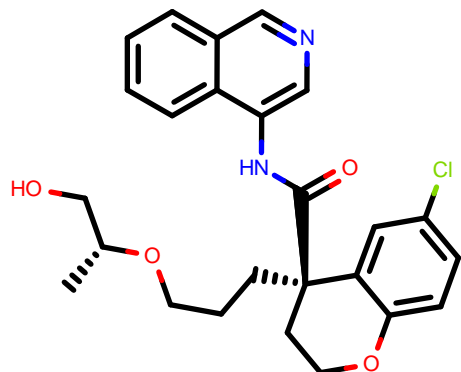
SMILES: C[C@@H](C1CC1)C(=O)N[C@@]2(CCOc3cc2cc3)C1C(=O)Nc4nnc5c4cccc5O

RUN: RUN4506

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.31

EN300-175186_4_2_1



CID: EN300-175186_4_2_1

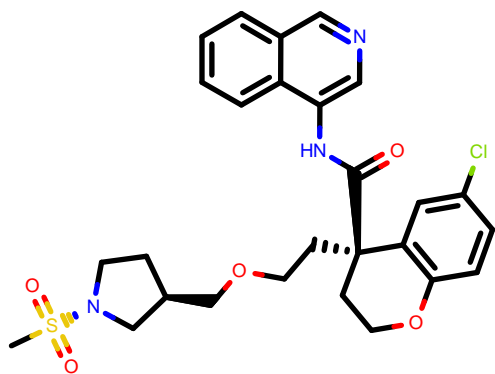
SMILES: C[C@H](CO)OCC[C@@]1(CCOc2c1cc3cc2)C1C(=O)Nc3nnc4c3cccc4

RUN: RUN4224

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.34

KAD-UNI-8a629cb0-1_2



CID: KAD-UNI-8a629cb0-1_2

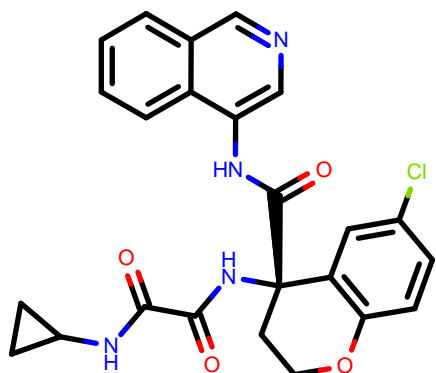
SMILES: CS(=O)(=O)N@1CC[C@@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN1976

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.48

EN300-78135_1_1_1



CID: EN300-78135_1_1_1

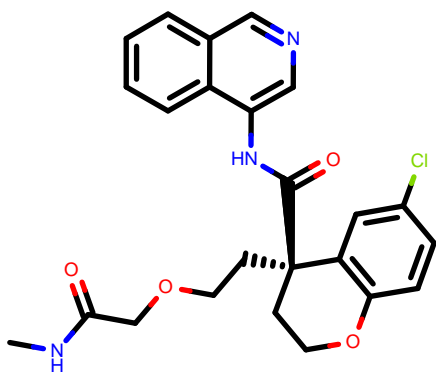
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NC5CC5

RUN: RUN3400

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.20

EN300-2977549_3_1_1



CID: EN300-2977549_3_1_1

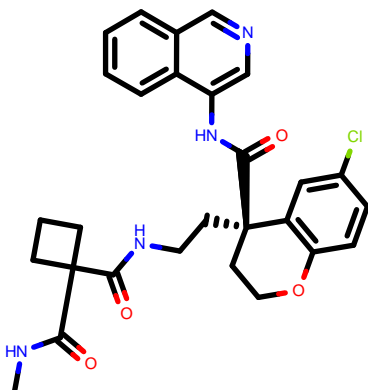
SMILES: CNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4156

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.20

EN300-70064_3_1_1



CID: EN300-70064_3_1_1

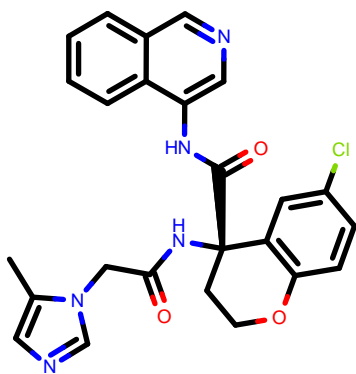
SMILES: CNC(=O)C1(CCC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5266

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.44

EDG-MED-90036822-43_1



CID: EDG-MED-90036822-43_1

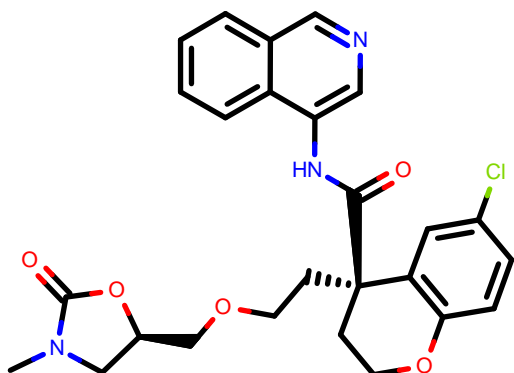
SMILES: Cc1cn[n1]CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1597

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.22

EN300-222969_3_1_1



CID: EN300-222969_3_1_1

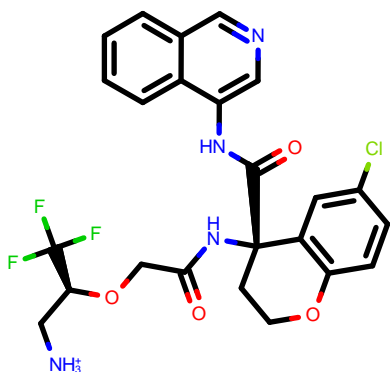
SMILES: CN1C[C@@H](OC1=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5010

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.33

EDG-MED-90036822-27_1



CID: EDG-MED-90036822-27_1

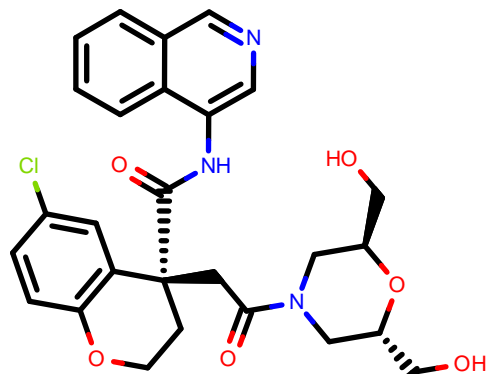
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@]5H(CN)C(F)(F)F

RUN: RUN1563

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.55

EN300-6735683_1_1_1



CID: EN300-6735683_1_1_1

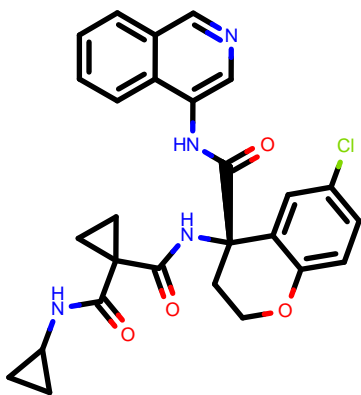
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H(C)C(O)CO

RUN: RUN3393

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.42

EN300-61636_1_1_1



CID: EN300-61636_1_1_1

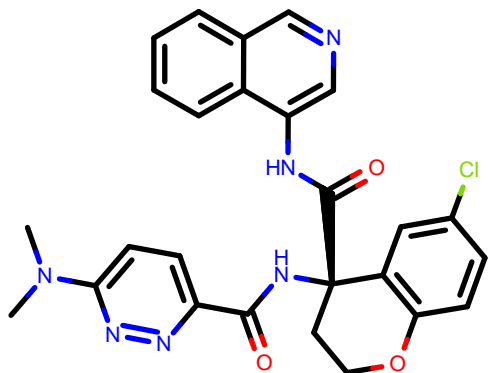
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)C5(CC5)C(=O)NC6CC6

RUN: RUN5049

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.30

EN300-7535922_1_1_1



CID: EN300-7535922_1_1_1

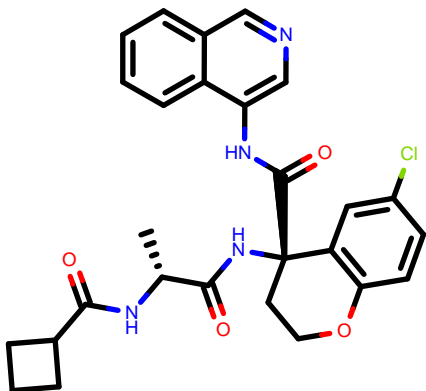
SMILES: CN(C)c1ccc(nn1)C(=O)N[C@@2](CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN7727

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.22

EN300-66082_1_2_1



CID: EN300-66082_1_2_1

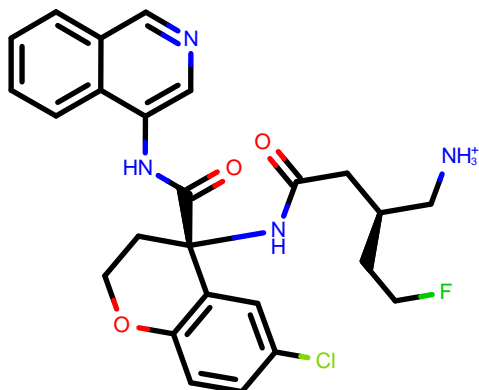
SMILES: C[C@H](C(=O)N[C@@1](CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4)NC(=O)C5CC5

RUN: RUN4191

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.33

EDG-MED-90036822-88_2



CID: EDG-MED-90036822-88_2

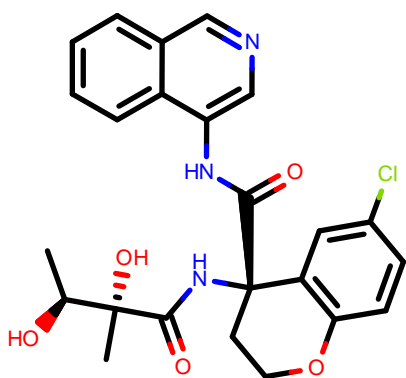
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)C[C@H](CCF)C[NH3+]

RUN: RUN1703

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.27

EN300-202922_1_3_1



CID: EN300-202922_1_3_1

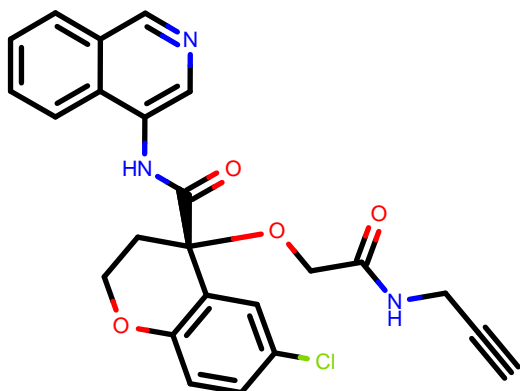
SMILES: C[C@@H]([C@](C)(C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)O)O

RUN: RUN6193

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.23

EN300-1659582_1_1_1



CID: EN300-1659582_1_1_1

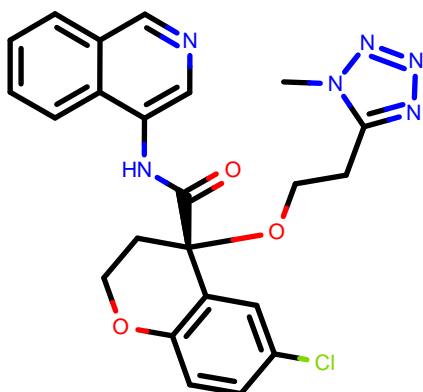
SMILES: C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN3839

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.20

EN300-365398_1_1_1



CID: EN300-365398_1_1_1

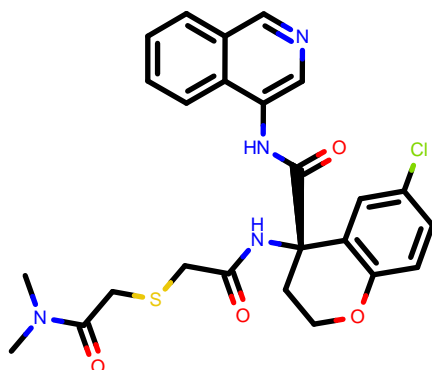
SMILES: Cn1c(nnn1)CCO[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4581

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.25

EN300-12139_1_1_1



CID: EN300-12139_1_1_1

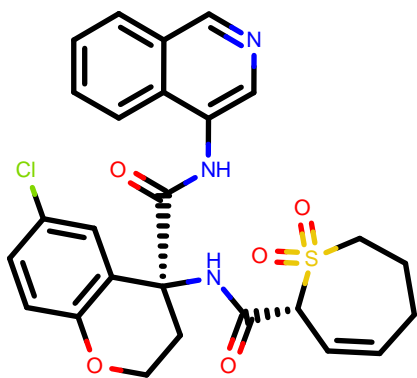
SMILES: CN(C)C(=O)CSCC(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN3480

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.31

EN300-6499531_1_2_1



CID: EN300-6499531_1_2_1

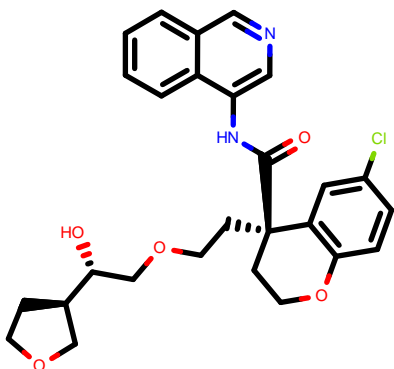
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCCC5S(=O)=O

RUN: RUN2881

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.27

EN300-1911992_3_2_1



CID: EN300-1911992_3_2_1

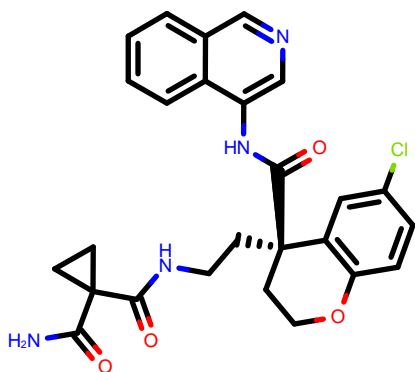
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5OCOC5O

RUN: RUN6759

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.36

EN300-69070_3_1_1



CID: EN300-69070_3_1_1

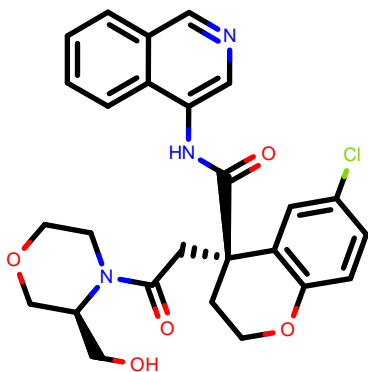
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(C)C5C(=O)N

RUN: RUN3454

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.37

EN300-154201_1_1_1



CID: EN300-154201_1_1_1

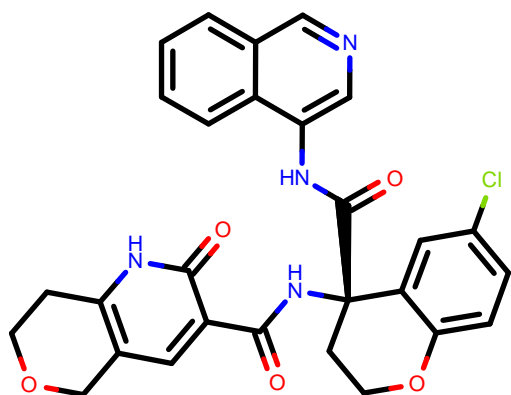
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO

RUN: RUN3838

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.34

EN300-383824_1_1_1



CID: EN300-383824_1_1_1

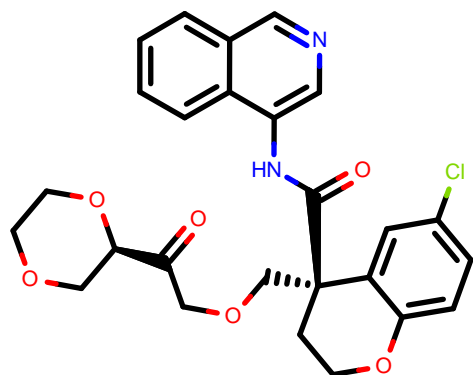
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c([nH]c5=O)CCOC6

RUN: RUN4243

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.31

EN300-6238494_2_2_1



CID: EN300-6238494_2_2_1

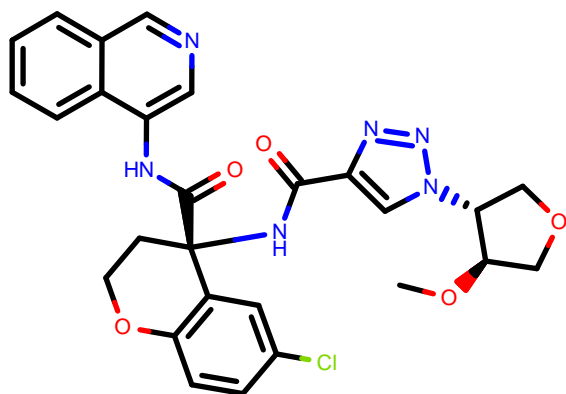
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)[C@H]5COCOC5

RUN: RUN3308

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.40

EN300-1273249_1_1_1



CID: EN300-1273249_1_1_1

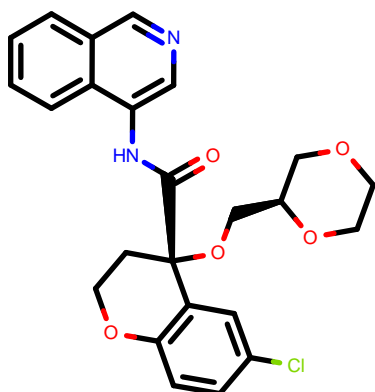
SMILES: CO[C@@H]1COC[C@H]1n2c[nH]2C(=O)NC@@3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccc6

RUN: RUN3586

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.28

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

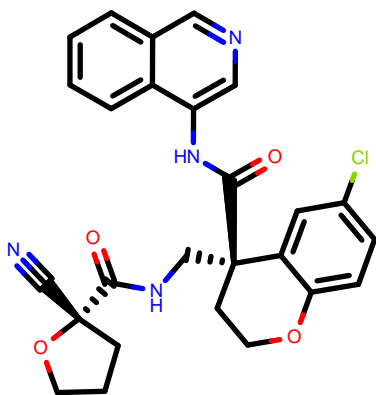
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5COCOC5

RUN: RUN3851

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.26

EN300-3710141_2_1_1



CID: EN300-3710141_2_1_1

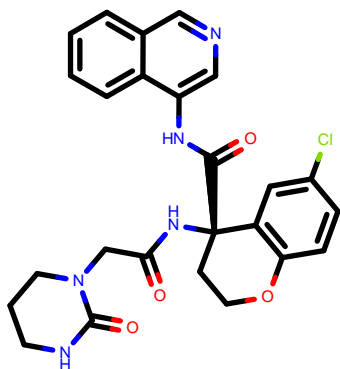
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN3493

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.31

EN300-36096_1_1_1



CID: EN300-36096_1_1_1

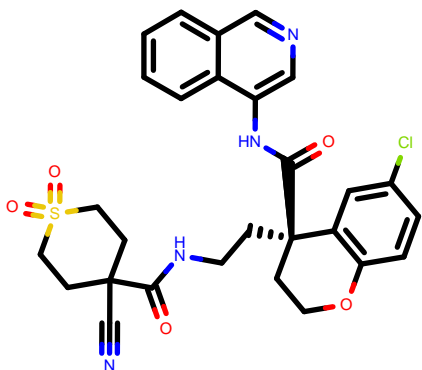
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)N5CCCC5=O

RUN: RUN5662

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.27

EN300-73967_3_1_1



CID: EN300-73967_3_1_1

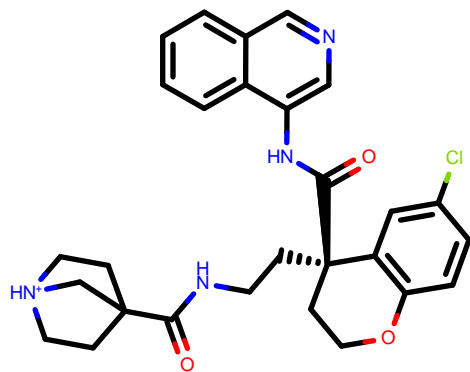
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCS(=O)(=O)CC5)C#N

RUN: RUN3870

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.38

EN300-313366_3_1_1



CID: EN300-313366_3_1_1

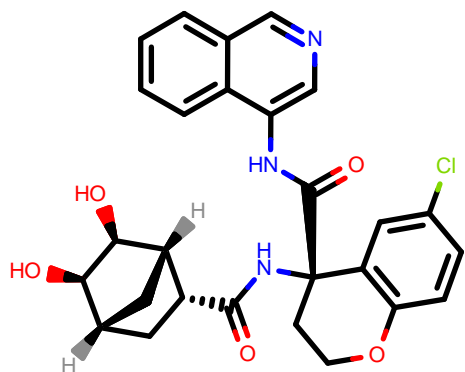
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CC[NH+]1(C5)CC6

RUN: RUN7566

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.29

EN300-6744028_1_1_1



CID: EN300-6744028_1_1_1

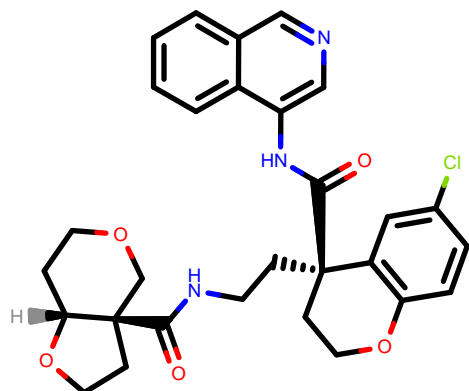
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)NC(=O)C@@H5[C@@H]6[C@@H]7[C@@H]8[C@@H]9[C@@H]9O

RUN: RUN5083

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.26

EN300-341337_3_1_1



CID: EN300-341337_3_1_1

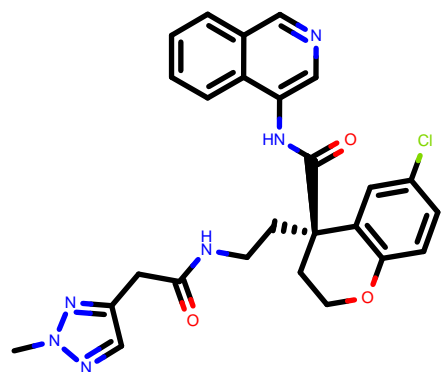
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)CNC(=O)C@@5[C@@H]6[C@@H]7O

RUN: RUN3592

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.30

EN300-755161_3_1_1



CID: EN300-755161_3_1_1

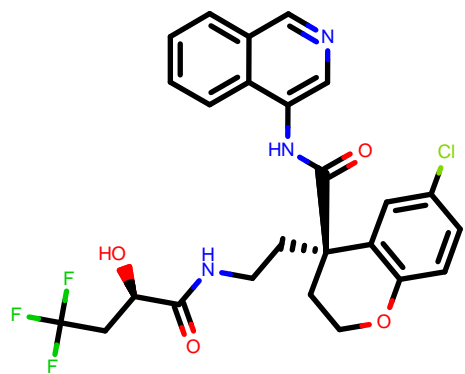
SMILES: Cn1nc(n1)CC(=O)NCC[C@@2](CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4300

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.30

EN300-1932013_3_1_1



CID: EN300-1932013_3_1_1

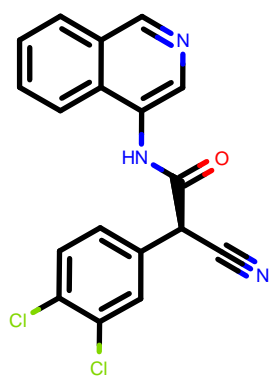
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)CCNC(=O)C@@H(C(F)(F)F)O

RUN: RUN5965

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.45

MAT-POS-fce787c2-8_1



CID: MAT-POS-fce787c2-8_1

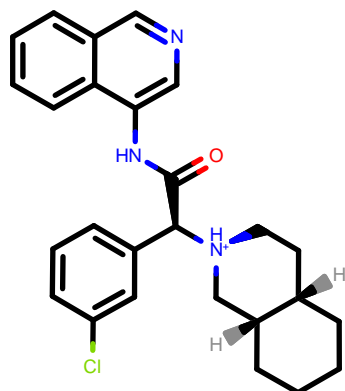
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C#N)c3ccc(c(c3)Cl)Cl

RUN: RUN1958

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.33

MIC-UNK-5a93dd5f-3_4



CID: MIC-UNK-5a93dd5f-3_4

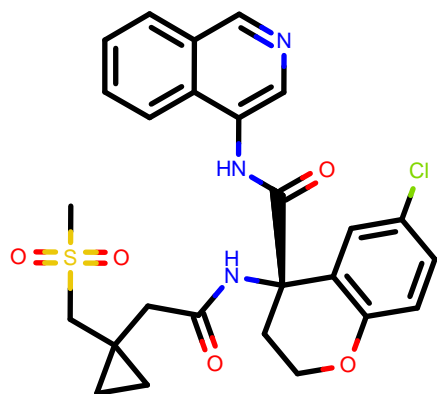
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c3)Cl)N@H+J4CC[C@@H]5CCCC[C@@H]5C4

RUN: RUN640

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.34

EN300-97904_1_1_1



CID: EN300-97904_1_1_1

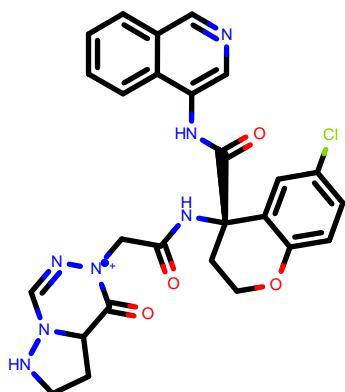
SMILES: CS(=O)(=O)CC1(CC1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN4422

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.35

KAD-UNI-8a629cb0-37_1



CID: KAD-UNI-8a629cb0-37_1

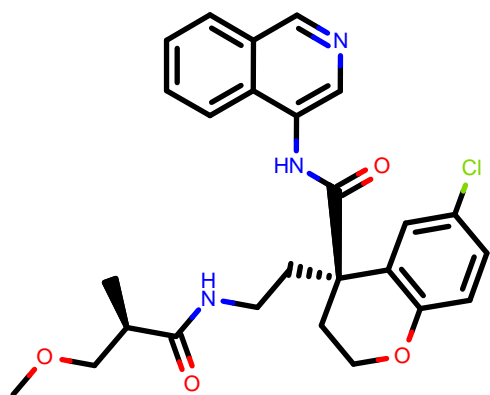
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)c6ccnn6cn5

RUN: RUN1955

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.33

EN300-69162_3_2_1



CID: EN300-69162_3_2_1

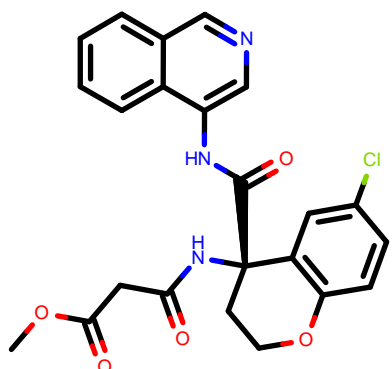
SMILES: C[C@H](COC)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7813

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.34

EN300-20668_1_1_1



CID: EN300-20668_1_1_1

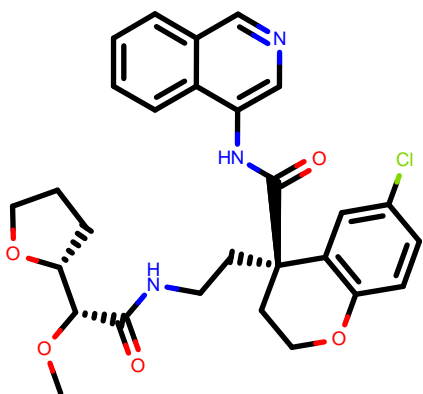
SMILES: COC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3927

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.21

EN300-6277108_3_4_1



CID: EN300-6277108_3_4_1

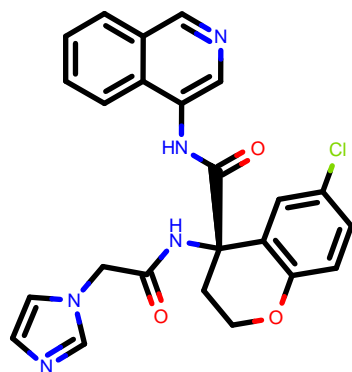
SMILES: CO[C@H]([C@H]1CCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3144

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.34

EN300-38979_1_1_1



CID: EN300-38979_1_1_1

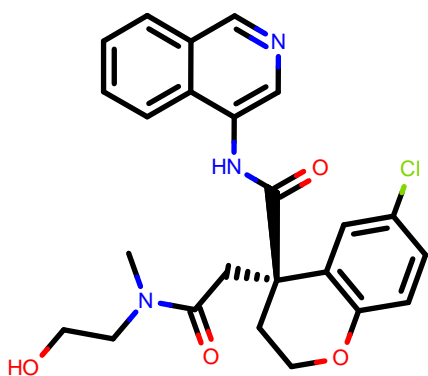
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc5

RUN: RUN3195

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.22

EN300-19342_1_1_1



CID: EN300-19342_1_1_1

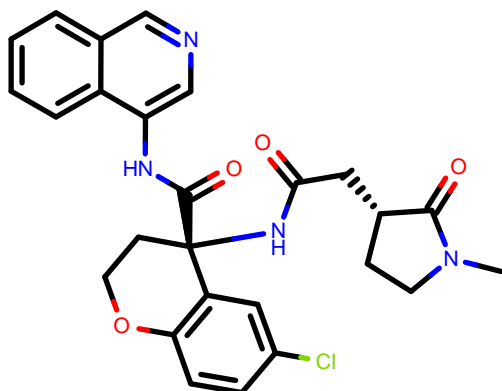
SMILES: CN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5408

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.31

EN300-378722_1_1_1



CID: EN300-378722_1_1_1

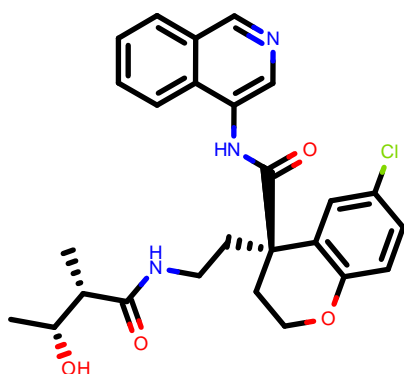
SMILES: CN1CC[C@@H](C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4671

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.24

EN300-7089802_3_1_1



CID: EN300-7089802_3_1_1

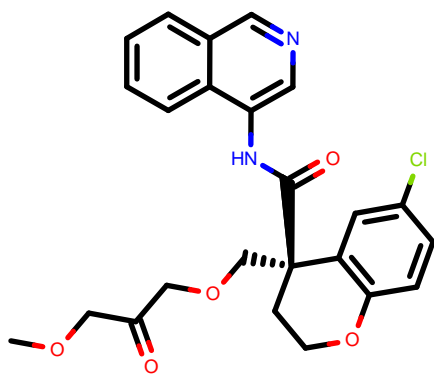
SMILES: C[C@@H](C[C@@H](C1=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3632

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.30

EN300-125140_2_1_1



CID: EN300-125140_2_1_1

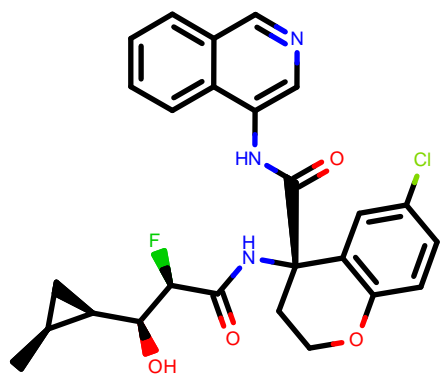
SMILES: COCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4427

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.28

EDG-MED-90036822-94_12



CID: EDG-MED-90036822-94_12

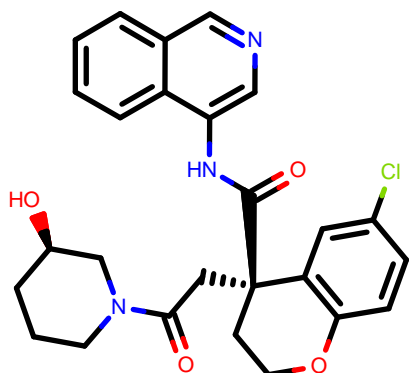
SMILES: C1C=H1C1C=H1[C@@H]1[C@@H]1[C@@H]1C1=O]N[C@@]2(CCOc3c2cc(cc3)C1=O)Nc4nc5c6c4ccc5)F)O

RUN: RUN1682

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.25

EN300-20284_1_2_1



CID: EN300-20284_1_2_1

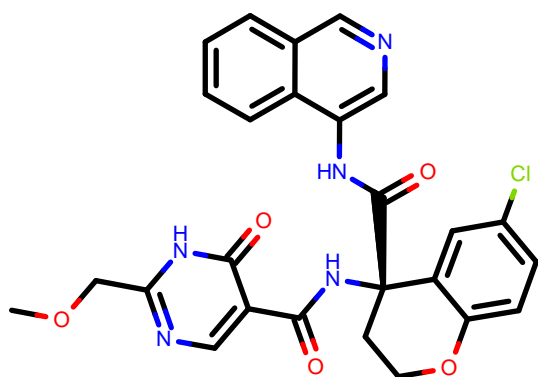
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C1)CC(=O)N5CC[C@H](C5)O

RUN: RUN4693

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.29

EN300-685492_1_1_1



CID: EN300-685492_1_1_1

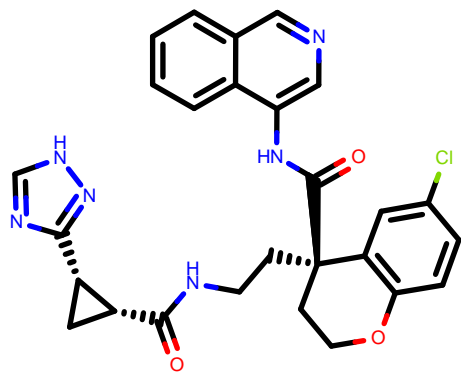
SMILES: COCc1[nH]c2(=O)c(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C1)C(=O)Nc4nc5c6c4ccc5

RUN: RUN6686

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.29

EN300-6477724_3_1_1



CID: EN300-6477724_3_1_1

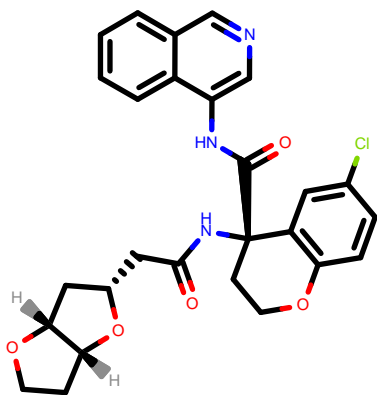
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)CNC1=O)C(=O)N5C[C@H](H)5n6

RUN: RUN3102

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.40

EN300-735519_1_6_1



CID: EN300-735519_1_6_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4cc3cc(c4)C)NC(=O)C@H5C[C@@H]6C@H5O5CCO6

RUN:

RUN3189

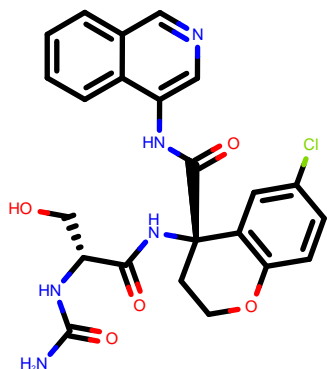
DDG (kcal/mol):

-1.86

dDDG (kcal/mol):

0.30

EN300-10170_1_1_1



CID: EN300-10170_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4cc3cc(c4)C)NC(=O)C@H]CO)NC(=O)N

RUN:

RUN4055

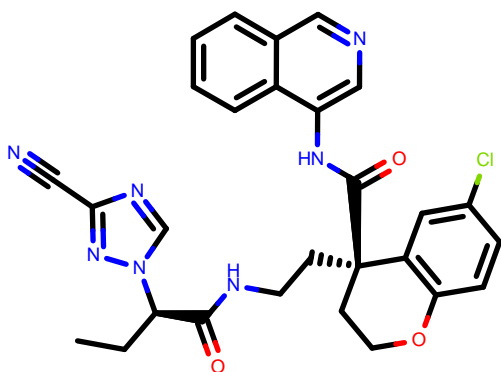
DDG (kcal/mol):

-1.86

dDDG (kcal/mol):

0.27

EN300-245264_3_2_1



CID: EN300-245264_3_2_1

SMILES:

CC[C@H](C(=O)NCC[C@@1(CCOc2c1cc(c2)Cl)C(=O)Nc3nc4c3ccoc4)n5nc(n5)C#N

RUN:

RUN2823

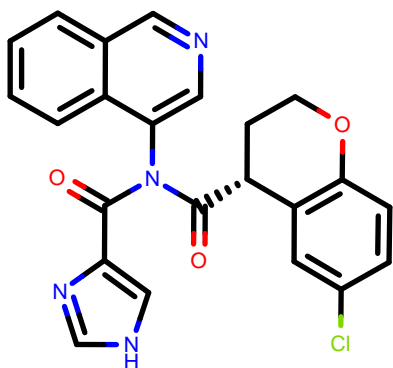
DDG (kcal/mol):

-1.86

dDDG (kcal/mol):

0.36

VLA-UCB-34f3ed0c-20_1



CID: VLA-UCB-34f3ed0c-20_1

SMILES:

c1ccc2c(c1)ncnc2N(C(=O)c3cnc[nH]3)C(=O)C@@H4CCOc5c4cc(cc5)Cl

RUN:

RUN601

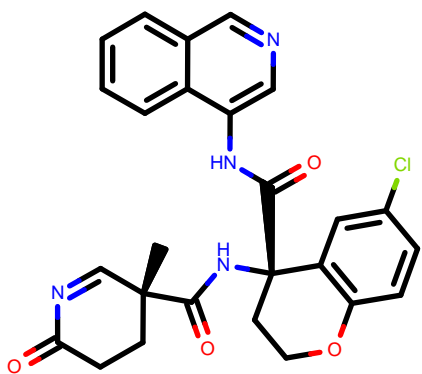
DDG (kcal/mol):

-1.86

dDDG (kcal/mol):

0.27

EN300-195924_1_2_1



CID: EN300-195924_1_2_1

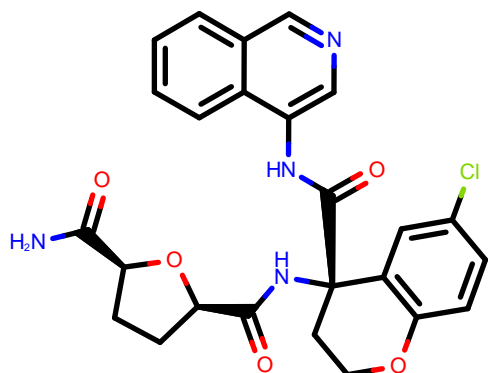
SMILES: C[C@]1(CCC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN5347

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.23

EN300-315238_1_1_1



CID: EN300-315238_1_1_1

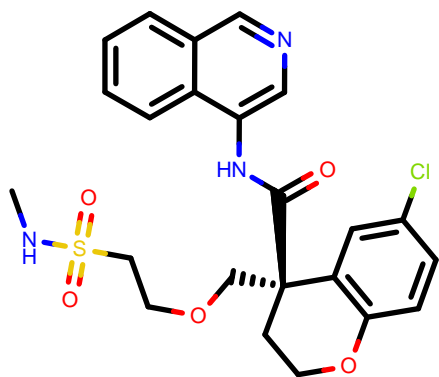
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC[C@H](O5)C(=O)N

RUN: RUN2859

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.30

EN300-6482967_2_1_1



CID: EN300-6482967_2_1_1

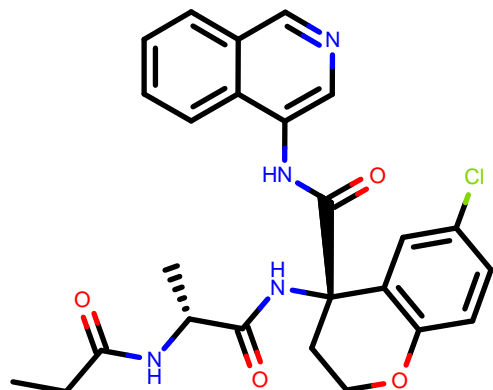
SMILES: CNS(=O)(=O)CCOC[C@]1(C)C(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccccc4

RUN: RUN3286

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.27

EN300-31148_1_2_1



CID: EN300-31148_1_2_1

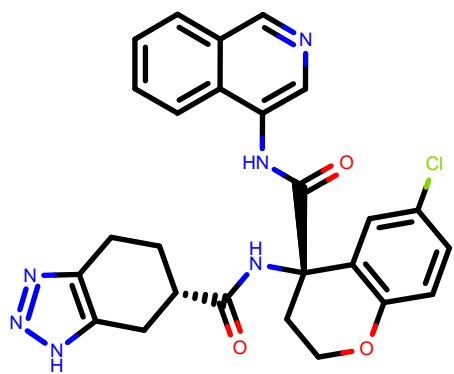
SMILES: CCC(=O)N[C@H](C)C(=O)N[C@]1(C)C(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccccc4

RUN: RUN4193

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.24

EN300-185729_1_2_1



CID: EN300-185729_1_2_1

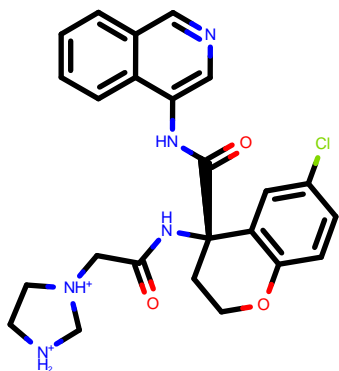
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5CCc6c(n1nH)n6)C5

RUN: RUN4978

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.28

EDG-MED-90036822-18_1



CID: EDG-MED-90036822-18_1

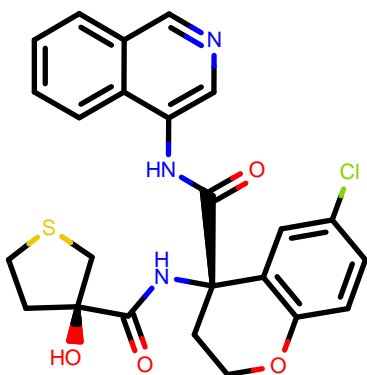
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5

RUN: RUN1553

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.22

EN300-122656_1_1_1



CID: EN300-122656_1_1_1

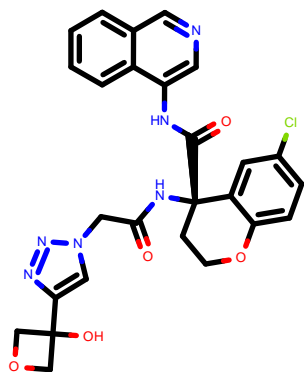
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCSC5)O

RUN: RUN3325

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.37

EN300-7445540_1_1_1



CID: EN300-7445540_1_1_1

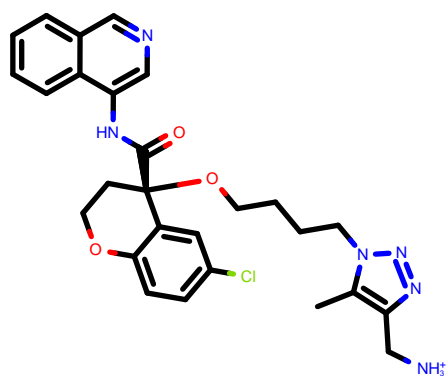
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(nn5)C6(COC6)O

RUN: RUN6179

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.29

ED_-GRI-5b13fbe2-63_1



CID: ED_-GRI-5b13fbe2-63_1

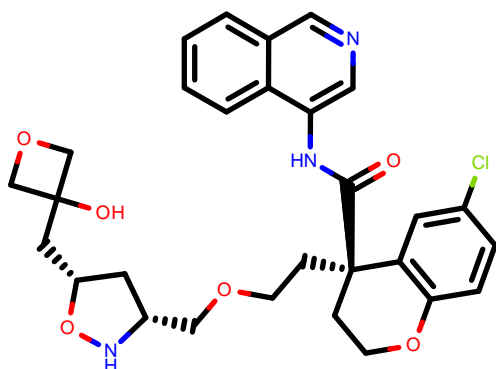
SMILES: Cc1c[nm]1CCCCO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c5c4ccoc5)C[NH3+]

RUN: RUN1518

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.45

EN300-7457160_3_1_2



CID: EN300-7457160_3_1_2

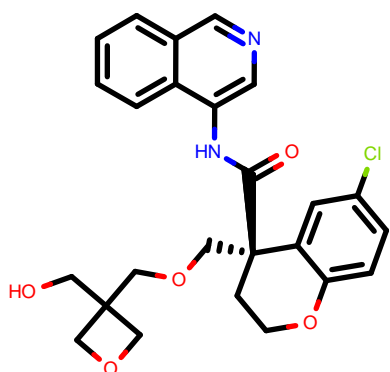
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)COCOC[C@@H]5O[C@@]5COC6O

RUN: RUN4017

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.35

EN300-102347_2_1_1



CID: EN300-102347_2_1_1

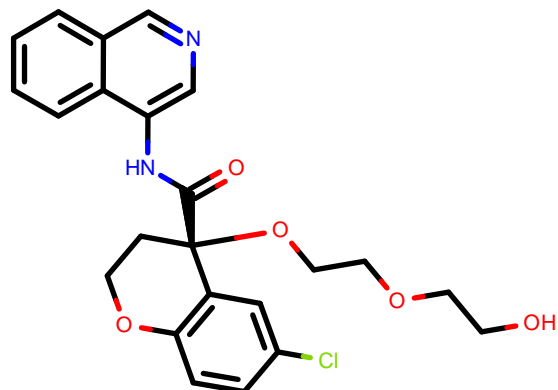
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5(COC5)CO

RUN: RUN4464

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.26

EN300-52467_1_1_1



CID: EN300-52467_1_1_1

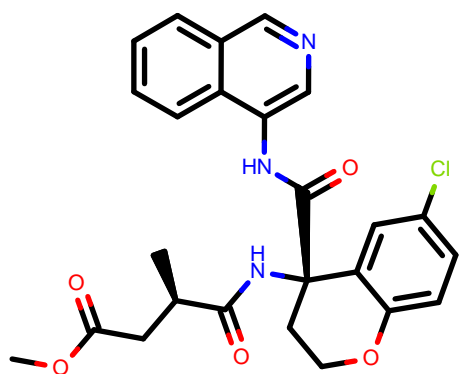
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN4787

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.23

EN300-106540_1_2_1



CID: EN300-106540_1_2_1

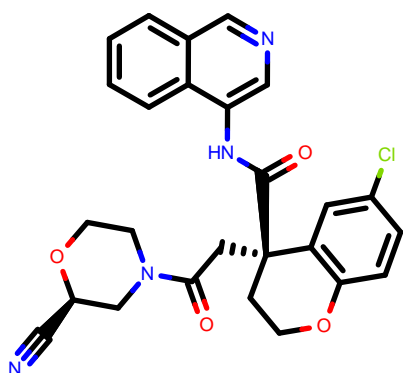
SMILES: C[C@H](CC(=O)OC)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4514

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.26

EN300-70489_1_1_1



CID: EN300-70489_1_1_1

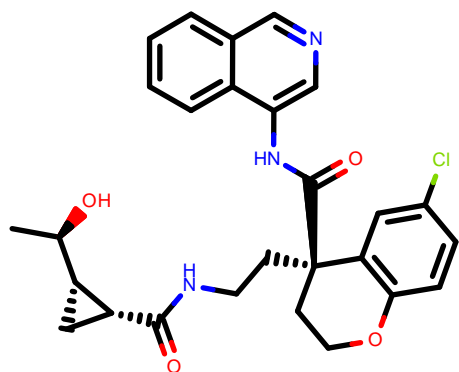
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)C#N

RUN: RUN3553

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.24

EN300-6729572_3_8_1



CID: EN300-6729572_3_8_1

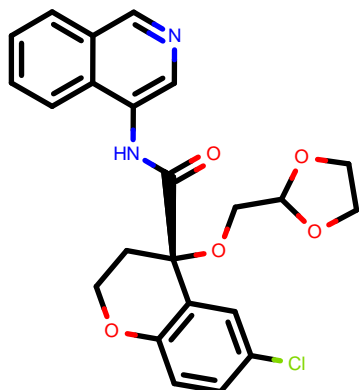
SMILES: C[C@H]([C@@H]1C[C@H]1C(=O)NCC)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5O

RUN: RUN3895

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.29

EN300-77092_1_1_1



CID: EN300-77092_1_1_1

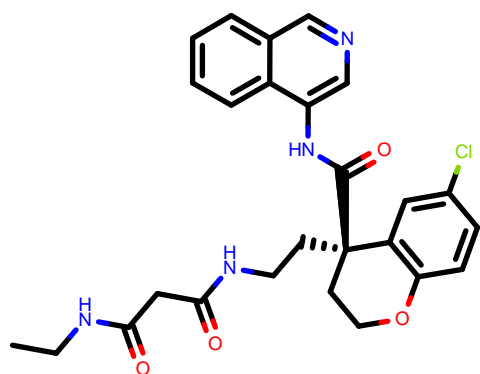
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5OCCO5

RUN: RUN5517

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.26

EN300-129455_3_1_1



CID: EN300-129455_3_1_1

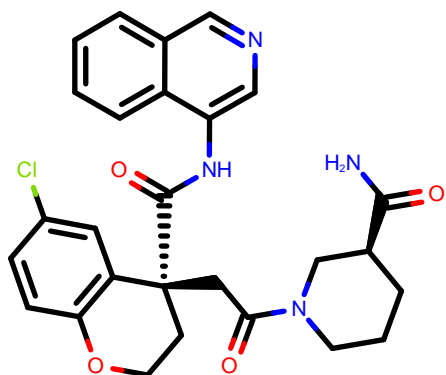
SMILES: CCNC(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN3853

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.33

EN300-1667084_1_1_1



CID: EN300-1667084_1_1_1

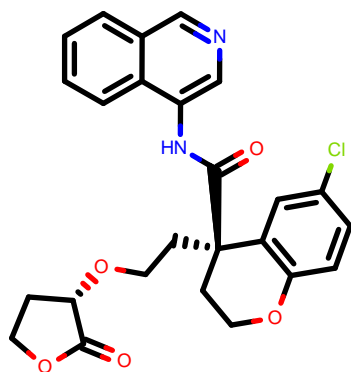
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC[C@@H](C5)C(=O)N

RUN: RUN5280

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.35

EN300-20496_3_2_1



CID: EN300-20496_3_2_1

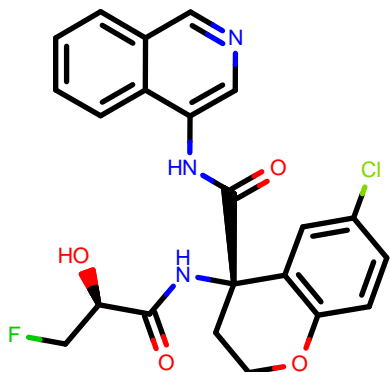
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@@H]5COOC5=O

RUN: RUN3049

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.26

EDG-MED-90036822-16_1



CID: EDG-MED-90036822-16_1

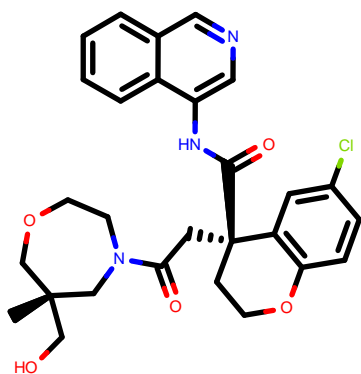
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](CF)O

RUN: RUN1550

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.23

EN300-224665_1_1_1



CID: EN300-224665_1_1_1

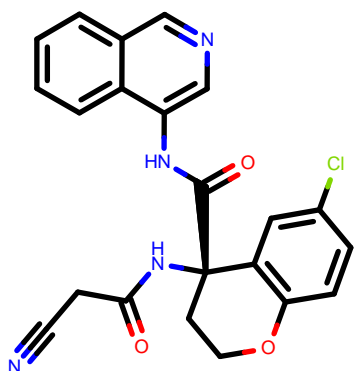
SMILES: C[C@@]1(CN(CCOC1)C(=O)C[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5)CO

RUN: RUN5865

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.36

EN300-19926_1_1_1



CID: EN300-19926_1_1_1

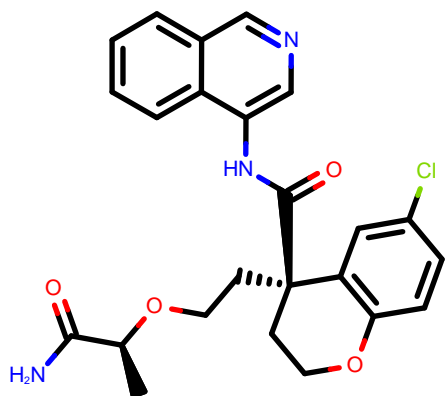
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)CC#N

RUN: RUN3857

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.17

EN300-17381_3_1_1



CID: EN300-17381_3_1_1

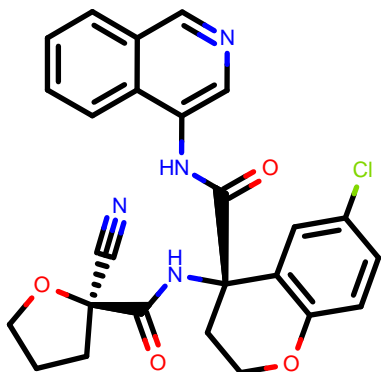
SMILES: C[C@@]([H])(C(=O)N)OCC[C@@]1(CCOC2c1cc(cc2)C)C(=O)Nc3ncnc4c3cccc4

RUN: RUN2975

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.26

EN300-3710141_1_2_1



CID: EN300-3710141_1_2_1

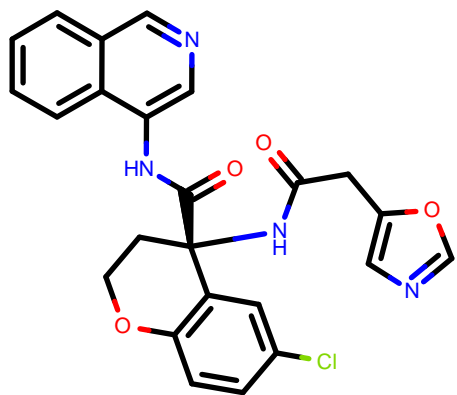
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)[C@@]5(CCCO5)C#N

RUN: RUN3435

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.28

EN300-6491117_1_1_1



CID: EN300-6491117_1_1_1

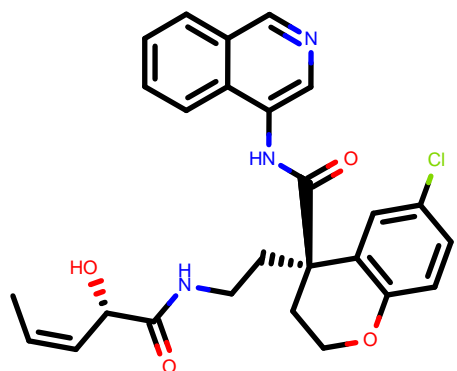
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5cnco5

RUN: RUN3226

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.21

EN300-300217_3_1_1



CID: EN300-300217_3_1_1

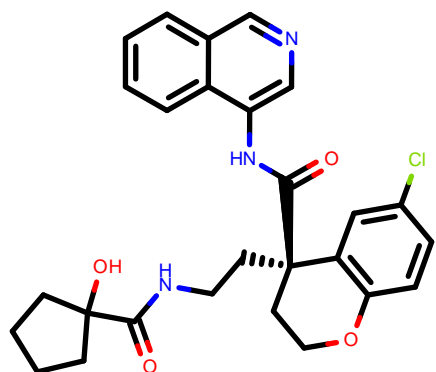
SMILES: C/C=C/[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3822

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.35

EN300-25960_3_1_1



CID: EN300-25960_3_1_1

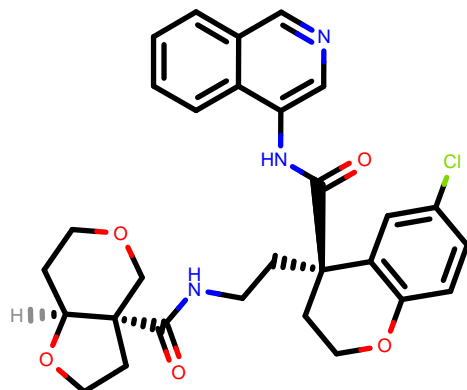
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCCC5)O

RUN: RUN4867

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.34

EN300-341337_3_4_1



CID: EN300-341337_3_4_1

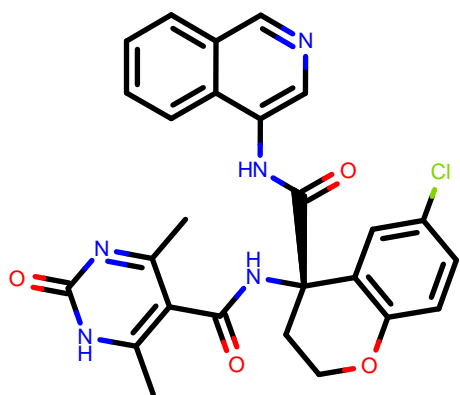
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]56COC[C@@H]5COC6

RUN: RUN6673

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.31

EN300-175506_1_1_1



CID: EN300-175506_1_1_1

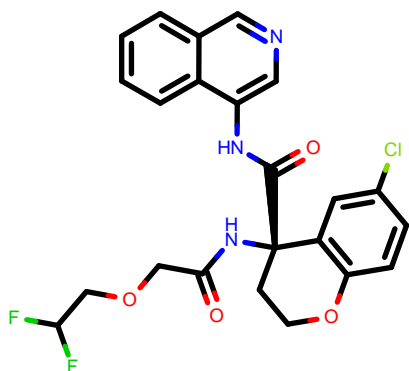
SMILES: Cc1c(c(nc(=O)[nH]1)C(=O)N)C@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3741

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.28

EN300-315792_1_1_1



CID: EN300-315792_1_1_1

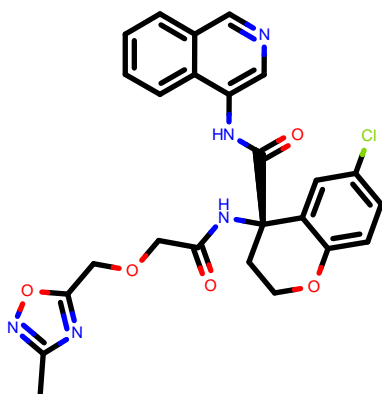
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F

RUN: RUN2866

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.23

EN300-77006_1_1_1



CID: EN300-77006_1_1_1

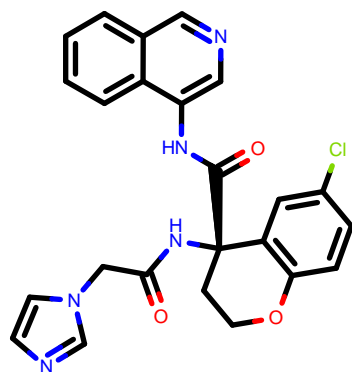
SMILES: Cc1nc(on1)COC(=O)N)C@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3771

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.47

EN300-38979_1_1_1



CID: EN300-38979_1_1_1

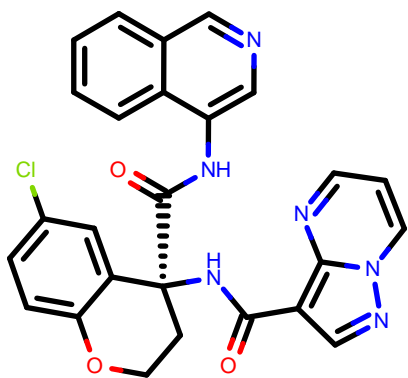
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5

RUN: RUN3447

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.20

EN300-29520_1_1_1



CID: EN300-29520_1_1_1

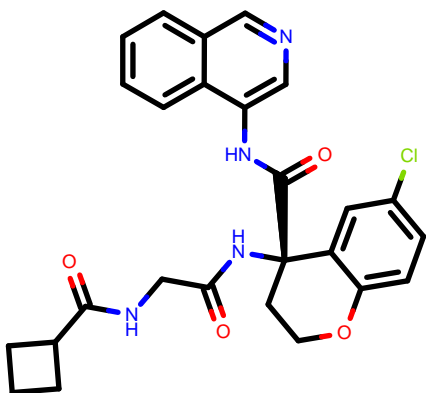
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5nccc6

RUN: RUN3639

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.24

EN300-62448_1_1_1



CID: EN300-62448_1_1_1

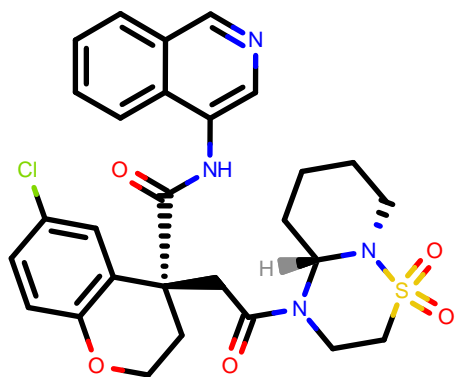
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)C5CCO5

RUN: RUN4625

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.25

ALP-UNI-3496895b-1_2



CID: ALP-UNI-3496895b-1_2

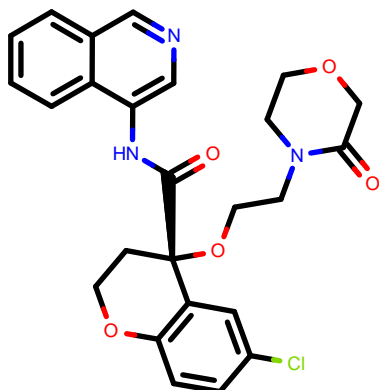
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C1=O)NS(=O)(=O)N1N@H[C@@H]5CCCC5

RUN: RUN2352

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.48

CHO-MSK-5891c1ff-6_1



CID: CHO-MSK-5891c1ff-6_1

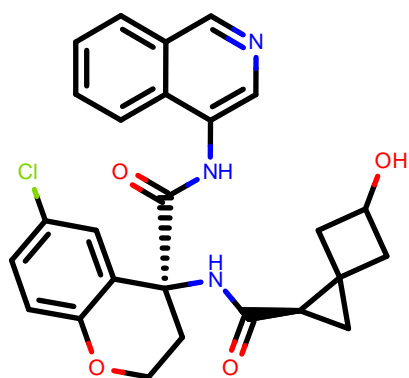
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOCC5=O

RUN: RUN1701

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.25

EN300-1717166_1_1_1



CID: EN300-1717166_1_1_1

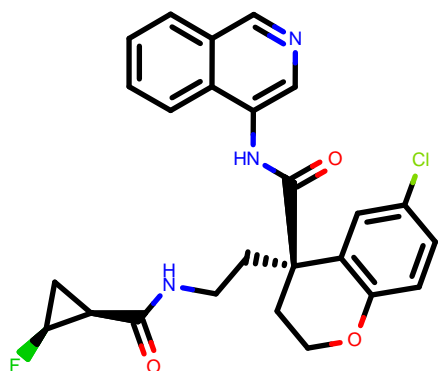
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC56CC(C)6O

RUN: RUN3456

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.28

EN300-1654606_3_1_1



CID: EN300-1654606_3_1_1

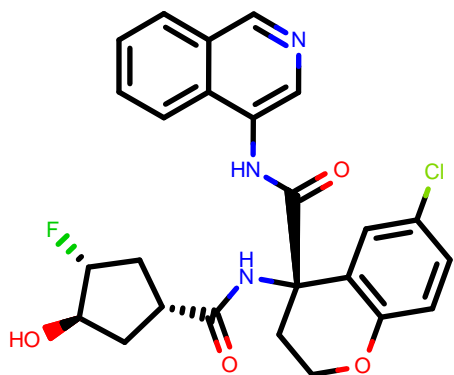
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN3426

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

EDG-MED-90036822-85_1



CID: EDG-MED-90036822-85_1

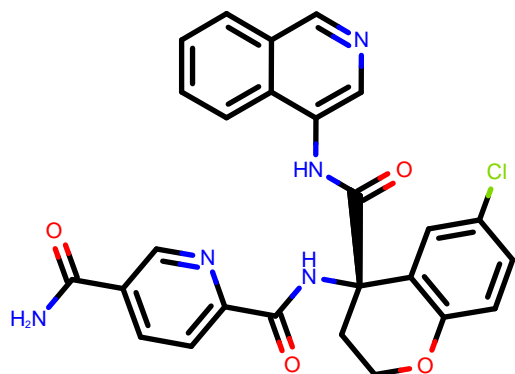
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H]5(F)O

RUN: RUN1660

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.26

EN300-58880_1_1_1



CID: EN300-58880_1_1_1

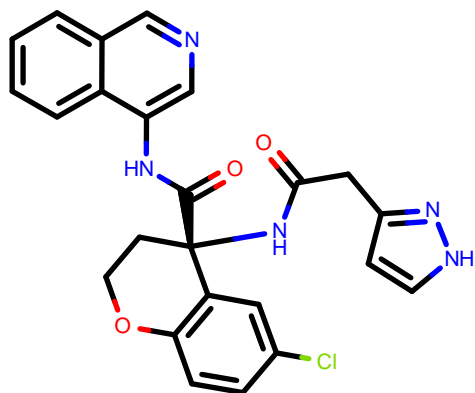
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(nc5)C(=O)N

RUN: RUN4500

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

VLA-UCB-34f3ed0c-4_1_1



CID: VLA-UCB-34f3ed0c-4_1_1

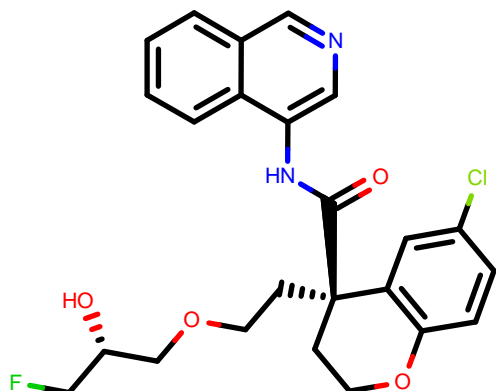
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cc[nH]5

RUN: RUN3934

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

EN300-1968342_3_2_1



CID: EN300-1968342_3_2_1

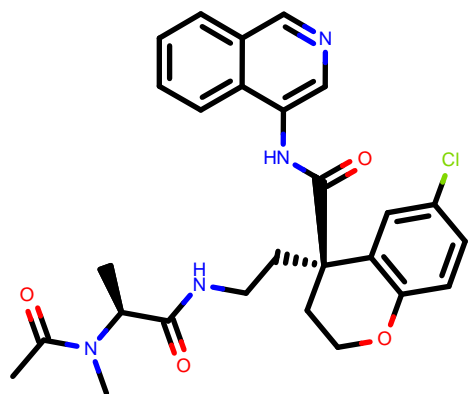
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN4030

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.34

EN300-863933_3_1_1



CID: EN300-863933_3_1_1

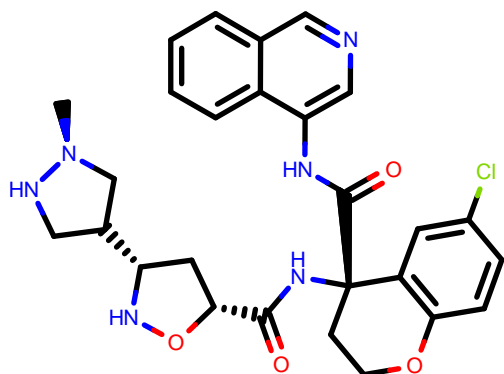
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4)N(C)C(=O)C

RUN: RUN3852

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.28

EN300-92605_1_2_1



CID: EN300-92605_1_2_1

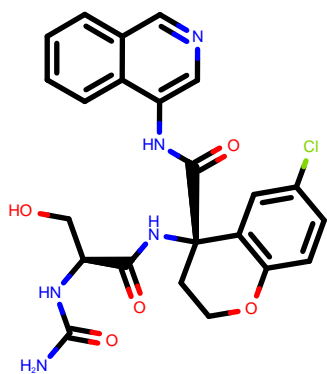
SMILES: Cn1cc[nH]1[C@@H]2[C@@H](ON2)C(=O)NC@@3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccoc6

RUN: RUN4280

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.32

EN300-10170_1_2_1



CID: EN300-10170_1_2_1

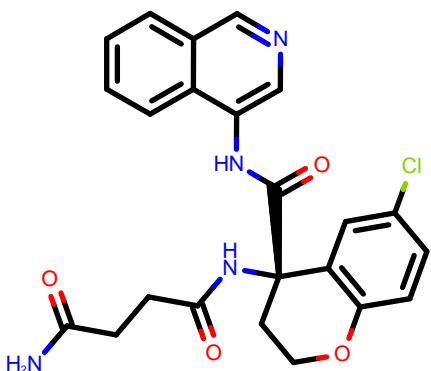
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](CO)NC(=O)N

RUN: RUN6443

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.23

EN300-178515_1_1_1



CID: EN300-178515_1_1_1

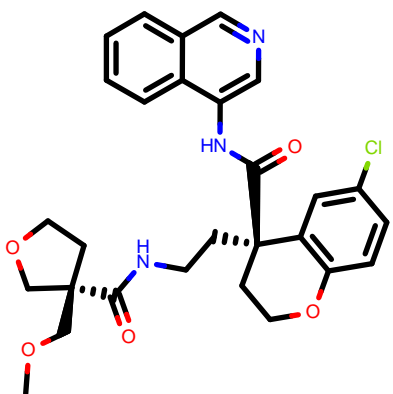
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCC(=O)N

RUN: RUN4801

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.23

EN300-248883_3_1_1



CID: EN300-248883_3_1_1

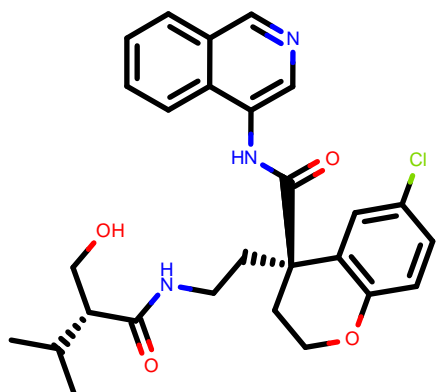
SMILES: COc[C@@]1(CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN3477

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.33

EN300-153257_3_2_1



CID: EN300-153257_3_2_1

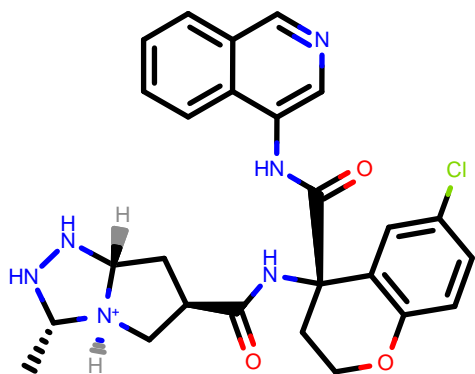
SMILES: CC(C)[C@H](CO)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3ccc4

RUN: RUN3819

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.32

EN300-6729747_1_1_3



CID: EN300-6729747_1_1_3

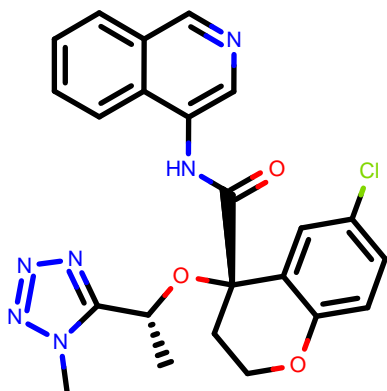
SMILES: C[C@@H]1N[N]C@H2[N@@H+]1C[C@@H]3C2C(-O)N[C@@]3(C)CCOc4c3cc(cc4)Cl[C@@]2O

RUN: RUN3156

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.44

EN300-173006_1_2_1



CID: EN300-173006_1_2_1

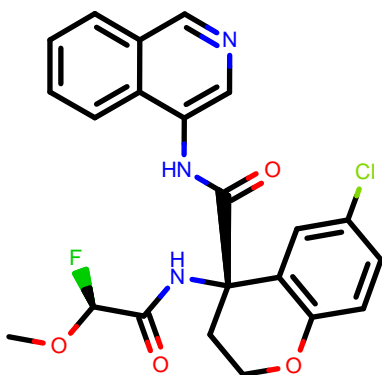
SMILES: C[C@@H](c1nnnn1C)O[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6136

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.23

EDG-MED-90036822-33_2



CID: EDG-MED-90036822-33_2

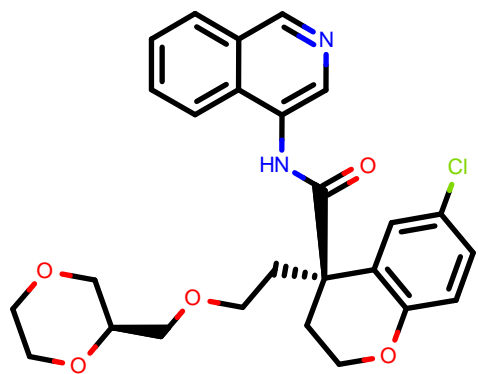
SMILES: CO[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)F

RUN: RUN1561

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.18

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

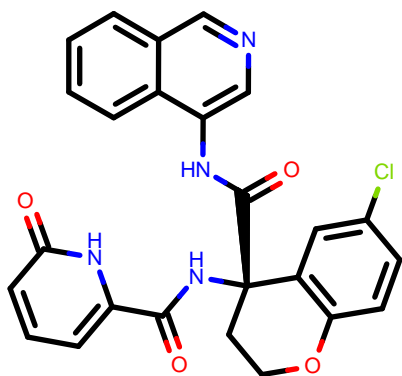
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)Cl)COC[C@@]@H]5COCOC5

RUN: RUN3113

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.32

EN300-34636_1_1_1



CID: EN300-34636_1_1_1

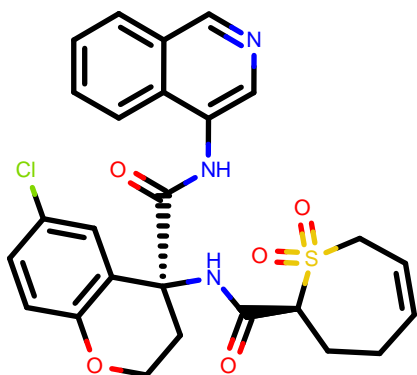
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cccc(=O)[nH]5

RUN: RUN5426

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.27

EN300-6499531_1_1_1



CID: EN300-6499531_1_1_1

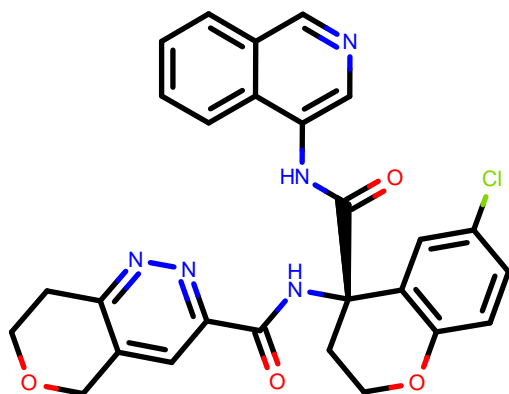
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5CSCC(=O)O5

RUN: RUN4536

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-7456641_1_1_1



CID: EN300-7456641_1_1_1

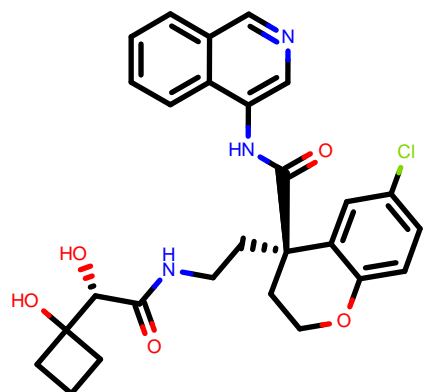
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c(n5)CCOC6

RUN: RUN3204

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.30

EN300-1073320_3_2_1



CID: EN300-1073320_3_2_1

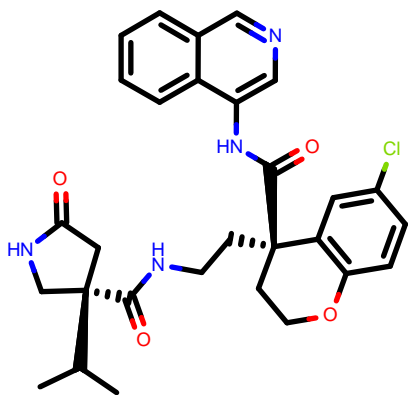
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5C(C5)O5

RUN: RUN7048

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.27

EN300-211203_3_1_1



CID: EN300-211203_3_1_1

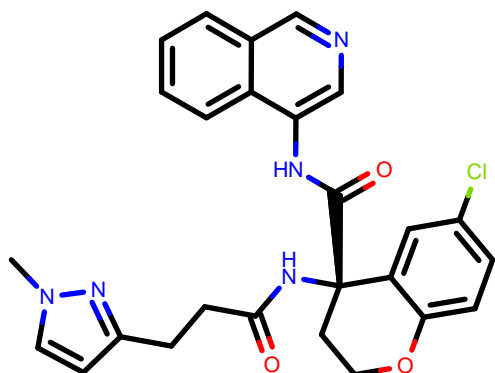
SMILES: CC(C)[C@@H]1(CC(=O)NC1)C(=O)NCC[C@H]2(CCOC3C2CC(C3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6089

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.29

EN300-92790_1_1_1



CID: EN300-92790_1_1_1

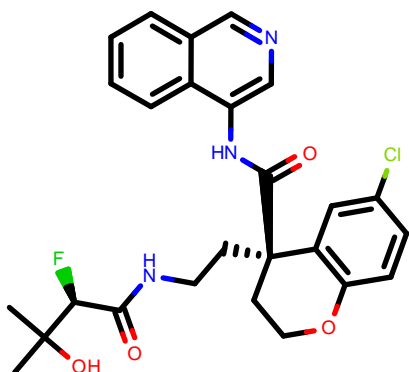
SMILES: Cn1ccc(n1)CCC(=O)N[C@H]2(CCOC3C2CC(C3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN2955

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.24

EN300-264744_3_2_1



CID: EN300-264744_3_2_1

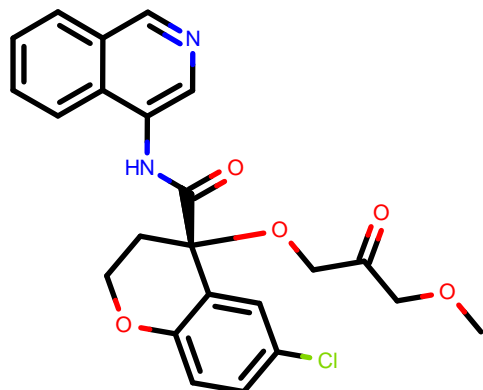
SMILES: CC(C)(C@H)(C(=O)NCC[C@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)F)O

RUN: RUN3685

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-125140_1_1_1



CID: EN300-125140_1_1_1

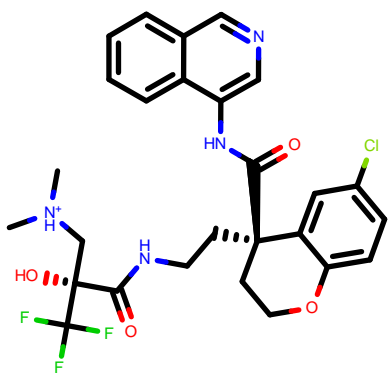
SMILES: COCC(=O)CO[C@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN4613

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.27

EN300-7459545_3_1_1



CID: EN300-7459545_3_1_1

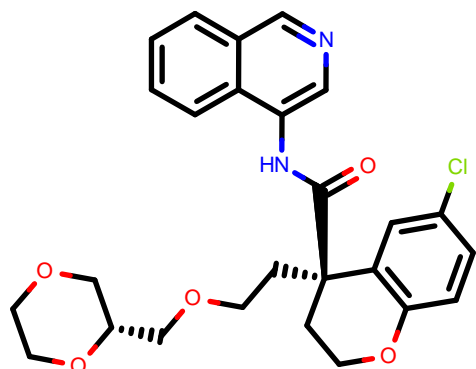
SMILES: CN(C)C[C@@]([C](=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)(C(F)(F)F)O

RUN: RUN3276

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.62

EN300-139167_3_2_1



CID: EN300-139167_3_2_1

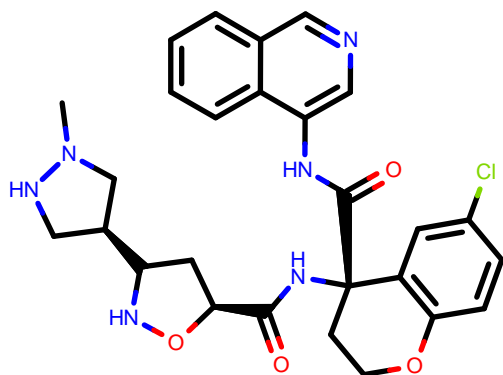
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]([C@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCOC5

RUN: RUN4100

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

ALP-UNI-dbbfd3db-13_1



CID: ALP-UNI-dbbfd3db-13_1

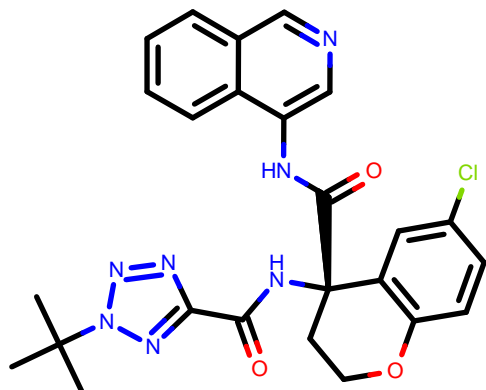
SMILES: Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN2629

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.24

EN300-268087_1_1_1



CID: EN300-268087_1_1_1

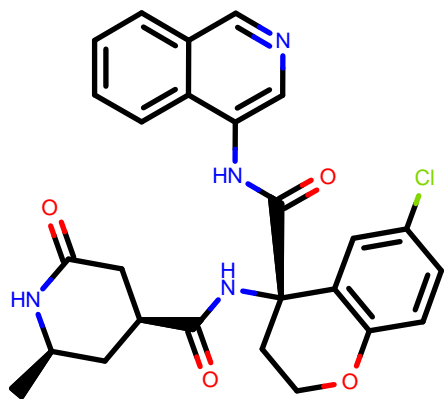
SMILES: CC(C)(C)n1nc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3014

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.24

EN300-7435400_1_1_1



CID: EN300-7435400_1_1_1

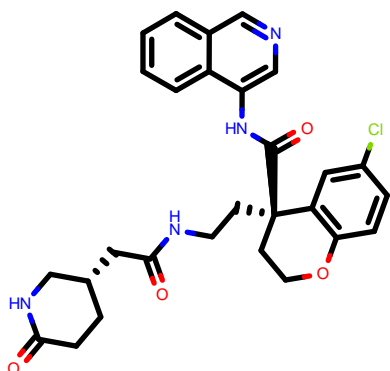
SMILES: C[C@@H]1C[C@@H](CC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3709

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.25

EN300-246992_3_1_1



CID: EN300-246992_3_1_1

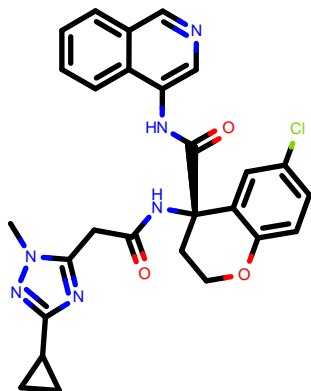
SMILES: c1ccc2c(c1)ncnc2N[C@@]([C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C)C(=O)Nc5ccc6c5ccc6

RUN: RUN4552

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.31

EN300-260418_1_1_1



CID: EN300-260418_1_1_1

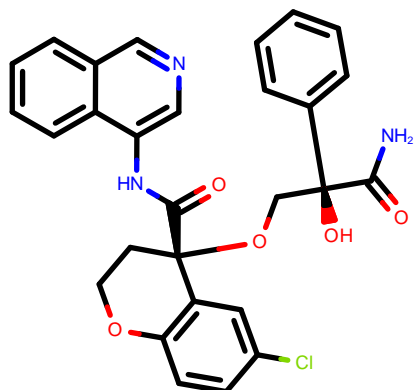
SMILES: Cn1c(nc(n1)C2CC2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN5634

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.31

EN300-248526_1_1_1



CID: EN300-248526_1_1_1

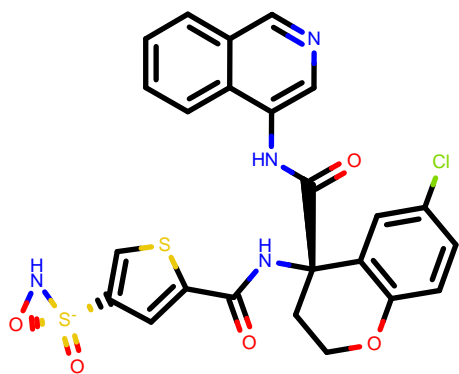
SMILES: c1ccc(cc1)[C@@]([C@]([C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C(=O)N)O

RUN: RUN7122

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.26

EN300-98099_1_1_1



CID: EN300-98099_1_1_1

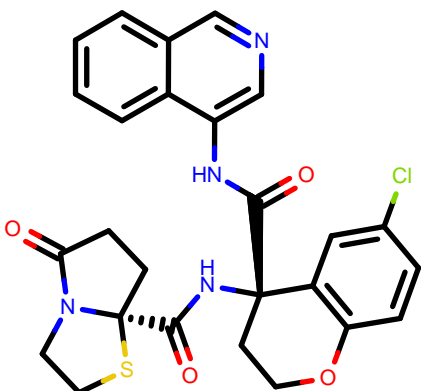
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(s5)S(=O)(=O)N

RUN: RUN4557

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.23

EN300-10334_1_1_1



CID: EN300-10334_1_1_1

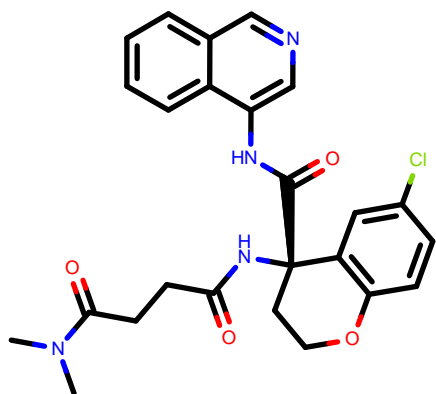
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCCC(=O)N5CCS6

RUN: RUN3914

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.31

EN300-176877_1_1_1



CID: EN300-176877_1_1_1

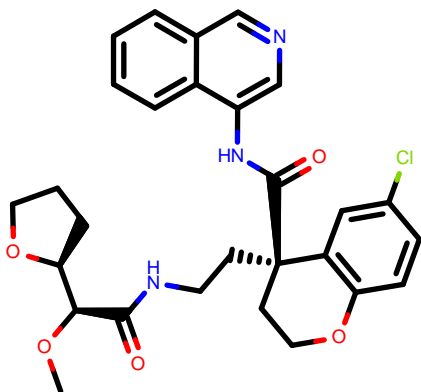
SMILES: CN(C)C(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4873

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.26

EN300-6277108_3_1_1



CID: EN300-6277108_3_1_1

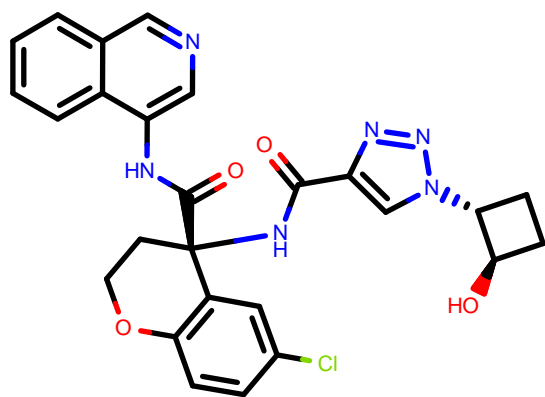
SMILES: CO[C@@H]1[C@@H](C@H)1CCCO1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN6746

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.35

EN300-316196_1_1_1



CID: EN300-316196_1_1_1

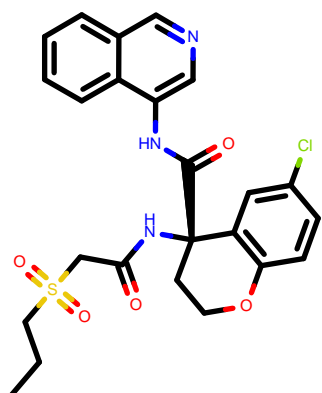
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C3CCOC3C(=O)N4C(=O)C5=CN=CN5[C@@H](O)C4

RUN: RUN3345

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.27

EN300-52325_1_1_1



CID: EN300-52325_1_1_1

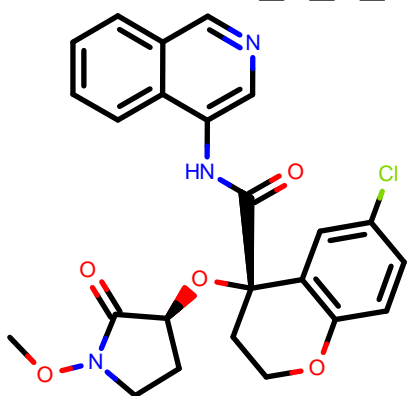
SMILES: CCCC(=O)(=O)CC(=O)N[C@@H](Cl)C1CCOC2c1cc(cc2)C1C(=O)Nc3cnc4c3cccc4

RUN: RUN3904

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.33

EN300-302058_1_1_1



CID: EN300-302058_1_1_1

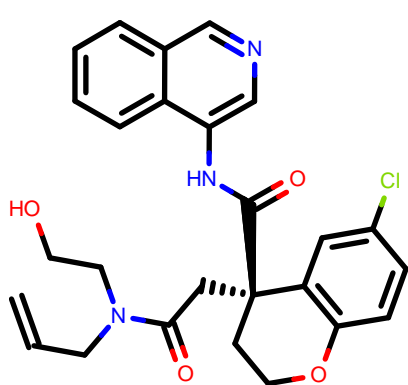
SMILES: CON1CC[C@@H](C1=O)O[C@@H](Cl)C2CCOC3c2cc(cc3)C1C(=O)Nc4cnc5c4cccc5

RUN: RUN4382

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.25

EN300-79536_1_1_1



CID: EN300-79536_1_1_1

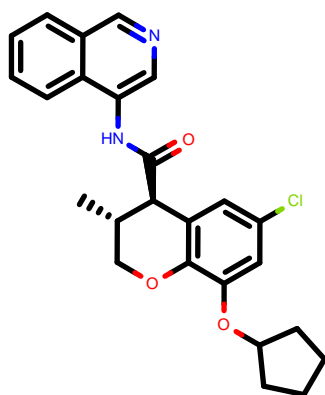
SMILES: C=CCN(CCO)C(=O)C[C@@H](Cl)C1CCOC2c1cc(cc2)C1C(=O)Nc3cnc4c3cccc4

RUN: RUN4793

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-4_1



CID: DAR-DIA-0d514e7d-4_1

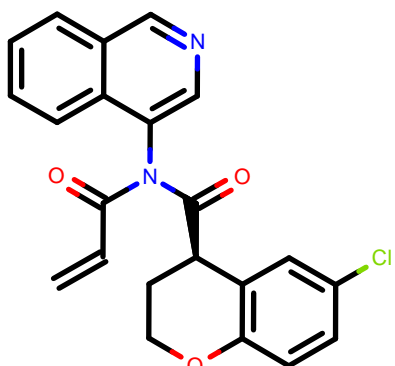
SMILES: C[C@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN793

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.21

MAT-POS-090737b9-1_1



CID: MAT-POS-090737b9-1_1

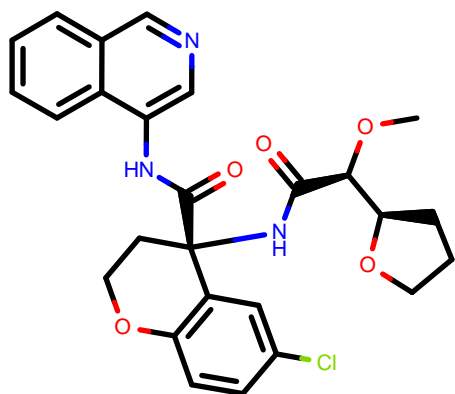
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN1995

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.16

EN300-6277108_1_3_1



CID: EN300-6277108_1_3_1

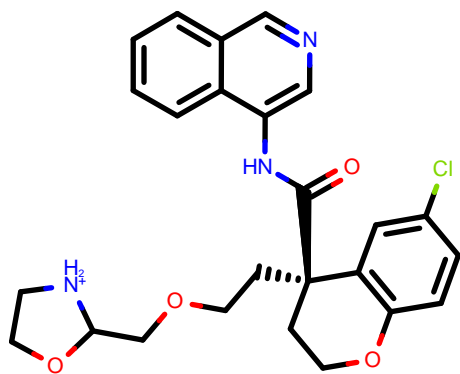
SMILES: CO[C@@H]([C@H]1CCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3669

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.28

EN300-317555_3_1_1



CID: EN300-317555_3_1_1

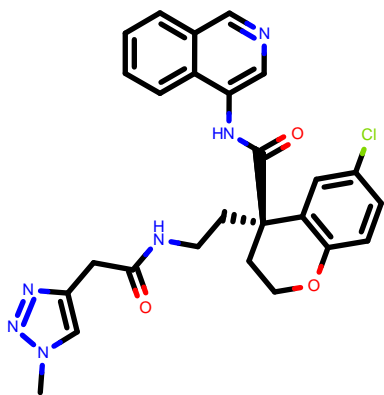
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5

RUN: RUN4543

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.21

EN300-1073264_3_1_1



CID: EN300-1073264_3_1_1

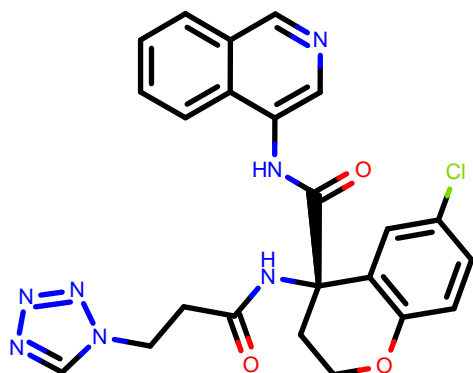
SMILES: Cn1cc(nn1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6865

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.29

EN300-191904_1_1_1



CID: EN300-191904_1_1_1

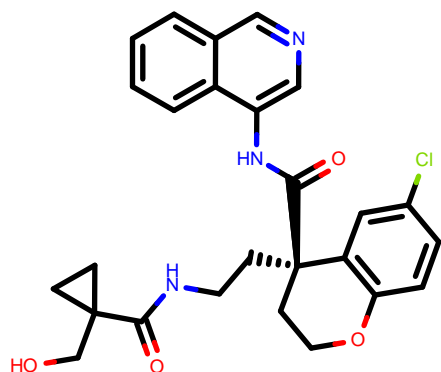
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ennn5

RUN: RUN3559

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.26

EN300-146174_3_1_1



CID: EN300-146174_3_1_1

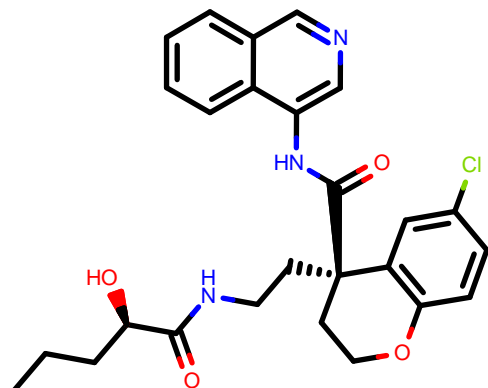
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)CO

RUN: RUN4260

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.27

EN300-300217_3_3_1



CID: EN300-300217_3_3_1

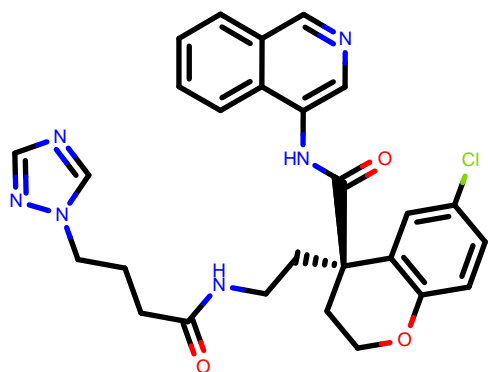
SMILES: C/C=C/[C@H](C)(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4O

RUN: RUN6615

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.33

EN300-316216_3_1_1



CID: EN300-316216_3_1_1

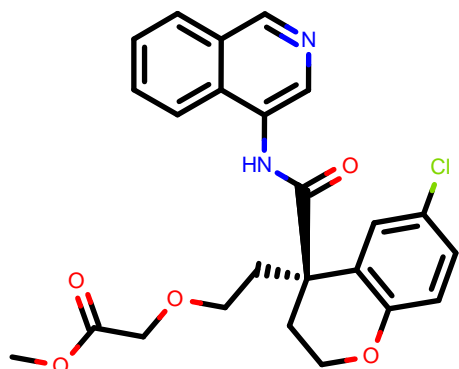
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CCCn5ncn5

RUN: RUN3677

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.33

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

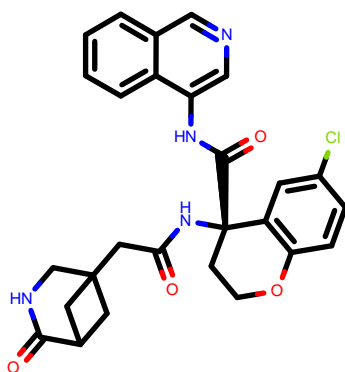
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4172

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-6487134_1_1_1



CID: EN300-6487134_1_1_1

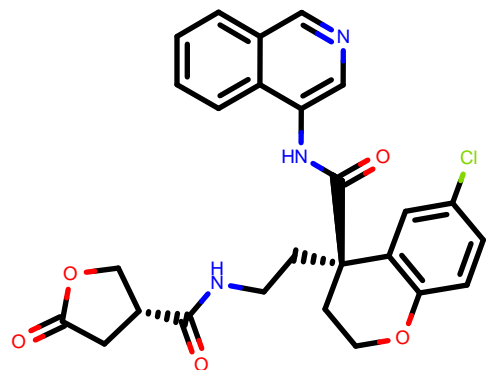
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)CC56CC(C5)C(=O)NC6

RUN: RUN3778

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.28

EN300-113234_3_1_1



CID: EN300-113234_3_1_1

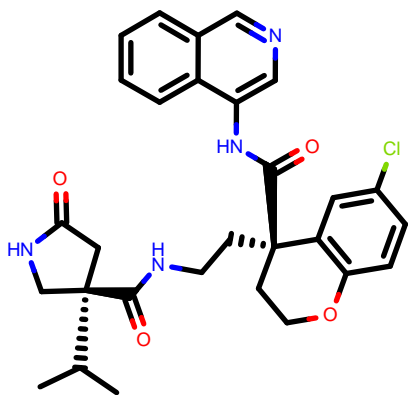
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@]5C(=O)OC5

RUN: RUN4258

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.35

EN300-211203_3_2_1



CID: EN300-211203_3_2_1

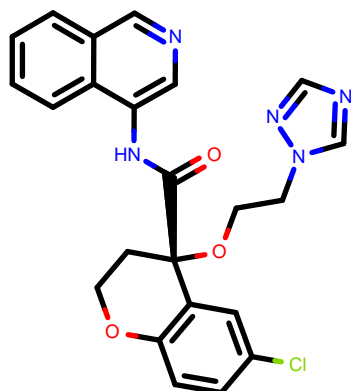
SMILES: CC(C)[C@H]1(CC(=O)NC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3743

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.36

EN300-6255179_1_1_1



CID: EN300-6255179_1_1_1

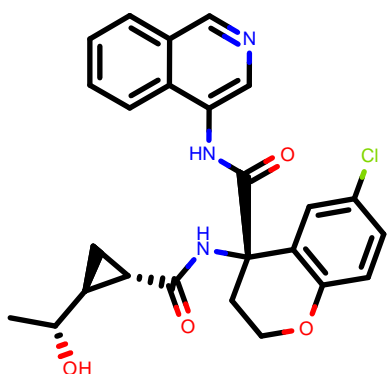
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cncn5

RUN: RUN4814

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.20

EN300-6729572_1_4_1



CID: EN300-6729572_1_4_1

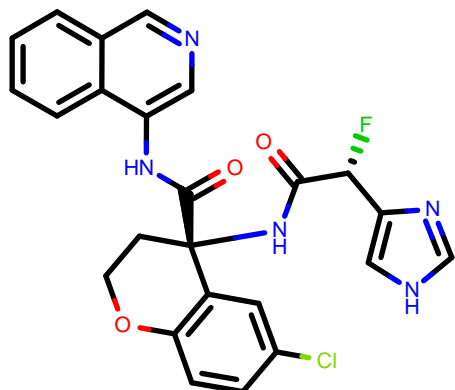
SMILES: C[C@H]1[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5O

RUN: RUN3223

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.23

EDG-MED-90036822-20_1



CID: EDG-MED-90036822-20_1

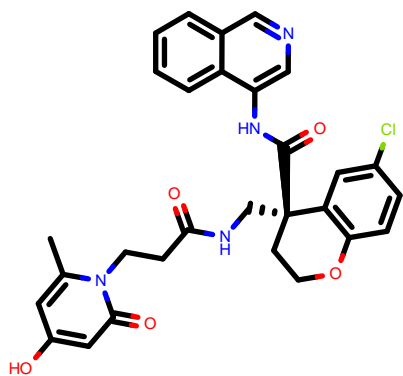
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5Cn5cnc(F)5

RUN: RUN1565

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-103435_2_1_1



CID: EN300-103435_2_1_1

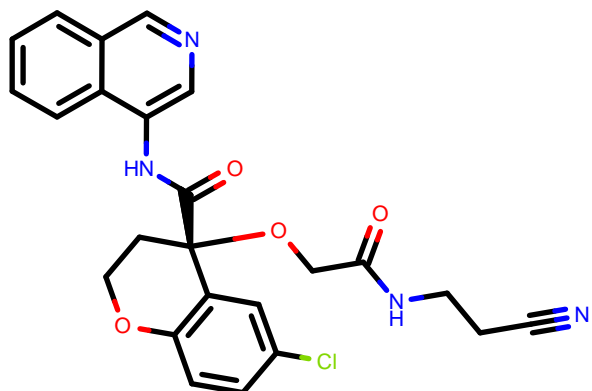
SMILES: Cc1cc(cc(=O)n1CCC(=O)NC[C@@]2(CCOC3C2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)[O-]

RUN: RUN2751

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.28

EN300-10895_1_1_1



CID: EN300-10895_1_1_1

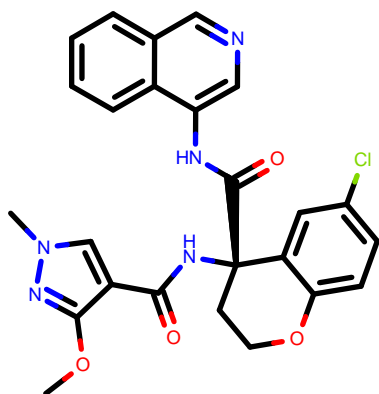
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)OCC(=O)NCCC#N

RUN: RUN4805

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.23

EN300-142957_1_1_1



CID: EN300-142957_1_1_1

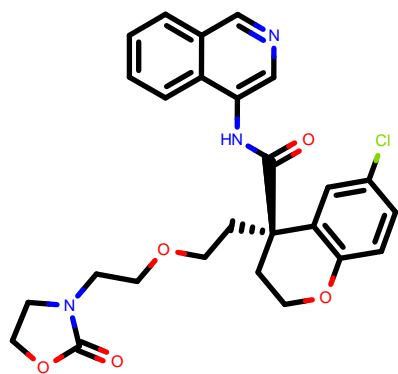
SMILES: Cn1cc(c(n1)OC)C(=O)N[C@@]2(CCOC3C2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3452

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.23

EN300-370967_3_1_1



CID: EN300-370967_3_1_1

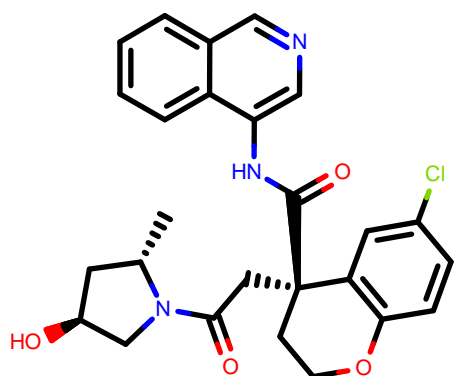
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)CCOCCN5COC5=O

RUN: RUN4033

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.26

EN300-173562_1_2_1



CID: EN300-173562_1_2_1

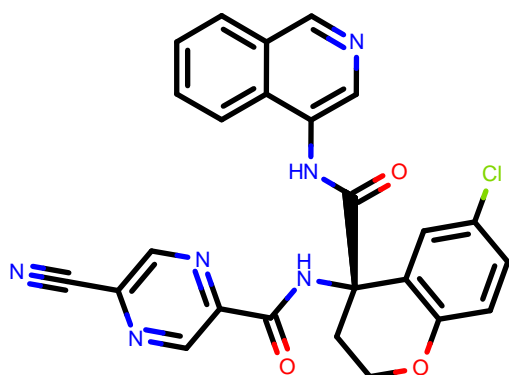
SMILES: C[C@H]1C[C@@H](CN1C(=O)C[C@]2(C)COCc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5O

RUN: RUN5676

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-149224_1_1_1



CID: EN300-149224_1_1_1

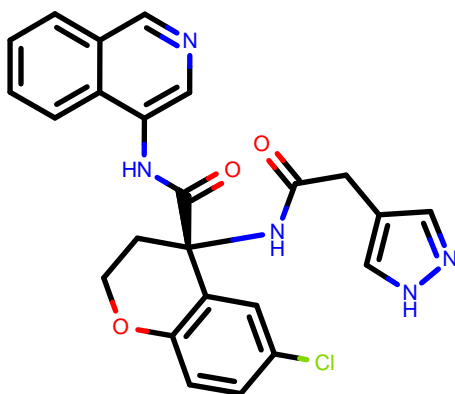
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)NC(=O)c5cnc(en5)C#N

RUN: RUN3245

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.24

EN300-1589101_1_1_1



CID: EN300-1589101_1_1_1

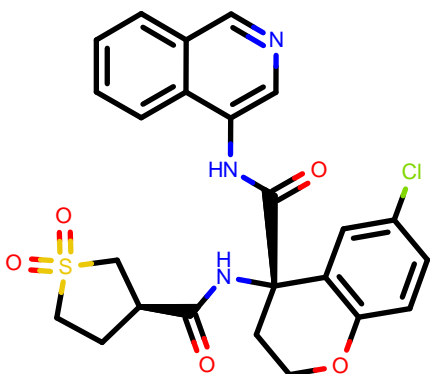
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)NC(=O)C5c[nH]c5

RUN: RUN2981

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.21

EN300-14437_1_2_1



CID: EN300-14437_1_2_1

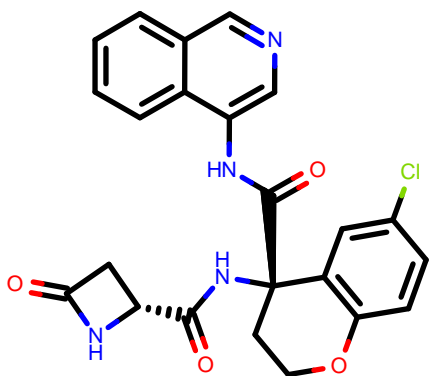
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)NC(=O)C5C(S(=O)(=O)C)C5

RUN: RUN4450

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-184266_1_1_1



CID: EN300-184266_1_1_1

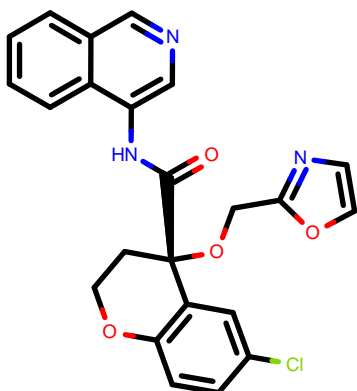
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5

RUN: RUN3151

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.20

EN300-317555_1_1_1



CID: EN300-317555_1_1_1

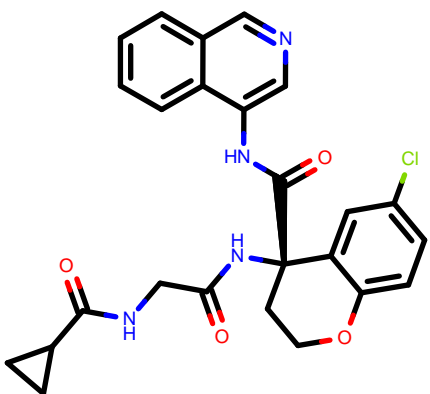
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5

RUN: RUN3804

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.22

EN300-36522_1_1_1



CID: EN300-36522_1_1_1

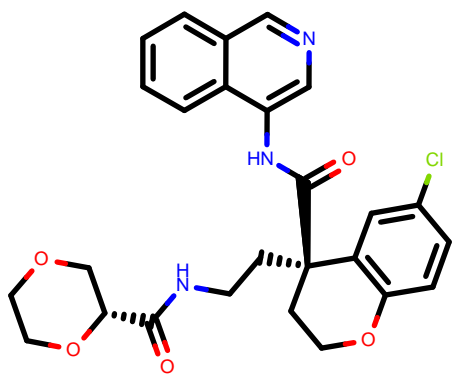
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)C5CCO5

RUN: RUN3266

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-36158_3_2_1



CID: EN300-36158_3_2_1

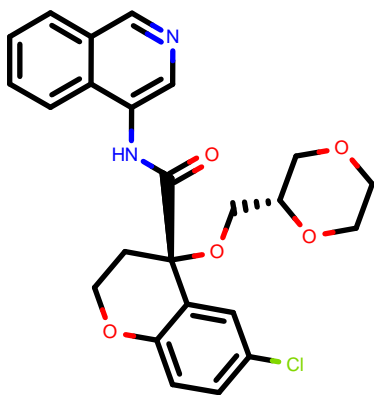
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5COC(CO)5

RUN: RUN4011

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.23

EN300-139167_1_1_1



CID: EN300-139167_1_1_1

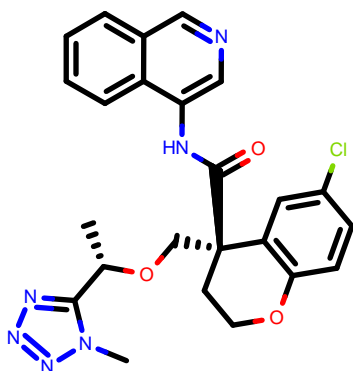
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c4)C)OC[C@@]5H5COCOC5

RUN: RUN4402

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.28

EN300-173006_2_1_1



CID: EN300-173006_2_1_1

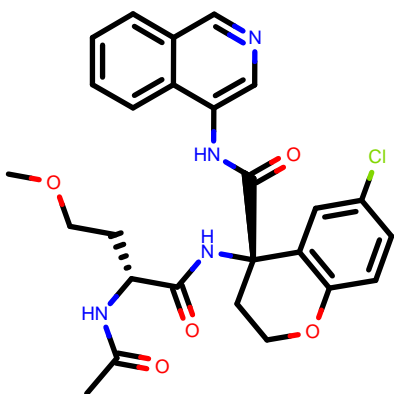
SMILES: C[C@@]H(c1nncn1C)OC[C@@]2(CCOc3c2cc(c3)C)C(=O)Nc4nnc5c4ccoc5

RUN: RUN3089

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.28

EN300-62074_1_2_1



CID: EN300-62074_1_2_1

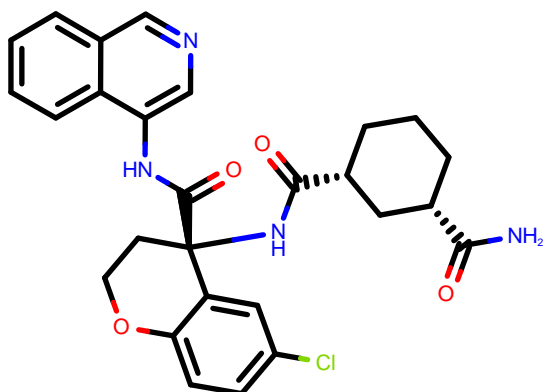
SMILES: CC(=O)N[C@@]H(COC)C(=O)N[C@@]1(CCOc2c1cc(c2)C)C(=O)Nc3nnc4c3ccoc4

RUN: RUN4520

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.27

EN300-90142_1_1_1



CID: EN300-90142_1_1_1

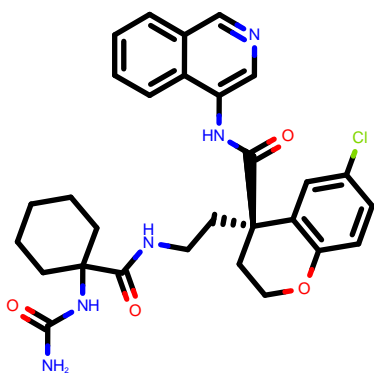
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c4)C)N[C@@]5C[C@@]6C[C@@]7C[C@@]6C[C@@]7C(=O)N

RUN: RUN3907

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.27

EN300-78368_3_1_1



CID: EN300-78368_3_1_1

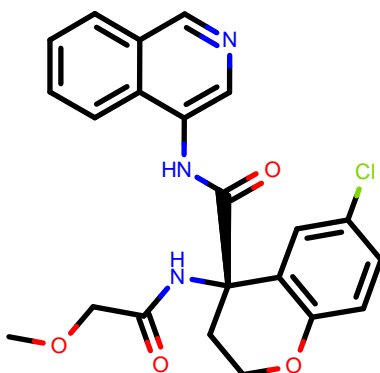
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCCC5)NC(=O)N

RUN: RUN6344

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.36

EN300-20233_1_1_1



CID: EN300-20233_1_1_1

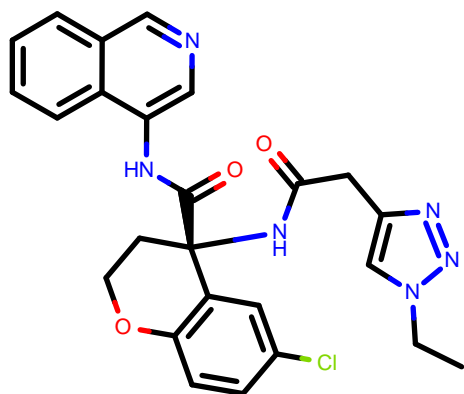
SMILES: COCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3461

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.23

EN300-717276_1_1_1



CID: EN300-717276_1_1_1

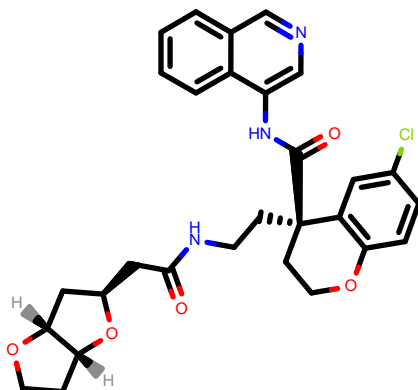
SMILES: CCn1cc(nn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4081

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-7355519_3_5_1



CID: EN300-7355519_3_5_1

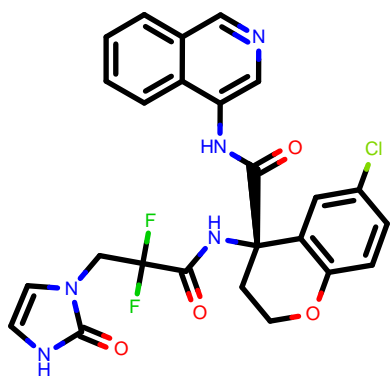
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@@H5C[C@@H]6[C@@H](O5)CCO6

RUN: RUN5254

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.33

EDG-MED-90036822-71_1



CID: EDG-MED-90036822-71_1

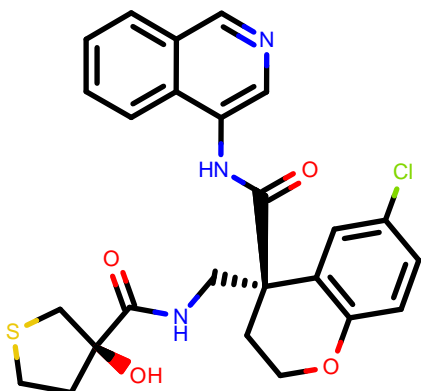
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(CN5CCNC5=O)F)F

RUN: RUN1662

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.30

EDJ-MED-40433386-3_1



CID: EDJ-MED-40433386-3_1

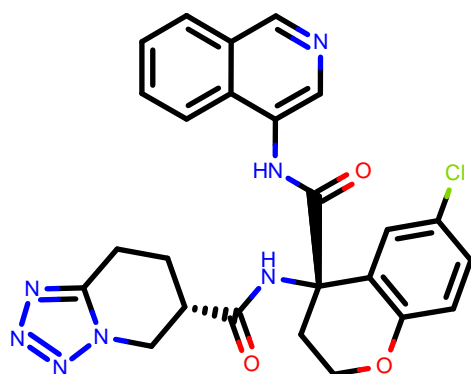
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@5(CCS5)O

RUN: RUN2407

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.39

EN300-269453_1_2_1



CID: EN300-269453_1_2_1

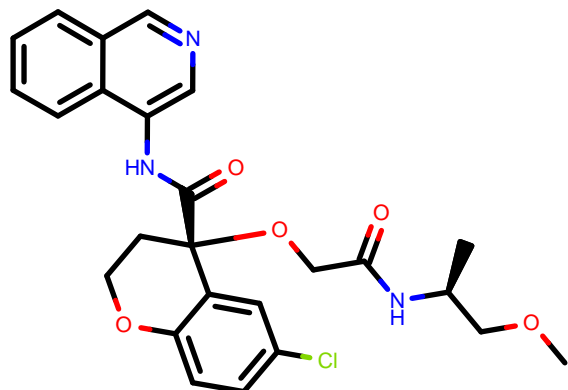
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@H]5CCc6n6nn6C5

RUN: RUN2938

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-02067_1_1_1



CID: EN300-02067_1_1_1

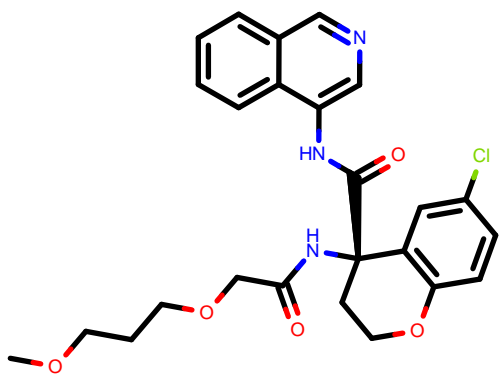
SMILES: C[C@@H](COC)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4

RUN: RUN4812

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.26

EN300-125769_1_1_1



CID: EN300-125769_1_1_1

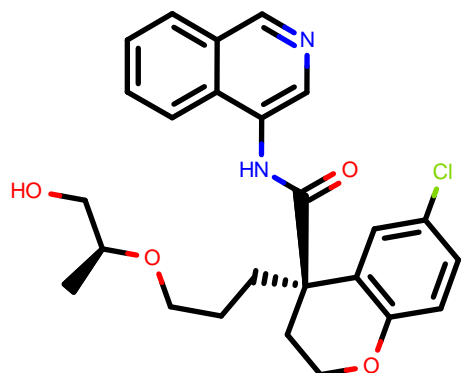
SMILES: COCCCCOC(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3262

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.28

EN300-175186_4_1_1



CID: EN300-175186_4_1_1

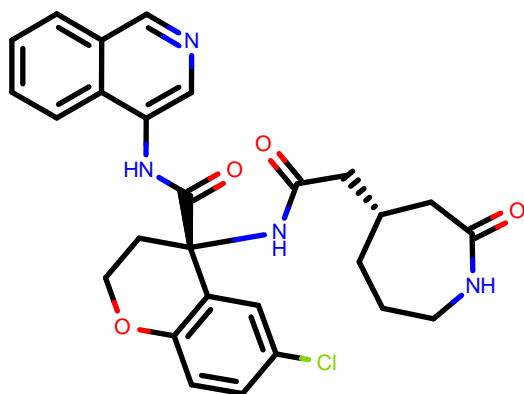
SMILES: C[C@@H](CO)OCCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3902

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.34

EN300-195590_1_2_1



CID: EN300-195590_1_2_1

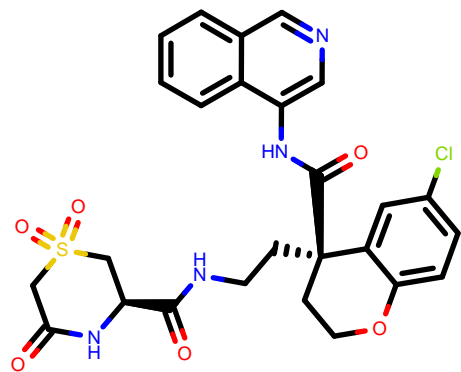
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]5CCNC(=O)C5

RUN: RUN4473

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.35

EN300-754584_3_1_1



CID: EN300-754584_3_1_1

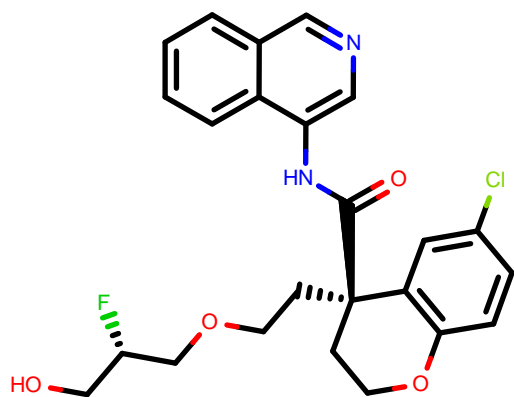
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H]5CS(=O)N5

RUN: RUN5226

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-1600517_3_2_1



CID: EN300-1600517_3_2_1

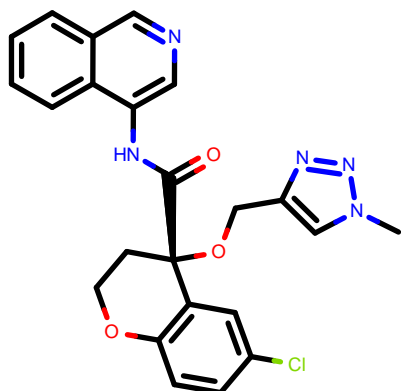
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)F

RUN: RUN3791

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.31

EN300-120282_1_1_1



CID: EN300-120282_1_1_1

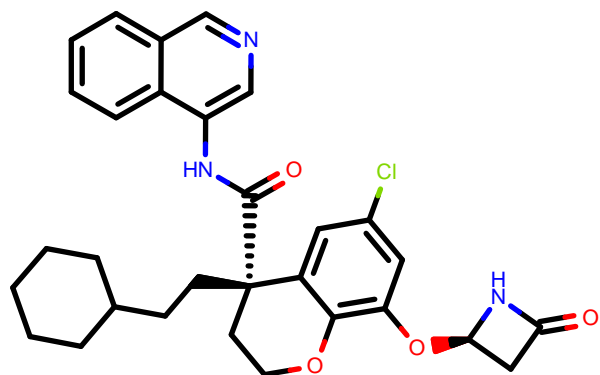
SMILES: Cn1cc(nn1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4786

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.19

VLA-UCB-05e51b3f-12_1



CID: VLA-UCB-05e51b3f-12_1

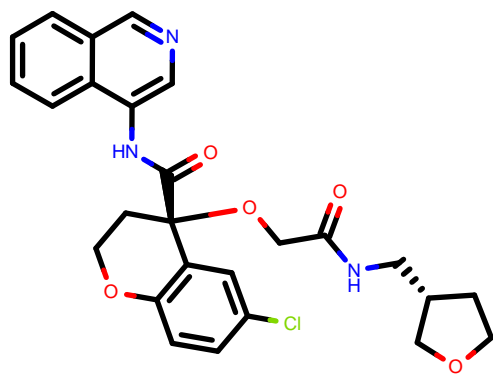
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C@@H)5CC(=O)N5)Cl)CCOC6CCCC6

RUN: RUN311

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.54

EN300-46832_1_1_1



CID: EN300-46832_1_1_1

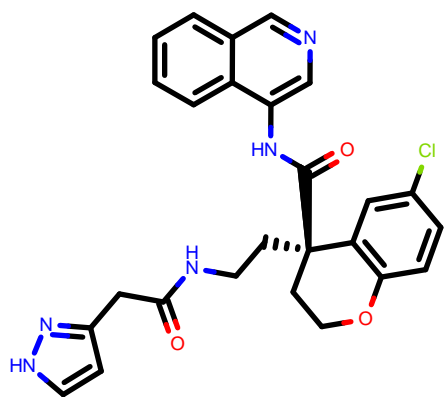
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCOC5

RUN: RUN4665

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.25

EN300-71405_3_1_1



CID: EN300-71405_3_1_1

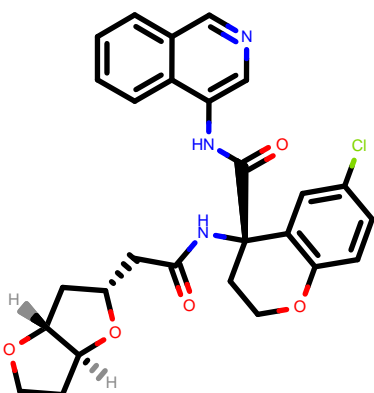
SMILES: c1ccc2c(c1)cnc2N[C@@H](C@@@3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5c[nH]5

RUN: RUN5277

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.28

EN300-735519_1_2_1



CID: EN300-735519_1_2_1

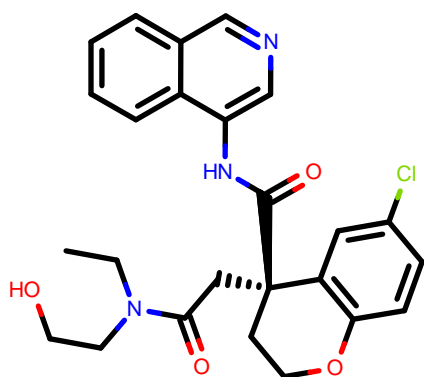
SMILES: c1ccc2c(c1)cnc2N[C@@H](C@@@3(CCOc4c3cc(cc4)C)N[C@@H]5C[C@@H]6C[C@@H]7O[C@H]5C[C@@H]67

RUN: RUN3737

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.26

EN300-74448_1_1_1



CID: EN300-74448_1_1_1

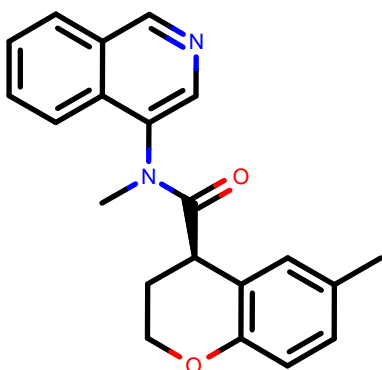
SMILES: CCN(CCO)C(=O)C[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN4929

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.29

MAK-UNK-3875bbc8-1_1



CID: MAK-UNK-3875bbc8-1_1

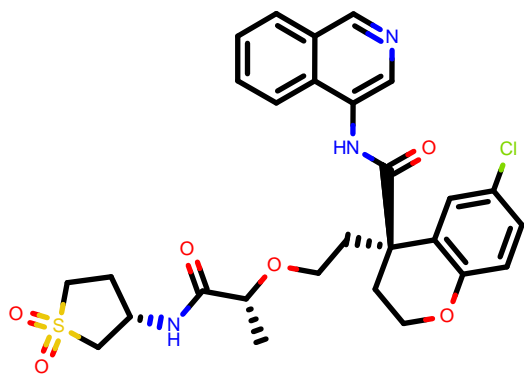
SMILES: Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)c3cnc4c3cccc4

RUN: RUN703

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.09

EN300-23318_3_4_1



CID: EN300-23318_3_4_1

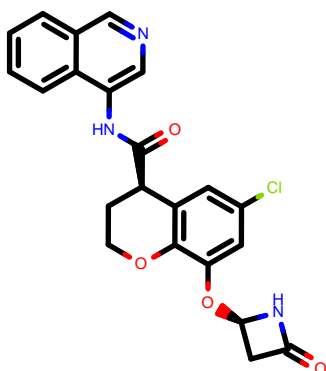
SMILES: C[C@H](Cl)C(=O)N[C@@H](CCS(=O)(=O)C1CC[C@H]2[C@@H](COC3C2C(=O)C3)C1)C(=O)N4CCCC4=O

RUN: RUN3060

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.29

VLA-UCB-50c39ae8-8_1



CID: VLA-UCB-50c39ae8-8_1

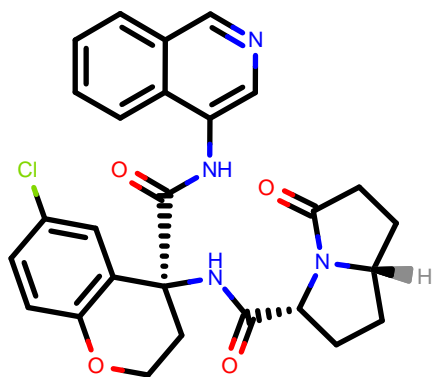
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](Cl)C3CCOC4C3C(=O)C4[C@@H]5CC(=O)N5Cl

RUN: RUN342

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.23

EN300-6479181_1_2_1



CID: EN300-6479181_1_2_1

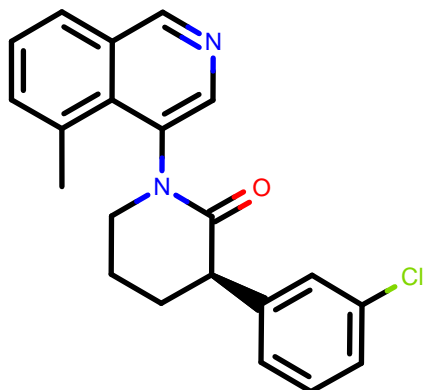
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](Cl)C3CCOC4C3C(=O)N4[C@@H]5CC[C@@H]6N5C(=O)C6

RUN: RUN3292

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.30

MIC-UNK-50cce87d-11_1



CID: MIC-UNK-50cce87d-11_1

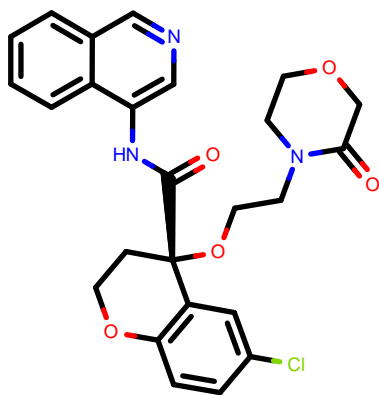
SMILES: Cc1cccc2c1c(cnc2)N3CCCC[C@@H](C3=O)c4cccc(c4)Cl

RUN: RUN566

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.35

EN300-219330_1_1_1



CID: EN300-219330_1_1_1

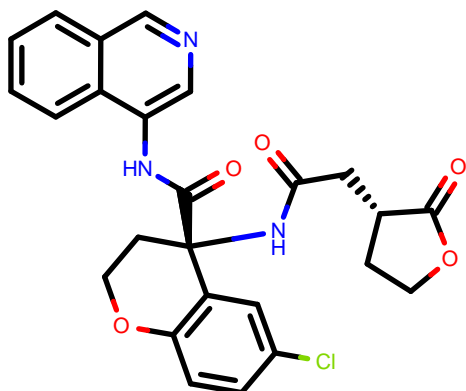
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOCC5=O

RUN: RUN3242

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.22

EN300-1072972_1_2_1



CID: EN300-1072972_1_2_1

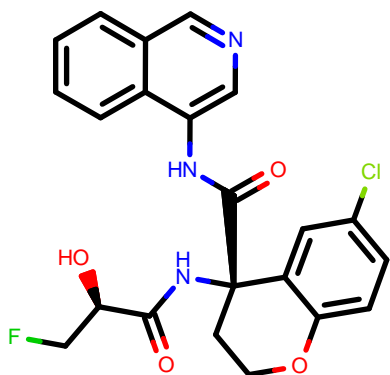
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCOCC5=O

RUN: RUN4008

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.23

EDG-MED-90036822-17_1



CID: EDG-MED-90036822-17_1

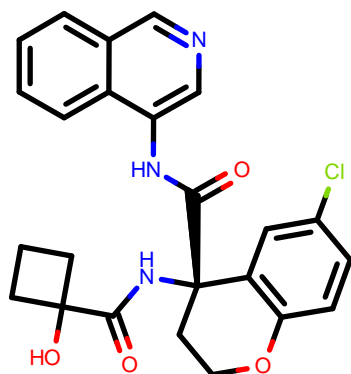
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CF)O

RUN: RUN1542

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.28

EN300-52009_1_1_1



CID: EN300-52009_1_1_1

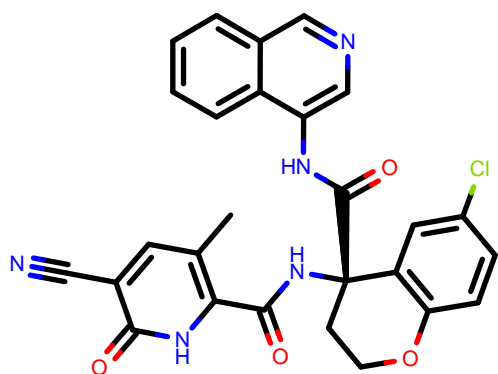
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)O

RUN: RUN3211

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.26

EN300-358956_1_1_1



CID: EN300-358956_1_1_1

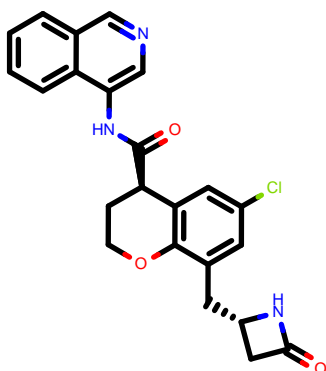
SMILES: Cc1cc(c(=O)[nH]c1C(=O)N)C@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)C#N

RUN: RUN4347

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.36

DAR-DIA-6a508060-5_3_1



CID: DAR-DIA-6a508060-5_3_1

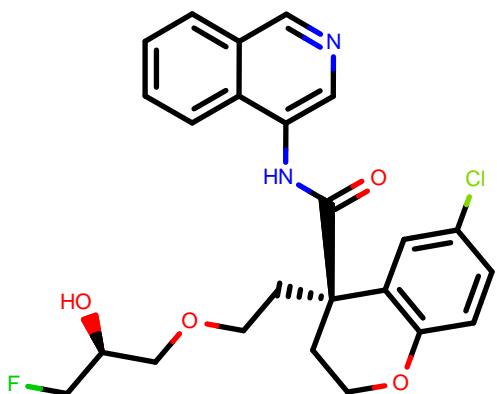
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C[C@@H]5CC(=O)N5)Cl

RUN: RUN3988

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.18

EN300-1968342_3_1_1



CID: EN300-1968342_3_1_1

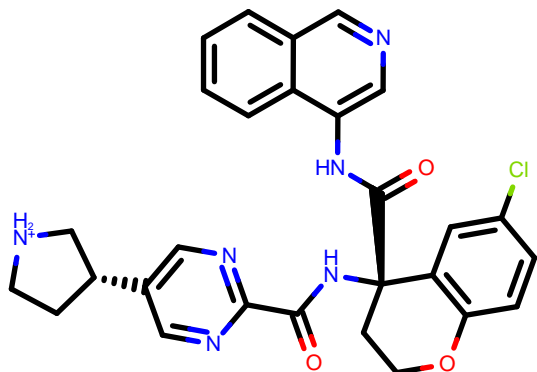
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CF)O

RUN: RUN2958

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.31

EDG-MED-90036822-104_1



CID: EDG-MED-90036822-104_1

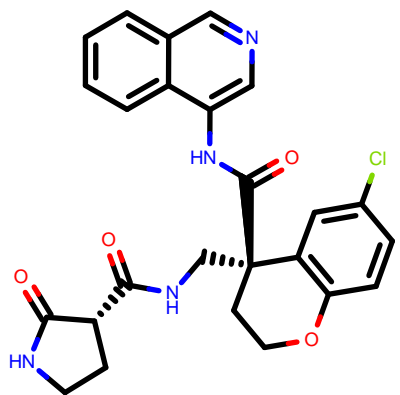
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nccn5)C#N

RUN: RUN1693

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.33

EN300-94945_2_1_1



CID: EN300-94945_2_1_1

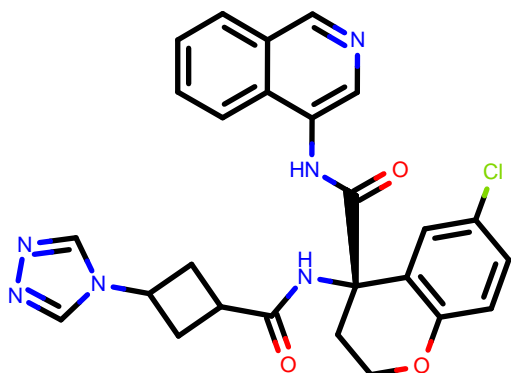
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CCNC5=O

RUN: RUN2914

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.20

EN300-1717596_1_1_1



CID: EN300-1717596_1_1_1

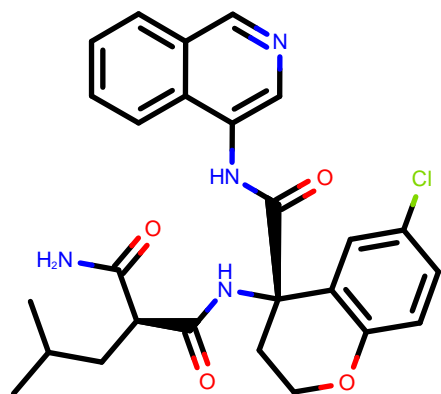
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5C(C)N5

RUN: RUN4270

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.35

EN300-250126_1_1_1



CID: EN300-250126_1_1_1

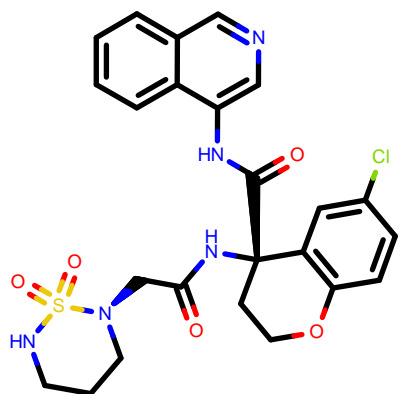
SMILES: CC(C)C[C@@H](C(=O)N)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccccc4

RUN: RUN2769

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.26

EN300-4726186_1_1_1



CID: EN300-4726186_1_1_1

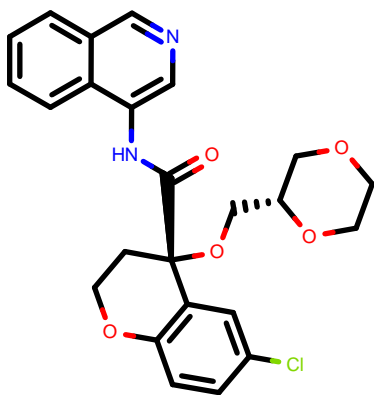
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)N[S](=O)(=O)C5CCNC5=O

RUN: RUN5310

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.43

EN300-139167_1_1_1



CID: EN300-139167_1_1_1

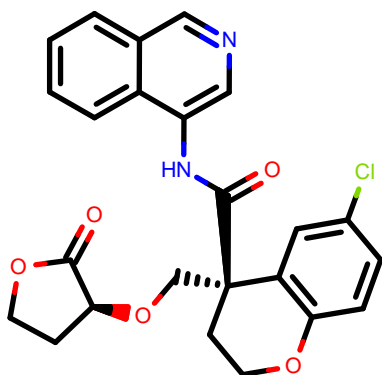
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCOC5

RUN: RUN4349

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.27

EDJ-MED-fcba3f31-8_1



CID: EDJ-MED-fcba3f31-8_1

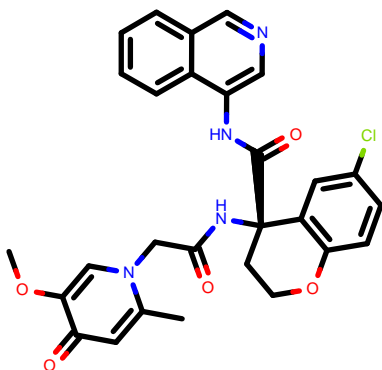
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5COCOC5=O

RUN: RUN2360

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.20

EN300-1271924_1_1_1



CID: EN300-1271924_1_1_1

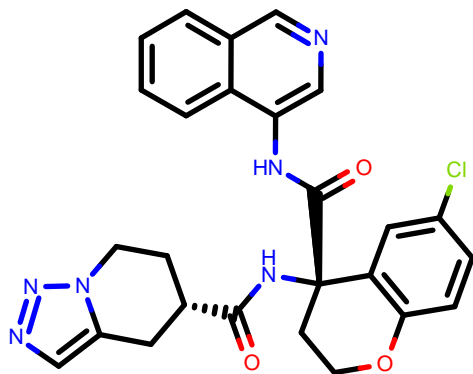
SMILES: Cc1cc(=O)c(cn1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)OC

RUN: RUN5058

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.30

EN300-7430501_1_2_1



CID: EN300-7430501_1_2_1

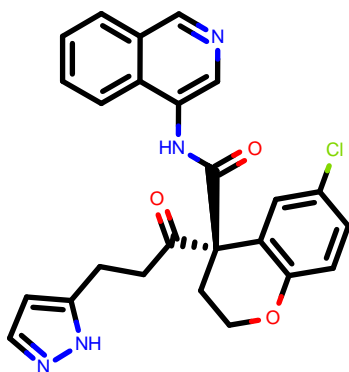
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCn6c(cnn6)C5

RUN: RUN2967

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-8_1_1



CID: VLA-UCB-34f3ed0c-8_1_1

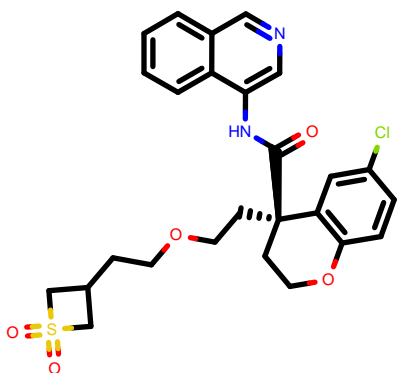
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]5

RUN: RUN3067

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.22

EN300-189563_3_1_1



CID: EN300-189563_3_1_1

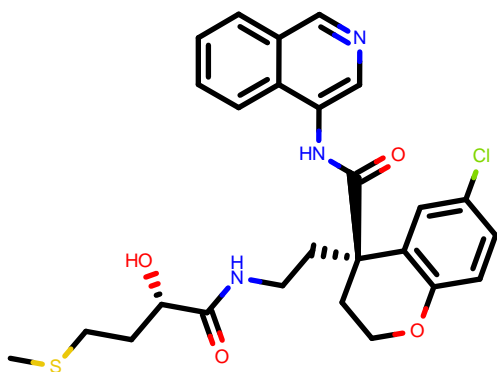
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCOCC5CS(=O)(=O)C5

RUN: RUN3584

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.28

EN300-103144_3_1_1



CID: EN300-103144_3_1_1

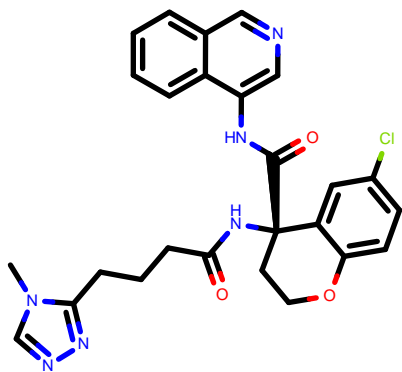
SMILES: CSCC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)O

RUN: RUN5516

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.44

EN300-6356960_1_1_1



CID: EN300-6356960_1_1_1

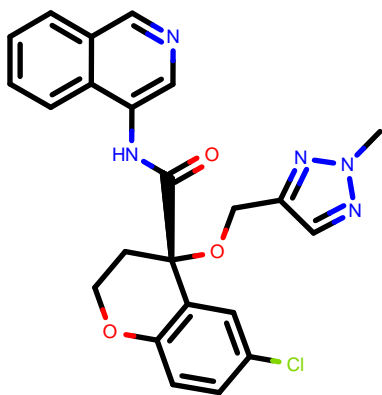
SMILES: Cn1cnc1CCCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4320

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.27

EN300-219020_1_1_1



CID: EN300-219020_1_1_1

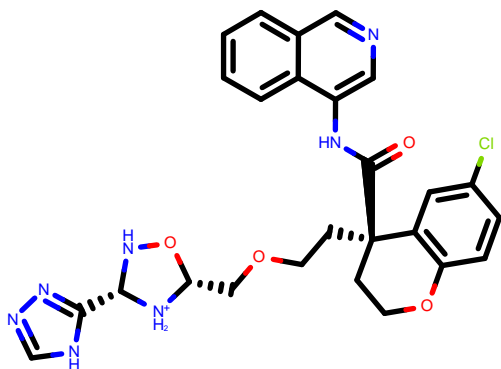
SMILES: Cn1ncc(n1)C(=O)C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4351

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.22

EN300-92031_3_1_1



CID: EN300-92031_3_1_1

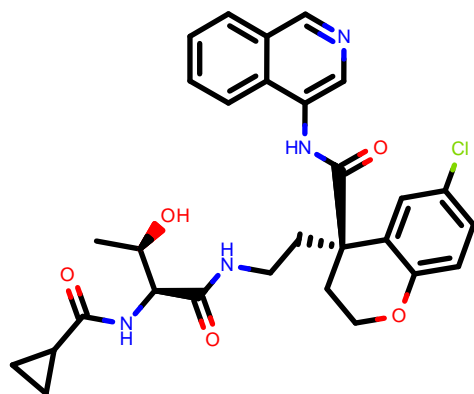
SMILES: c1ccc2c(c1)ncc2NC(=O)C@]3(CCOc4c3cc(cc4)C)CCOC]C@]H]5[NH2+]C@]H]N]O]c]6]H]n]r]6

RUN: RUN3309

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.70

EN300-96362_3_2_1



CID: EN300-96362_3_2_1

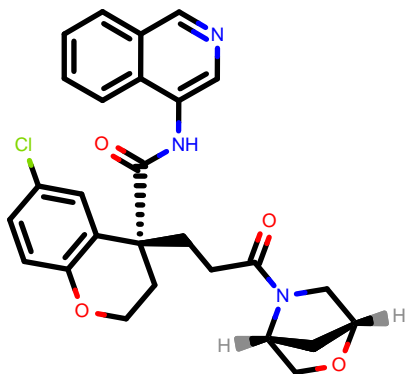
SMILES: C]C@]H]([C@]H]C]1=O)NC]C]@]1]([CO]c2c1cc(cc2)C]1=O)Nc3ncc4c3cccc4]N]C]1=O]C]5C]C]5]O

RUN: RUN4255

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.43

EN300-321789_2_1_1



CID: EN300-321789_2_1_1

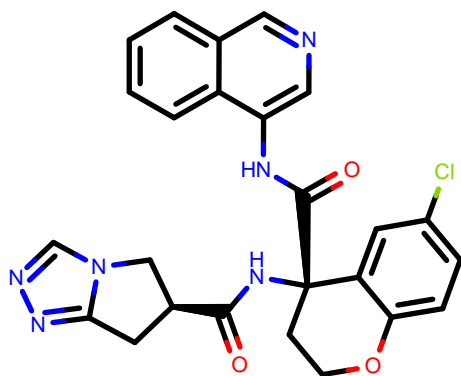
SMILES: c1ccc2c(c1)ncc2NC(=O)C@]3(CCOc4c3cc(cc4)C)CCC(=O)N5C]C@]H]6C]C@]H]5C]O]6

RUN: RUN6424

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.23

EN300-6745453_1_2_1



CID: EN300-6745453_1_2_1

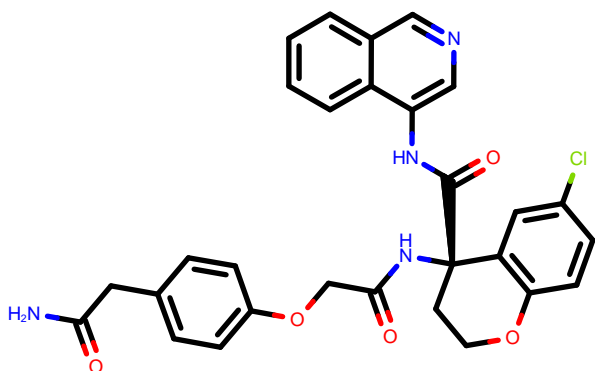
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5Cc6nncn6C5

RUN: RUN4550

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.31

EN300-50514_1_1_1



CID: EN300-50514_1_1_1

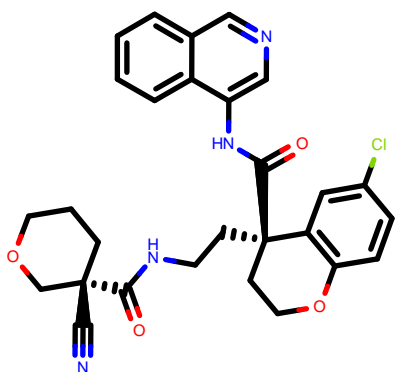
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)COc5ccc(cc5)CC(=O)N

RUN: RUN3443

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.35

EN300-301925_3_2_1



CID: EN300-301925_3_2_1

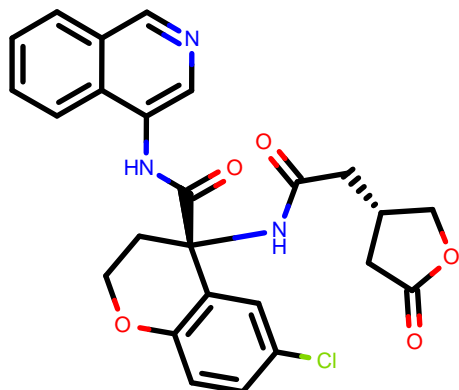
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5[C@@]6(CCCOC6)C#N

RUN: RUN3125

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.25

EN300-109535_1_2_1



CID: EN300-109535_1_2_1

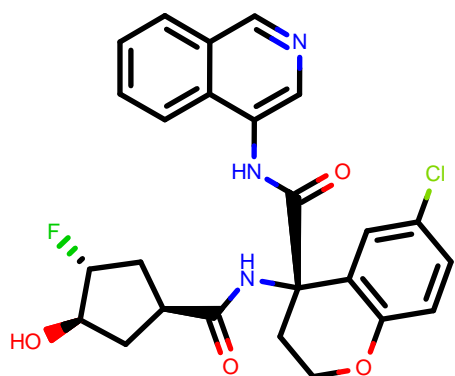
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)OC5

RUN: RUN3903

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.21

EDG-MED-90036822-85_2



CID: EDG-MED-90036822-85_2

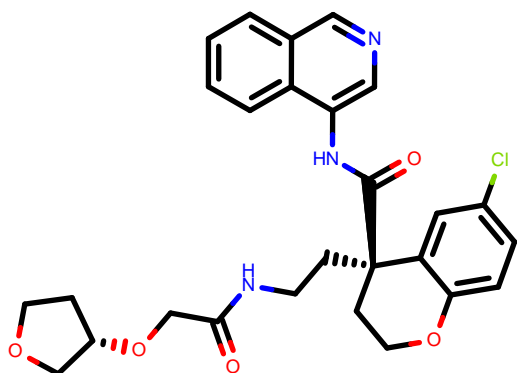
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)NC(=O)[C@H]5CC@@HC5(F)O

RUN: RUN1658

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.24

EN300-99391_3_2_1



CID: EN300-99391_3_2_1

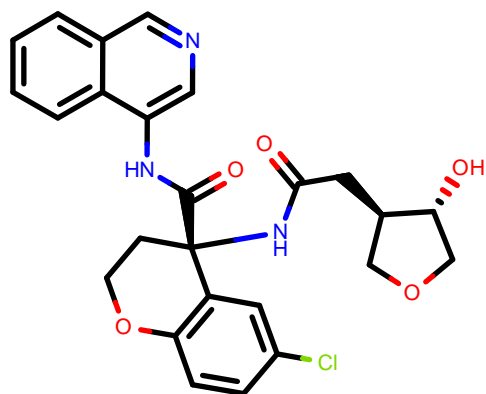
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CCNC(=O)CO[C@H]5CCOC5

RUN: RUN5480

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.27

EN300-1708882_1_1_1



CID: EN300-1708882_1_1_1

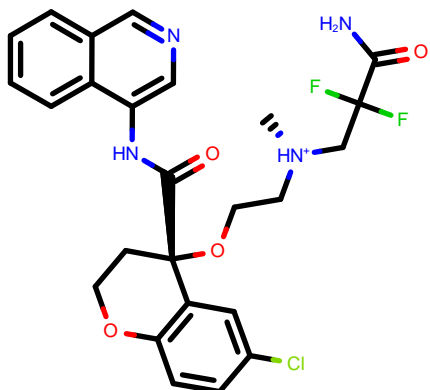
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)NC(=O)[C@H]5COC(C@H)5O

RUN: RUN3799

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.22

ED_-GRI-5b13fbe2-34_2



CID: ED_-GRI-5b13fbe2-34_2

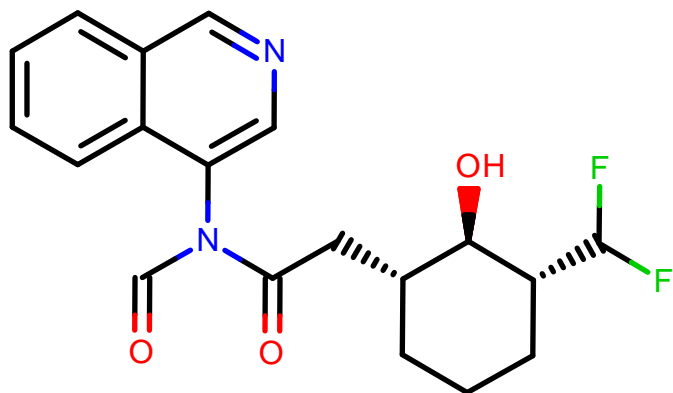
SMILES: C[N@@]([CCO][C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4cccoc4)CC(C(=O)N)(F)F

RUN: RUN1443

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.31

MAK-UNK-c749d764-28_4



CID: MAK-UNK-c749d764-28_4

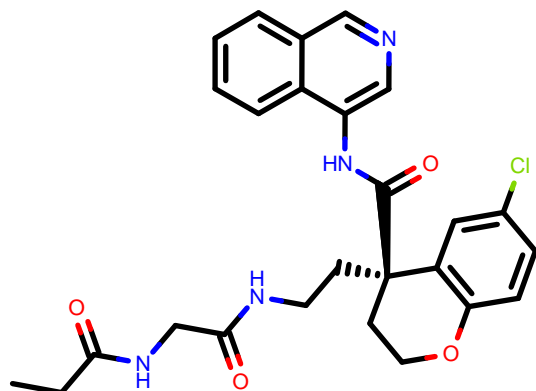
SMILES: c1ccc2c(c1)cncc2N(C=O)C(=O)C[C@H]3CCCC[C@H]1[C@@H]3O)C(F)F

RUN: RUN989

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.34

EN300-31099_3_1_1



CID: EN300-31099_3_1_1

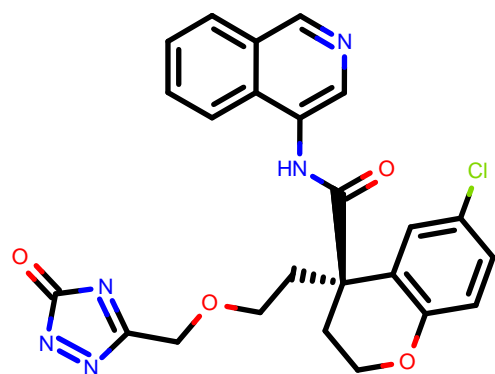
SMILES: CCC(=O)NCC(=O)NCC[C@]1(C)C(CO)C2C1CC(=O)C(=O)Nc3ccc4c3ccc4

RUN: RUN5833

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-73772_3_1_1



CID: EN300-73772_3_1_1

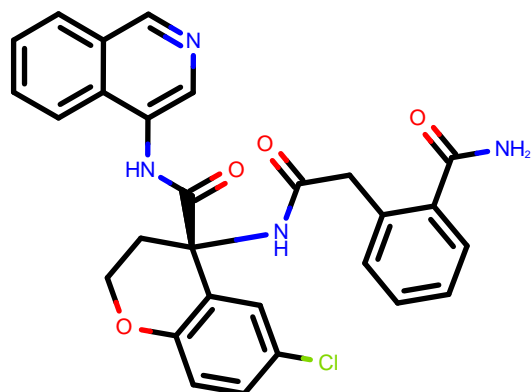
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4C3CC(=O)C(=O)Nc5[nH]c(=O)[nH]n5

RUN: RUN3358

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.23

EN300-121144_1_1_1



CID: EN300-121144_1_1_1

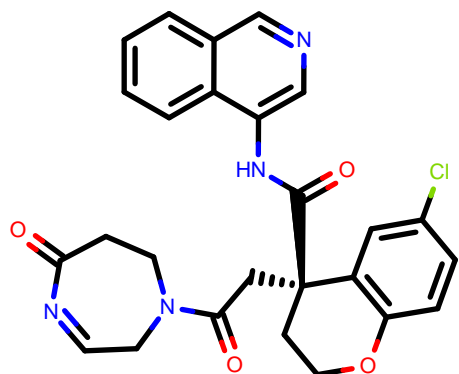
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4C3CC(=O)C(=O)Nc5ccc6c5C(=O)N

RUN: RUN4672

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-69107_1_1_1



CID: EN300-69107_1_1_1

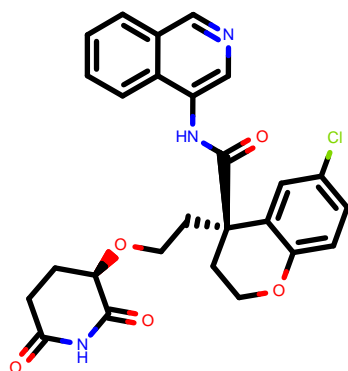
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(=O)NCS

RUN: RUN2902

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-120920_3_1_1



CID: EN300-120920_3_1_1

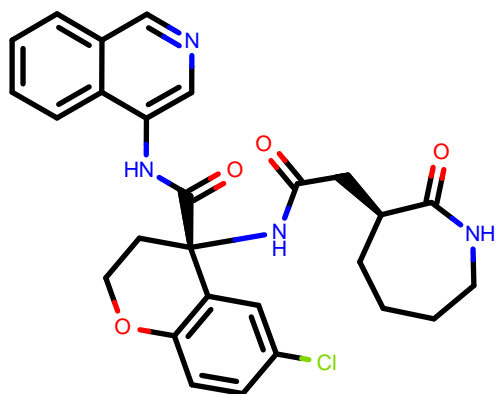
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@]5NCCC(=O)NCS=O

RUN: RUN4076

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.25

EN300-198633_1_1_1



CID: EN300-198633_1_1_1

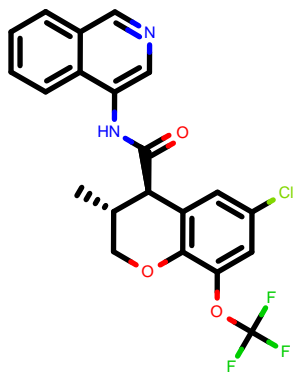
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5NCCC(=O)NCS=O

RUN: RUN3304

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-18_1_1



CID: DAR-DIA-0d514e7d-18_1_1

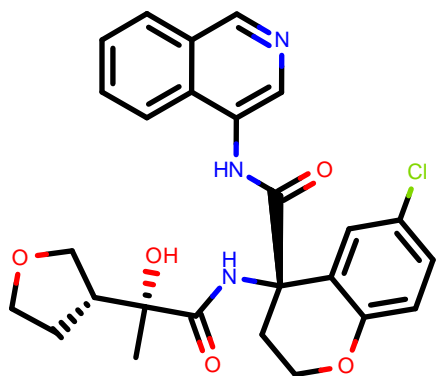
SMILES: C[C@H]1COc2c(cc(cc2OC(F)(F)F)Cl)[C@@]3(C)NCC(=O)Nc3cncc4c3cccc4

RUN: RUN4737

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.16

EN300-217494_1_1_1



CID: EN300-217494_1_1_1

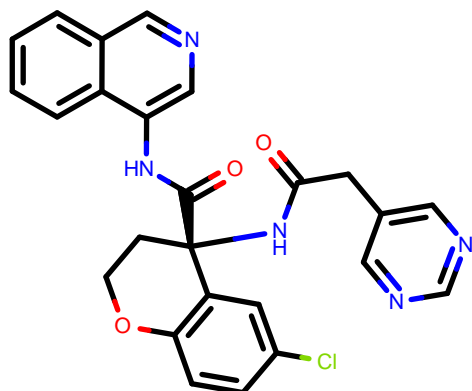
SMILES: C[C@@]([C@@H]1CCOC1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN3496

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-185751_1_1_1



CID: EN300-185751_1_1_1

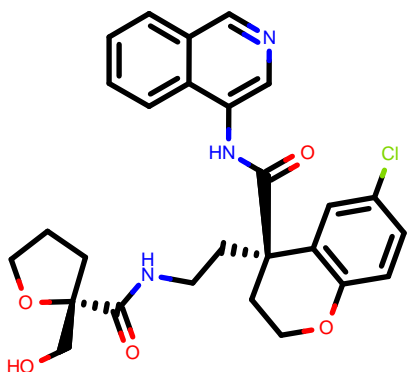
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cncc5

RUN: RUN4780

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.21

EN300-1425677_3_2_1



CID: EN300-1425677_3_2_1

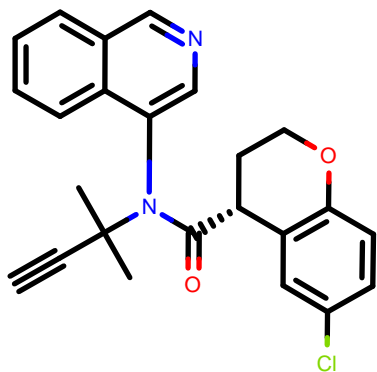
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCCO5)CO

RUN: RUN4635

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.38

DAR-DIA-5ff57136-14_1_1



CID: DAR-DIA-5ff57136-14_1_1

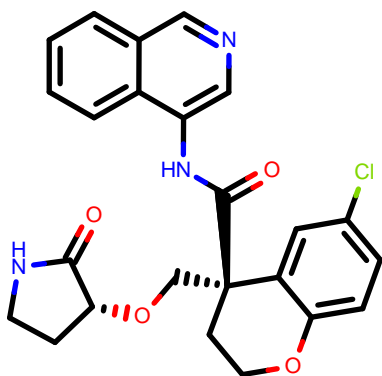
SMILES: CC(C)(C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN5433

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.19

EN300-6736413_2_1_1



CID: EN300-6736413_2_1_1

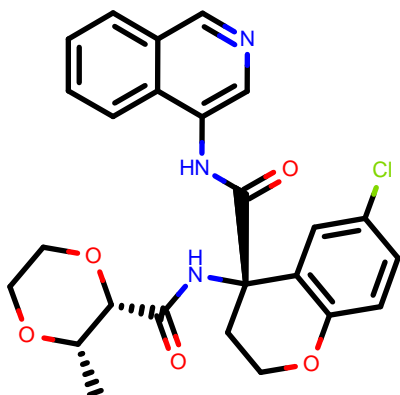
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCNC5=O

RUN: RUN4701

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-299215_1_1_1



CID: EN300-299215_1_1_1

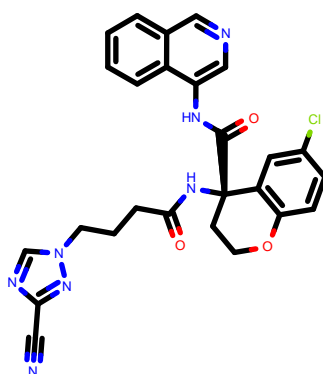
SMILES: C[C@H]1[C@H](OCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN2767

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.26

EN300-245265_1_1_1



CID: EN300-245265_1_1_1

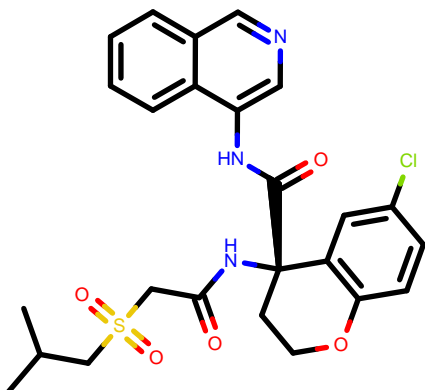
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ncnc5C#N

RUN: RUN3203

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.31

EN300-42243_1_1_1



CID: EN300-42243_1_1_1

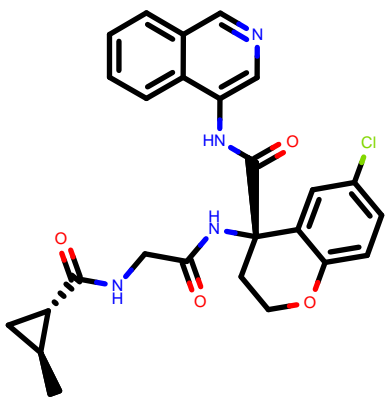
SMILES: CC(C)CS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN: RUN2812

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.25

EN300-30768_1_2_1



CID: EN300-30768_1_2_1

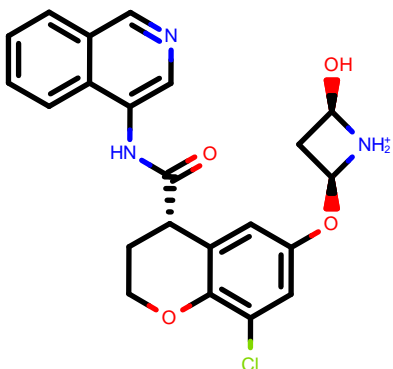
SMILES: C[C@H]1C[C@@H]1C(=O)NCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4610

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.30

FRA-DIA-b66f7109-3_2_1



CID: FRA-DIA-b66f7109-3_2_1

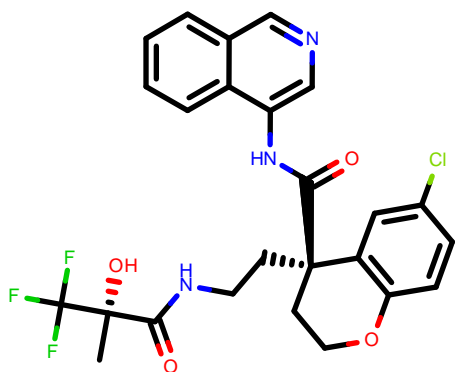
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOCc4c3cc(cc4Cl)O[C@H]5C[C@H]([NH2+][5]O

RUN: RUN3341

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.52

EN300-159633_3_2_1



CID: EN300-159633_3_2_1

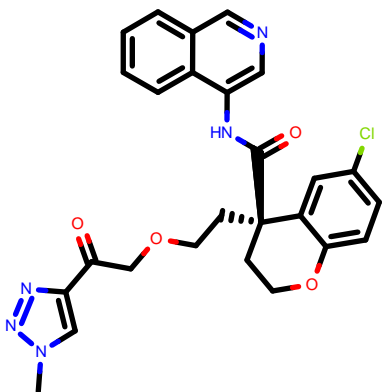
SMILES: C[C@](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)(C(F)(F)F)O

RUN: RUN4018

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.33

EN300-263153_3_1_1



CID: EN300-263153_3_1_1

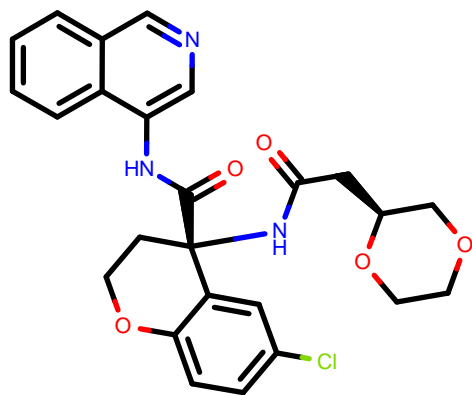
SMILES: Cn1cc(nn1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4622

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.29

EN300-731622_1_2_1



CID: EN300-731622_1_2_1

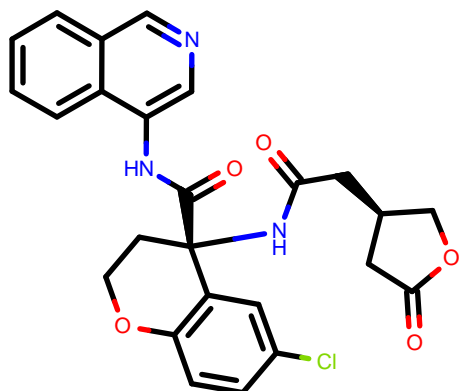
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5COCOC5

RUN: RUN3772

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.26

EN300-109535_1_1_1



CID: EN300-109535_1_1_1

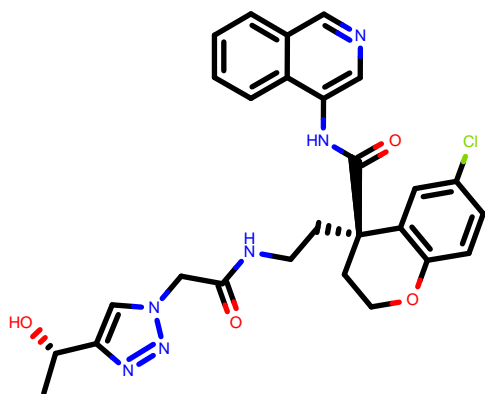
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5OC(=O)O5

RUN: RUN7166

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-109540_3_1_1



CID: EN300-109540_3_1_1

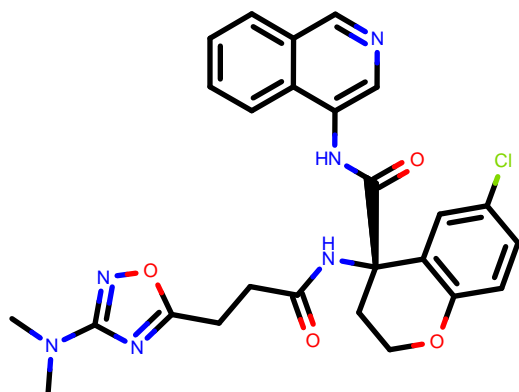
SMILES: C[C@@H](c1cn(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccoc5)O

RUN: RUN3163

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.30

EN300-152913_1_1_1



CID: EN300-152913_1_1_1

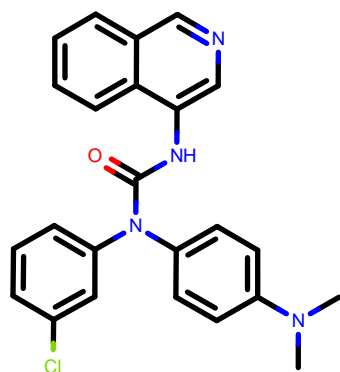
SMILES: CN(C)c1nc(on1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccoc5

RUN: RUN3711

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.30

FRA-DIA-13af2da5-1_1



CID: FRA-DIA-13af2da5-1_1

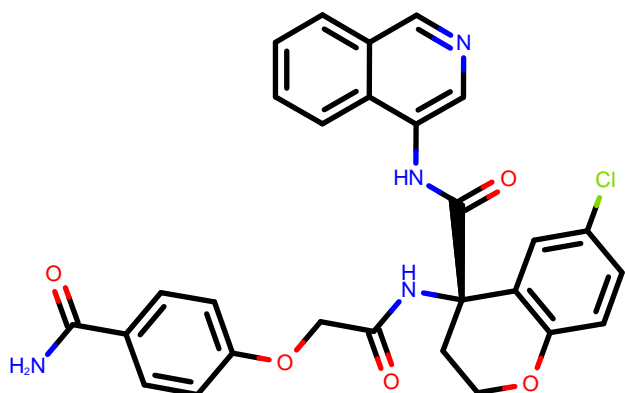
SMILES: CN(C)c1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN449

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.30

ALP-UNI-dbbfd3db-5_1



CID: ALP-UNI-dbbfd3db-5_1

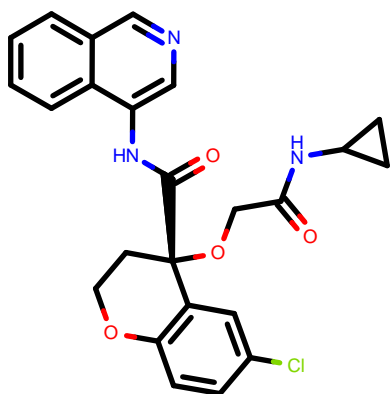
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)COc5ccc(cc5)C(=O)N

RUN: RUN2633

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.28

EN300-1253178_1_1_1



CID: EN300-1253178_1_1_1

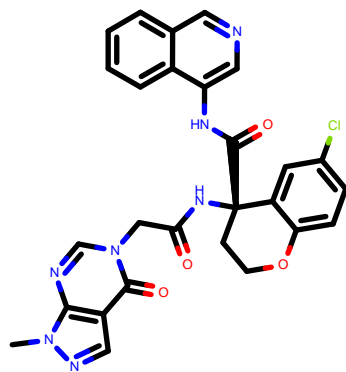
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN: RUN4417

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.18

ALP-UNI-dbbfd3db-16_1



CID: ALP-UNI-dbbfd3db-16_1

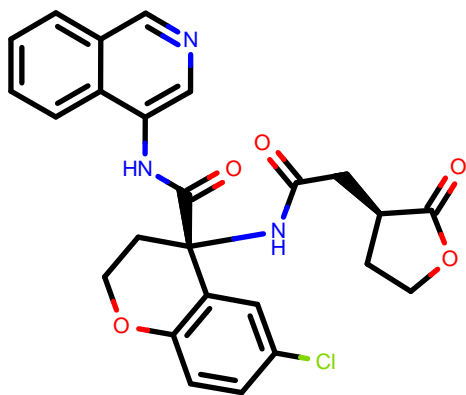
SMILES: Cn1c2c(cn1)c(=O)n(cn2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccccc6

RUN: RUN2617

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EN300-1072972_1_1_1



CID: EN300-1072972_1_1_1

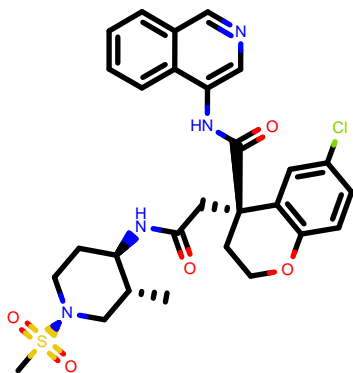
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)NC(=O)[C@H]5CCOC5=O

RUN: RUN3660

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

ALP-UNI-3496895b-5_5



CID: ALP-UNI-3496895b-5_5

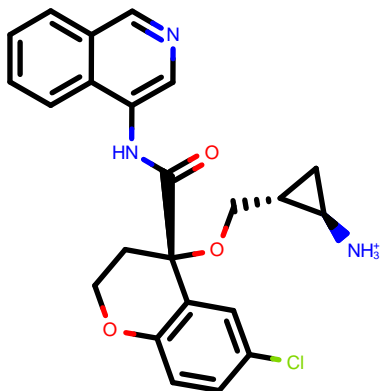
SMILES: C[C@@H]1C[N@@]1CC[C@@H]1NC(=O)[C@]2(CCOc3c2cc(c3)C)C(=O)Nc4ncoc5c4ccccc5S(=O)(=O)C

RUN: RUN2392

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.45

ED_-GRI-5b13fbe2-69_3



CID: ED_-GRI-5b13fbe2-69_3

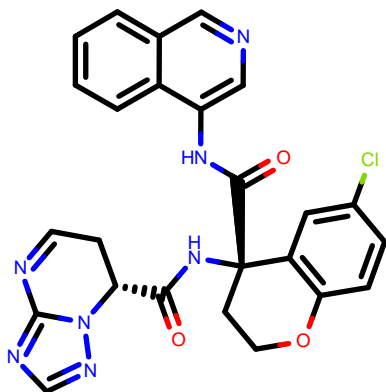
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)OC)C(=O)[C@H]5[C@H]5[NH3+]

RUN: RUN1463

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.26

EN300-28262_1_1_2



CID: EN300-28262_1_1_2

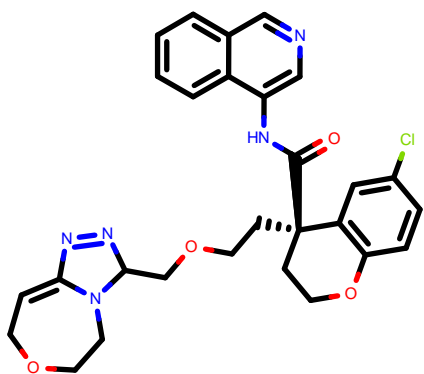
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)NC(=O)[C@H]5CC=Nc6f5nc6

RUN: RUN6514

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.34

EN300-310888_3_1_1



CID: EN300-310888_3_1_1

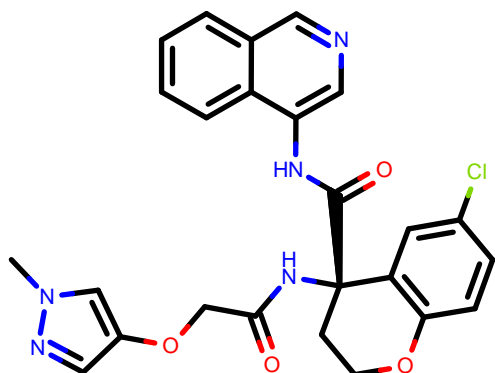
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nn6n5COCOC6

RUN: RUN4950

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.33

EN300-201553_1_1_1



CID: EN300-201553_1_1_1

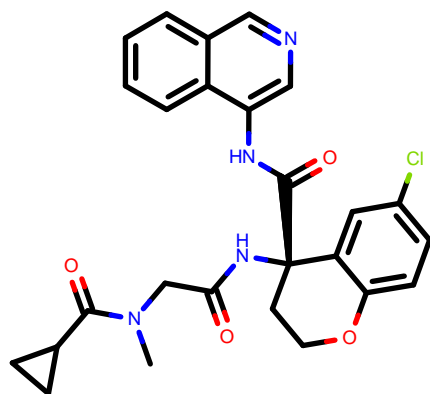
SMILES: C[n+1]cc(c[nH]1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN5411

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EN300-31146_1_1_1



CID: EN300-31146_1_1_1

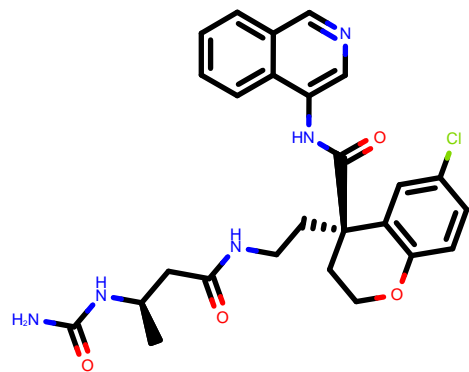
SMILES: CN(CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c4c3ccc4)C(=O)C5CC5

RUN: RUN6191

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.24

EN300-268198_3_2_1



CID: EN300-268198_3_2_1

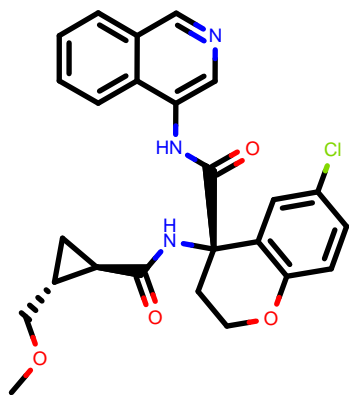
SMILES: C[C@@H](CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c4c3ccc4)NC(=O)N

RUN: RUN4949

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.27

EN300-705386_1_1_1



CID: EN300-705386_1_1_1

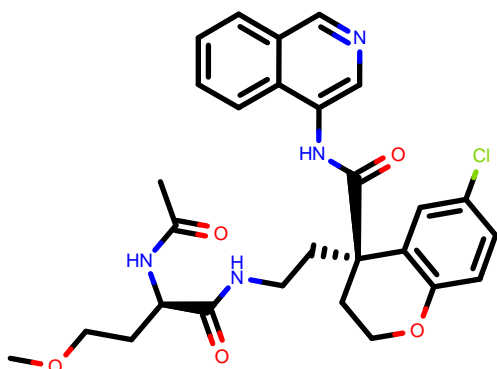
SMILES: COC[C@@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3429

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.23

EN300-62074_3_2_1



CID: EN300-62074_3_2_1

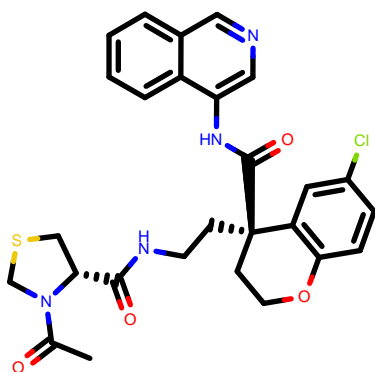
SMILES: CC(=O)N[C@@H](CCOC)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN6369

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.31

EN300-56202_3_1_1



CID: EN300-56202_3_1_1

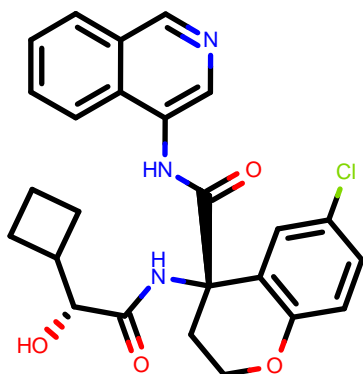
SMILES: CC(=O)N1CSC[C@@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN4336

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.31

EN300-249764_1_1_1



CID: EN300-249764_1_1_1

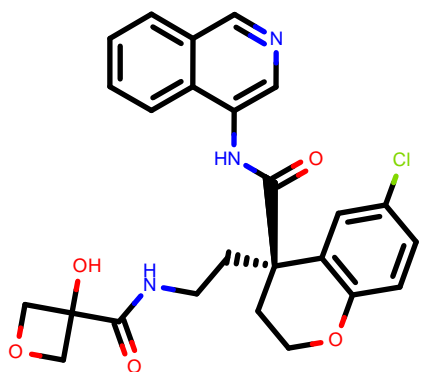
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](C5CC5)O

RUN: RUN3789

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.23

EN300-101443_3_1_1



CID: EN300-101443_3_1_1

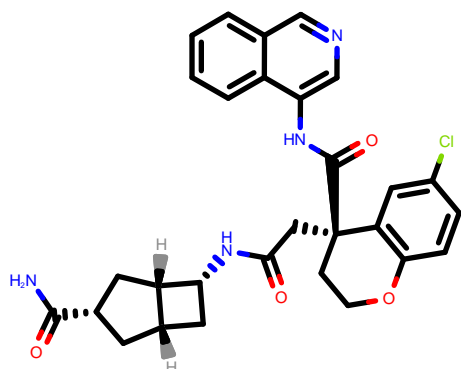
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(COC5)O

RUN: RUN6455

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-4_1



CID: EDJ-MED-d203f206-4_1

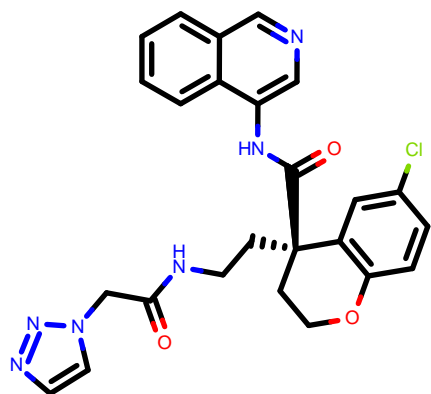
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5[C@@]6(C)C[C@H]5C6=O

RUN: RUN2416

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.31

EN300-100467_3_1_1



CID: EN300-100467_3_1_1

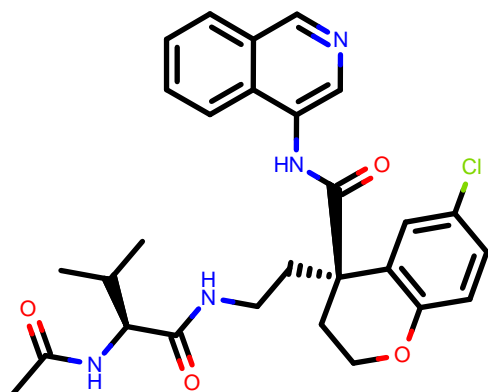
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnn5

RUN: RUN2863

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.28

EN300-16582_3_1_1



CID: EN300-16582_3_1_1

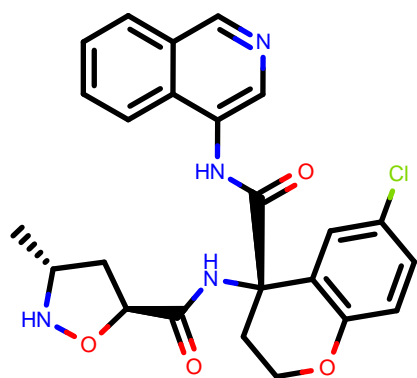
SMILES: CC(C)[C@@H](C=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4NC(=O)C

RUN: RUN5533

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.40

EN300-92447_1_1_1



CID: EN300-92447_1_1_1

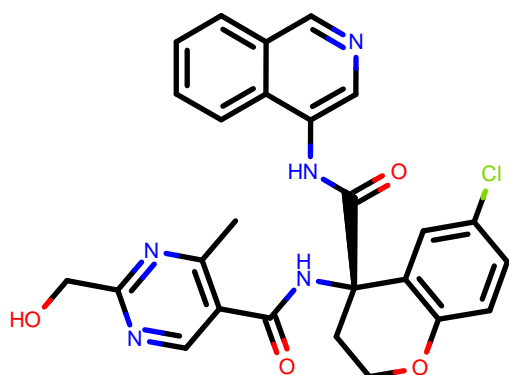
SMILES: C[C@@H]1C[C@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3430

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.30

EN300-6497975_1_1_1



CID: EN300-6497975_1_1_1

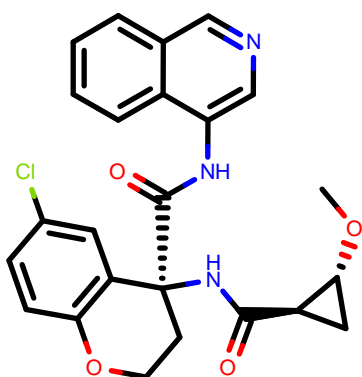
SMILES: Cc1c(nc(n1)CO)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4627

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.26

EN300-650518_1_1_1



CID: EN300-650518_1_1_1

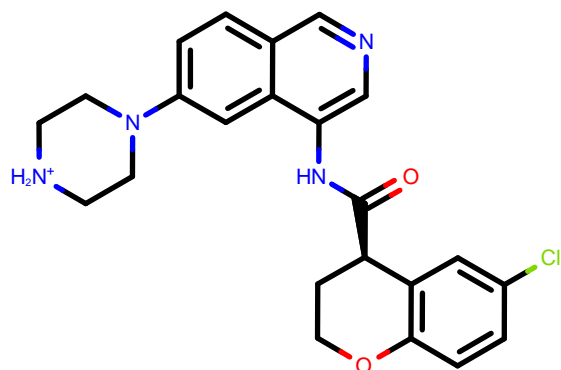
SMILES: CO[C@@H]1C[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4853

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.23

MAK-UNK-8be7dca9-4_1



CID: MAK-UNK-8be7dca9-4_1

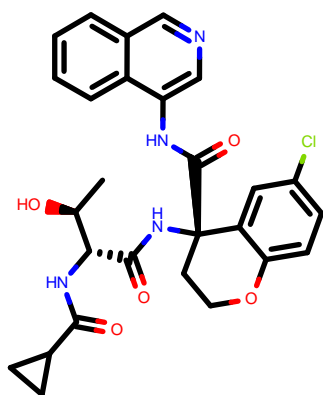
SMILES: c1cc2nccc(c2cc1N3CC[NH2+]CC3)NC(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN: RUN440

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.09

EN300-96362_1_3_1



CID: EN300-96362_1_3_1

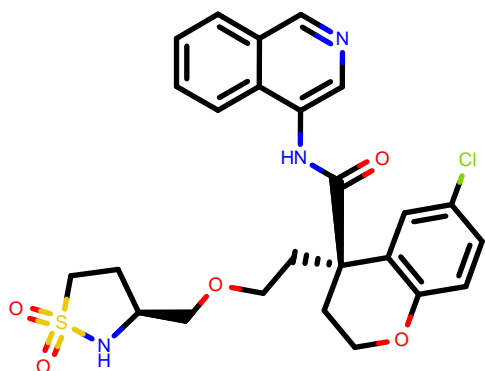
SMILES: C[C@@H](C[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(c2)Cl)C(=O)Nc3ncoc4c3ccoc4N[C@@H](C)C(=O)C5CC5)O

RUN: RUN4488

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.30

EN300-1699871_3_1_1



CID: EN300-1699871_3_1_1

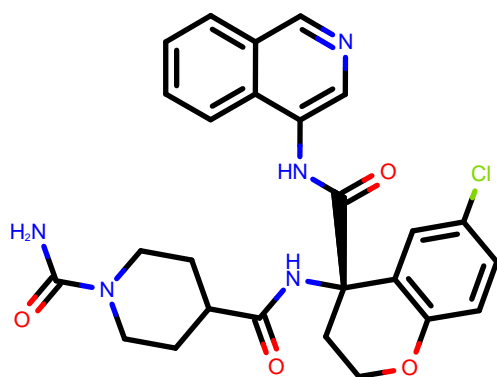
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H](C)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5SCCS(=O)(=O)N5

RUN: RUN5182

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.27

EN300-13489_1_1_1



CID: EN300-13489_1_1_1

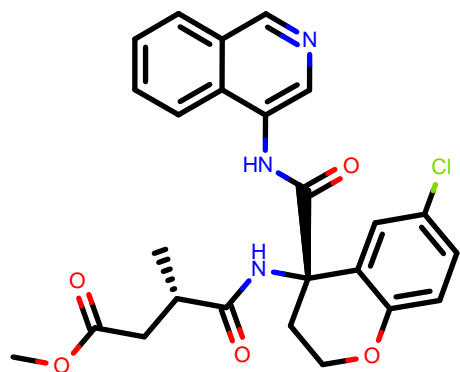
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H](C)[C@@H]3(CCOc4c3cc(cc4)Cl)N[C@@H](C)C(=O)C5CCN(CC5)C(=O)N

RUN: RUN2922

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.31

EN300-106540_1_1_1



CID: EN300-106540_1_1_1

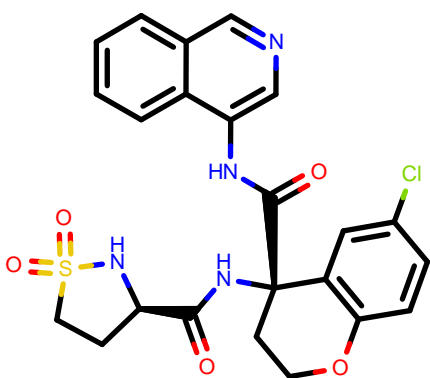
SMILES: C[C@@H](C[C@@H](C(=O)OC)C(=O)N[C@@H]1(CCOc2c1cc(c2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5549

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.24

EN300-45049_1_2_1



CID: EN300-45049_1_2_1

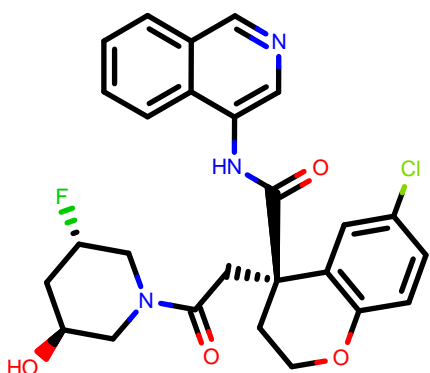
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCS(=O)(=O)N5

RUN: RUN5648

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.28

EN300-270422_1_1_1



CID: EN300-270422_1_1_1

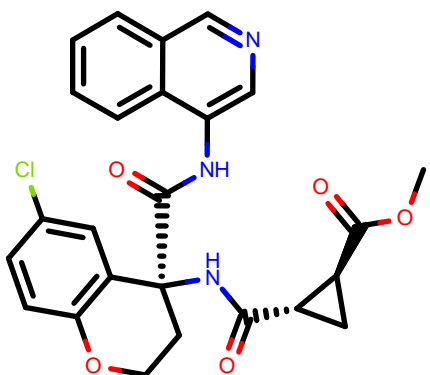
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C[C@@]3(C)F)O

RUN: RUN3234

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.41

EN300-66764_1_2_1



CID: EN300-66764_1_2_1

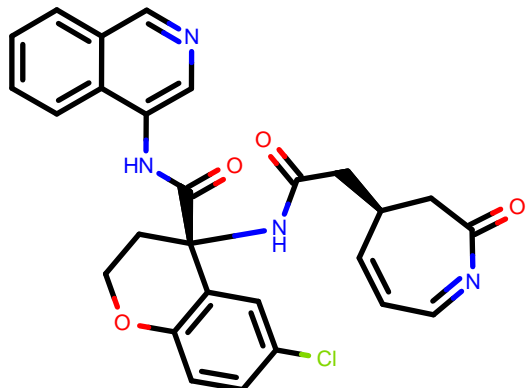
SMILES: COC(=O)[C@H]1C[C@@]2(CO)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5899

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.24

EN300-195590_1_1_1



CID: EN300-195590_1_1_1

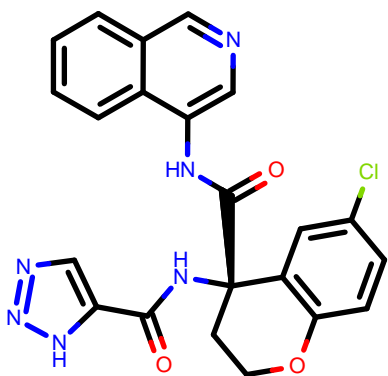
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@]4(C)NCC(=O)C5

RUN: RUN5613

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.26

EN300-31998_1_1_1



CID: EN300-31998_1_1_1

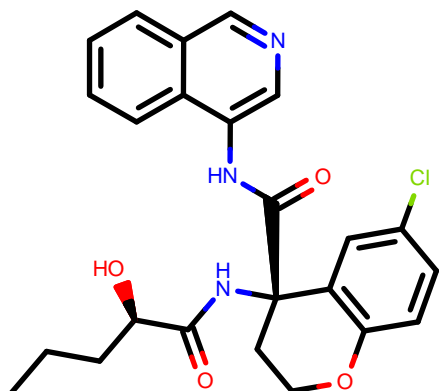
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]n5

RUN: RUN2787

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.20

EN300-300217_1_3_1



CID: EN300-300217_1_3_1

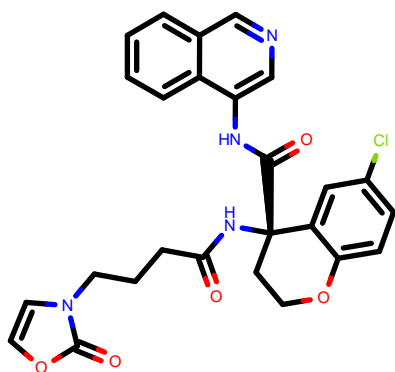
SMILES: C/C=C/[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN2845

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.24

EN300-45182_1_1_1



CID: EN300-45182_1_1_1

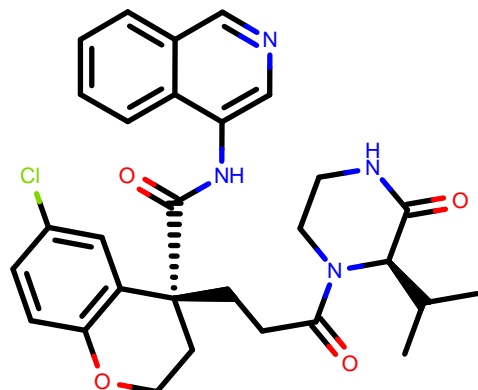
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCN5COC5=O

RUN: RUN3110

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.31

EN300-67791_2_1_1



CID: EN300-67791_2_1_1

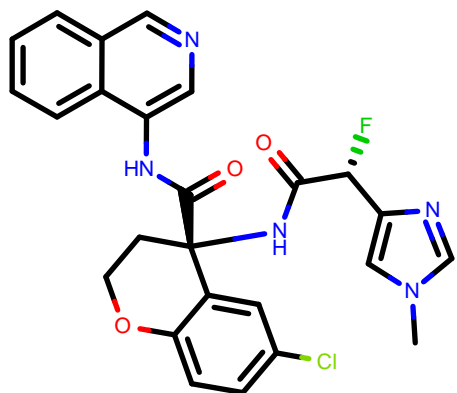
SMILES: CC(C)[C@@H]1C(=O)NCCN1C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7790

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.40

EDG-MED-90036822-25_2



CID: EDG-MED-90036822-25_2

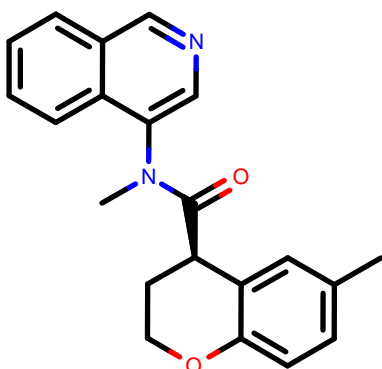
SMILES: Cn1cc(nc1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)F

RUN: RUN1583

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.22

MAK-UNK-3875bbc8-1_1_1



CID: MAK-UNK-3875bbc8-1_1_1

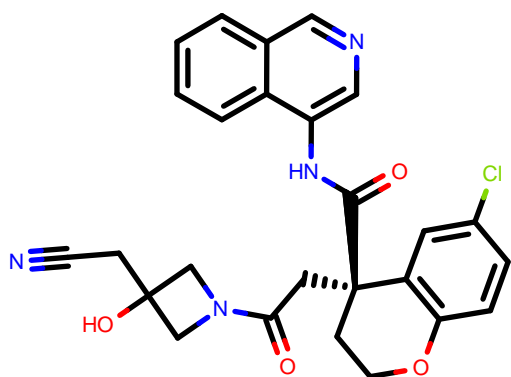
SMILES: Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)c3ccc4c3cccc4

RUN: RUN4944

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.11

EN300-155823_1_1_1



CID: EN300-155823_1_1_1

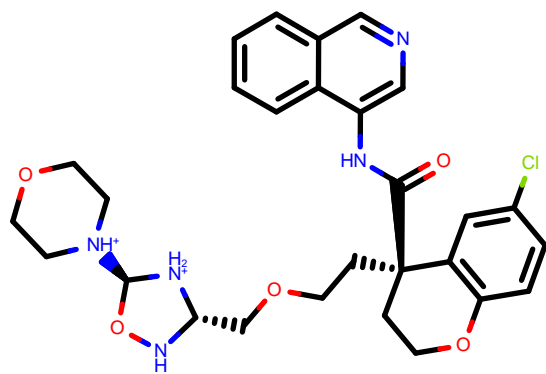
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CC#N)O

RUN: RUN4916

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.24

EN300-1608590_3_1_2



CID: EN300-1608590_3_1_2

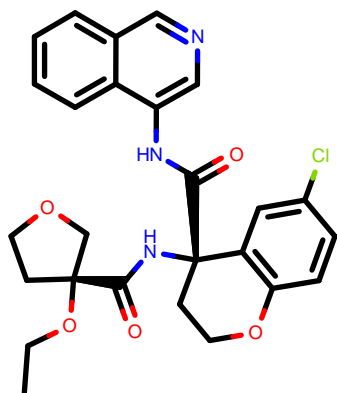
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5NCC5[NH+]1CCOCC1

RUN: RUN4647

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.56

EN300-259694_1_1_1



CID: EN300-259694_1_1_1

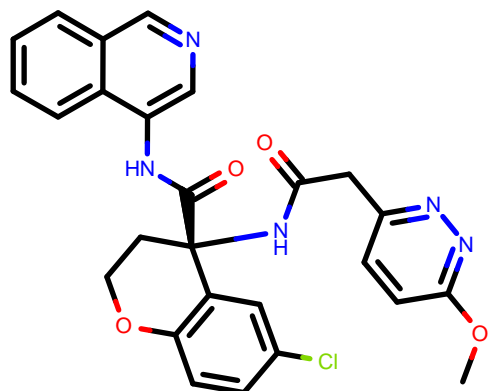
SMILES: CCOC@ @]1(CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN7493

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.32

EN300-7540889_1_1_1



CID: EN300-7540889_1_1_1

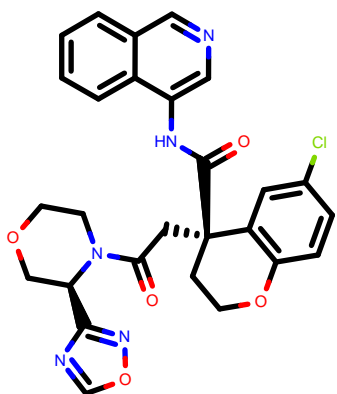
SMILES: COc1ccc(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3037

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.31

EN300-122849_1_1_1



CID: EN300-122849_1_1_1

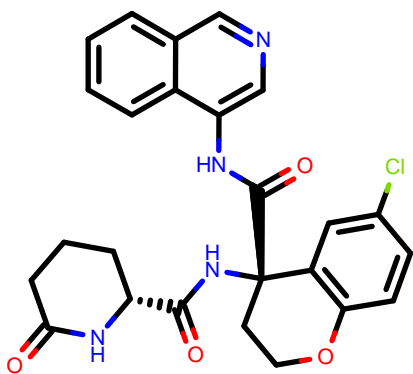
SMILES: c1ccc2c(c1)nc2NC(=O)[C@ @]3(CCOc4c3cc(cc4)Cl)C(=O)N5CCOC[C@ @]H]5c6nc6

RUN: RUN3126

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.37

EN300-146491_1_1_1



CID: EN300-146491_1_1_1

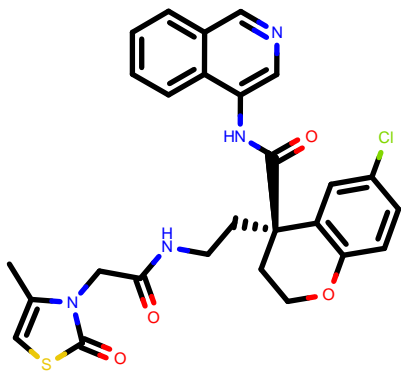
SMILES: c1ccc2c(c1)nc2NC(=O)[C@ @]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCC(=O)N5

RUN: RUN3281

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.25

EN300-12067_3_1_1



CID: EN300-12067_3_1_1

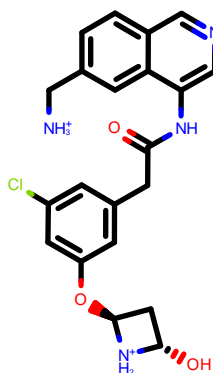
SMILES: Cc1csc(=O)n1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccoc5

RUN: RUN3070

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.29

ALF-EVA-0b412456-5_2



CID: ALF-EVA-0b412456-5_2

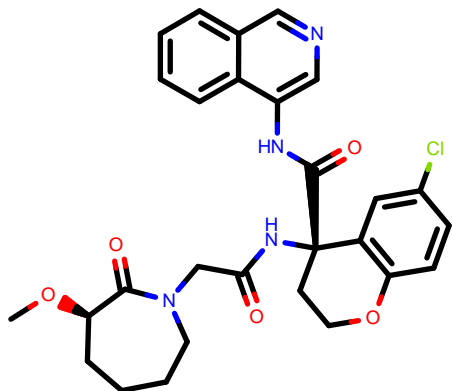
SMILES: c1cc2cncc(e2cc1C[NH3+])NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4

RUN: RUN2571

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.48

EN300-259847_1_1_1



CID: EN300-259847_1_1_1

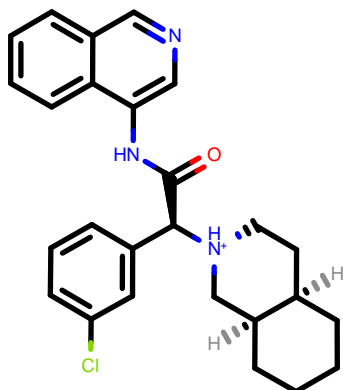
SMILES: CO[C@@H]1CCCC(C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN4900

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

MIC-UNK-5a93dd5f-3_14



CID: MIC-UNK-5a93dd5f-3_14

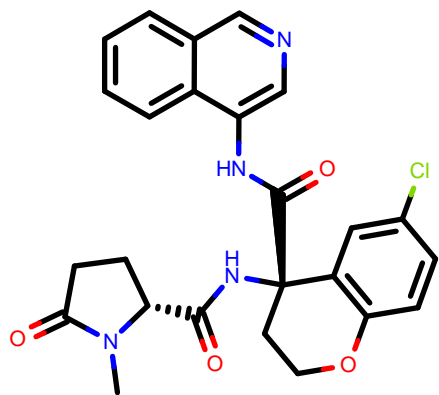
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)[N@@H]4CC[C@H]5CCCC[C@H]5C4

RUN: RUN657

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.36

EN300-343787_1_1_1



CID: EN300-343787_1_1_1

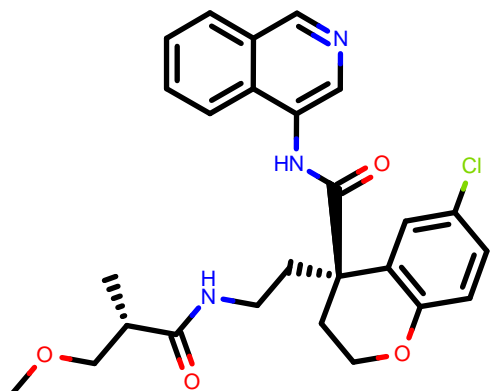
SMILES: CN1[C@H](CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN3489

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-69162_3_1_1



CID: EN300-69162_3_1_1

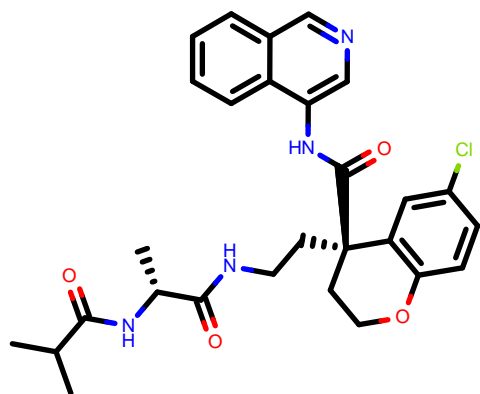
SMILES: C[C@@H](COC)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4

RUN: RUN3622

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

EN300-31184_3_2_1



CID: EN300-31184_3_2_1

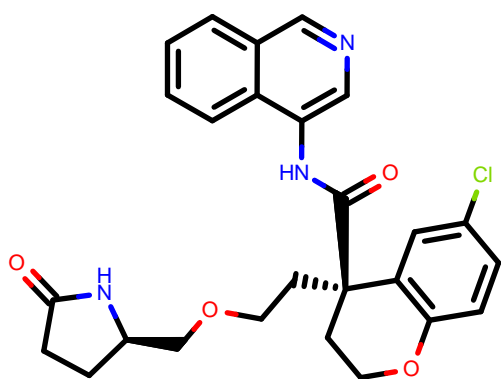
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4)N(C)C(C)C

RUN: RUN4027

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.32

EN300-195756_3_2_1



CID: EN300-195756_3_2_1

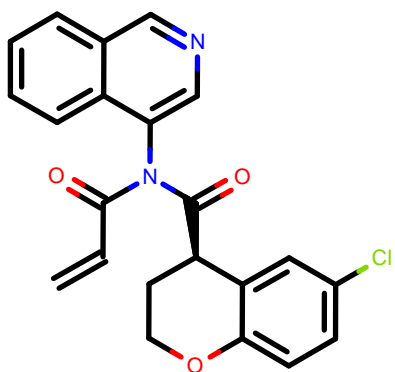
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCCC(=O)N5

RUN: RUN3810

DDG (kcal/mol): -1.69

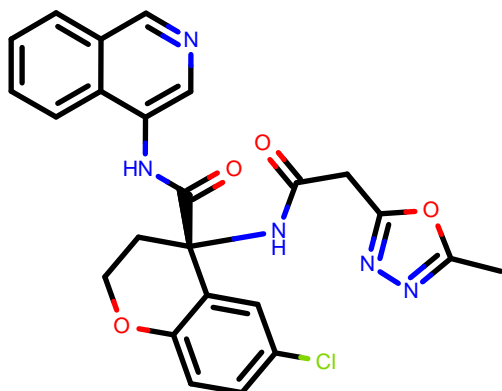
dDDG (kcal/mol): 0.25

VLA-UCB-50c39ae8-7_1



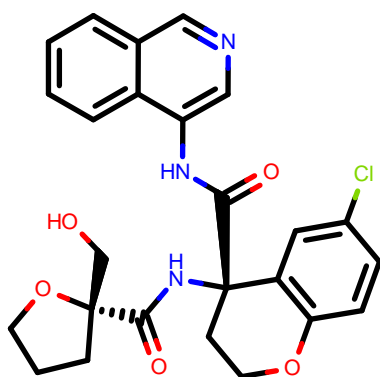
CID:	VLA-UCB-50c39ae8-7_1
SMILES:	<chem>C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN343
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.16

EN300-64193_1_1_1



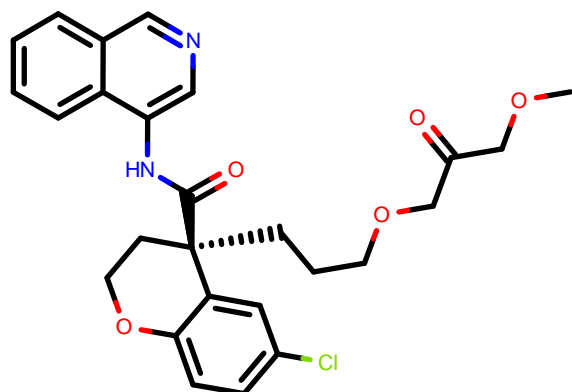
CID:	EN300-64193_1_1_1
SMILES:	<chem>Cc1nnc(o1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN5167
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.24

EN300-1425677_1_1_1



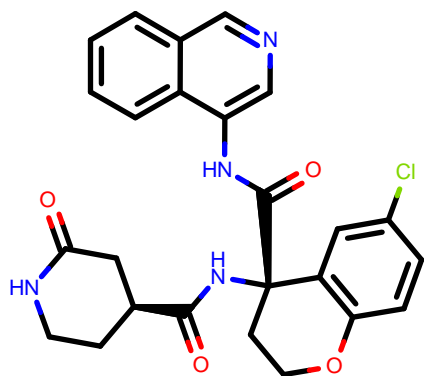
CID:	EN300-1425677_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCOC5)CO</chem>
RUN:	RUN2837
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.25

EN300-125140_4_1_1



CID:	EN300-125140_4_1_1
SMILES:	<chem>COCC(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN4727
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.29

EN300-107493_1_2_1



CID: EN300-107493_1_2_1

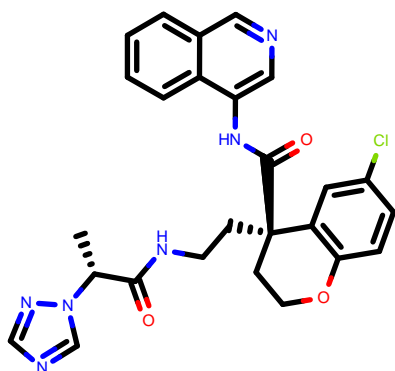
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCNC(=O)C5

RUN: RUN3628

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.25

EN300-30397_3_2_1



CID: EN300-30397_3_2_1

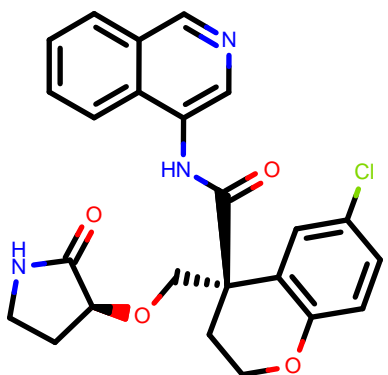
SMILES: C[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)n5enrn5

RUN: RUN3692

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.41

EDJ-MED-fcba3f31-7_1



CID: EDJ-MED-fcba3f31-7_1

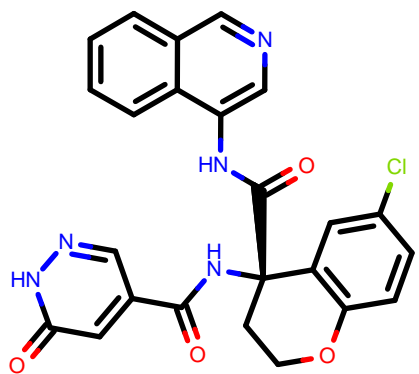
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O

RUN: RUN2339

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.20

EN300-159634_1_1_1



CID: EN300-159634_1_1_1

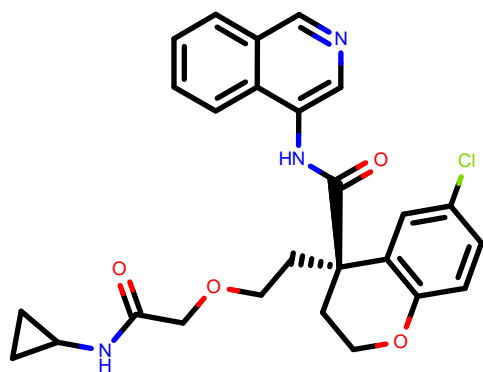
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]jnc5

RUN: RUN4994

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-1253178_3_1_1



CID: EN300-1253178_3_1_1

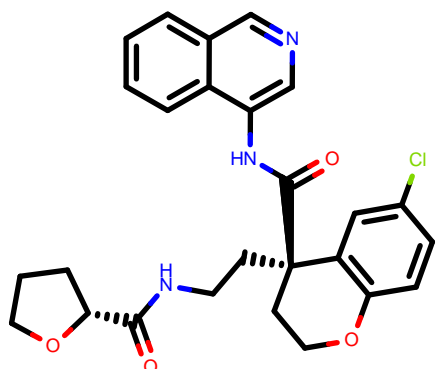
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NC5CC5

RUN: RUN5341

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.26

EN300-116234_3_1_1



CID: EN300-116234_3_1_1

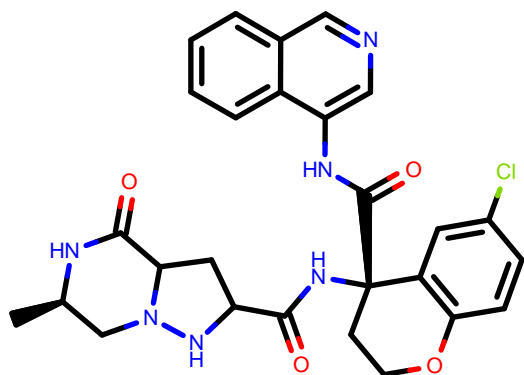
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5

RUN: RUN4928

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-265285_1_1_1



CID: EN300-265285_1_1_1

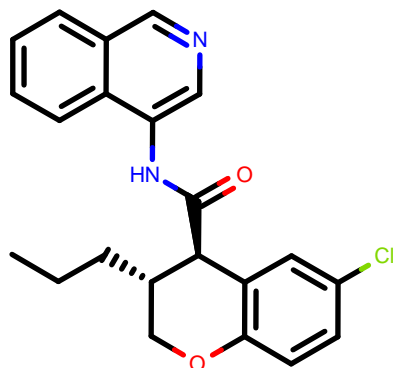
SMILES: C[C@@]1[C@H]1Cn2c(cc(n2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccc6)C(=O)N1

RUN: RUN4775

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

EDJ-MED-e4b030d8-6_1



CID: EDJ-MED-e4b030d8-6_1

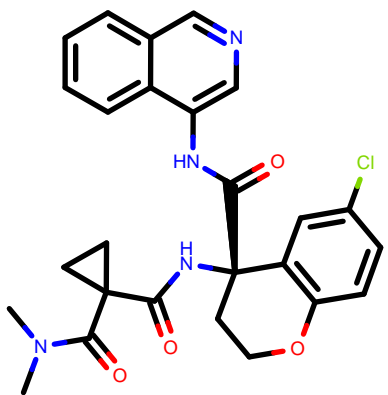
SMILES: CCC[C@H]1COc2ccc(cc2[C@@]3[C@@]3(=O)Nc3ncoc4c3ccc4)Cl

RUN: RUN254

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.10

EN300-180875_1_1_1



CID: EN300-180875_1_1_1

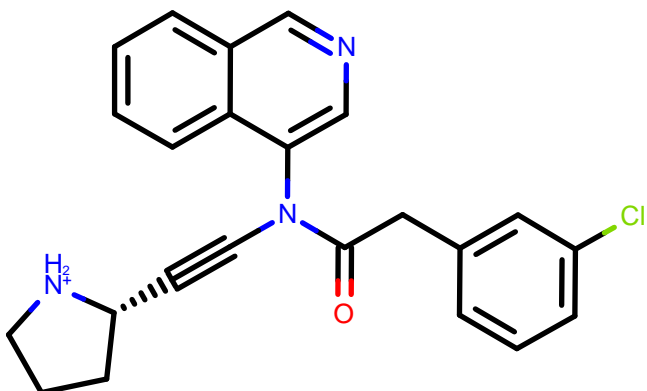
SMILES: CN(C)C(=O)C1(CC1)C(=O)N[C@]2(COCc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN4535

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.31

DAR-DIA-076fb6ea-9_1



CID: DAR-DIA-076fb6ea-9_1

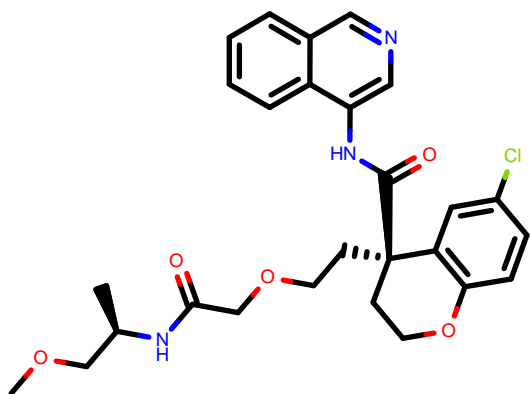
SMILES: c1ccc2c(c1)nccc2N(C#C[C@]([H])3CCCC[NH2+](3)C(=O)Cc4cccc(c4)Cl

RUN: RUN1273

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.35

EN300-02067_3_2_1



CID: EN300-02067_3_2_1

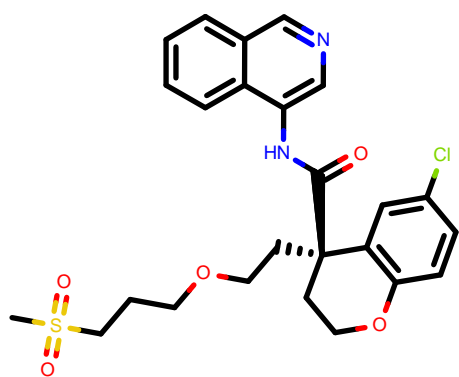
SMILES: C[C@]([H])(COC)NC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6976

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-68794_3_1_1



CID: EN300-68794_3_1_1

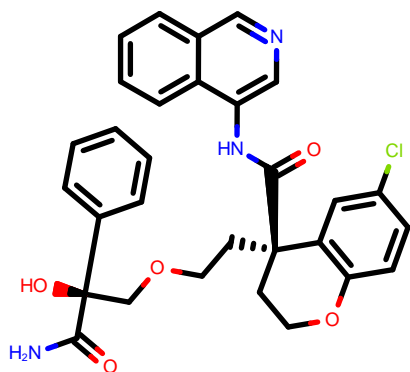
SMILES: CS(=O)(=O)CCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6094

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-248526_3_2_1



CID: EN300-248526_3_2_1

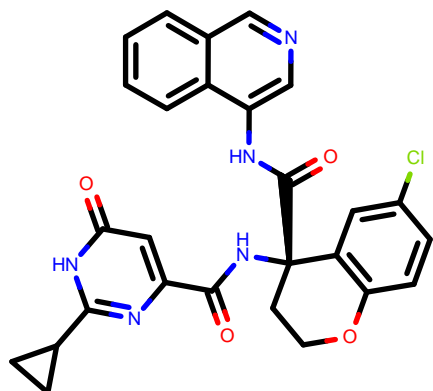
SMILES: c1ccc(cc1)[C@@]([C@@]([C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C(=O)N)O

RUN: RUN2973

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.34

EN300-204239_1_1_1



CID: EN300-204239_1_1_1

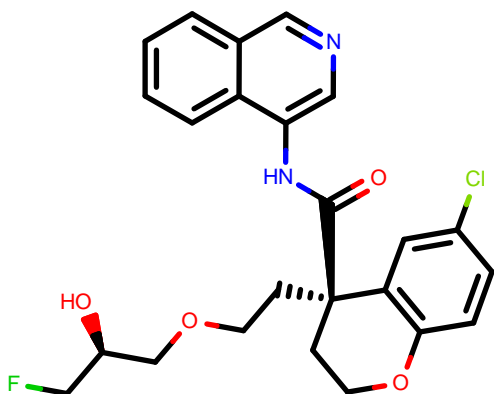
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]([C@@]([C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]c1n5)C6CC6

RUN: RUN4315

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.22

EN300-1968342_3_1_1



CID: EN300-1968342_3_1_1

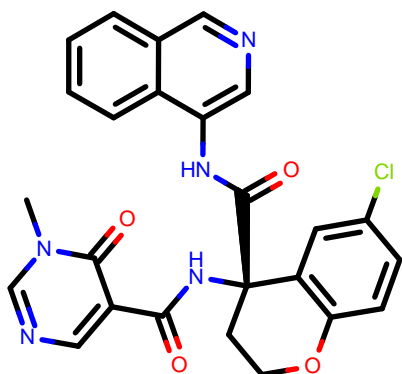
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]([C@@]([C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]([C@@]3)F)O

RUN: RUN4606

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.35

EN300-295132_1_1_1



CID: EN300-295132_1_1_1

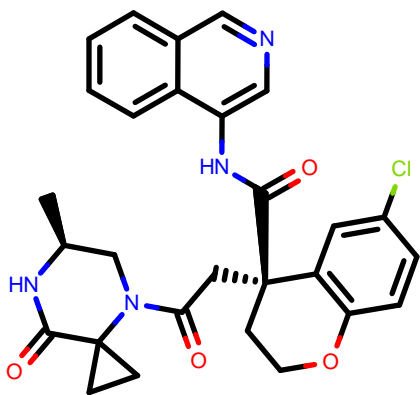
SMILES: Cn1cncc(c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3387

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.26

EN300-7542429_1_2_1



CID: EN300-7542429_1_2_1

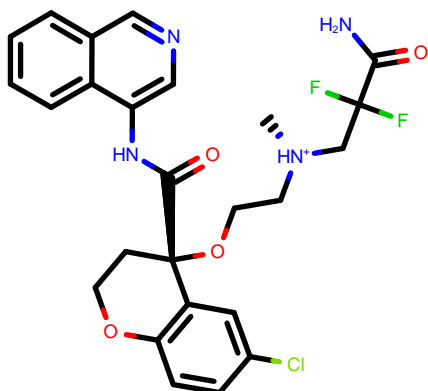
SMILES: C[C@H]1CN(C2(CC2)C(=O)N1)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN3423

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.38

ED_-GRI-5b13fbe2-34_1



CID: ED_-GRI-5b13fbe2-34_1

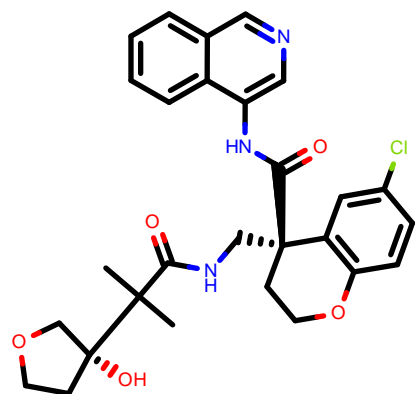
SMILES: C[N@]([CCO][C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)CC(C(=O)N)(F)F

RUN: RUN1446

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.33

EN300-1630093_2_2_1



CID: EN300-1630093_2_2_1

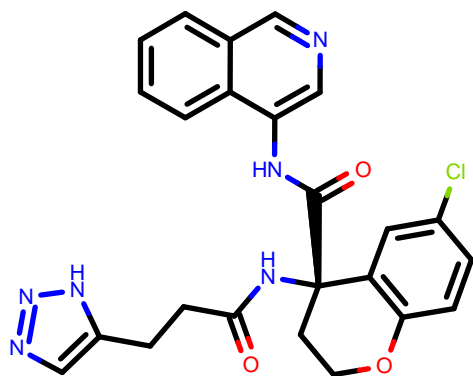
SMILES: CC(C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)[C@]5(CCOCS)O

RUN: RUN7325

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.28

EN300-244947_1_1_1



CID: EN300-244947_1_1_1

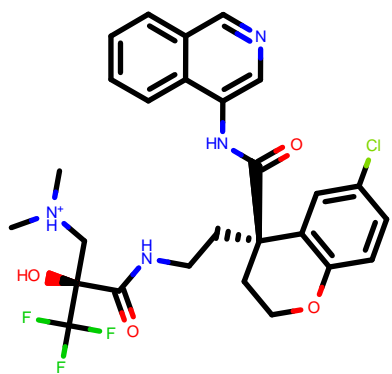
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5cn[nH]5

RUN: RUN3864

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.24

EN300-7459545_3_2_1



CID: EN300-7459545_3_2_1

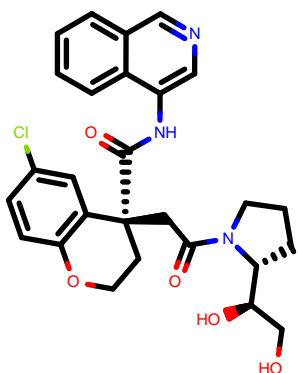
SMILES: CN(C)C[C@@](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)(C(F)F)F)O

RUN: RUN3651

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.52

EN300-7459540_1_1_1



CID: EN300-7459540_1_1_1

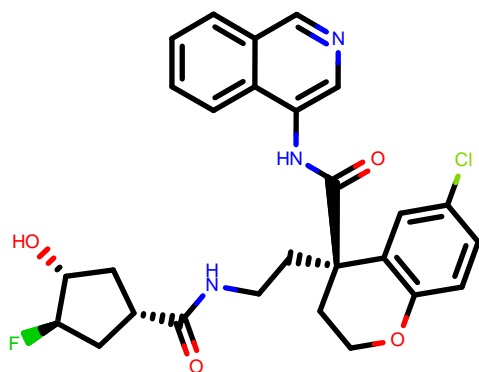
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)NCC(C)C@H5[C@@H]6(CO)O

RUN: RUN7042

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.36

EN300-7461217_3_2_1



CID: EN300-7461217_3_2_1

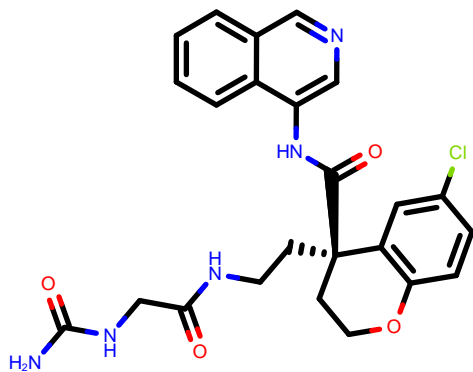
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5[C@@H]6(C)F)O

RUN: RUN5038

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.28

EN300-10397_3_1_1



CID: EN300-10397_3_1_1

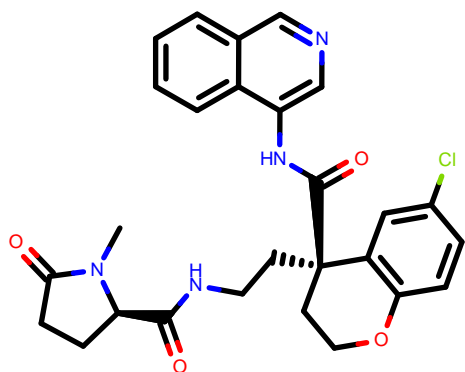
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)NCC(=O)N

RUN: RUN5461

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.26

EN300-343787_3_1_1



CID: EN300-343787_3_1_1

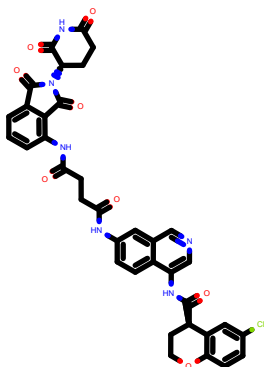
SMILES: CN1[C@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5809

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.32

DAR-DIA-9e4459de-15_6



CID: DAR-DIA-9e4459de-15_6

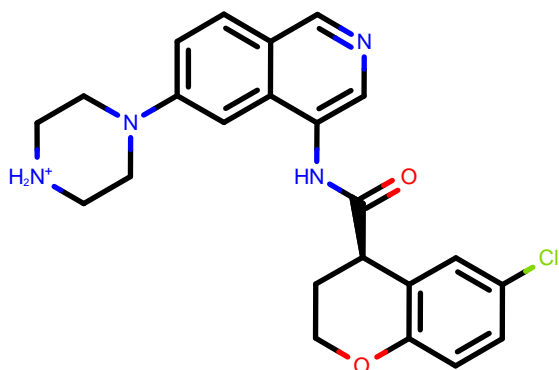
SMILES: c1cc2c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)ncnc4NC(=O)C[C@]5(CCOc6c5cc(cc6)Cl)C(=O)Nc7c7ccc1c7nc1=O

RUN: RUN1318

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.33

MAK-UNK-8be7dca9-4_1_1



CID: MAK-UNK-8be7dca9-4_1_1

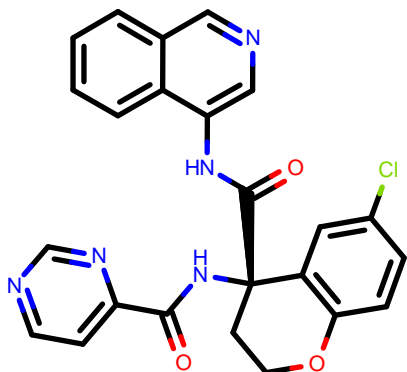
SMILES: c1cc2cnc(c2cc1N3CC[NH2+][CC3])NC(=O)[C@]4(CCOc5c4cc(cc5)Cl)C

RUN: RUN5625

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.09

EN300-111006_1_1_1



CID: EN300-111006_1_1_1

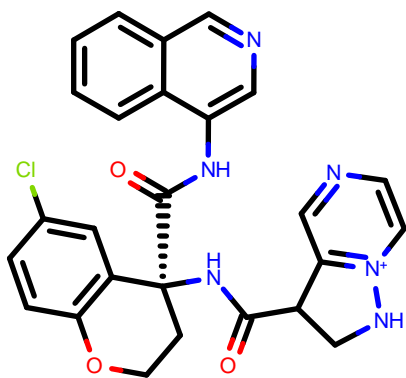
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccncc5

RUN: RUN3005

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.18

EN300-131572_1_1_1



CID: EN300-131572_1_1_1

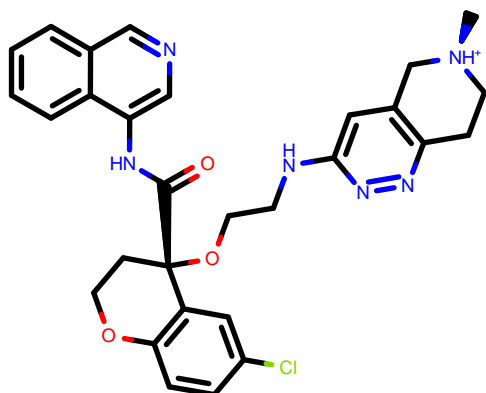
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn6c5cnc6

RUN: RUN4322

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.22

ED_-GRI-5b13fbe2-67_2



CID: ED_-GRI-5b13fbe2-67_2

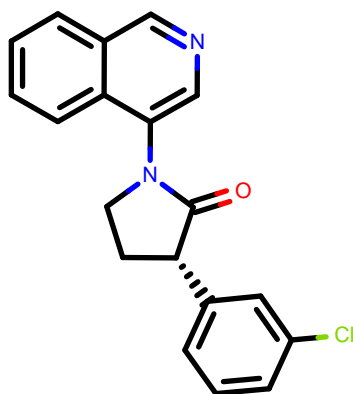
SMILES: C[N@H+]1CCc2c(ccn2)NCCO[C@]3(CCOc4c3cc(cc4)O)C(=O)Nc5cnc6c5cnc6

RUN: RUN1480

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.34

EDG-MED-5d232de5-8_1



CID: EDG-MED-5d232de5-8_1

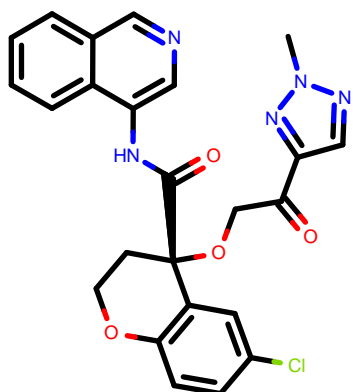
SMILES: c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN2186

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.28

EN300-204935_1_1_1



CID: EN300-204935_1_1_1

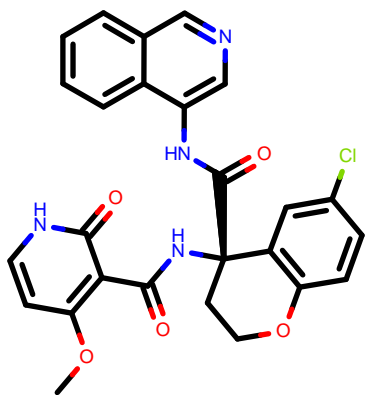
SMILES: Cn1ncc(n1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6060

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.29

EN300-156318_1_1_1



CID: EN300-156318_1_1_1

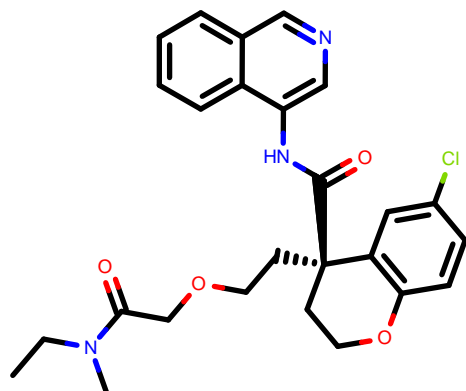
SMILES: COc1cc[nH]c(=O)c1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3484

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.27

EN300-1253122_3_1_1



CID: EN300-1253122_3_1_1

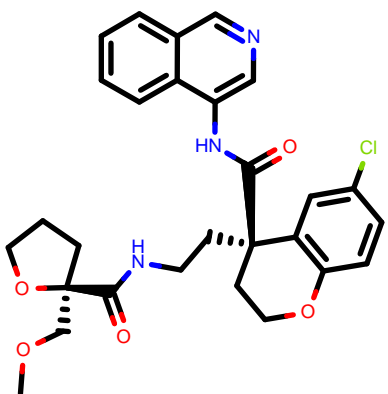
SMILES: CCN(C)C(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3597

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.27

EN300-1301381_3_2_1



CID: EN300-1301381_3_2_1

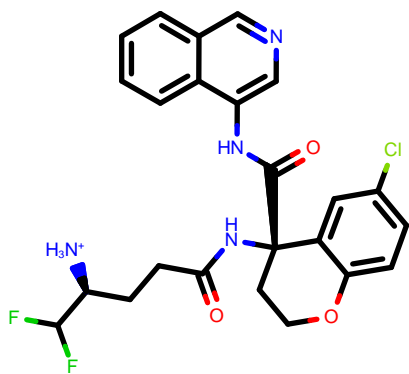
SMILES: COC[C@@]1(CCCO1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4969

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.29

EDG-MED-90036822-57_1



CID: EDG-MED-90036822-57_1

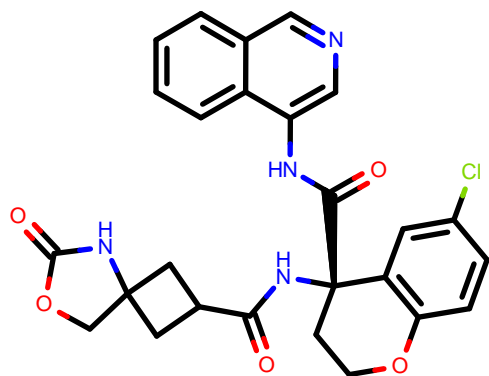
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@@]H(C)(F)F

RUN: RUN1607

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.43

EN300-7447185_1_1_1



CID: EN300-7447185_1_1_1

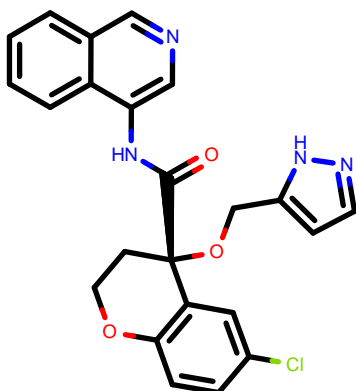
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC6(C5)COC(=O)N6

RUN: RUN3415

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-57_1



CID: ED_-GRI-5b13fbe2-57_1

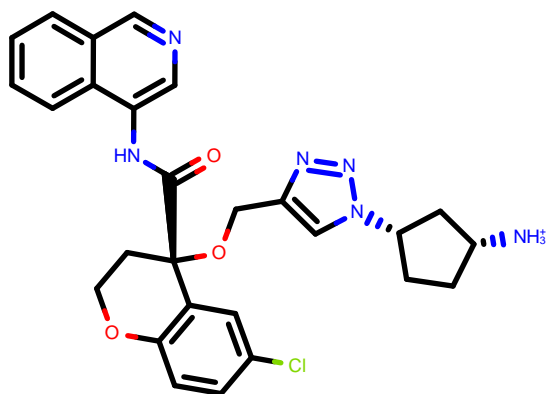
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn[nH]5

RUN: RUN1428

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.17

ED_-GRI-5b13fbe2-64_1



CID: ED_-GRI-5b13fbe2-64_1

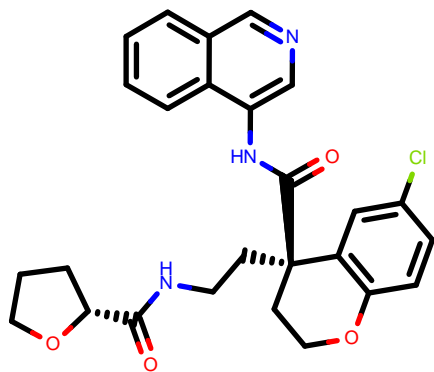
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5c[nH]5[C@@H]6CC[C@H]6C[NH3+]

RUN: RUN1470

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.34

EN300-21009_3_2_1



CID: EN300-21009_3_2_1

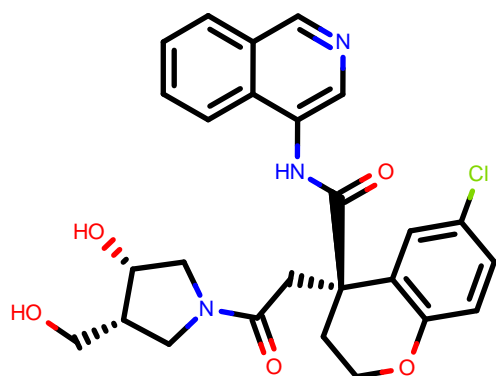
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCO5

RUN: RUN4287

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.25

EN300-248521_1_1_1



CID: EN300-248521_1_1_1

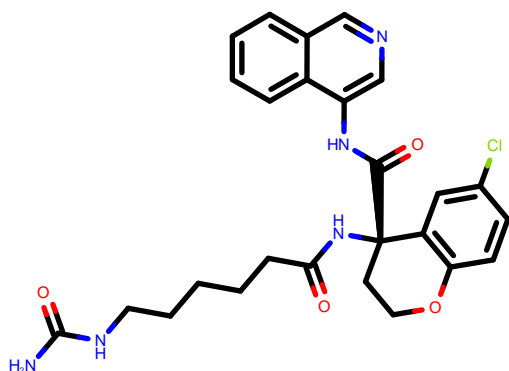
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H]5C[C@@H]5O5CO

RUN: RUN5927

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.36

EN300-13252_1_1_1



CID: EN300-13252_1_1_1

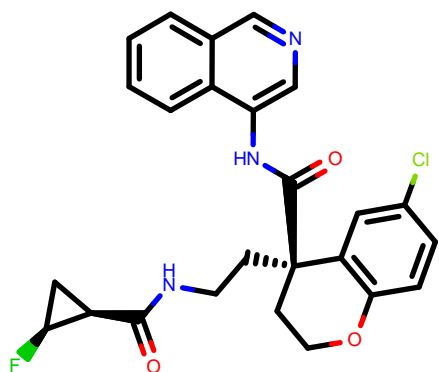
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCCCNC(=O)N

RUN: RUN6388

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.28

EN300-1654606_3_1_1



CID: EN300-1654606_3_1_1

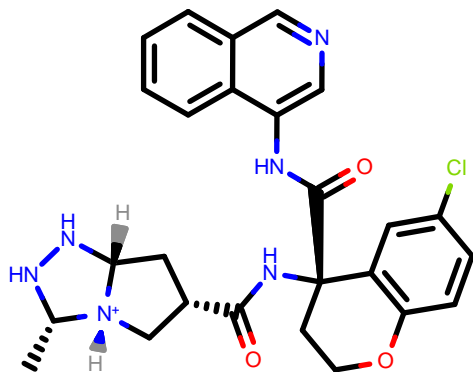
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]4[C@@]4H5C[C@@]4H5F

RUN: RUN3948

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.23

EN300-6729747_1_2_1



CID: EN300-6729747_1_2_1

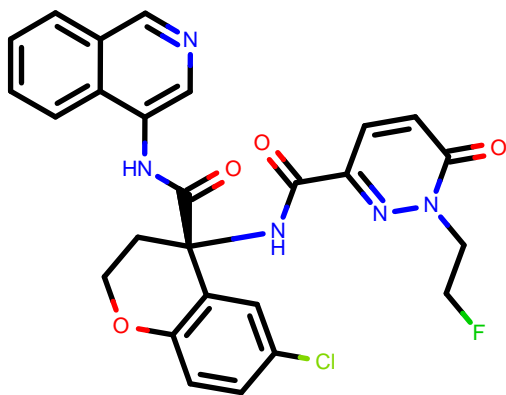
SMILES: C[C@@]1N[C@@H]2N[C@@H]1C[C@@H]2C[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H]5C[C@@H]5O5CCCC5

RUN: RUN5123

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.43

EN300-263456_1_1_1



CID: EN300-263456_1_1_1

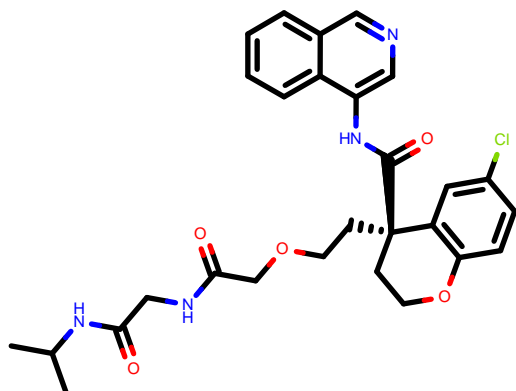
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(=O)n(n5)CCF

RUN: RUN3038

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.22

EN300-23221_3_1_1



CID: EN300-23221_3_1_1

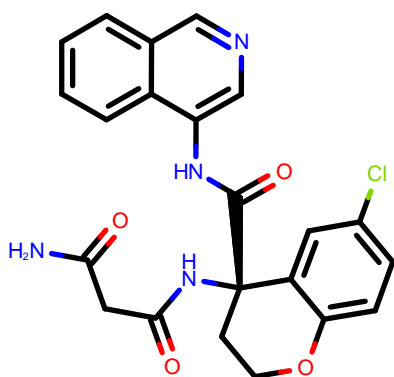
SMILES: CC(C)NC(=O)CNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN6493

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.31

EN300-82179_1_1_1



CID: EN300-82179_1_1_1

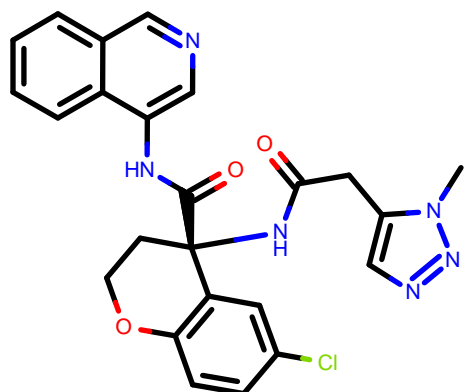
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)N

RUN: RUN3727

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.19

EN300-6486855_1_1_1



CID: EN300-6486855_1_1_1

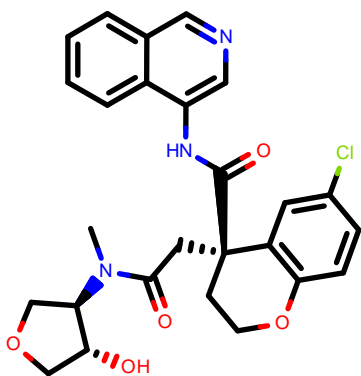
SMILES: Cn1c(cnn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4588

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.25

EN300-371682_1_1_1



CID: EN300-371682_1_1_1

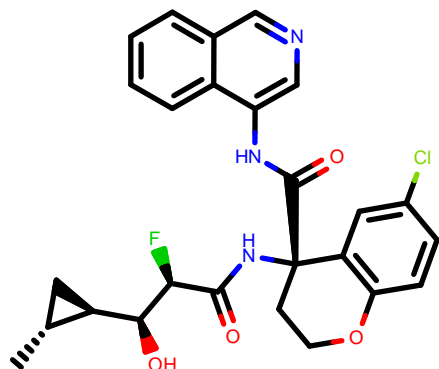
SMILES: CN[C@@H]1COC[C@H]1O)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3952

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.32

EDG-MED-90036822-94_11



CID: EDG-MED-90036822-94_11

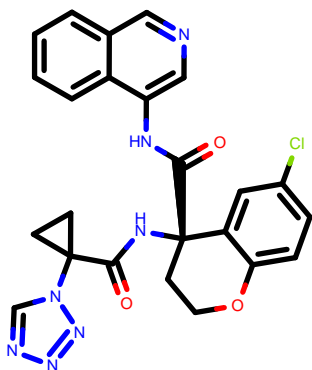
SMILES: C[C@@H]1C[C@@H]1[C@@H]2[C@H](C(=O)N[C@@]3(CCOc4c2cc(cc4)C)C(=O)Nc5ccc6c4ccc6)F)O

RUN: RUN1685

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.26

EN300-263085_1_1_1



CID: EN300-263085_1_1_1

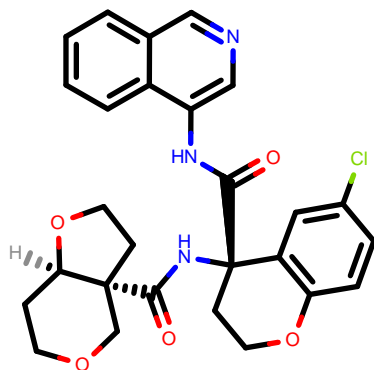
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C(C5)n6cnnn6

RUN: RUN2952

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.20

EN300-341337_1_1_1



CID: EN300-341337_1_1_1

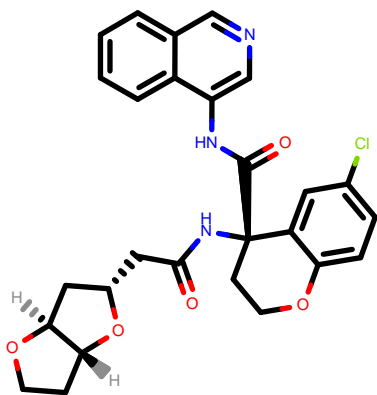
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]56CCO[C@@H]5CCO6

RUN: RUN3908

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.26

EN300-735519_1_8_1



CID: EN300-735519_1_8_1

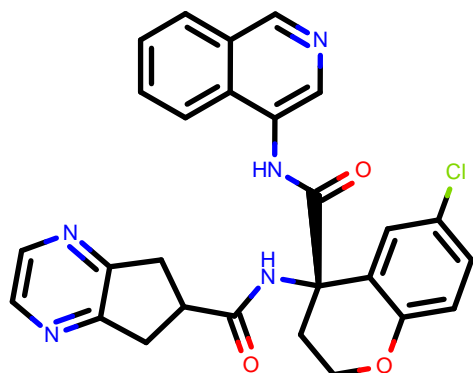
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)C1NC(=O)C[C@@H]5C[C@H]6[C@@H]O5CCO6

RUN: RUN4784

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.24

EN300-2011576_1_1_1



CID: EN300-2011576_1_1_1

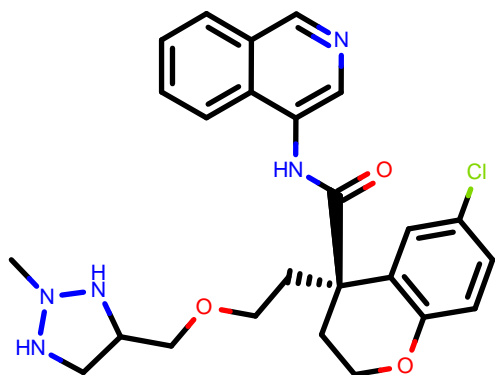
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4C3CC1(C)C1NC(=O)C5C6c6(ncn6)C5

RUN: RUN5956

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.24

EN300-219020_3_1_1



CID: EN300-219020_3_1_1

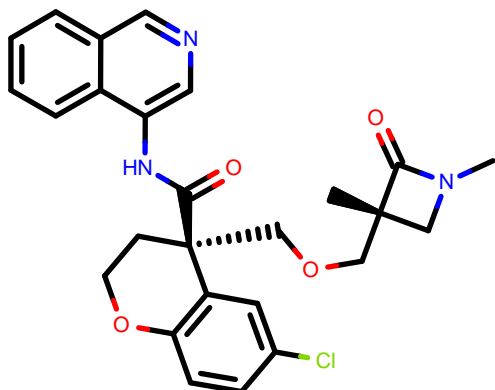
SMILES: Cn1ncc(n1)COC[C@@]2(C)C(CO)C3C2CC1(C)C1NC(=O)Nc4cnc5c4cccc5

RUN: RUN4184

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.27

EN300-1273362_2_1_1



CID: EN300-1273362_2_1_1

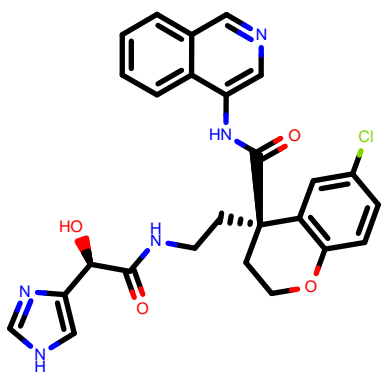
SMILES: C[C@@]1(C)NC(C1=O)C)COC[C@@]2(C)C(CO)C3C2CC1(C)C1NC(=O)Nc4cnc5c4cccc5

RUN: RUN3671

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.31

EN300-254121_3_1_1



CID: EN300-254121_3_1_1

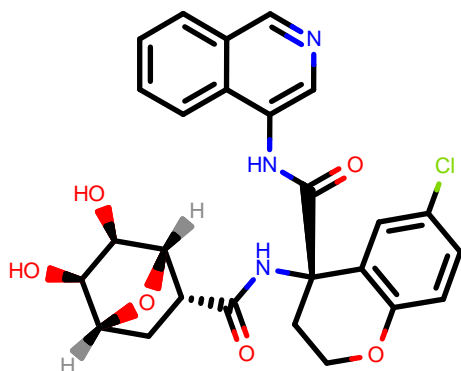
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C@H](c5nc[nH]5)O

RUN: RUN5315

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.31

EN300-6764836_1_7_1



CID: EN300-6764836_1_7_1

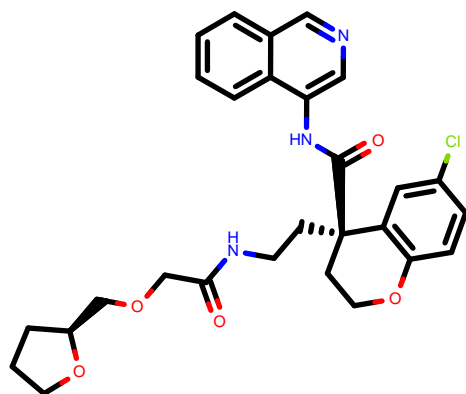
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@H]5C[C@@H]6[C@H](C)C=H5O6)O

RUN: RUN4965

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.25

EN300-60033_3_1_1



CID: EN300-60033_3_1_1

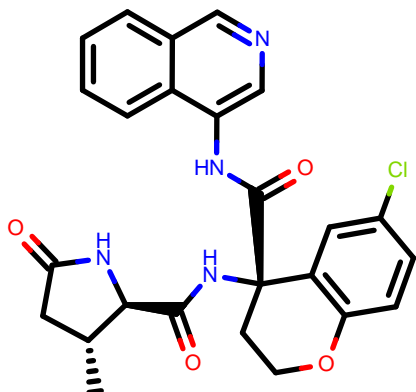
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)COC[C@@H]5CCCC5

RUN: RUN4894

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.33

EN300-155362_1_3_1



CID: EN300-155362_1_3_1

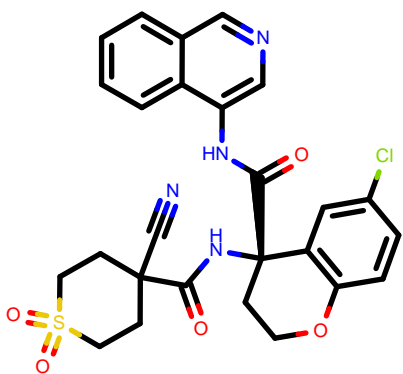
SMILES: C[C@@H]1CC(=O)N[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN4620

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.23

EN300-73967_1_1_1



CID: EN300-73967_1_1_1

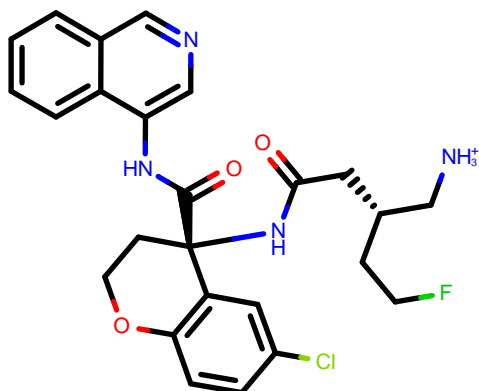
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)C5(CCS(=O)(=O)C)C#N

RUN: RUN6405

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.32

EDG-MED-90036822-88_1



CID: EDG-MED-90036822-88_1

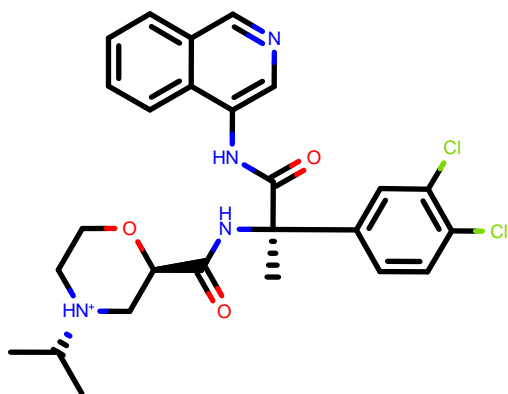
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H](CCF)C[NH3+]

RUN: RUN1681

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.30

MAT-POS-e9e99895-2_7



CID: MAT-POS-e9e99895-2_7

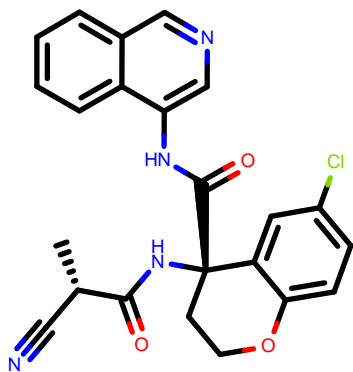
SMILES: CC(C)[N@@H+]1CCO[C@@H](C1)C(=O)N[C@@]2(C)C(=O)C2c3cc(c(c2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN2087

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.51

EDG-MED-90036822-80_1



CID: EDG-MED-90036822-80_1

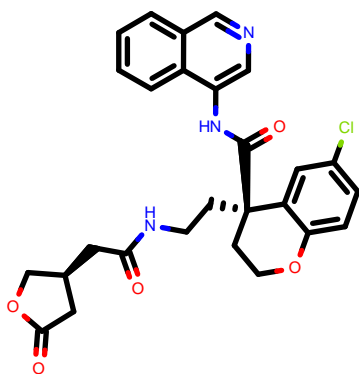
SMILES: C[C@@H](C#N)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN1623

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.15

EN300-109535_3_2_1



CID: EN300-109535_3_2_1

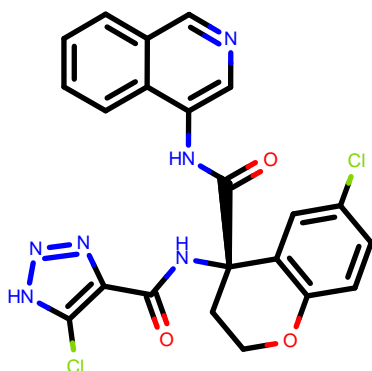
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@@H]5CC(=O)OC5

RUN: RUN4297

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.28

EN300-149013_1_1_1



CID: EN300-149013_1_1_1

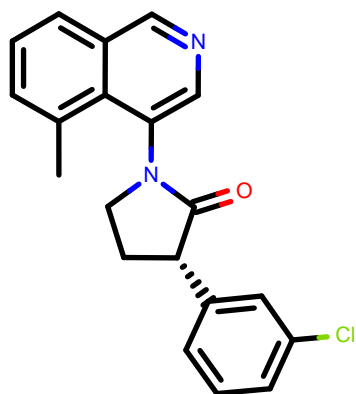
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]n5Cl

RUN: RUN3546

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.22

MIC-UNK-50cce87d-7_2



CID: MIC-UNK-50cce87d-7_2

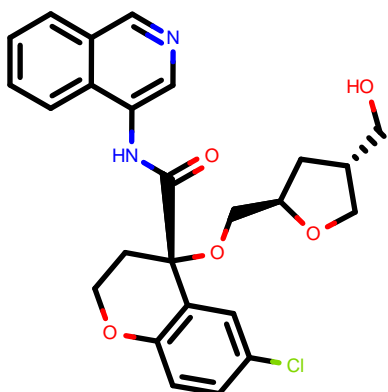
SMILES: Cc1cccc2c1c(cnc2)N3CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN553

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.25

EN300-6494158_1_2_1



CID: EN300-6494158_1_2_1

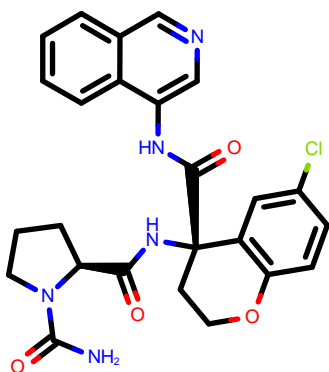
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@@H](CO)CO

RUN: RUN3526

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.30

EN300-87536_1_1_1



CID: EN300-87536_1_1_1

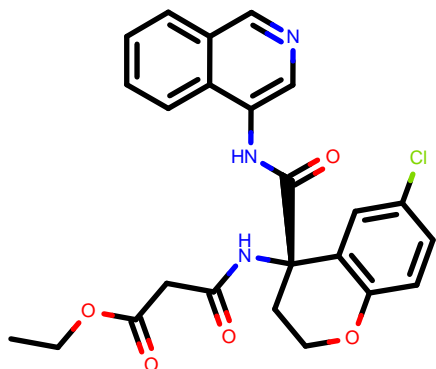
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5CNCN5C(=O)N

RUN: RUN6864

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.27

EN300-41828_1_1_1



CID: EN300-41828_1_1_1

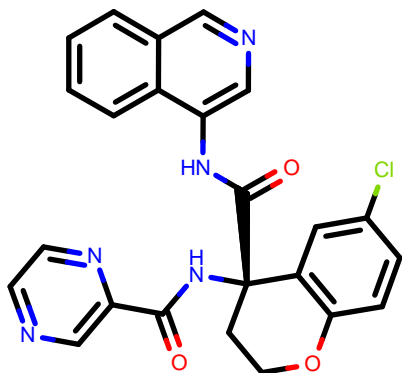
SMILES: CCOC(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN5542

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.20

EN300-19900_1_1_1



CID: EN300-19900_1_1_1

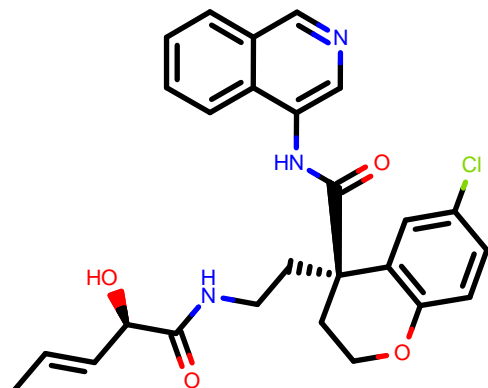
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nccn5

RUN: RUN2727

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.20

EN300-300217_3_4_1



CID: EN300-300217_3_4_1

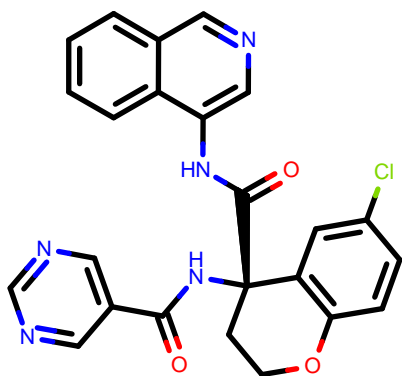
SMILES: C/C=C/[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4)O

RUN: RUN4924

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.36

EN300-64297_1_1_1



CID: EN300-64297_1_1_1

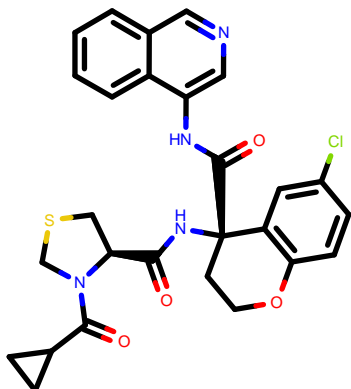
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnc5

RUN: RUN4690

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.20

EN300-18928_1_1_1



CID: EN300-18928_1_1_1

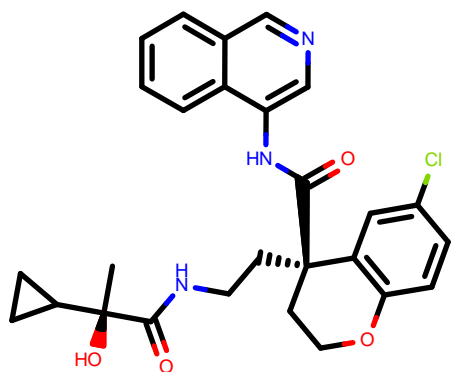
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CSCN5C(=O)C6CC6

RUN: RUN5885

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.31

EN300-118760_3_1_1



CID: EN300-118760_3_1_1

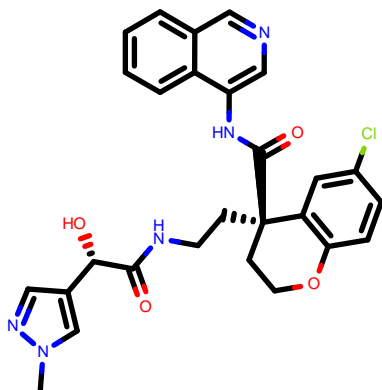
SMILES: C[C@@](C1CC1)(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN3947

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.38

EN300-198540_3_1_1



CID: EN300-198540_3_1_1

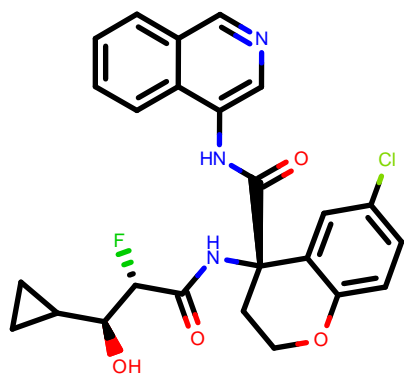
SMILES: Cn1cc(cn1)[C@@]3(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN6584

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.31

EDG-MED-90036822-78_4



CID: EDG-MED-90036822-78_4

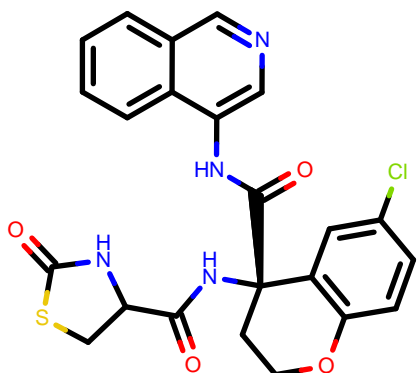
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@H](C5CC5)O)F

RUN: RUN1659

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.22

EN300-133915_1_1_1



CID: EN300-133915_1_1_1

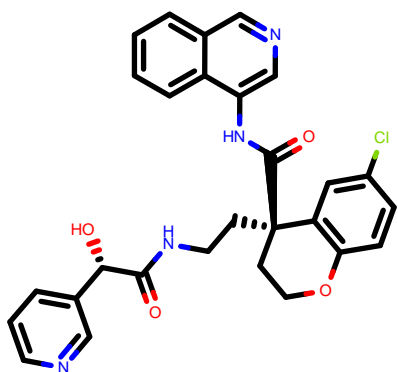
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CSCC(=O)N

RUN: RUN6528

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-134855_3_2_1



CID: EN300-134855_3_2_1

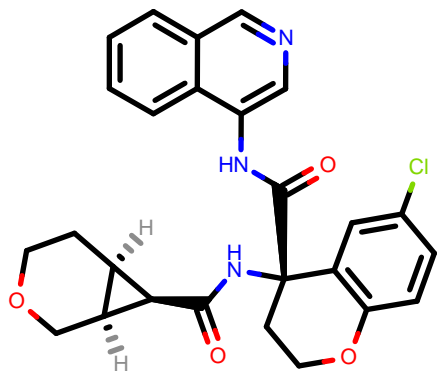
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](c5ccncc5)O

RUN: RUN5586

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.30

EN300-1644723_1_3_1



CID: EN300-1644723_1_3_1

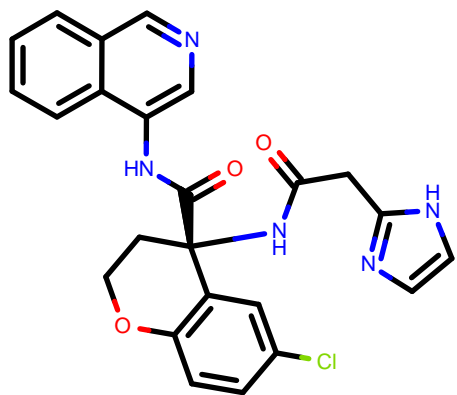
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]([C@H]([C@@]4(C)COC4)C)C(=O)O

RUN: RUN4460

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.28

EDG-MED-90036822-31_1



CID: EDG-MED-90036822-31_1

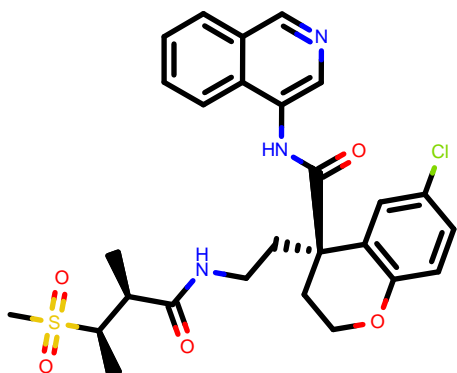
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5[nH]cn5

RUN: RUN1535

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.22

EN300-182725_3_2_1



CID: EN300-182725_3_2_1

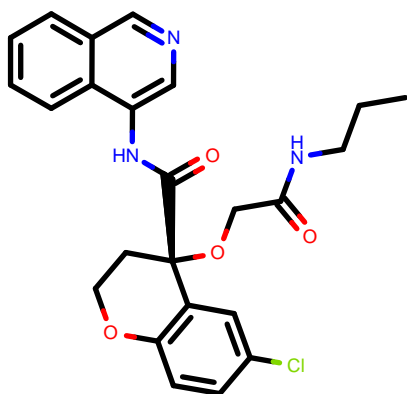
SMILES: C[C@@H](C[C@@H](C)[Si](=O)(=O)C)C(=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN5618

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.43

EN300-17184_1_1_1



CID: EN300-17184_1_1_1

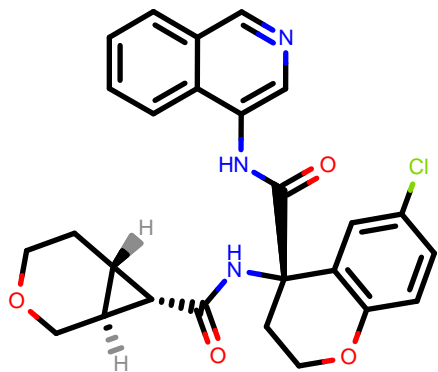
SMILES: C=CCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN5670

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.19

EN300-1644723_1_2_1



CID: EN300-1644723_1_2_1

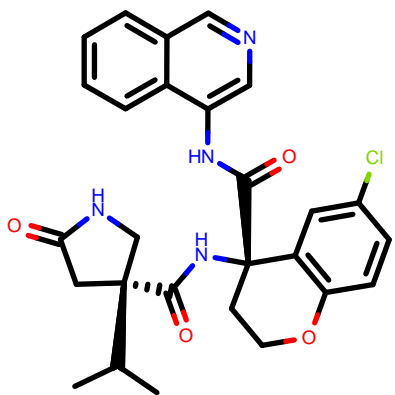
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]6[C@@H]5COC6

RUN: RUN5173

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.22

EN300-211203_1_2_1



CID: EN300-211203_1_2_1

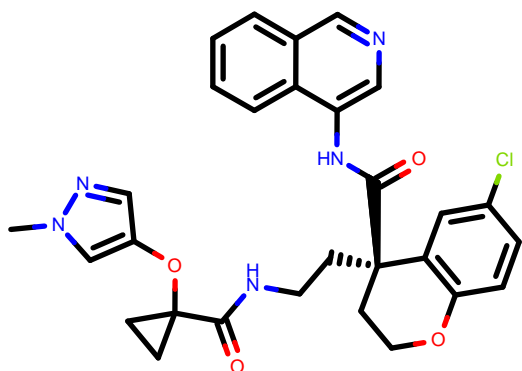
SMILES: CC(C)[C@]1(CC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5122

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-7352812_3_1_1



CID: EN300-7352812_3_1_1

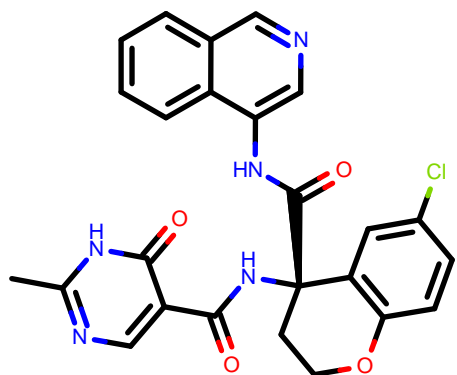
SMILES: Cn1cc(en1)OC2(CC2)C(=O)NCC[C@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN4020

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.34

EN300-67267_1_1_1



CID: EN300-67267_1_1_1

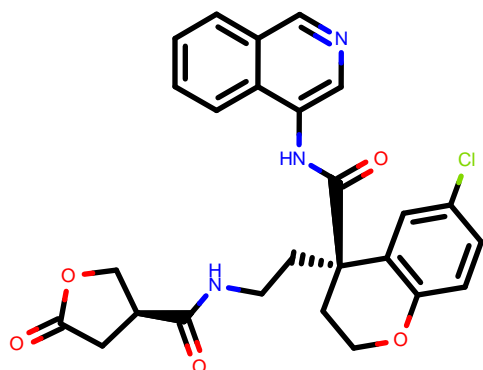
SMILES: Cc1[nH]c(=O)c(en1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4226

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.27

EN300-113234_3_2_1



CID: EN300-113234_3_2_1

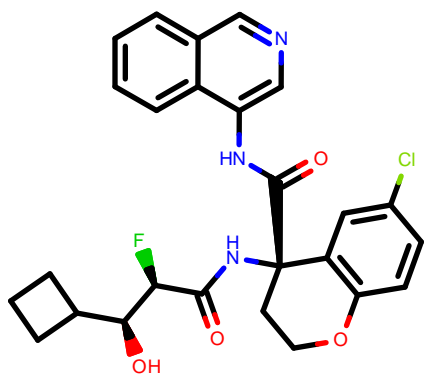
SMILES: c1ccc2c(c1)cnoc2NC(=O)[C@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CC(=O)OC5

RUN: RUN4821

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

EDG-MED-90036822-99_3



CID: EDG-MED-90036822-99_3

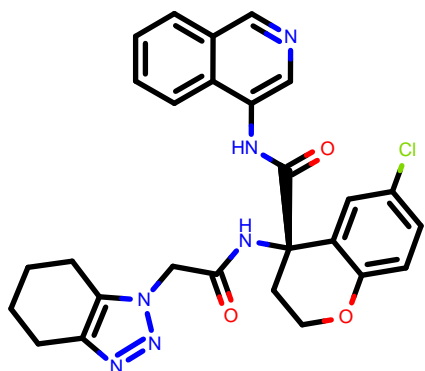
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@@H](C5CC5)O)F

RUN: RUN1692

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.26

EN300-223187_1_1_1



CID: EN300-223187_1_1_1

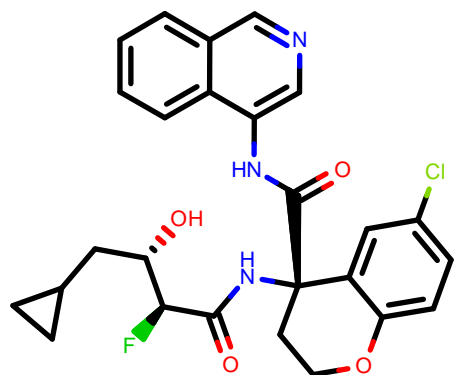
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c6c(nn5)CCCC6

RUN: RUN3478

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

EDG-MED-90036822-108_4



CID: EDG-MED-90036822-108_4

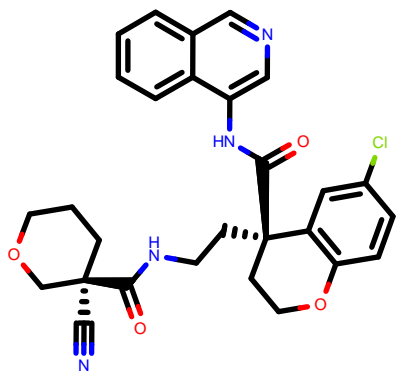
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@@H](C5CC5)O)F

RUN: RUN1754

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

EN300-301925_3_1_1



CID: EN300-301925_3_1_1

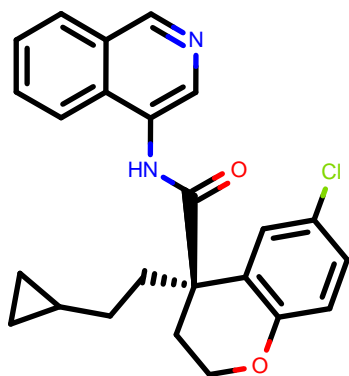
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN2997

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.29

ALP-POS-477dc5b7-3_1_1



CID: ALP-POS-477dc5b7-3_1_1

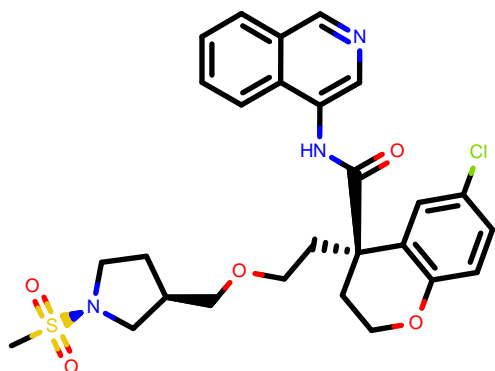
SMILES: c1ccc2c(e1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CC5

RUN: RUN5937

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.21

KAD-UNI-8a629cb0-1_1



CID: KAD-UNI-8a629cb0-1_1

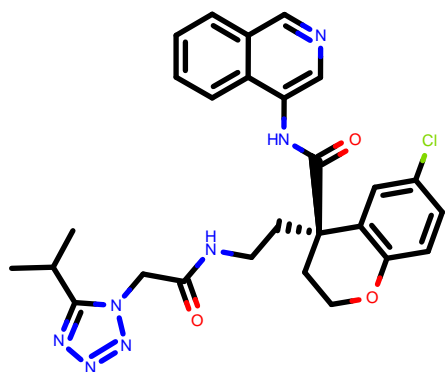
SMILES: CS(=O)(=O)N@@]1CC[C@H](C1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2029

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.40

EN300-96933_3_1_1



CID: EN300-96933_3_1_1

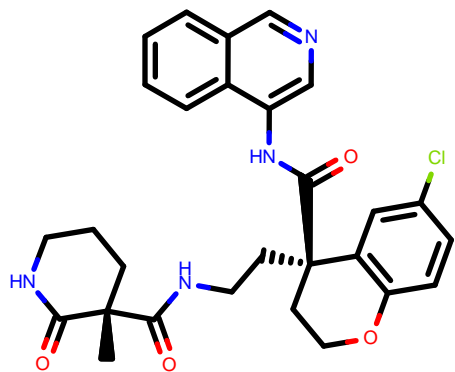
SMILES: CC(C)c1n[nH]1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4276

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.42

EN300-178876_3_1_1



CID: EN300-178876_3_1_1

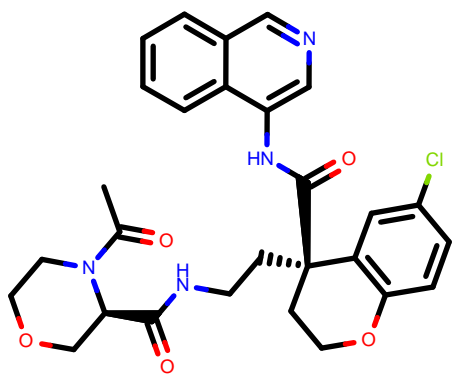
SMILES: C[C@@]1(CCCN1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5109

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.40

EN300-116313_3_1_1



CID: EN300-116313_3_1_1

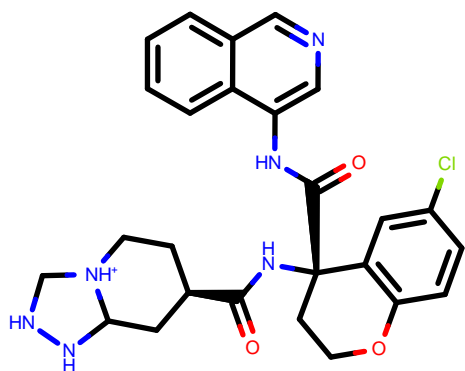
SMILES: CC(=O)N1CCOC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4487

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.31

EN300-6474341_1_1_1



CID: EN300-6474341_1_1_1

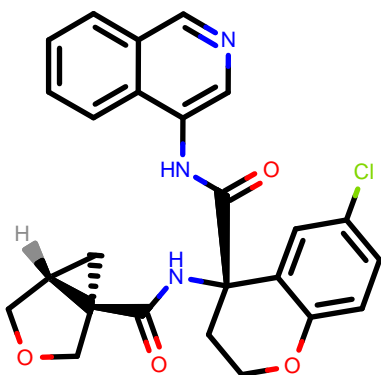
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCN6enncc65

RUN: RUN5577

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.24

EN300-263669_1_1_1



CID: EN300-263669_1_1_1

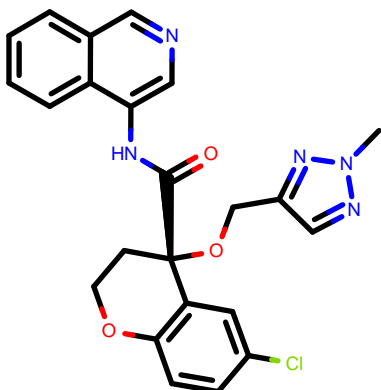
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56C[C@H]5COC6

RUN: RUN4339

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.23

EN300-219020_1_1_1



CID: EN300-219020_1_1_1

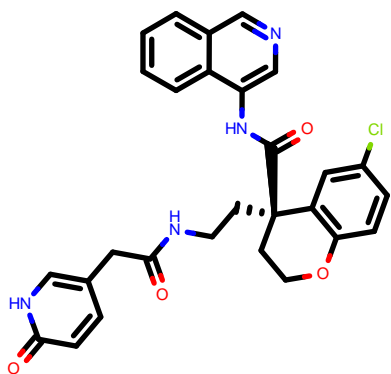
SMILES: Cn1ncc(n1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4875

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.20

EN300-189672_3_1_1



CID: EN300-189672_3_1_1

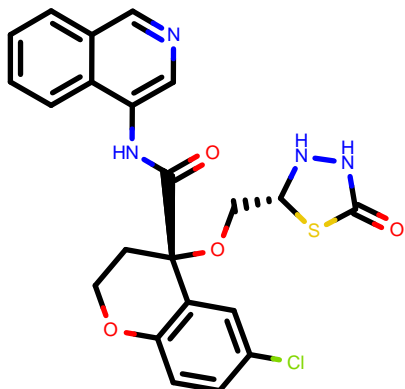
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(=O)[nH]c5

RUN: RUN4247

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.31

EN300-171766_1_1_1



CID: EN300-171766_1_1_1

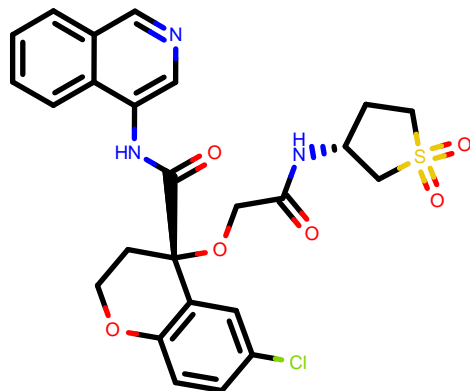
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]H5NNC(=O)S5

RUN: RUN3540

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.20

EN300-05512_1_1_1



CID: EN300-05512_1_1_1

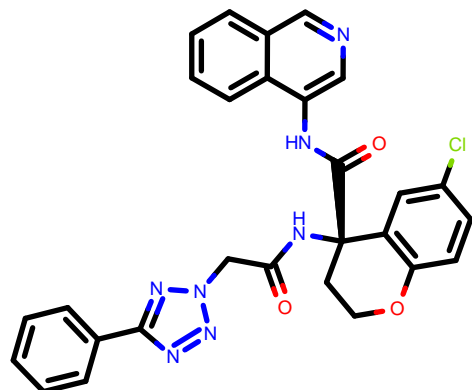
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@]H5SCS(=O)(=O)C5

RUN: RUN3470

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.32

EN300-08065_1_1_1



CID: EN300-08065_1_1_1

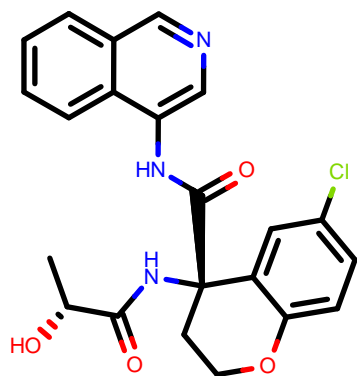
SMILES: c1ccc(cc1)c2nnn(n2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN4683

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.27

EN300-77464_1_1_1



CID: EN300-77464_1_1_1

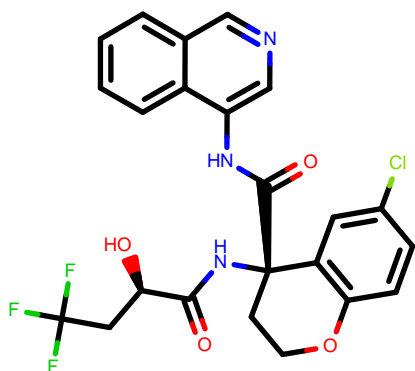
SMILES: C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN4524

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.19

EN300-1932013_1_1_1



CID: EN300-1932013_1_1_1

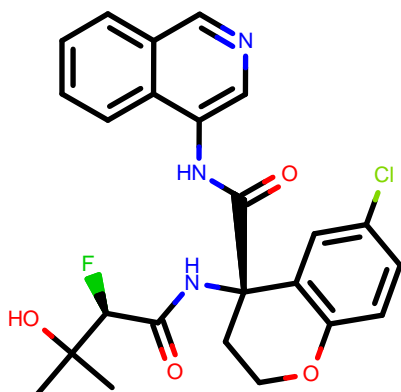
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)[C@@]H(CC(F)(F)F)O

RUN: RUN2927

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.30

EN300-264744_1_2_1



CID: EN300-264744_1_2_1

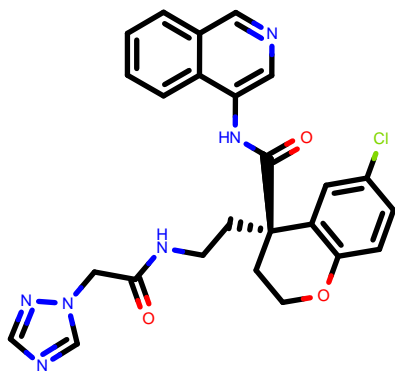
SMILES: CC(C)[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)F)O

RUN: RUN4257

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.20

EN300-06654_3_1_1



CID: EN300-06654_3_1_1

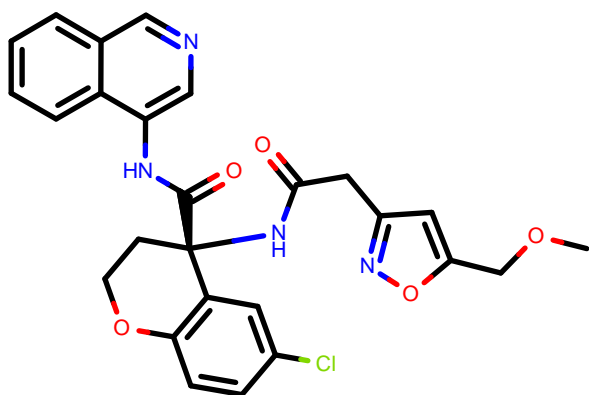
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)Cn5cncn5

RUN: RUN4558

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.25

EN300-6477475_1_1_1



CID: EN300-6477475_1_1_1

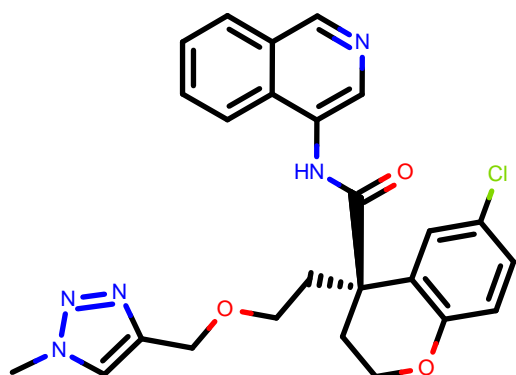
SMILES: COCc1cc(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6279

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.24

EN300-120282_3_1_1



CID: EN300-120282_3_1_1

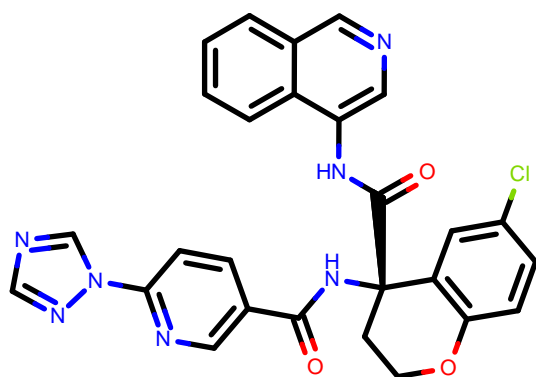
SMILES: Cn1cc(nn1)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3465

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.25

EN300-27261_1_1_1



CID: EN300-27261_1_1_1

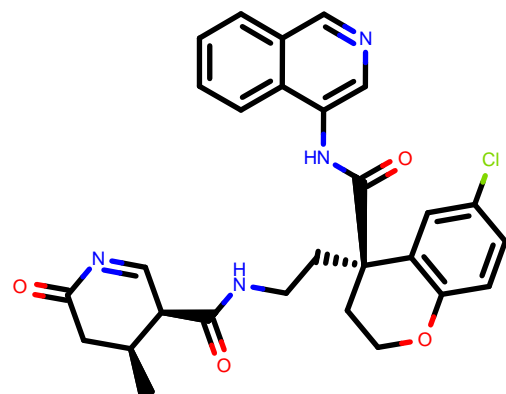
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(nc5)n6cnc6

RUN: RUN7510

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.23

EN300-95698_3_4_1



CID: EN300-95698_3_4_1

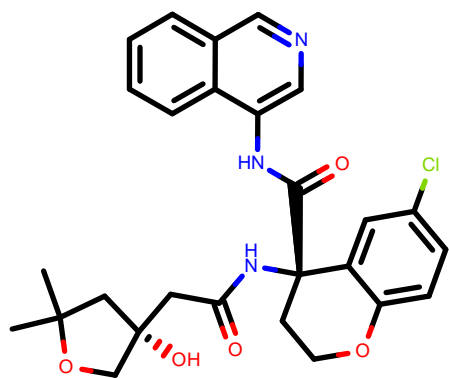
SMILES: C[C@H]1CC(=O)NC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN5760

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.33

EN300-360158_1_2_1



CID: EN300-360158_1_2_1

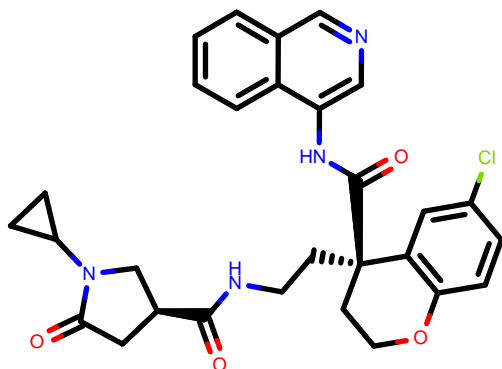
SMILES: CC1(C)C@](CO1)(CC(=O)N[C@@]2(CCOC3C2C(C)C)C(=O)Nc4nc5c4ccc5O)C

RUN: RUN3383

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.28

EN300-12440_3_2_1



CID: EN300-12440_3_2_1

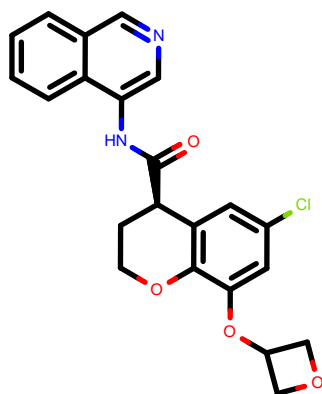
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3C(C)C(C)CNC1=O[C@@H]5CC(=O)N(C5)C6C6

RUN: RUN4451

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.43

EDJ-MED-e4b030d8-4_1_1



CID: EDJ-MED-e4b030d8-4_1_1

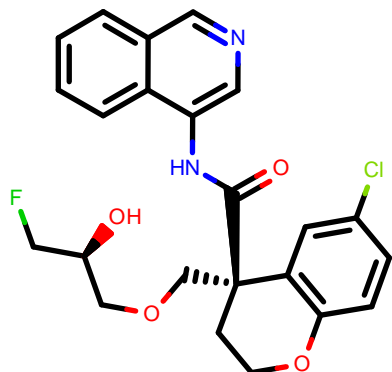
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3C(C)C(C)CNC1=O[C@@H]5COC5)C

RUN: RUN3965

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.19

EN300-1968342_2_1_1



CID: EN300-1968342_2_1_1

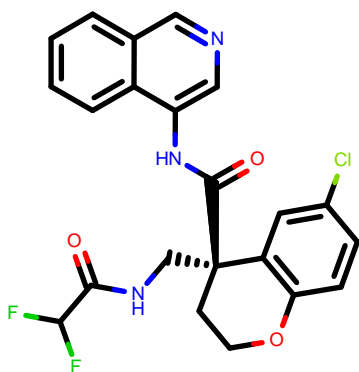
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3C(C)C(C)CNC1=O[C@@H](CF)O

RUN: RUN3650

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.28

EN300-19507_2_1_1



CID: EN300-19507_2_1_1

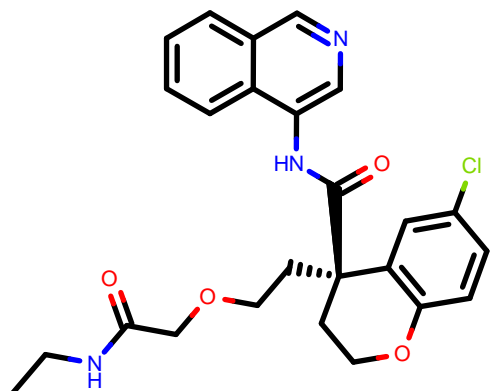
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(F)F

RUN: RUN5759

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.21

EN300-7003350_3_1_1



CID: EN300-7003350_3_1_1

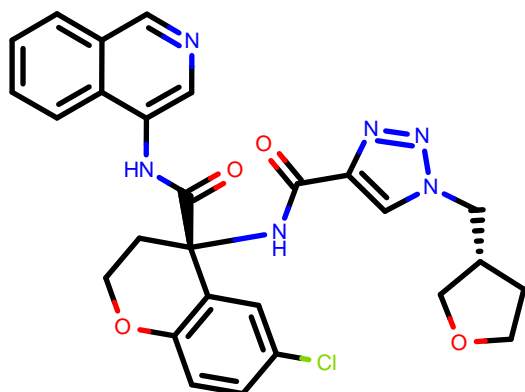
SMILES: CCNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3833

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.25

EN300-317272_1_1_1



CID: EN300-317272_1_1_1

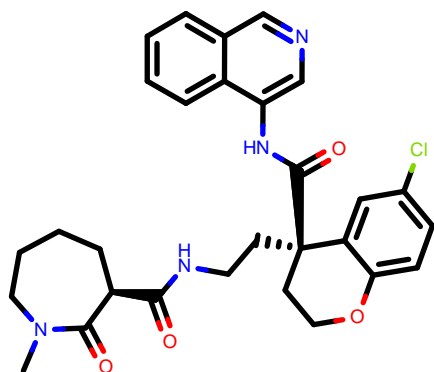
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@]6OCOC6

RUN: RUN7490

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.30

EN300-304695_3_2_1



CID: EN300-304695_3_2_1

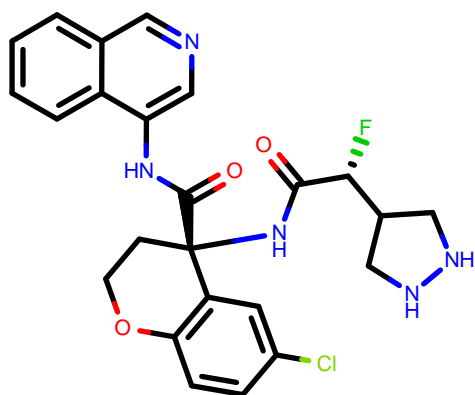
SMILES: CN1CCCC[C@@H](C1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN6140

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.39

EDG-MED-90036822-8_1



CID: EDG-MED-90036822-8_1

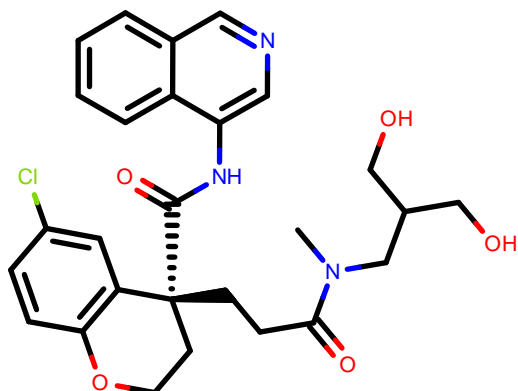
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5c[nH]nc5)F

RUN: RUN1547

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.22

EN300-1654957_2_1_1



CID: EN300-1654957_2_1_1

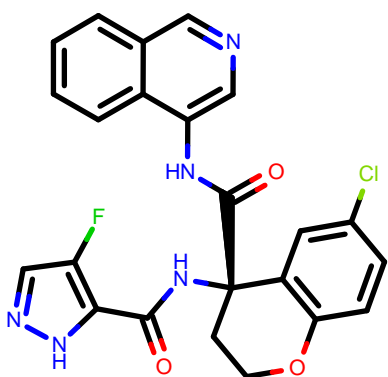
SMILES: CN(CC(CO)CO)C(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN5373

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.25

EDG-MED-90036822-32_1



CID: EDG-MED-90036822-32_1

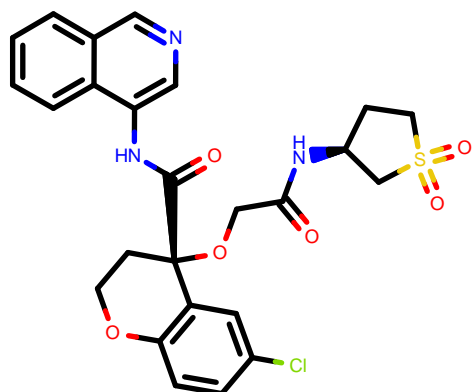
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5c[nH]j5)F

RUN: RUN1552

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.23

EN300-05512_1_2_1



CID: EN300-05512_1_2_1

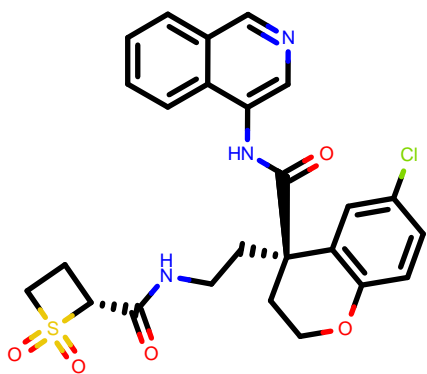
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5SCCS(=O)(=O)C5

RUN: RUN7170

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.32

EN300-1387104_3_2_1



CID: EN300-1387104_3_2_1

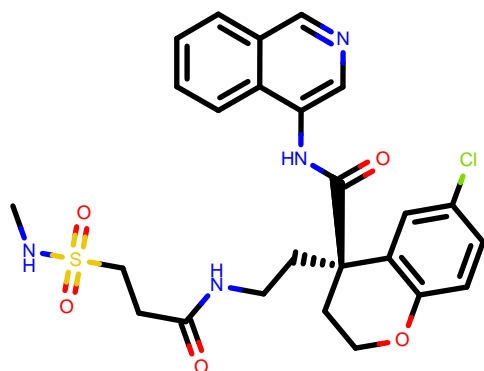
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCSS(=O)=O

RUN: RUN5159

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.29

EN300-123205_3_1_1



CID: EN300-123205_3_1_1

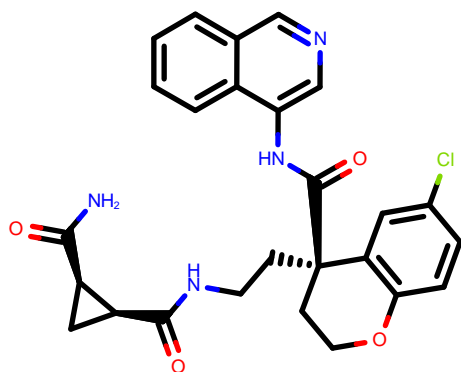
SMILES: CNS(=O)(=O)CCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN4619

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.33

EN300-331941_3_1_1



CID: EN300-331941_3_1_1

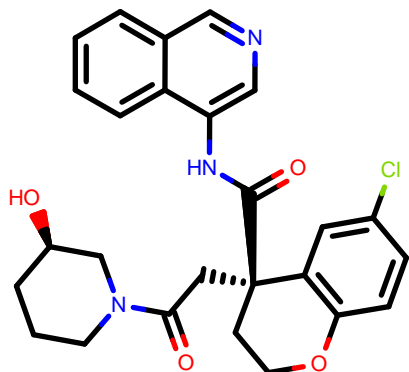
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@H]5C(=O)N

RUN: RUN3964

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.29

EDJ-MED-d203f206-26_1



CID: EDJ-MED-d203f206-26_1

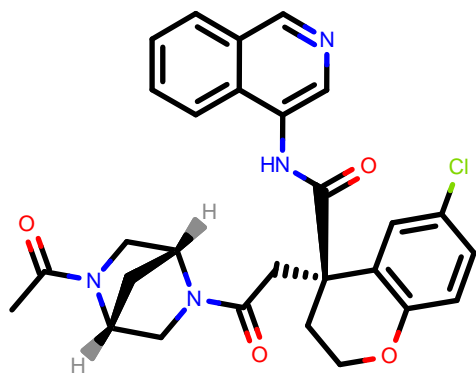
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O

RUN: RUN2410

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.26

KAD-UNI-80f122c8-2_2



CID: KAD-UNI-80f122c8-2_2

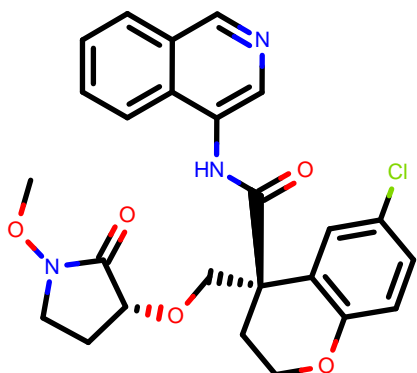
SMILES: CC(=O)N1C[C@@H]2C[C@@H]1CN2C(=O)C[C@@]3(C)COC4=C3C(=O)C(Cl)=O)N5COC6=C5C=CC=C6

RUN: RUN2201

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.32

EN300-302058_2_2_1



CID: EN300-302058_2_2_1

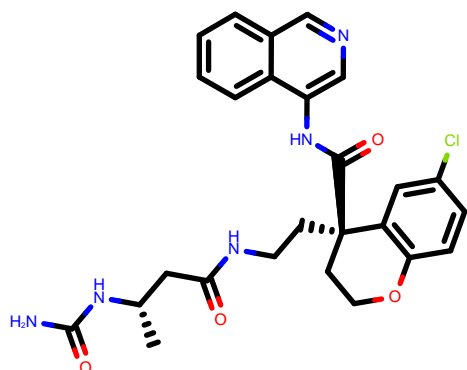
SMILES: CON1CC[C@@H](C1=O)OC[C@@]2(C)COC3=C2C(=O)C(Cl)=O)N4COC5=C4C=CC=C5

RUN: RUN5502

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.27

EN300-268198_3_1_1



CID: EN300-268198_3_1_1

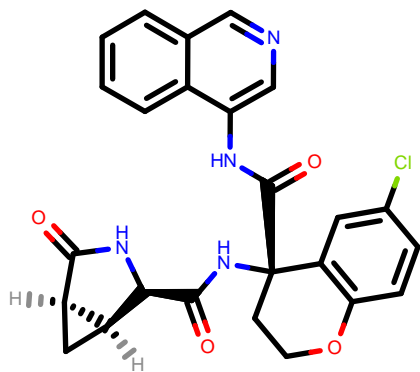
SMILES: C[C@@H](CC(=O)NCC[C@@]1(C)COC2=C1C(=O)C(Cl)=O)N3COC4=C3C=CC=C4)N(=O)N

RUN: RUN4848

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.30

EN300-6766359_1_1_1



CID: EN300-6766359_1_1_1

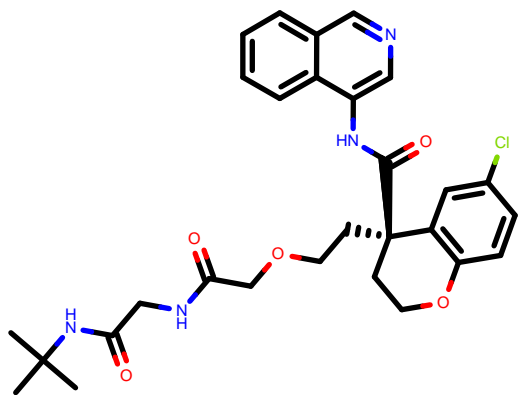
SMILES: C1C=CC2=C1)NCC2(=O)C[C@@]3(C)COC4=C3C(=O)C(Cl)=O)N5C(=O)C(=O)N5C(=O)N

RUN: RUN6045

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.21

EN300-48760_3_1_1



CID: EN300-48760_3_1_1

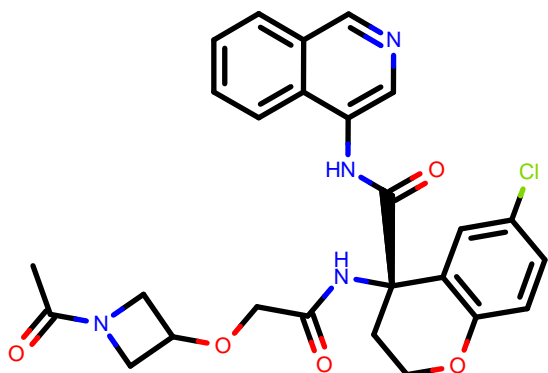
SMILES: CC(C)(C)NC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6069

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.28

EN300-259004_1_1_1



CID: EN300-259004_1_1_1

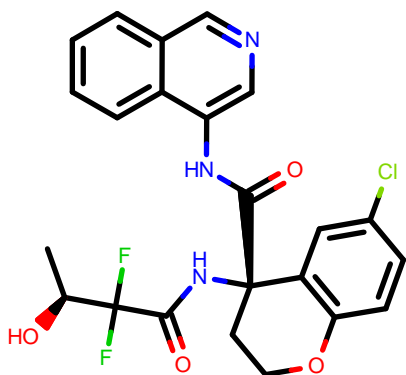
SMILES: CC(=O)N1CC(C1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5734

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.32

EN300-185398_1_1_1



CID: EN300-185398_1_1_1

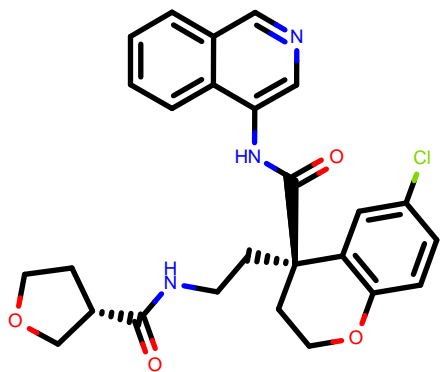
SMILES: C[C@@H](C(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)(F)F)O

RUN: RUN4061

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.19

EN300-170463_3_1_1



CID: EN300-170463_3_1_1

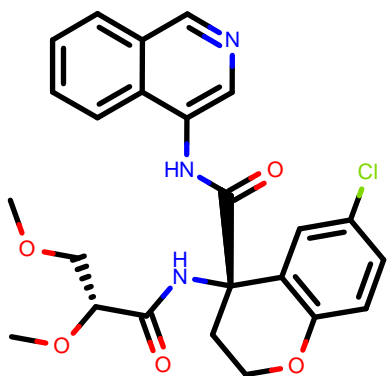
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5

RUN: RUN4696

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.27

EN300-305282_1_2_1



CID: EN300-305282_1_2_1

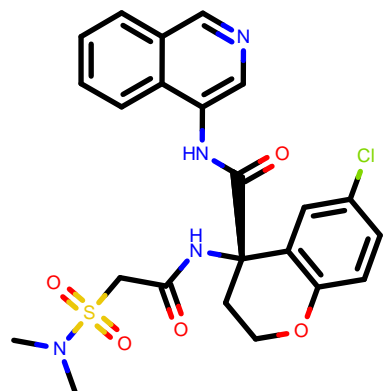
SMILES: COC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC

RUN: RUN3552

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.33

EN300-133128_1_1_1



CID: EN300-133128_1_1_1

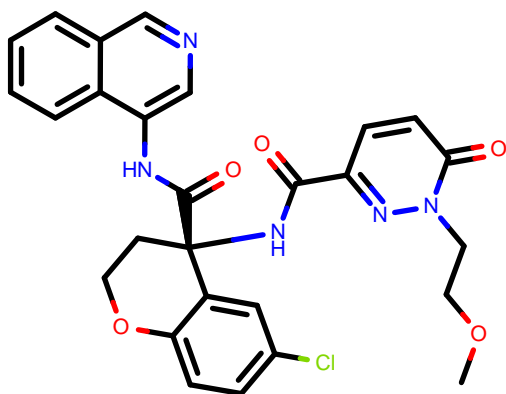
SMILES: CN(C)S(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3135

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.25

EN300-23417_1_1_1



CID: EN300-23417_1_1_1

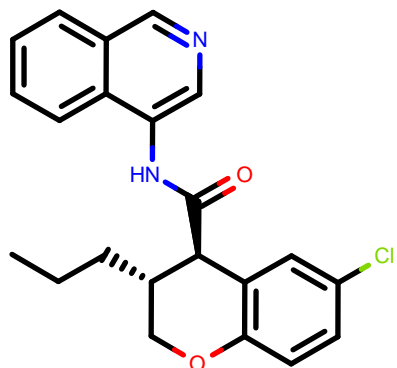
SMILES: COCCn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2841

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.32

EDJ-MED-e4b030d8-6_1_1



CID: EDJ-MED-e4b030d8-6_1_1

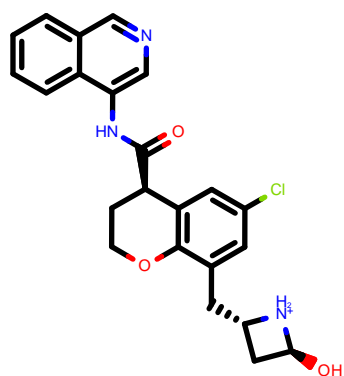
SMILES: CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN3915

DDG (kcal/mol): -1.60

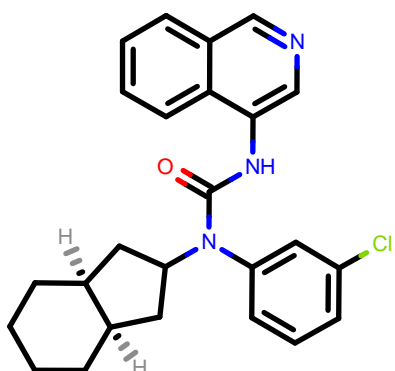
dDDG (kcal/mol): 0.09

DAR-DIA-6a508060-5_3



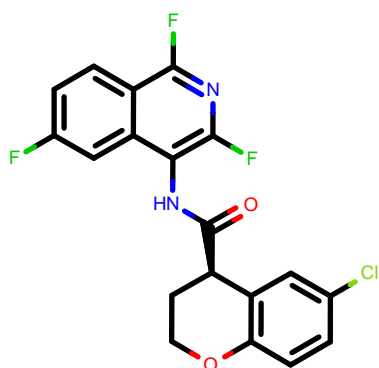
CID:	DAR-DIA-6a508060-5_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4C[C@H]5CC(=O)N5)Cl</chem>
RUN:	RUN301
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.17

MIC-UNK-cdc2493e-5_1



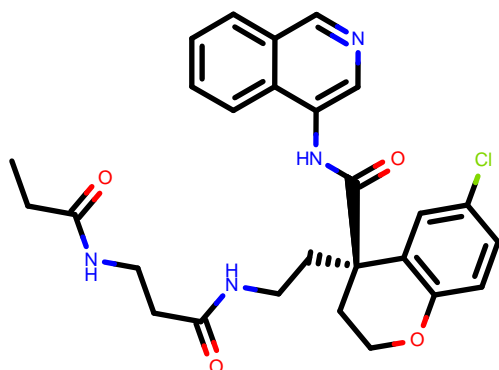
CID:	MIC-UNK-cdc2493e-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCCC[C@H]5C4</chem>
RUN:	RUN455
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.30

JOH-SUS-a69c159d-7_1_1



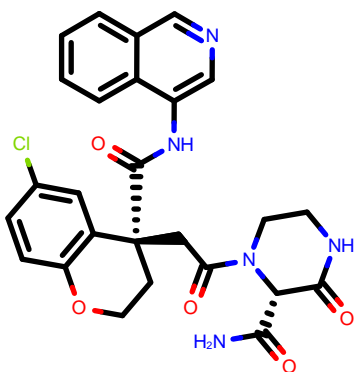
CID:	JOH-SUS-a69c159d-7_1_1
SMILES:	<chem>c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN3521
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.11

EN300-31186_3_1_1



CID:	EN300-31186_3_1_1
SMILES:	<chem>CCC(=O)NCCC(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4</chem>
RUN:	RUN7148
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.33

EN300-7473032_1_1_1



CID: EN300-7473032_1_1_1

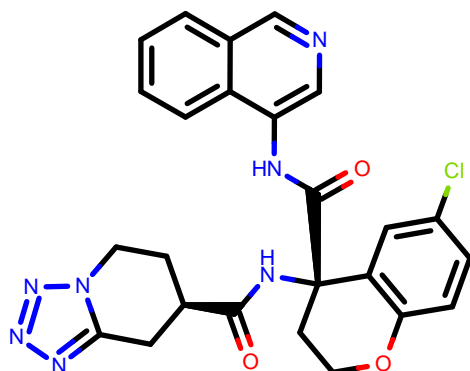
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)[C@@]H5C(=O)N

RUN: RUN5256

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.34

EN300-1653482_1_1_1



CID: EN300-1653482_1_1_1

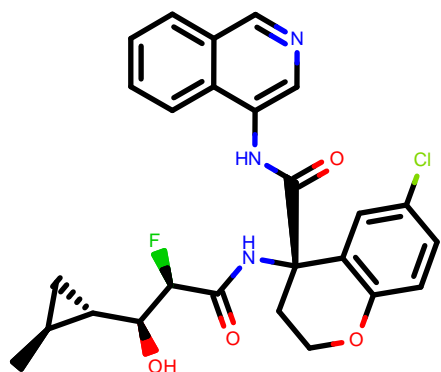
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]H5Cn6c(nnn6)C5

RUN: RUN4563

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.25

EDG-MED-90036822-94_10



CID: EDG-MED-90036822-94_10

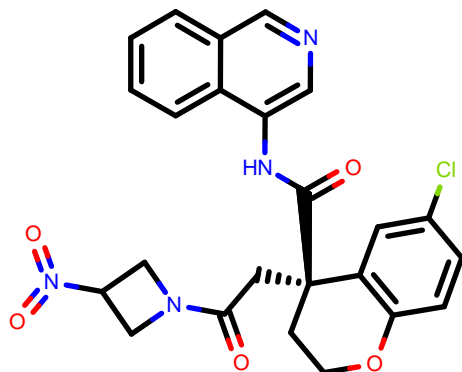
SMILES: C[C@@H]1[C@@]2[C@@]3[C@@]3(CCOc4c3cc(cc4)C)C1(=O)N4cnc5c6ccccc5F)O

RUN: RUN1710

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.23

EN300-7461023_1_1_1



CID: EN300-7461023_1_1_1

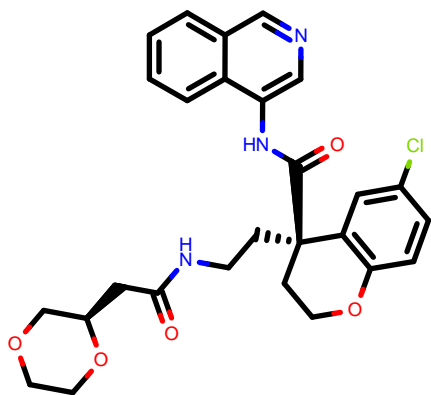
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)N(=O)=O

RUN: RUN3689

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.26

EN300-731622_3_1_1



CID: EN300-731622_3_1_1

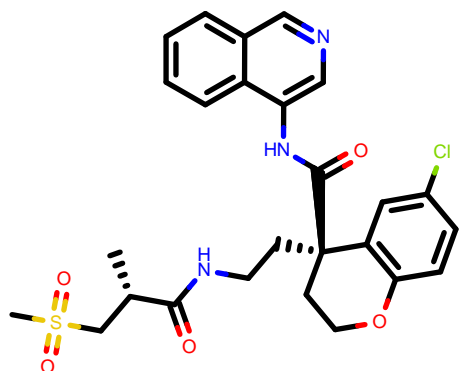
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5COCOC5

RUN: RUN6017

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.29

EN300-97699_3_1_1



CID: EN300-97699_3_1_1

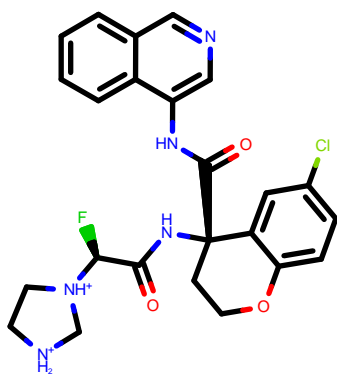
SMILES: C[C@@H](CS(=O)(=O)C(=O)N)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6395

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.34

EDG-MED-90036822-36_1



CID: EDG-MED-90036822-36_1

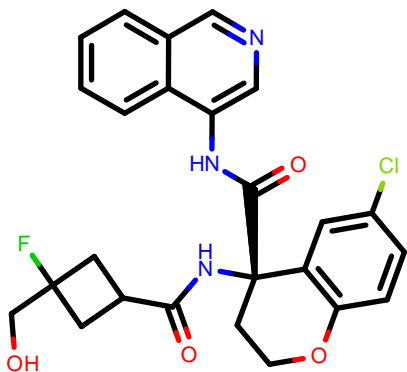
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](n5ccnc5)F

RUN: RUN1575

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

EDG-MED-90036822-76_1



CID: EDG-MED-90036822-76_1

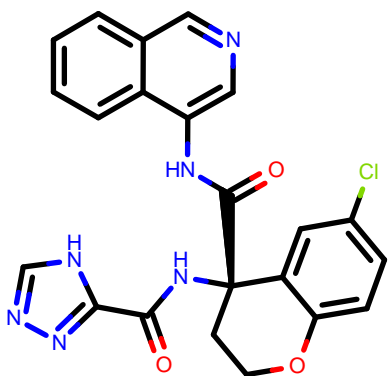
SMILES: c1cc2c(c1)cnc2NC(=O)[C@@]3(C4C(CCC(C4)Cl)OCC3)NC(=O)[C@@H]5C[C@@](C5)(F)CO)c1

RUN: RUN1661

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.21

EN300-100741_1_1_1



CID: EN300-100741_1_1_1

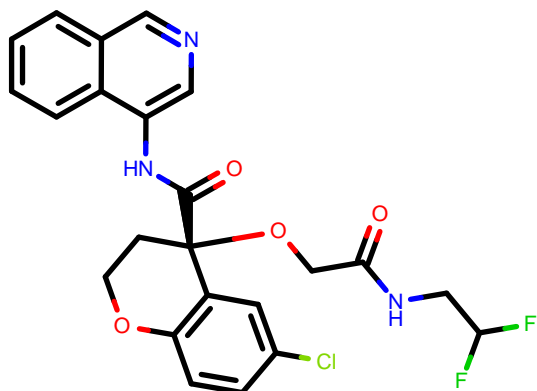
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]nnc5

RUN: RUN4163

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.19

CHO-MSK-5891c1ff-9_1



CID: CHO-MSK-5891c1ff-9_1

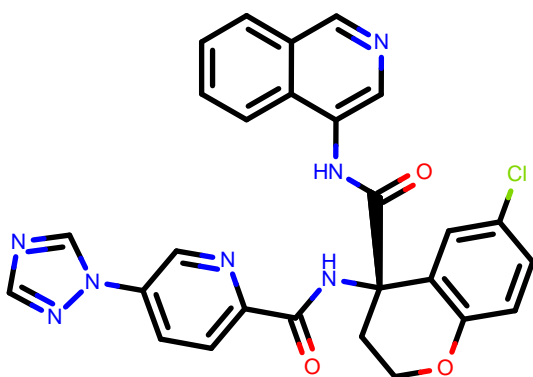
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCC(F)F

RUN: RUN1808

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

EN300-195855_1_1_1



CID: EN300-195855_1_1_1

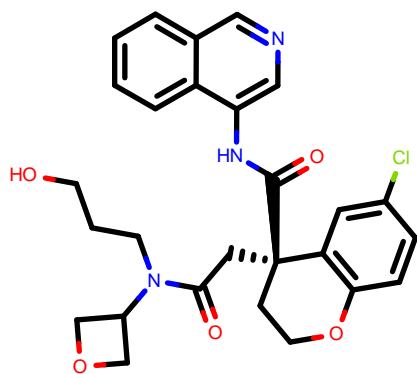
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccoc(n5)n6cnnc6

RUN: RUN7183

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.21

EN300-1725529_1_1_1



CID: EN300-1725529_1_1_1

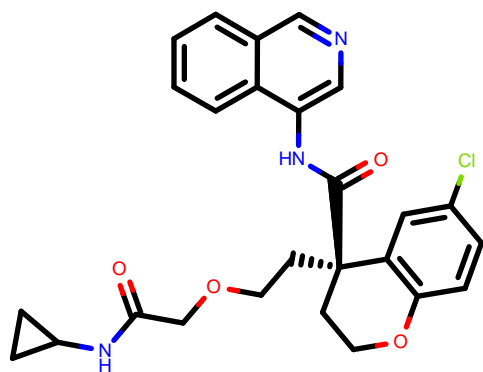
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5OCOS5

RUN: RUN4093

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.31

EN300-1253178_3_1_1



CID: EN300-1253178_3_1_1

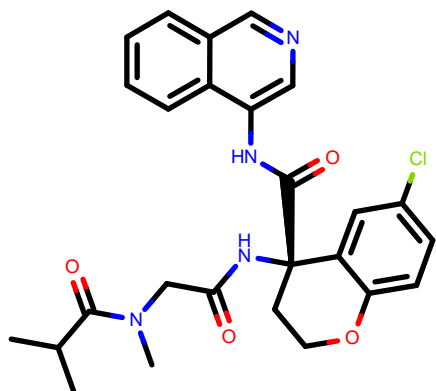
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOC(=O)NC5OC5

RUN: RUN3652

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.28

EN300-31145_1_1_1



CID: EN300-31145_1_1_1

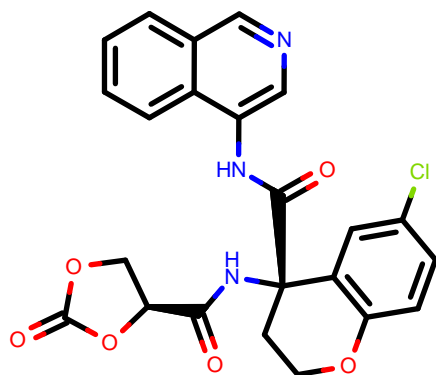
SMILES: CC(C)C(=O)N(C)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5590

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.23

EN300-5253939_1_1_1



CID: EN300-5253939_1_1_1

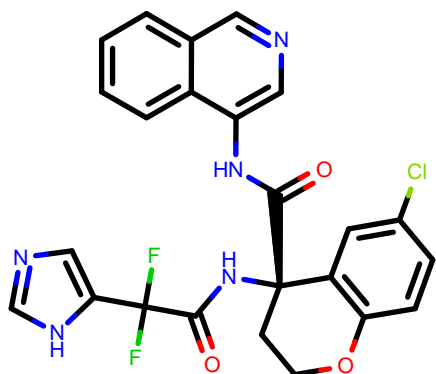
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H5COC(=O)O5

RUN: RUN4664

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.18

EDG-MED-90036822-67_1



CID: EDG-MED-90036822-67_1

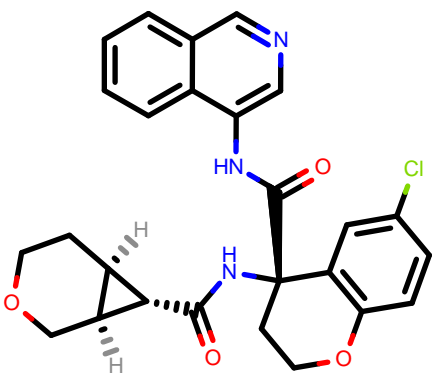
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(F)(F)F

RUN: RUN1653

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.28

EN300-1644723_1_4_1



CID: EN300-1644723_1_4_1

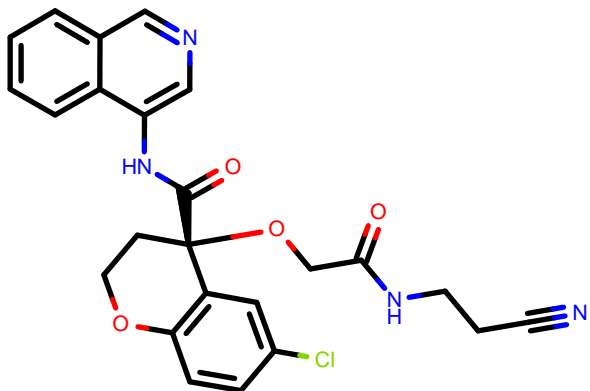
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](C(=O)C1=O)C(=O)C(=O)C1=O

RUN: RUN2904

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

CHO-MSK-5891c1ff-11_1



CID: CHO-MSK-5891c1ff-11_1

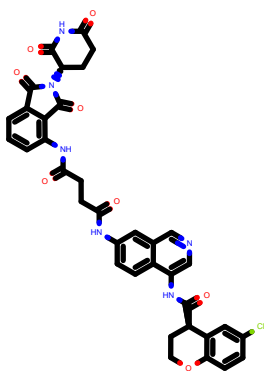
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](C(=O)C1=O)C(=O)C1=O

RUN: RUN1759

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.25

DAR-DIA-9e4459de-15_7



CID: DAR-DIA-9e4459de-15_7

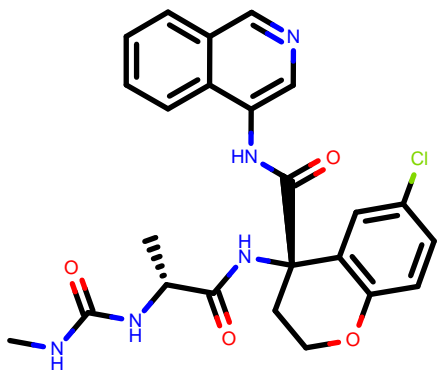
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](C(=O)C1=O)C(=O)C1=O

RUN: RUN1379

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.27

EN300-1258964_1_2_1



CID: EN300-1258964_1_2_1

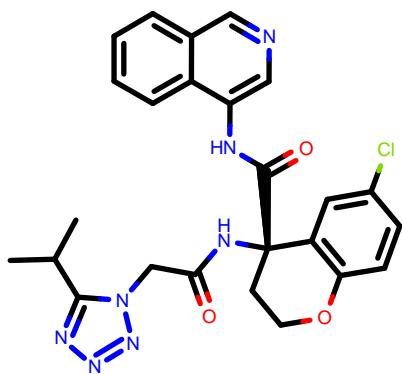
SMILES: C[C@@H](C(=O)N[C@@]1(C(=O)C1=O)C(=O)C(=O)C1=O

RUN: RUN6578

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.24

EN300-96933_1_1_1



CID: EN300-96933_1_1_1

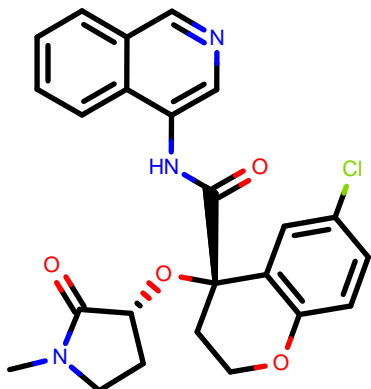
SMILES: CC(C)c1nncn1CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6546

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.27

EN300-98648_1_2_1



CID: EN300-98648_1_2_1

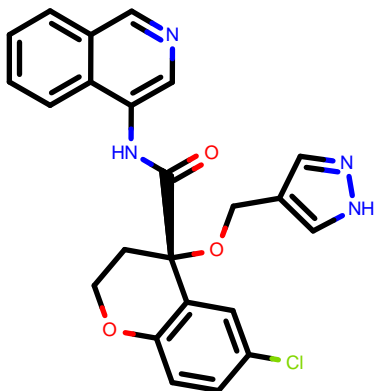
SMILES: CN1CC[C@H](C1=O)O[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7488

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.21

EDJ-MED-28ec730d-4_1_1



CID: EDJ-MED-28ec730d-4_1_1

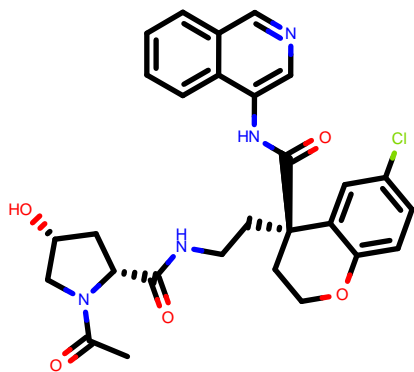
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCc5c[nH]nc5

RUN: RUN4710

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.22

EN300-158260_3_1_1



CID: EN300-158260_3_1_1

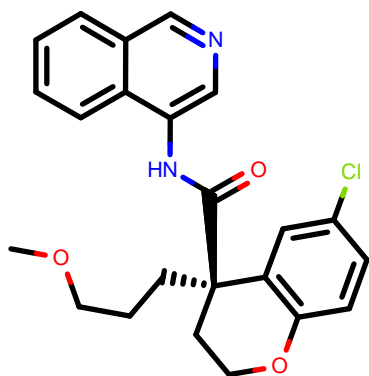
SMILES: CC(=O)N1C[C@@H](C1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5O

RUN: RUN4501

DDG (kcal/mol): -1.58

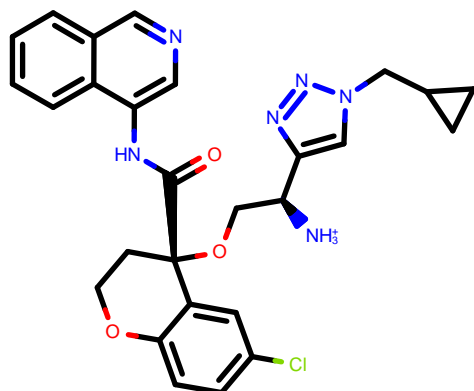
dDDG (kcal/mol): 0.33

EDJ-MED-28ec730d-1_1



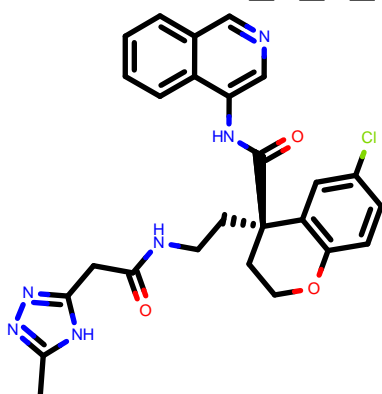
CID:	EDJ-MED-28ec730d-1_1
SMILES:	<chem>COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN590
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.22

ED_-GRI-5b13fbe2-18_1



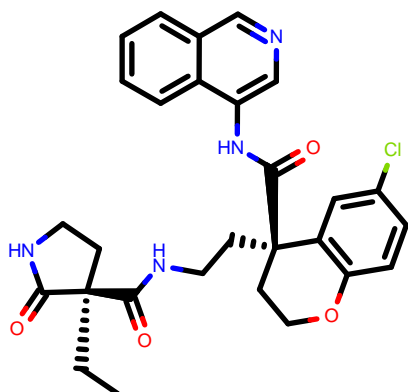
CID:	ED_-GRI-5b13fbe2-18_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5cn[nH]5)COC6C(=O)N4H34</chem>
RUN:	RUN1486
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.35

EN300-119126_3_1_1



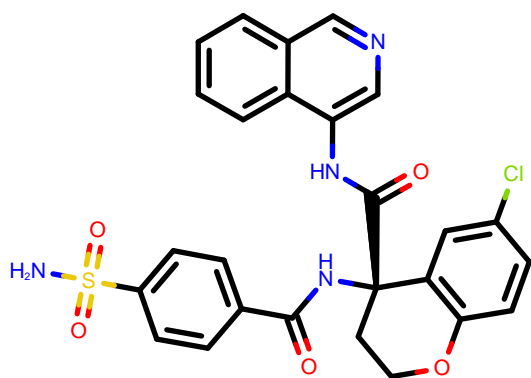
CID:	EN300-119126_3_1_1
SMILES:	<chem>Cc1[nH]nc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN6278
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.29

EN300-304135_3_2_1



CID:	EN300-304135_3_2_1
SMILES:	<chem>CC[C@]1(CCN1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN3663
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.34

EN300-16248_1_1_1



CID: EN300-16248_1_1_1

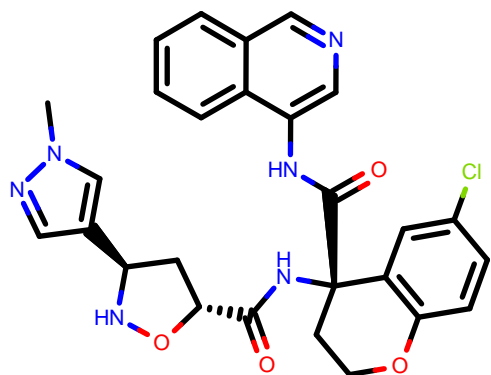
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5ccc(cc5)S(=O)(=O)N

RUN: RUN4889

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.32

EN300-92605_1_2_2



CID: EN300-92605_1_2_2

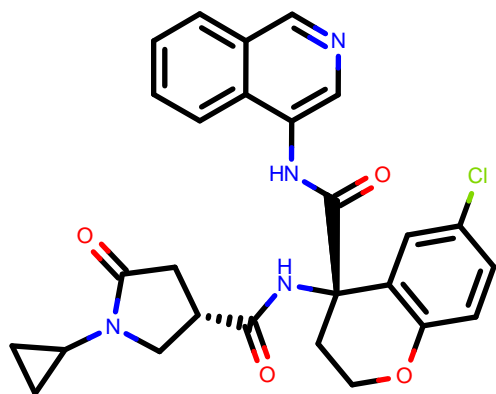
SMILES: Cn1cc[n1][C@H]2[C@@H](O)N2C(=O)NC@@3(CCOc4c3cc(cc4Cl)NC(=O)Nc5ncoc5c6ccccc6

RUN: RUN4251

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.36

EN300-12440_1_2_1



CID: EN300-12440_1_2_1

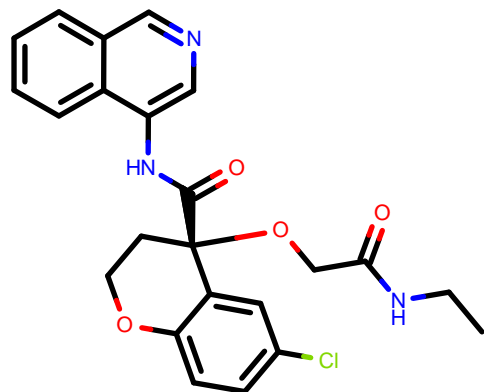
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@H]5CC(=O)N(C5)C6CC6

RUN: RUN6980

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.30

EN300-7003350_1_1_1



CID: EN300-7003350_1_1_1

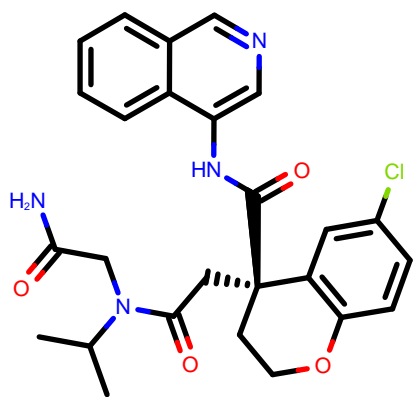
SMILES: CCNC(=O)CO[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3580

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.19

EN300-35450_1_1_1



CID: EN300-35450_1_1_1

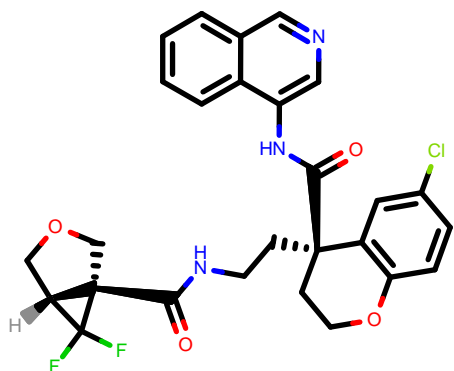
SMILES: CC(C)N(CC(=O)N)C(=O)C[C@]1(C)COCc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN4960

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.26

EN300-6738732_3_1_1



CID: EN300-6738732_3_1_1

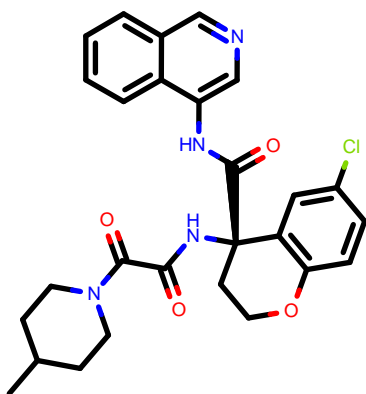
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)CCNC(=O)[C@H]5COC(F)F

RUN: RUN4494

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.23

EN300-137784_1_1_1



CID: EN300-137784_1_1_1

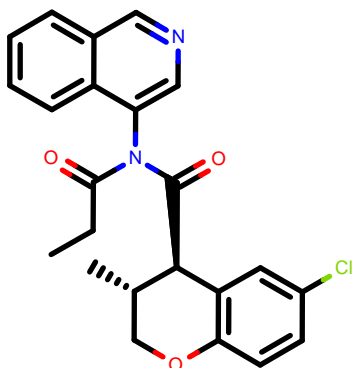
SMILES: CC1CCN(CC1)C(=O)N[C@@]2(C)COCc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4385

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.31

DAR-DIA-5ff57136-2_1



CID: DAR-DIA-5ff57136-2_1

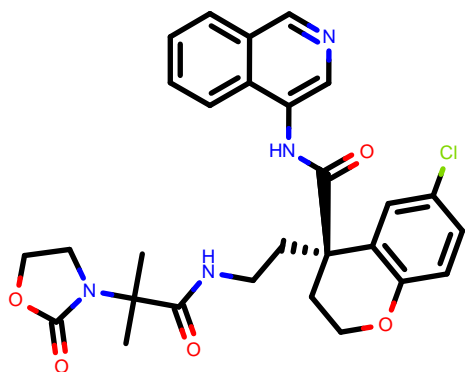
SMILES: C[C@H]1COCc2ccc(cc2[C@@H]1C(=O)N(c3cnc4c3cccc4)C(=O)C=C)Cl

RUN: RUN1236

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.20

EN300-96175_3_1_1



CID: EN300-96175_3_1_1

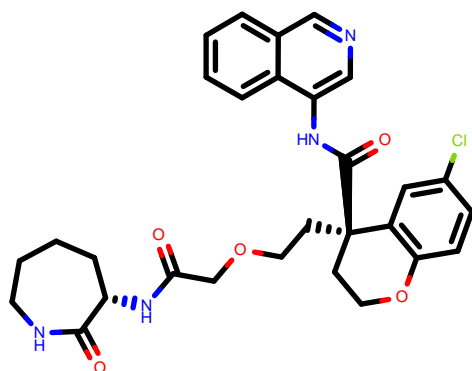
SMILES: CC(C)(C(=O)NCC[C@]1(CCOC2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)N5CCOC5=O

RUN: RUN5537

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.46

EN300-37195_3_2_1



CID: EN300-37195_3_2_1

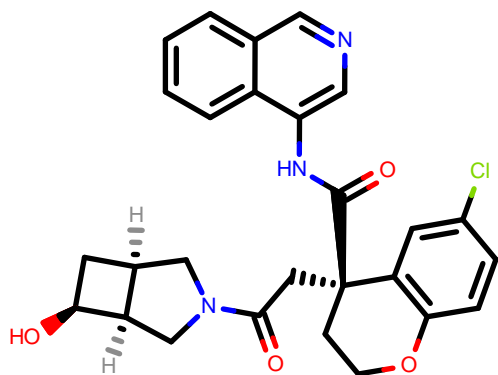
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)C(=O)N[C@@H]5CCCCNC5=O

RUN: RUN7401

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.32

EN300-305294_1_1_1



CID: EN300-305294_1_1_1

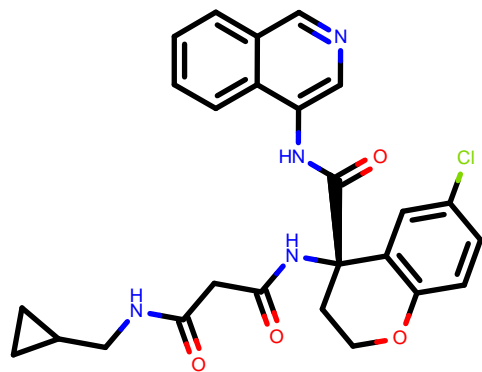
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)C(=O)N5C[C@@H]6C[C@@H]1[C@@H]5C[C@@H]6C5=O

RUN: RUN3379

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.30

EN300-178829_1_1_1



CID: EN300-178829_1_1_1

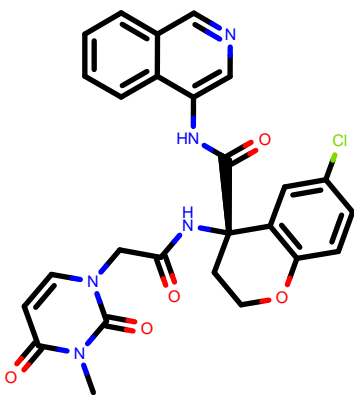
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)CC(=O)NCC5CC5

RUN: RUN5087

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.25

ALP-UNI-dbbfd3db-18_1



CID: ALP-UNI-dbbfd3db-18_1

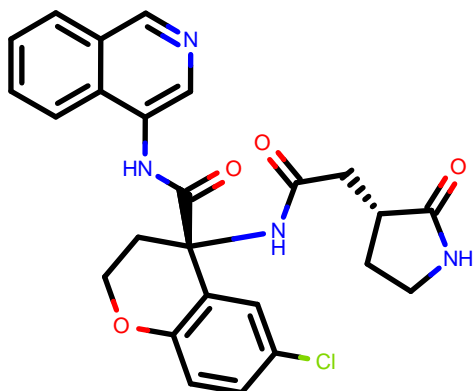
SMILES: Cn1c(=O)ccn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2646

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.29

EN300-343474_1_2_1



CID: EN300-343474_1_2_1

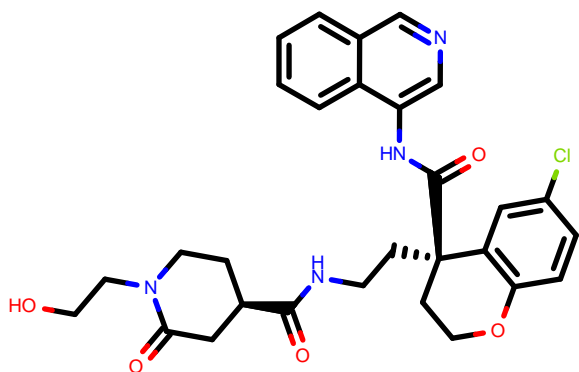
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)C[C@H]5CCNC5=O

RUN: RUN5747

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.26

EN300-1723663_3_1_1



CID: EN300-1723663_3_1_1

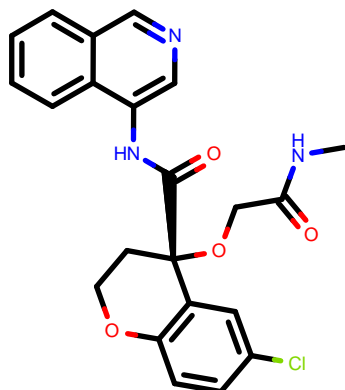
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)C[C@H]5CCNC(=O)C5CO

RUN: RUN4120

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.34

EN300-2977549_1_1_1



CID: EN300-2977549_1_1_1

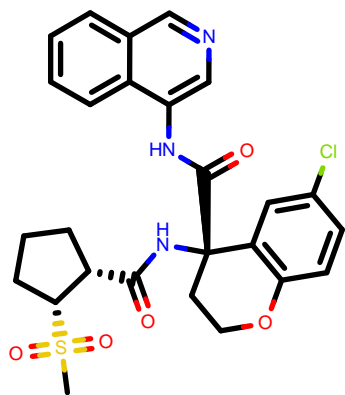
SMILES: CNC(=O)CO[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5151

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.18

EN300-1387145_1_1_1



CID: EN300-1387145_1_1_1

SMILES:

CS(=O)(=O)C@H1C[C@@H]2C[C@@H]1C(=O)NC@2(COC3C2c2c(cc3)C)C(=O)Nc4nc5c4ccccc5

RUN:

RUN3149

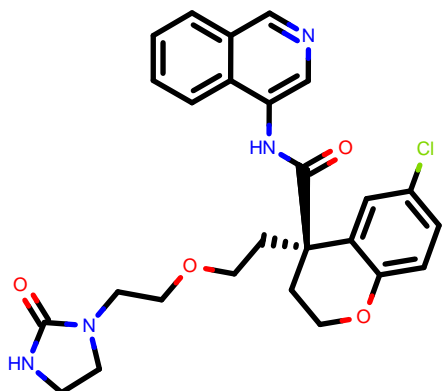
DDG (kcal/mol):

-1.56

dDDG (kcal/mol):

0.31

EN300-214800_3_1_1



CID: EN300-214800_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCOC5NCCNC5=O

RUN:

RUN3808

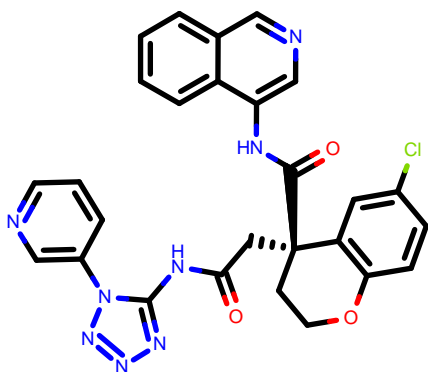
DDG (kcal/mol):

-1.56

dDDG (kcal/mol):

0.31

EDJ-MED-d203f206-17_1



CID: EDJ-MED-d203f206-17_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CC(=O)Nc5nnnn5c6ccccc6

RUN:

RUN2437

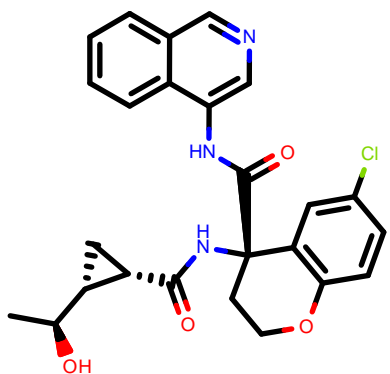
DDG (kcal/mol):

-1.56

dDDG (kcal/mol):

0.30

EN300-6729572_1_1_1



CID: EN300-6729572_1_1_1

SMILES:

C[C@@H]1C[C@H]1C[C@@H]2[C@@H]1C(=O)NC@2(COC3C2c2c(cc3)C)C(=O)Nc4nc5c4ccccc5O

RUN:

RUN3679

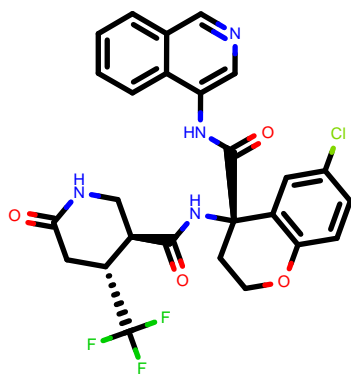
DDG (kcal/mol):

-1.56

dDDG (kcal/mol):

0.27

EN300-208959_1_3_1



CID: EN300-208959_1_3_1

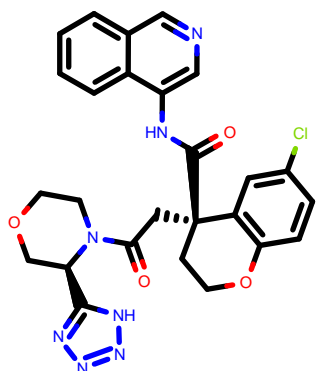
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@@H5CN(C)O[C@@H]5C(F)(F)F

RUN: RUN5084

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.27

EDJ-MED-d203f206-14_1



CID: EDJ-MED-d203f206-14_1

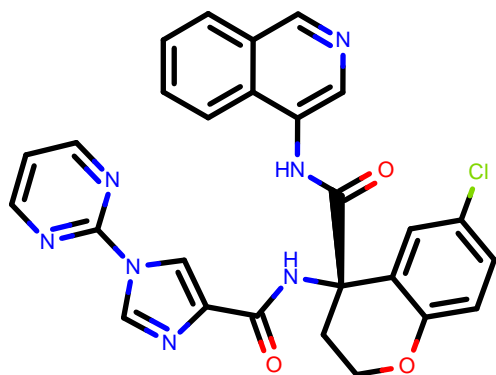
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCOC[C@@H]5c6n[n-]n6

RUN: RUN2400

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.39

EN300-261056_1_1_1



CID: EN300-261056_1_1_1

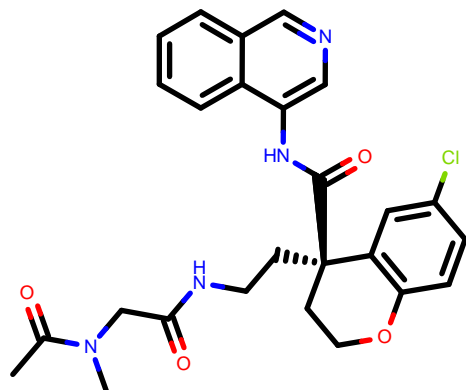
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(cn5)c6nccn6

RUN: RUN3777

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.21

EN300-33657_3_1_1



CID: EN300-33657_3_1_1

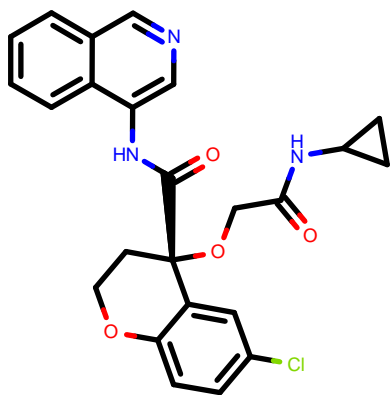
SMILES: CC(=O)N(C)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN: RUN5968

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.25

CHO-MSK-5891c1ff-8_1



CID: CHO-MSK-5891c1ff-8_1

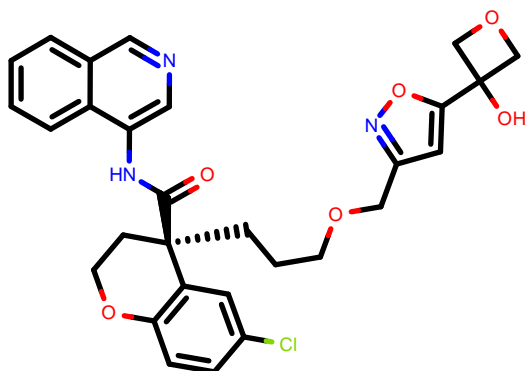
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCC(=O)NC5CC5

RUN: RUN1718

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.19

EN300-7457159_4_1_1



CID: EN300-7457159_4_1_1

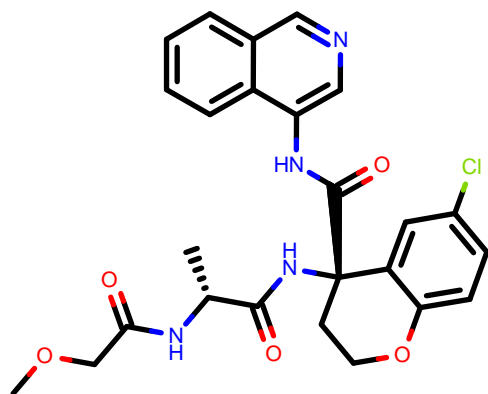
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCCOCc5cc(on5)C6(COC6)O

RUN: RUN4721

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.37

EN300-31183_1_2_1



CID: EN300-31183_1_2_1

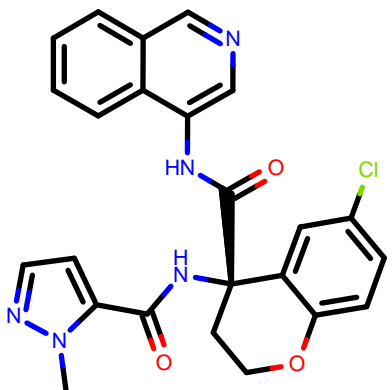
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3nccc4c3ccc4NC(=O)COC

RUN: RUN4099

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-31077_1_1_1



CID: EN300-31077_1_1_1

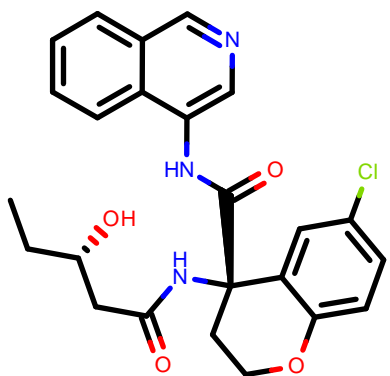
SMILES: Cn1c(ccn1)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4032

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.20

EN300-224741_1_1_1



CID: EN300-224741_1_1_1

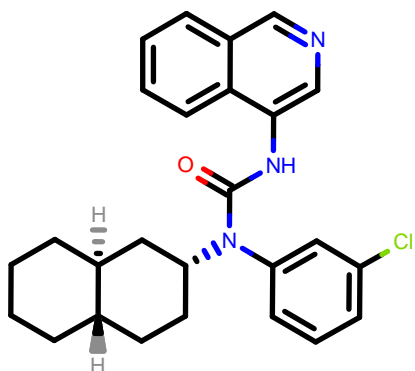
SMILES: CC[C@@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN3505

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.22

MIC-UNK-cdc2493e-8_5



CID: MIC-UNK-cdc2493e-8_5

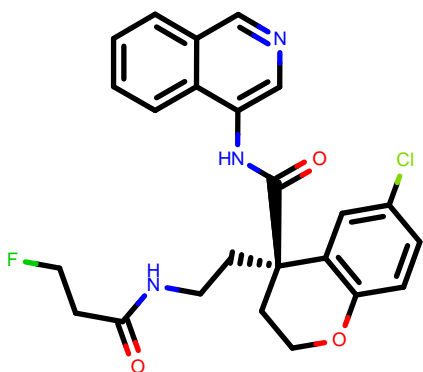
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3ccccc3Cl)[C@@H]4CC[C@@H]5CCCC[C@@H]5C4

RUN: RUN475

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.45

EN300-97758_3_1_1



CID: EN300-97758_3_1_1

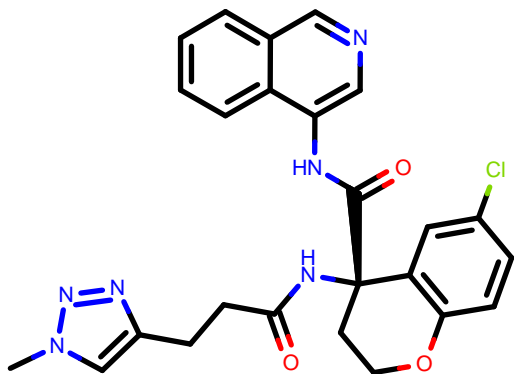
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCF

RUN: RUN3222

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.25

EN300-306047_1_1_1



CID: EN300-306047_1_1_1

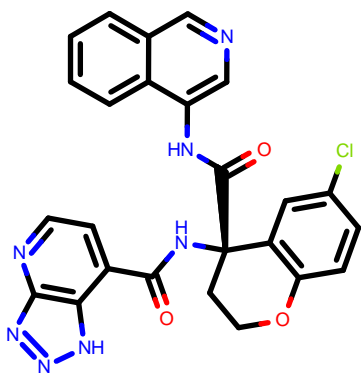
SMILES: Cn1cc(nn1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4910

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.26

EN300-188377_1_1_1



CID: EN300-188377_1_1_1

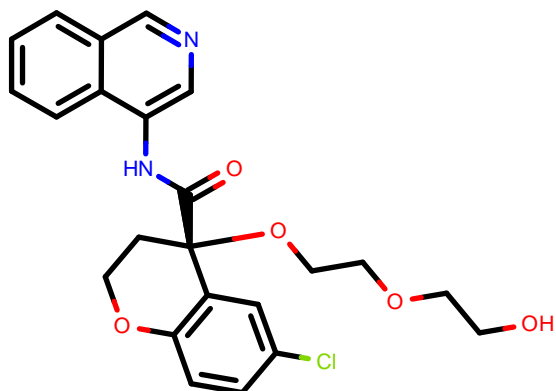
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6c5n[nH]6

RUN: RUN4170

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.24

EN300-52467_1_1_1



CID: EN300-52467_1_1_1

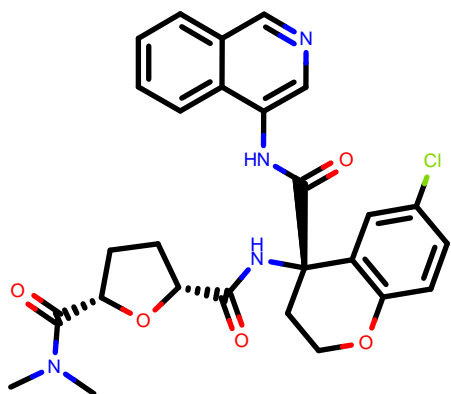
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN6766

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.24

EN300-314890_1_1_1



CID: EN300-314890_1_1_1

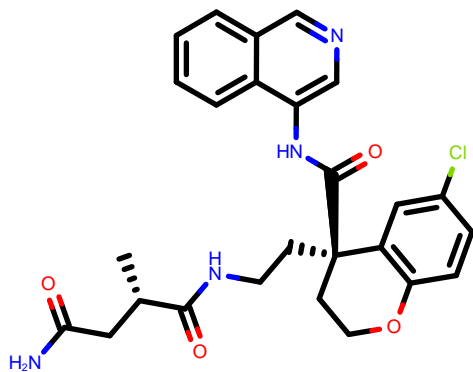
SMILES: CN(C)C(=O)[C@@H]1CC[C@@H]1O[C@@]2(C)C(=O)NC(=O)[C@@]3(C)C(=O)Nc4nc5c4ccccc5

RUN: RUN5415

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.38

EN300-202757_3_1_1



CID: EN300-202757_3_1_1

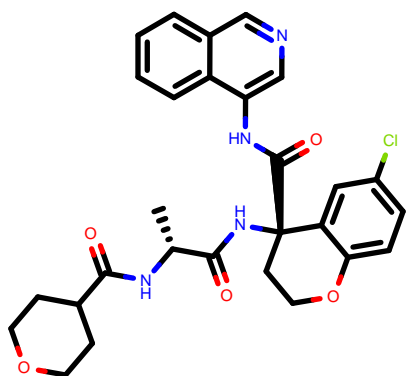
SMILES: C[C@@H](CC(=O)N)C(=O)NCC[C@@]1(C)COC2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccccc4

RUN: RUN3960

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.28

EN300-73102_1_2_1



CID: EN300-73102_1_2_1

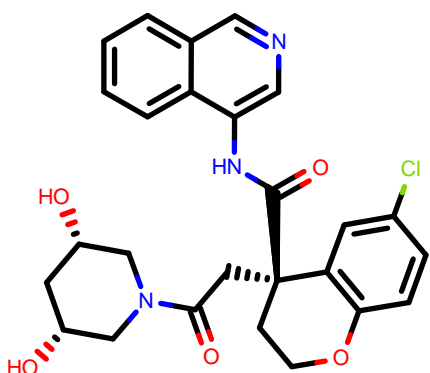
SMILES: C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCOCC5

RUN: RUN6072

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.43

EN300-96886_1_1_1



CID: EN300-96886_1_1_1

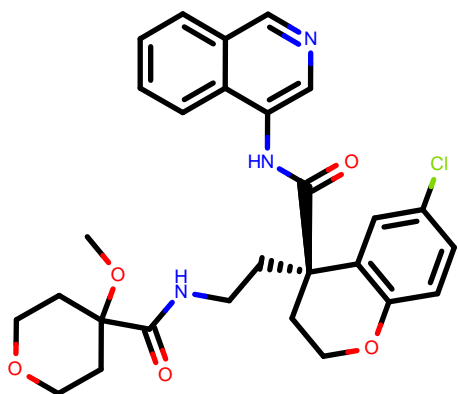
SMILES: c1ccc2c(c1)ncnc2N[C@@]1(CO)N[C@@]2(CCOC3c1cc(cc3)C)C(=O)N5C[C@@]1(C)C[C@@]2(O)O

RUN: RUN5069

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.28

EN300-204133_3_1_1



CID: EN300-204133_3_1_1

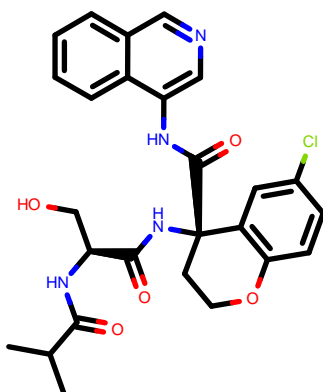
SMILES: OCC1(CCOC1)C(=O)NCC[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4089

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.32

EN300-212266_1_1_1



CID: EN300-212266_1_1_1

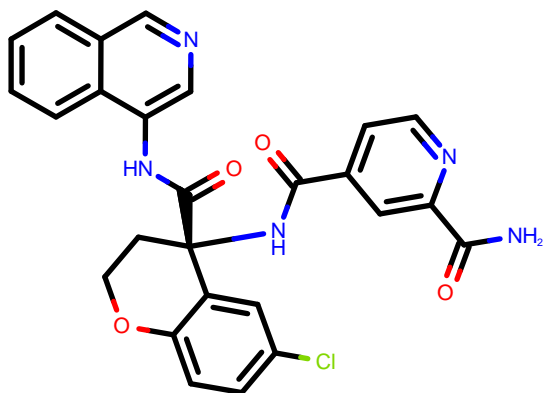
SMILES: CC(C)C(=O)N[C@@]1(CO)C(=O)N[C@@]2(CCOC2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN3130

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.31

EN300-102071_1_1_1



CID: EN300-102071_1_1_1

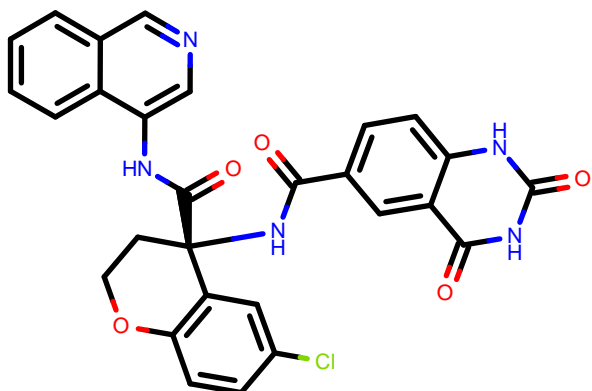
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnc(c5)C(=O)N

RUN: RUN2734

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.25

EN300-1723214_1_1_1



CID: EN300-1723214_1_1_1

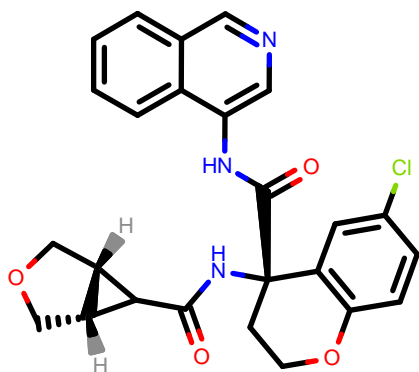
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6nc(c5)C(=O)Nc7cnc8c7c8

RUN: RUN3613

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.26

EN300-257945_1_1_1



CID: EN300-257945_1_1_1

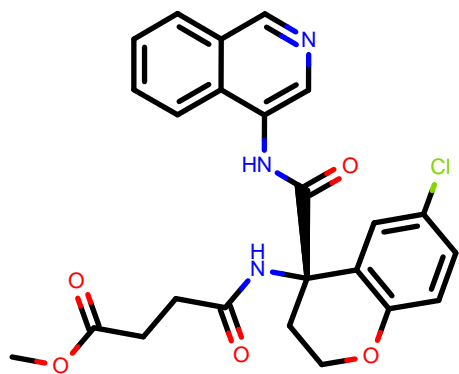
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C@H)6[C@@]3(H)5COC6

RUN: RUN3367

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.23

EN300-24949_1_1_1



CID: EN300-24949_1_1_1

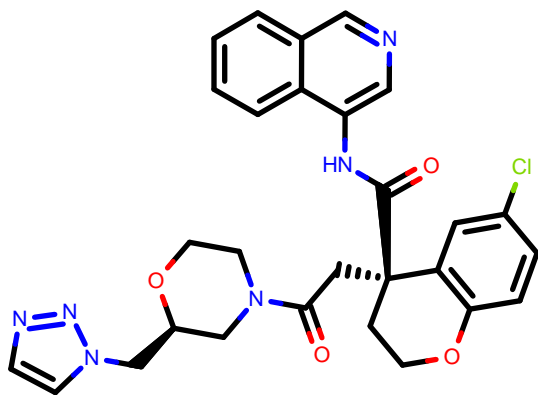
SMILES: COC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN3942

DDG (kcal/mol): -1.55

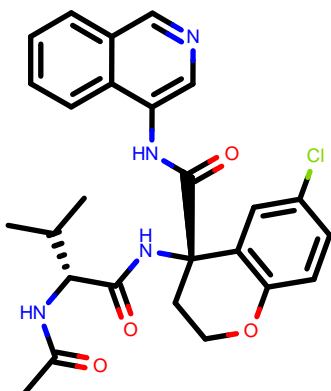
dDDG (kcal/mol): 0.24

EDJ-MED-d203f206-24_1



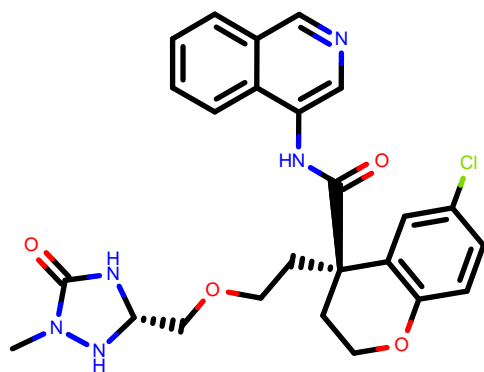
CID:	EDJ-MED-d203f206-24_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)Cn6cnn6</chem>
RUN:	RUN2431
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.33

EN300-318284_1_1_1



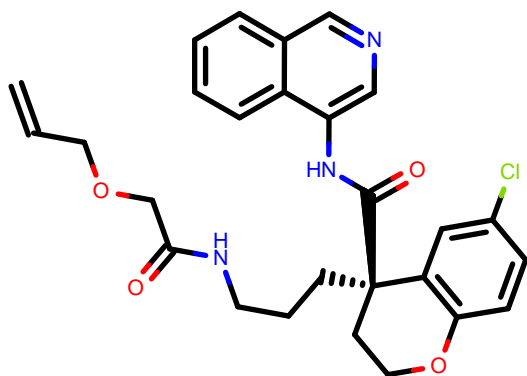
CID:	EN300-318284_1_1_1
SMILES:	<chem>CC(C)[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)C</chem>
RUN:	RUN2776
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.23

EN300-124918_3_1_1



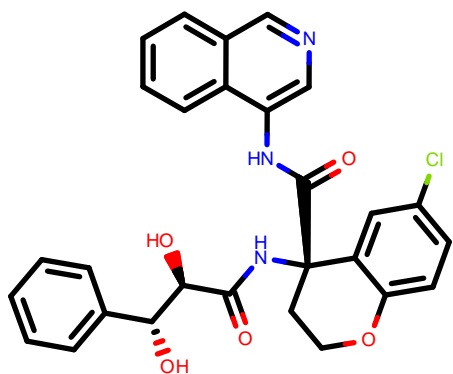
CID:	EN300-124918_3_1_1
SMILES:	<chem>CN1C(=O)N[C@@H](C1)[NH2+][1]COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5</chem>
RUN:	RUN4436
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.30

EN300-44821_4_1_1



CID:	EN300-44821_4_1_1
SMILES:	<chem>C=CCOCC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN6347
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.29

EN300-2923949_1_4_1



CID: EN300-2923949_1_4_1

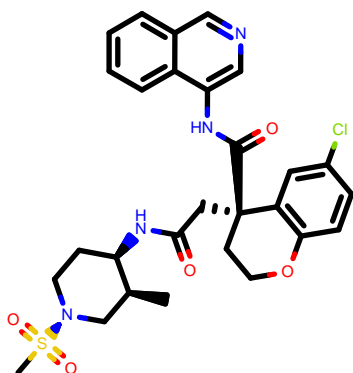
SMILES: c1ccc(cc1)[C@H]([C@H](C(=O)N[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5)O)O

RUN: RUN3336

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

ALP-POS-5bb456a5-1_14



CID: ALP-POS-5bb456a5-1_14

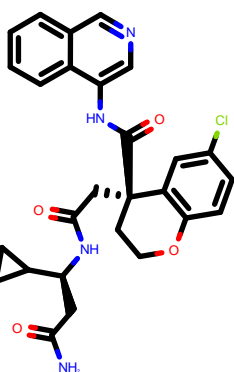
SMILES: C[C@H]1C[N@@]2(C)C[C@@H]1NC(=O)[C@@]3(CCOc4c2cc(c4)Cl)CC(=O)N[C@@]5(C)C(=O)N5C(=O)S(=O)(=O)C

RUN: RUN2264

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.37

EN300-85413_1_1_1



CID: EN300-85413_1_1_1

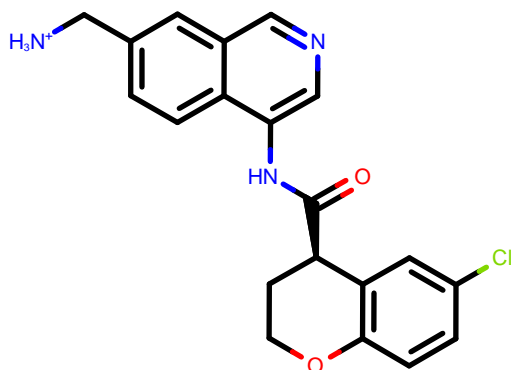
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(O)c4c3cc(cc4)Cl)CC(=O)N[C@@]5(C)C(=O)N5C(=O)C

RUN: RUN3467

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.32

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

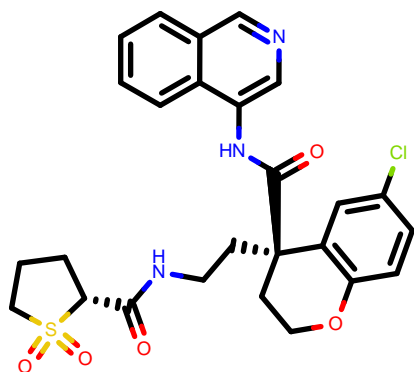
SMILES: c1cc2c(cc1C[NH3+])cnc2NC(=O)[C@@]3(C)C(O)c4c3cc(cc4)Cl

RUN: RUN413

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.11

EN300-88656_3_2_1



CID: EN300-88656_3_2_1

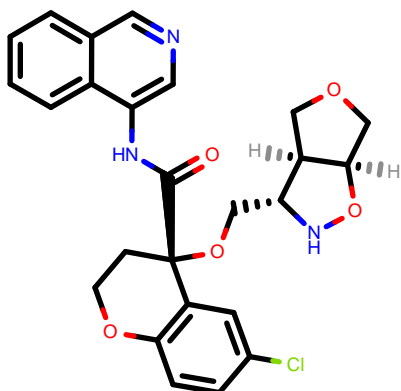
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCS5(=O)=O

RUN: RUN6033

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.28

EN300-7436306_1_1_1



CID: EN300-7436306_1_1_1

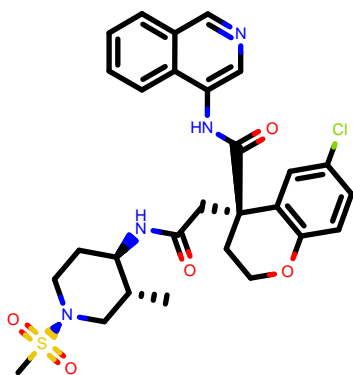
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@]5[H]C@H6COC[C@H]6ON5

RUN: RUN5304

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.22

ALP-POS-5bb456a5-1_13



CID: ALP-POS-5bb456a5-1_13

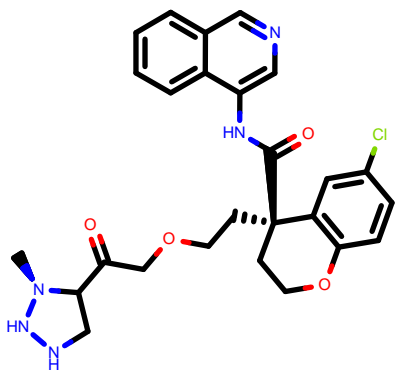
SMILES: C[C@@]1(C)[N@@]2(C)[C@H]1NC(=O)C[C@@]3(COCc4c3cc(cc4)Cl)Nc4ncoc5c4ccc5(S(=O)(=O)=O)C

RUN: RUN2282

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.43

EN300-204936_3_1_1



CID: EN300-204936_3_1_1

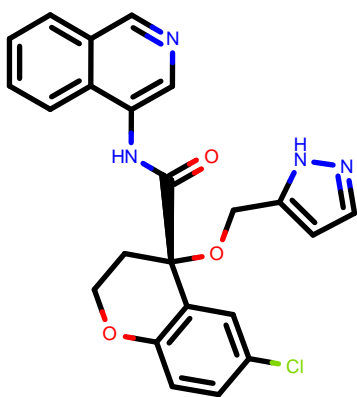
SMILES: Cn1c(cnn1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN4010

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.30

EDG-MED-4c68219f-15_1



CID: EDG-MED-4c68219f-15_1

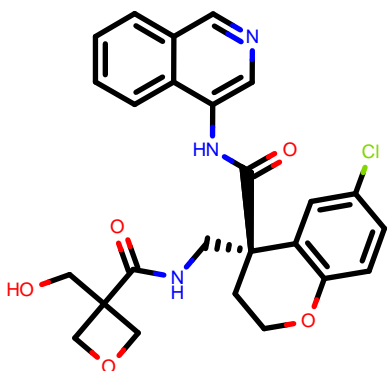
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn[nH]5

RUN: RUN1493

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.16

EN300-105693_2_1_1



CID: EN300-105693_2_1_1

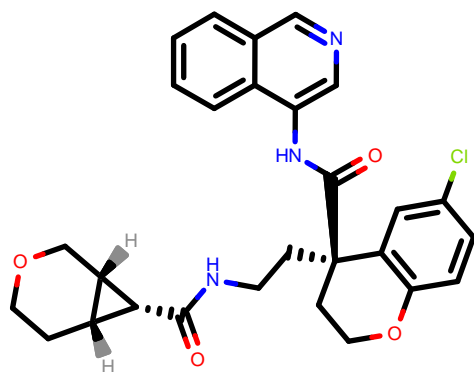
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COC5)CO

RUN: RUN3554

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

EN300-1644723_3_3_1



CID: EN300-1644723_3_3_1

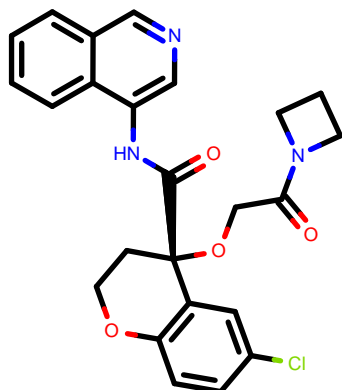
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(C)C[C@H]6[C@@H]5C[C@H]6

RUN: RUN3207

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.31

CHO-MSK-5891c1ff-10_1



CID: CHO-MSK-5891c1ff-10_1

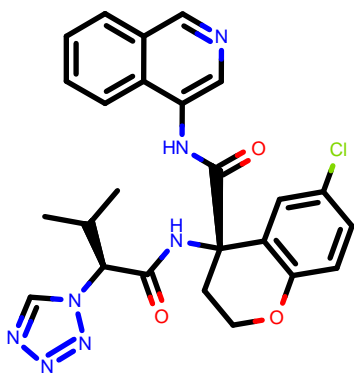
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC5

RUN: RUN1704

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.19

EN300-297561_1_1_1



CID: EN300-297561_1_1_1

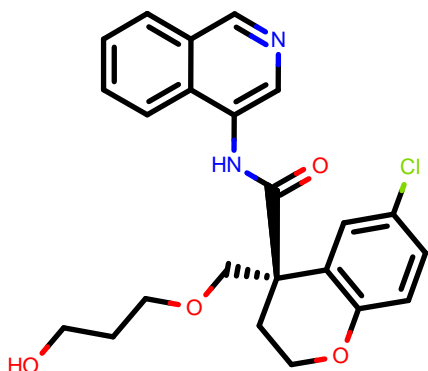
SMILES: CC(C)C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)n5nnn5

RUN: RUN3468

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.23

EN300-221518_2_1_1



CID: EN300-221518_2_1_1

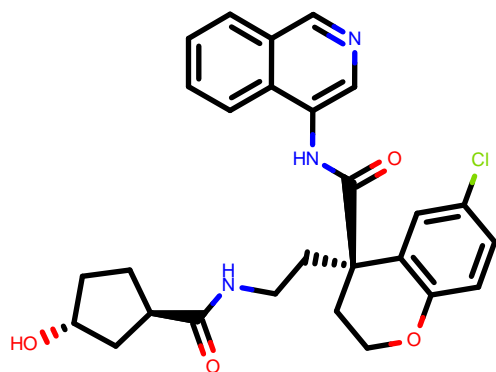
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(C)CO

RUN: RUN4570

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.25

EN300-321597_3_1_1



CID: EN300-321597_3_1_1

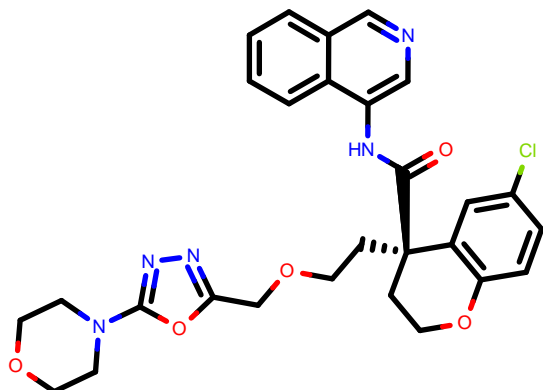
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5C[C@H](C5)O

RUN: RUN7038

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

EN300-6486576_3_1_1



CID: EN300-6486576_3_1_1

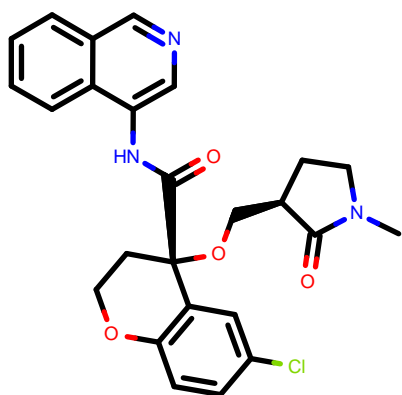
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nnc(o5)N6COC6

RUN: RUN4151

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.32

EN300-260816_1_1_1



CID: EN300-260816_1_1_1

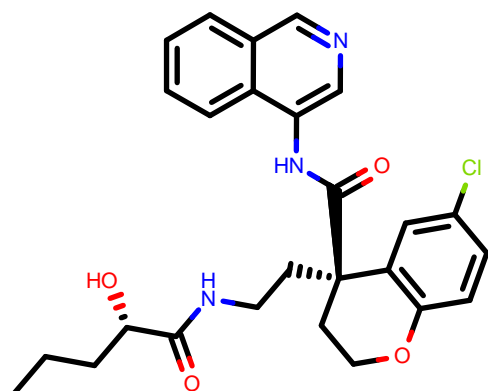
SMILES: CN1CC[C@@H](C1=O)C(=O)C2[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN3891

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.25

EN300-219531_3_1_1



CID: EN300-219531_3_1_1

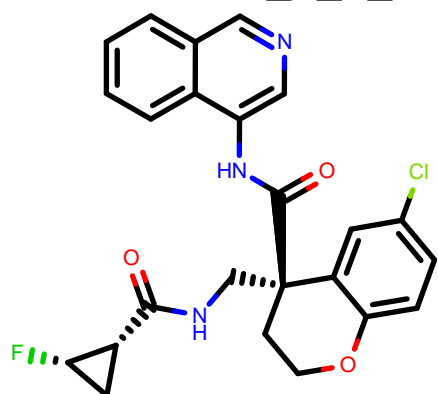
SMILES: CCC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O

RUN: RUN3576

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.33

EN300-97300_2_1_1



CID: EN300-97300_2_1_1

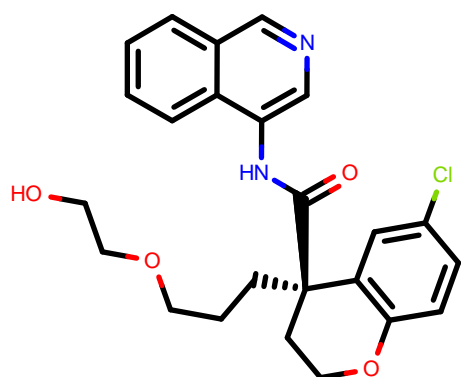
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN6222

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-21258_4_1_1



CID: EN300-21258_4_1_1

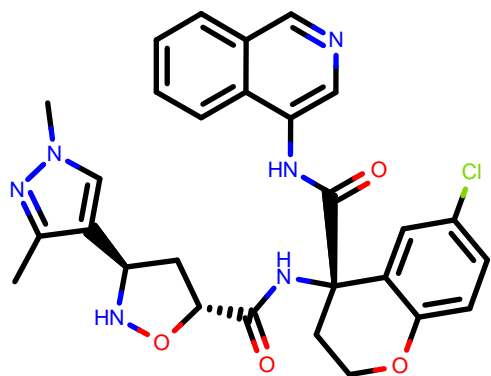
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN7318

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.40

EN300-92684_1_2_2



CID: EN300-92684_1_2_2

SMILES:

Cc1c([nH]1)C(C@H)C(C@@H)(ON2C(=O)N(C)C3(CCOc4ccc(cc4)C)C(=O)Nc5ccc6c5ccc6

RUN:

RUN3026

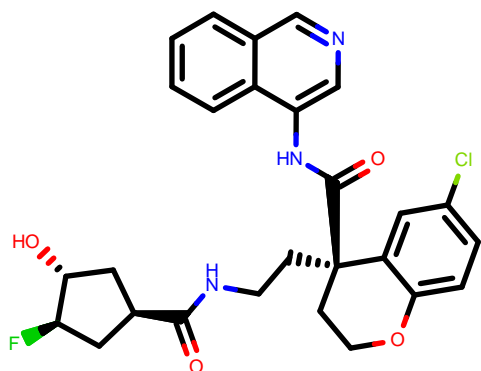
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.40

EN300-7461217_3_1_1



CID: EN300-7461217_3_1_1

SMILES:

c1ccc2c(c1)nc2NC(=O)[C@@]3(C)C(COc4ccc(cc4)O)CCNC(=O)[C@@H]5C[C@@H](C5)F(O)

RUN:

RUN5601

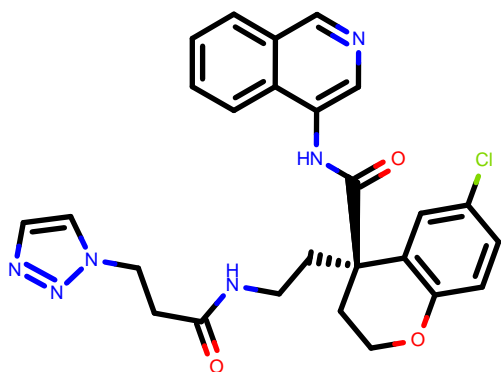
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.30

EN300-28871_3_1_1



CID: EN300-28871_3_1_1

SMILES:

c1ccc2c(c1)nc2NC(=O)[C@@]3(C)C(COc4ccc(cc4)O)CCNC(=O)Cn5ccnn5

RUN:

RUN3078

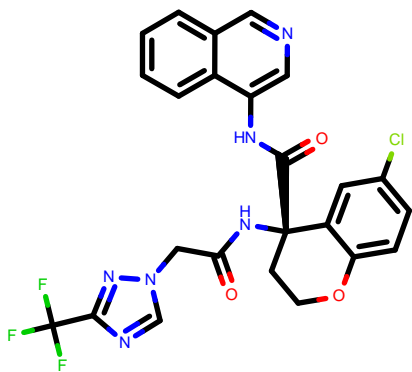
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.27

EN300-7385389_1_1_1



CID: EN300-7385389_1_1_1

SMILES:

c1ccc2c(c1)nc2NC(=O)[C@@]3(C)C(COc4ccc(cc4)O)NC(=O)Cn5cnc(n5)C(F)(F)F

RUN:

RUN4580

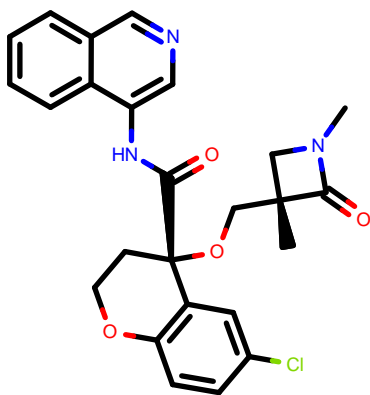
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.29

EN300-1273362_1_2_1



CID: EN300-1273362_1_2_1

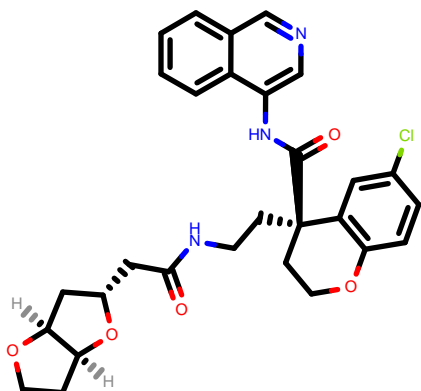
SMILES: C[C@]1(CN(C1=O)C)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4380

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.25

EN300-7355519_3_4_1



CID: EN300-7355519_3_4_1

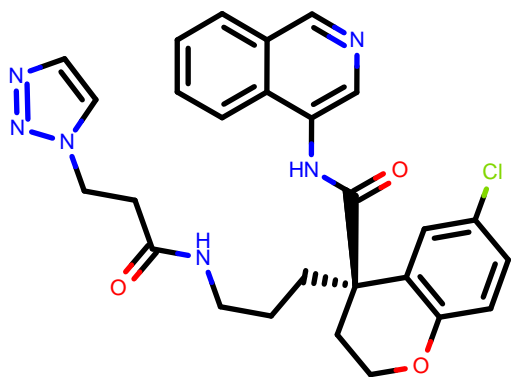
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCNC(=O)C[C@@H]5C[C@@H]6[C@@H]5O[C@H]6O

RUN: RUN4930

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.32

EN300-28871_4_1_1



CID: EN300-28871_4_1_1

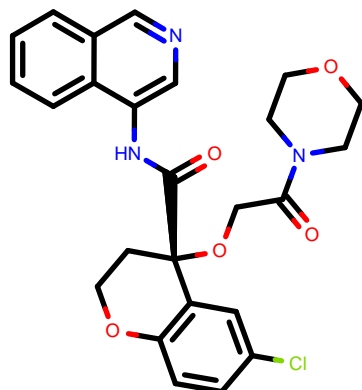
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCNC(=O)CCN5Cnnc5

RUN: RUN5575

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.32

EN300-1241327_1_1_1



CID: EN300-1241327_1_1_1

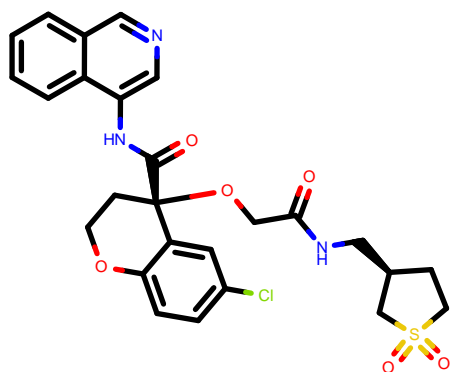
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCOCC5

RUN: RUN4943

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.26

EN300-47606_1_2_1



CID: EN300-47606_1_2_1

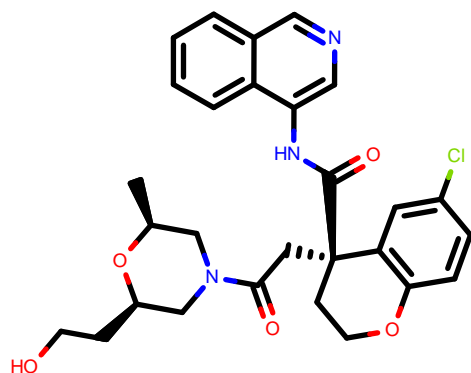
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5SCCS(=O)(=O)C5

RUN: RUN7794

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.40

EN300-212814_1_4_1



CID: EN300-212814_1_4_1

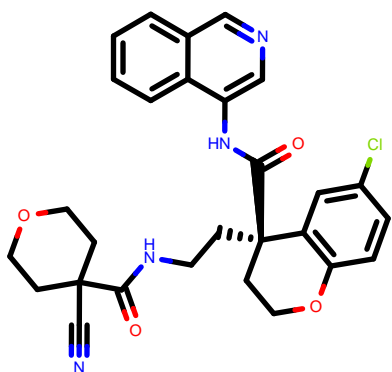
SMILES: C[C@H]1CN[C@H](O1)CCO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN5236

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.30

EN300-74089_3_1_1



CID: EN300-74089_3_1_1

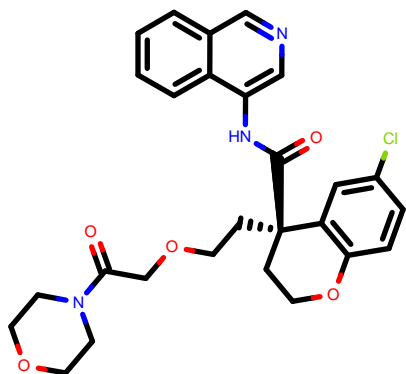
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCOCC5)C#N

RUN: RUN3769

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.38

EN300-1241327_3_1_1



CID: EN300-1241327_3_1_1

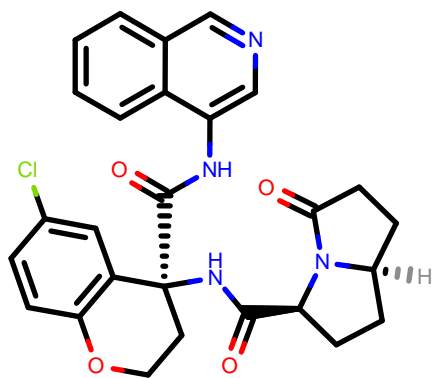
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5

RUN: RUN5307

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.28

EN300-6479181_1_3_1



CID: EN300-6479181_1_3_1

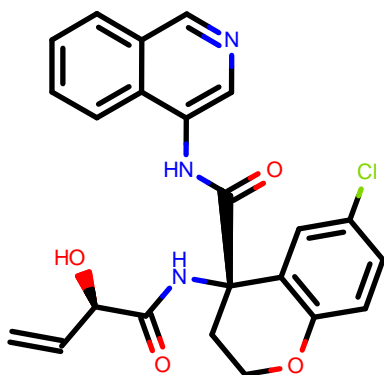
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3[C@@H](CCOc4c3cc(c4)C)NC(=O)C@H5CC[C@@H]6NSC1=O)CC6

RUN: RUN4071

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.31

EN300-181492_1_2_1



CID: EN300-181492_1_2_1

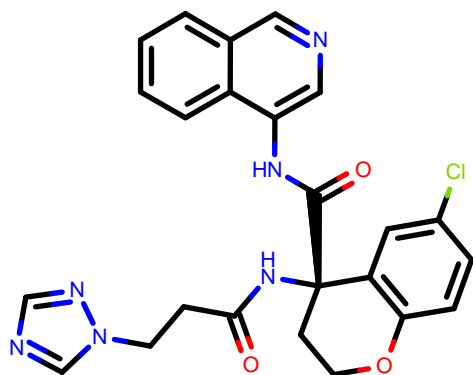
SMILES: C=C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN3167

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.23

EN300-26147_1_1_1



CID: EN300-26147_1_1_1

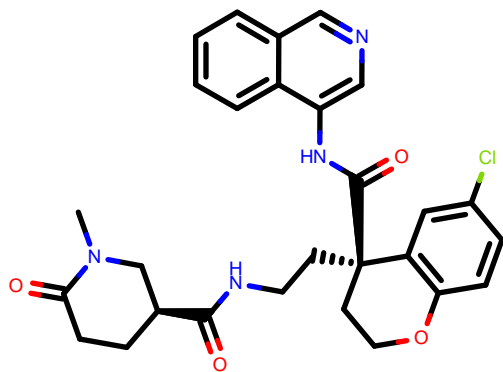
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ncn5

RUN: RUN5308

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-52983_3_2_1



CID: EN300-52983_3_2_1

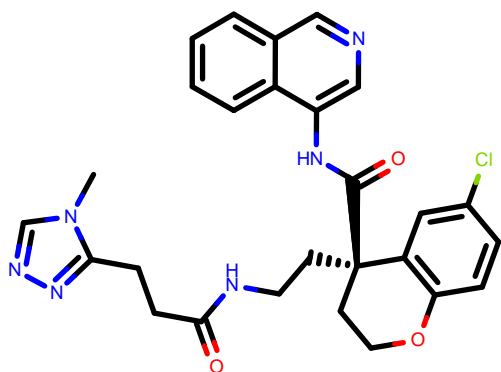
SMILES: CN1C[C@H](CCC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN6929

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.32

EN300-1138792_3_1_1



CID: EN300-1138792_3_1_1

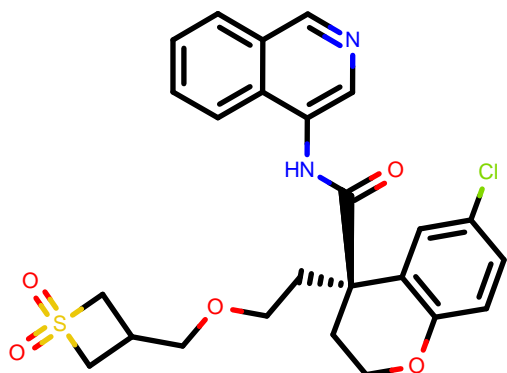
SMILES: Cn1cnc1CCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3401

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.33

EN300-5638430_3_1_1



CID: EN300-5638430_3_1_1

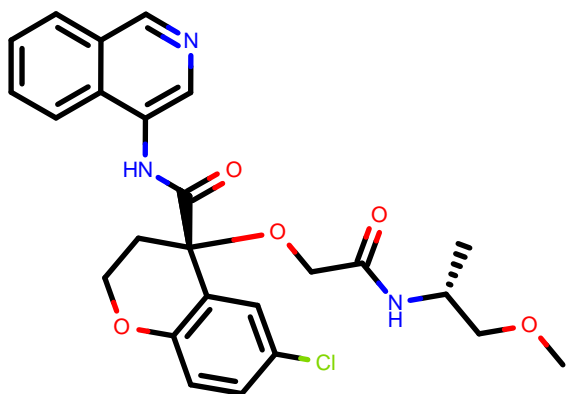
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5CS(=O)=O=C5

RUN: RUN3905

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.31

EN300-02067_1_2_1



CID: EN300-02067_1_2_1

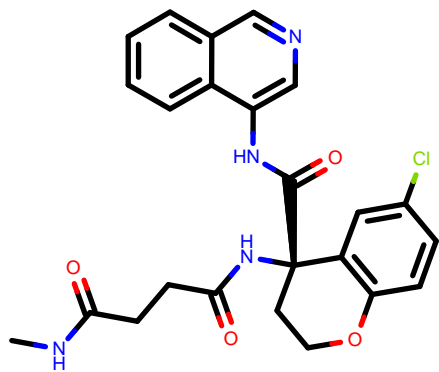
SMILES: C[C@H](COC)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN6831

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.27

EN300-1081277_1_1_1



CID: EN300-1081277_1_1_1

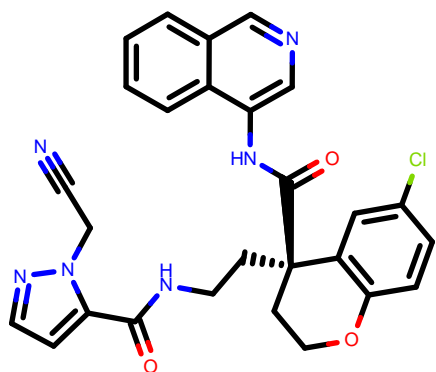
SMILES: CNC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN4507

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-373791_3_1_1



CID: EN300-373791_3_1_1

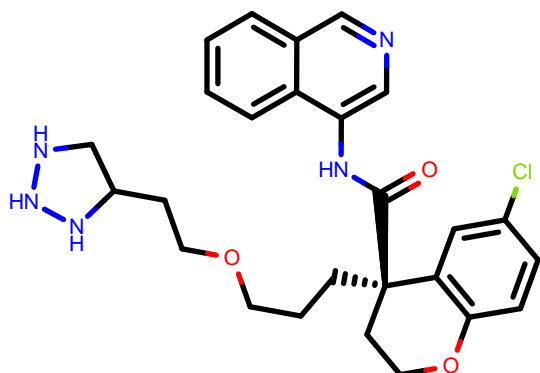
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cnnc5C#N

RUN: RUN4345

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.29

EN300-222357_4_1_1



CID: EN300-222357_4_1_1

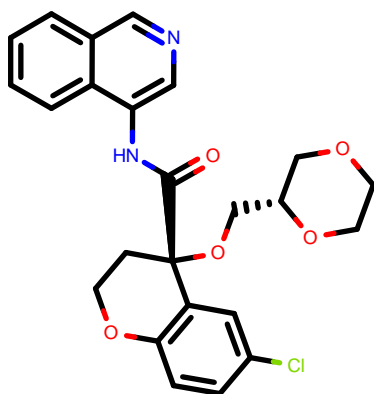
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCc5cn[nH]5

RUN: RUN7368

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.35

EN300-139167_1_1_1



CID: EN300-139167_1_1_1

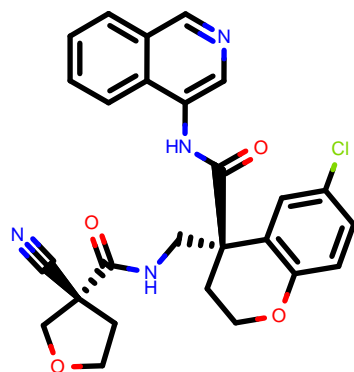
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@]5H5COCCO5

RUN: RUN3444

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

EN300-261210_2_1_1



CID: EN300-261210_2_1_1

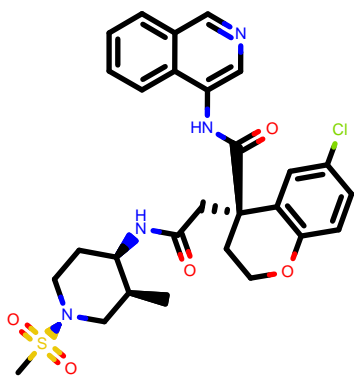
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCOCC5)C#N

RUN: RUN3028

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.30

ALP-UNI-3496895b-5_6



CID: ALP-UNI-3496895b-5_6

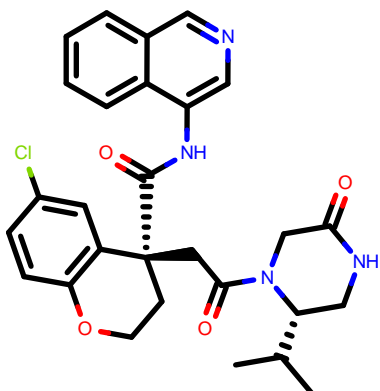
SMILES: C1C@H1C[N+]([O-])C(C1=O)C(C@2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5)S(=O)(=O)C

RUN: RUN2391

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.35

EN300-2983332_1_2_1



CID: EN300-2983332_1_2_1

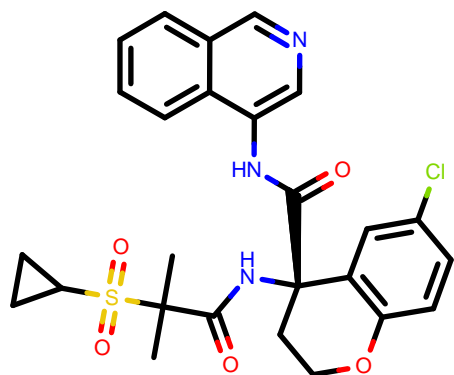
SMILES: CC(C)[C@H]1CNC(=O)CN1C(=O)C(C@2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5)

RUN: RUN7114

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

EN300-193399_1_1_1



CID: EN300-193399_1_1_1

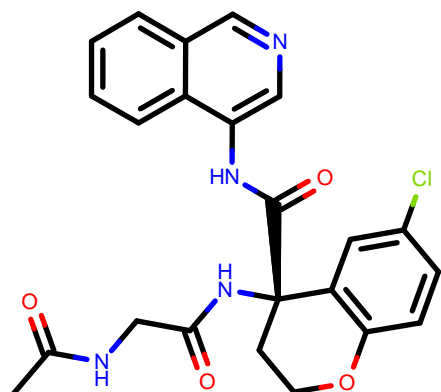
SMILES: CC(C)(C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nc4c3ccc4)S(=O)(=O)C5CC5

RUN: RUN4006

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.32

EN300-18561_1_1_1



CID: EN300-18561_1_1_1

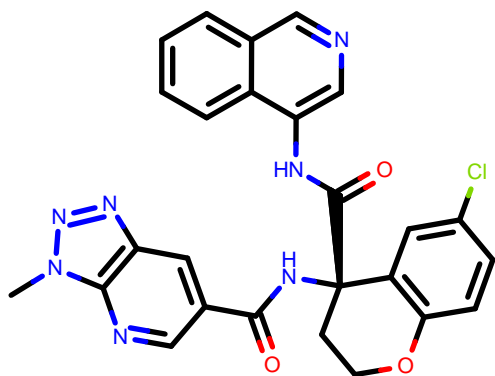
SMILES: CC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nc4c3ccc4

RUN: RUN6370

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-128431_1_1_1



CID: EN300-128431_1_1_1

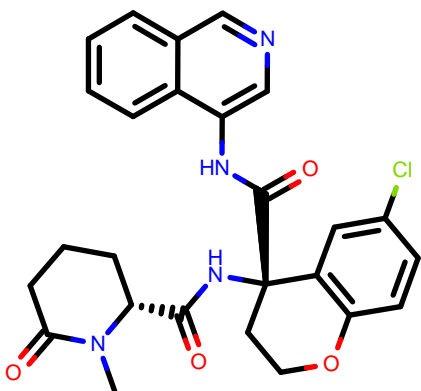
SMILES: Cn1c2c(cc(cn2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccc6)nn1

RUN: RUN6731

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.24

EN300-325738_1_2_1



CID: EN300-325738_1_2_1

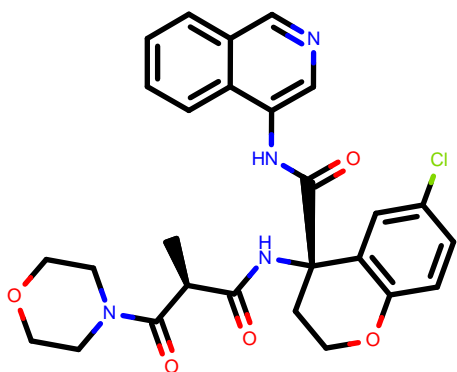
SMILES: CN1C@H](CCCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN3488

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.23

EN300-2855057_1_1_1



CID: EN300-2855057_1_1_1

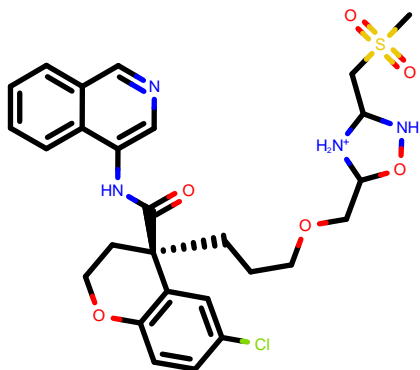
SMILES: C[C@@H](Cl)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccc4)C(=O)N5CCOCC5

RUN: RUN6000

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.29

EN300-94900_4_1_1



CID: EN300-94900_4_1_1

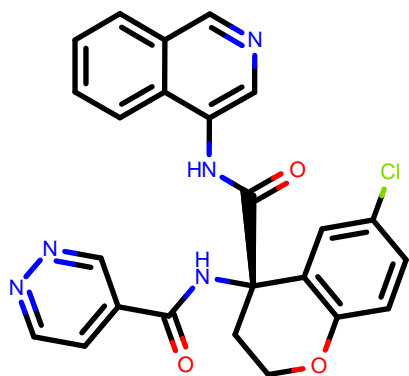
SMILES: CS(=O)(=O)Cc1nc(on1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN4354

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.33

EN300-75875_1_1_1



CID: EN300-75875_1_1_1

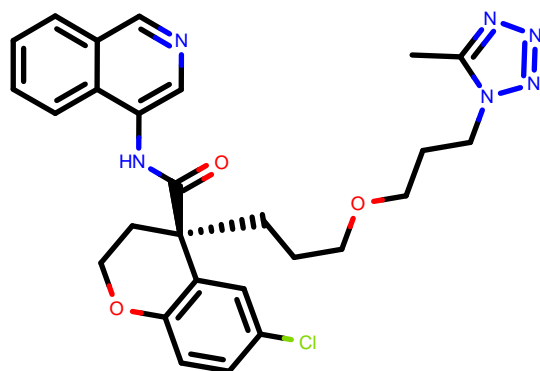
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5

RUN: RUN4346

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-197715_4_1_1



CID: EN300-197715_4_1_1

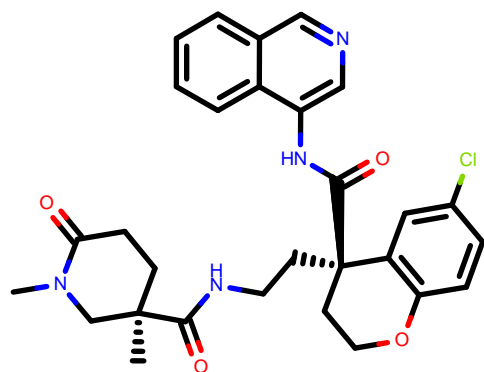
SMILES: Cc1nmm1CCOCCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5466

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.34

EN300-6734171_3_2_1



CID: EN300-6734171_3_2_1

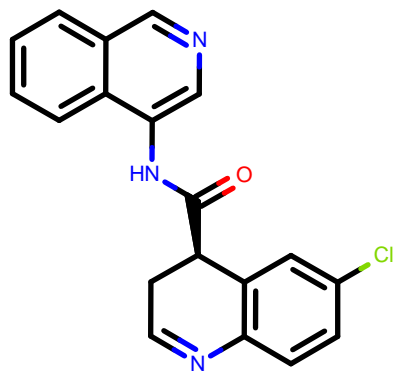
SMILES: C[C@@]1(CCC(=O)N(C1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3725

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.43

BEN-BAS-c2bc0d80-1_1



CID: BEN-BAS-c2bc0d80-1_1

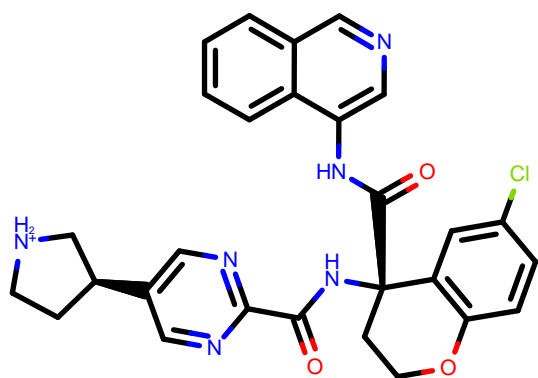
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H]3CC=Nc4c3cc(cc4)Cl

RUN: RUN997

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.28

EDG-MED-90036822-104_2



CID: EDG-MED-90036822-104_2

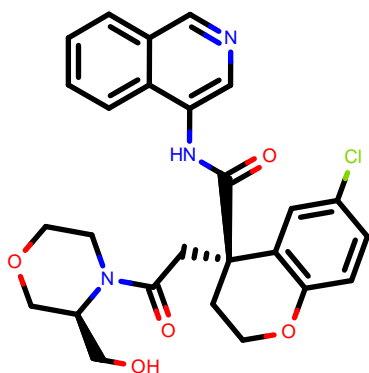
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C]N(C(=O)c5nc6c(c5)C@H)CC[NH2+]c6

RUN: RUN1689

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.39

EN300-154201_1_1_1



CID: EN300-154201_1_1_1

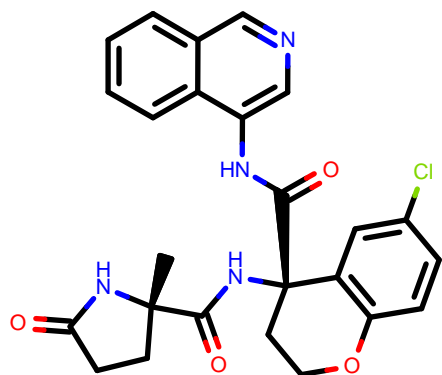
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc(cc4)C]C(=O)N5CCOC[C@@]3H5CO

RUN: RUN2999

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.31

EN300-370280_1_1_1



CID: EN300-370280_1_1_1

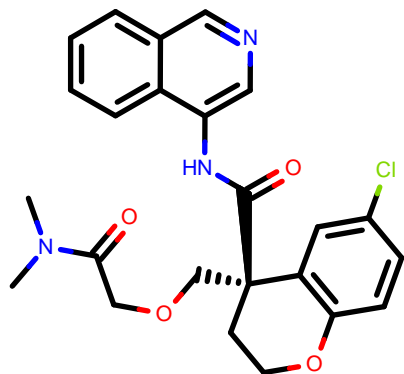
SMILES: C[C@@]1(CCC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN7029

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.23

EN300-216063_2_1_1



CID: EN300-216063_2_1_1

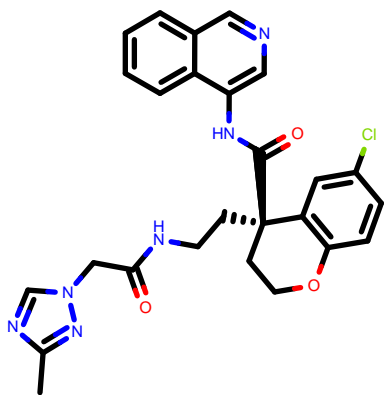
SMILES: CN(C)C(=O)COC[C@@]1(C)COCc2c1cc(cc2)C]C(=O)Nc3nccc4c3cccc4

RUN: RUN4197

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.20

EN300-7473354_3_1_1



CID: EN300-7473354_3_1_1

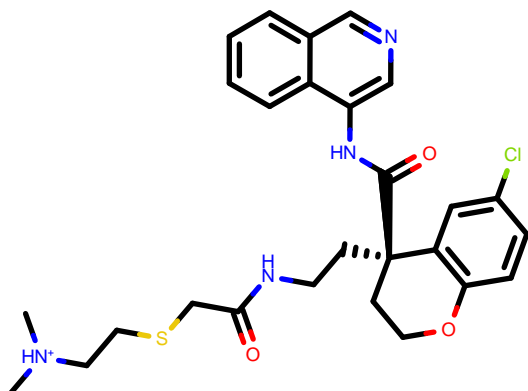
SMILES: Cc1nnc(n1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3611

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.38

EN300-1708620_3_1_1



CID: EN300-1708620_3_1_1

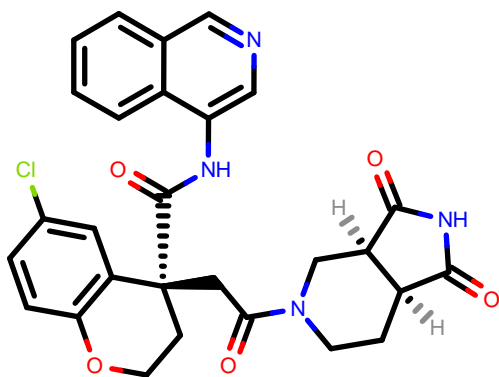
SMILES: C[NH+](C)CCSCC(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4319

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.37

EDJ-MED-d203f206-35_1



CID: EDJ-MED-d203f206-35_1

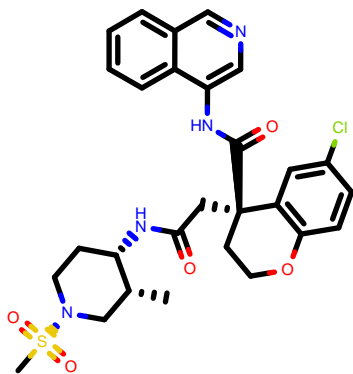
SMILES: c1ccc2c(c1)ncnc2N(C(=O)C[C@]3(C)CCOC4c3cc(cc4)Cl)C(=O)N5CC[C@H]6[C@@H](C5)C(=O)N6c7=O

RUN: RUN2421

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.27

ALP-UNI-3496895b-5_1



CID: ALP-UNI-3496895b-5_1

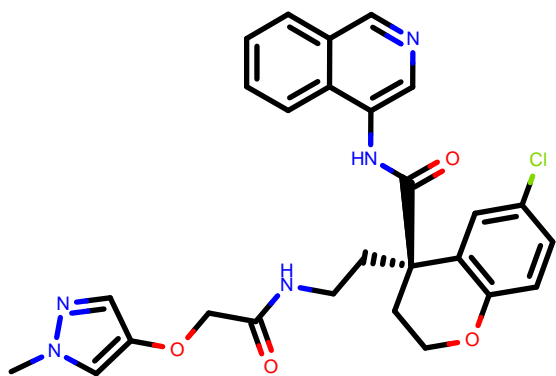
SMILES: C[C@@H]1CN(C)CC[C@@H]1NC(=O)C[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5S(=O)(=O)C

RUN: RUN2397

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.37

EN300-201553_3_1_1



CID: EN300-201553_3_1_1

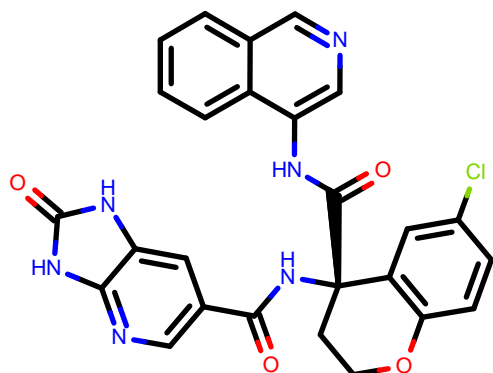
SMILES: Cn1cc(en1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccoc5

RUN: RUN3614

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.35

EN300-214552_1_1_1



CID: EN300-214552_1_1_1

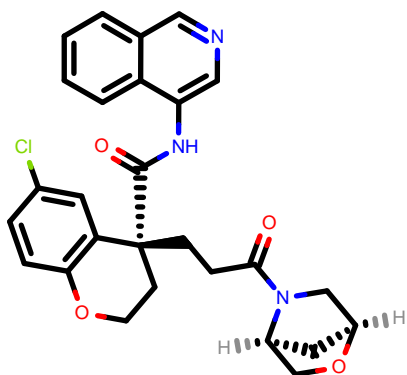
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cc6c([nH]c(=O)[nH]6)nc5

RUN: RUN5521

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.30

EN300-321790_2_1_1



CID: EN300-321790_2_1_1

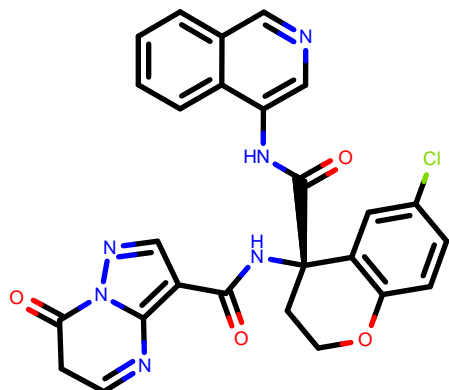
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@@H]6C[C@H]5OC6

RUN: RUN6660

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.27

EN300-203940_1_1_1



CID: EN300-203940_1_1_1

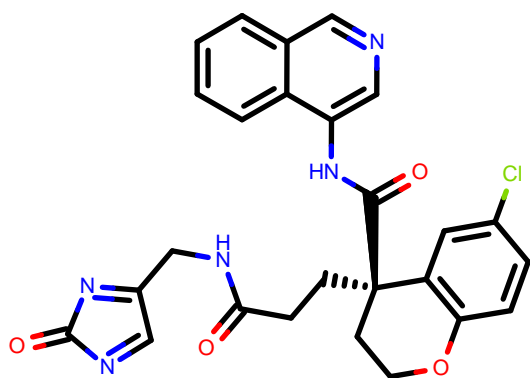
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]6c5nccoc6=O

RUN: RUN4366

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.26

EN300-260603_2_1_1



CID: EN300-260603_2_1_1

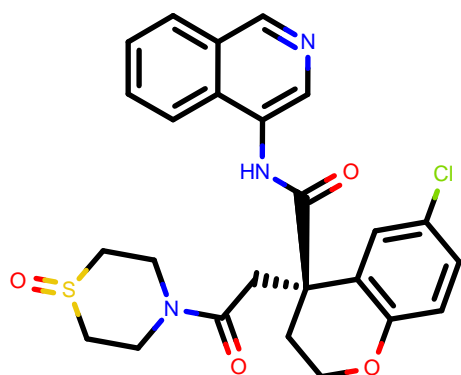
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)NCc5c[nH]c(=O)[nH]5

RUN: RUN7064

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.29

EDJ-MED-d203f206-37_1



CID: EDJ-MED-d203f206-37_1

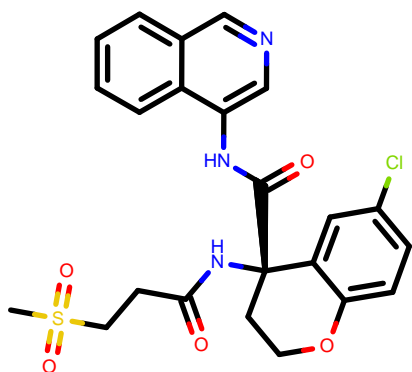
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CCS(=O)CC5

RUN: RUN2424

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.34

EN300-31387_1_1_1



CID: EN300-31387_1_1_1

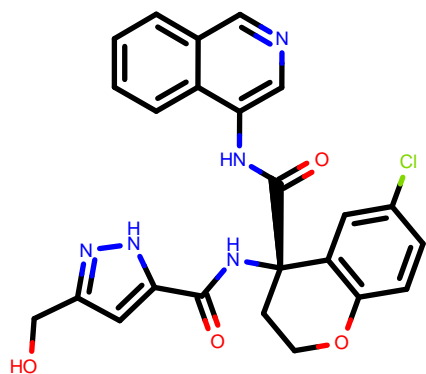
SMILES: CS(=O)(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5733

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.26

EN300-658865_1_1_1



CID: EN300-658865_1_1_1

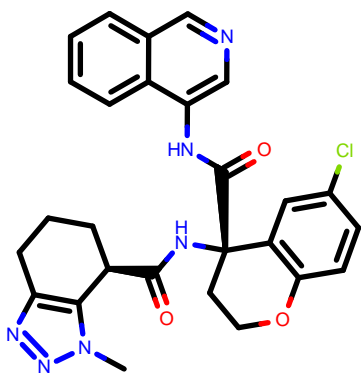
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cc[nH]5)CO

RUN: RUN3556

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.21

EN300-1664865_1_2_1



CID: EN300-1664865_1_2_1

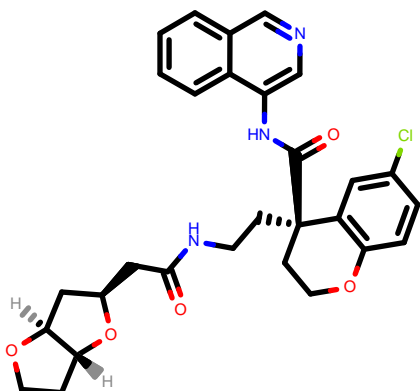
SMILES: Cn1c2c(nn1)CC[C@H]2C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN5438

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.25

EN300-7355519_3_7_1



CID: EN300-7355519_3_7_1

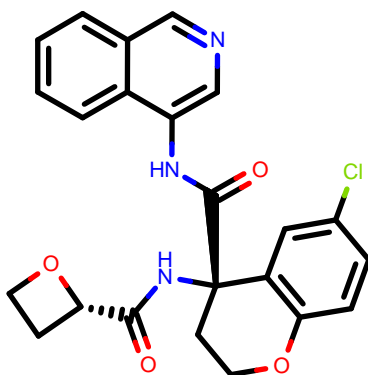
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@@]4(C)C[C@@]5(C)O[C@]4(C)O5

RUN: RUN5469

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.36

EN300-85760_1_1_1



CID: EN300-85760_1_1_1

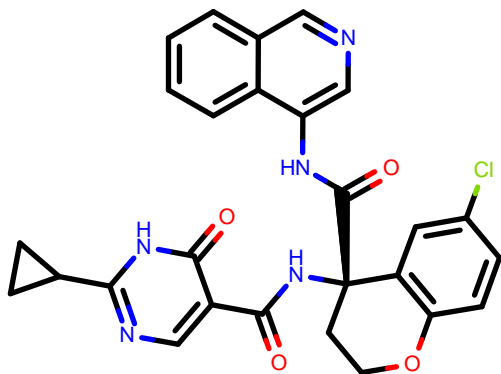
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(C)O[C@]4(C)O5

RUN: RUN4745

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.24

EN300-118045_1_1_1



CID: EN300-118045_1_1_1

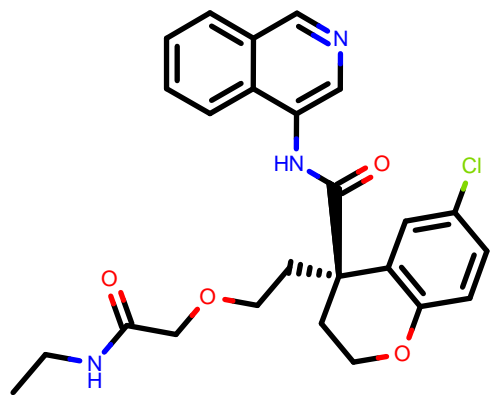
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6[nH]c5=O)C6CC6

RUN: RUN7705

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.36

EN300-7003350_3_1_1



CID: EN300-7003350_3_1_1

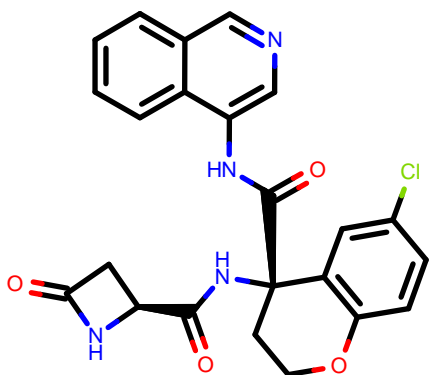
SMILES: CCNC(=O)COCC[C@]1(C)C(CO)C2c1cc(cc2)C(=O)Nc3ccc4c3ccc4

RUN: RUN4026

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.23

EN300-101505_1_1_1



CID: EN300-101505_1_1_1

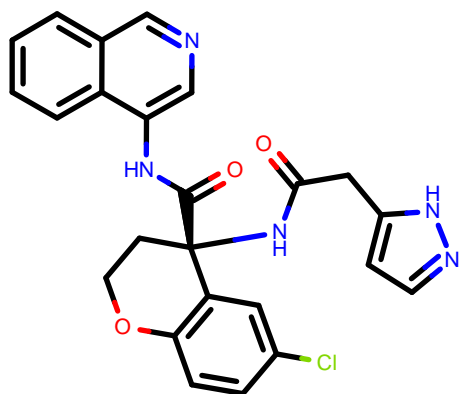
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(=O)Nc5c[nH]5

RUN: RUN5523

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.22

EN300-71405_1_1_1



CID: EN300-71405_1_1_1

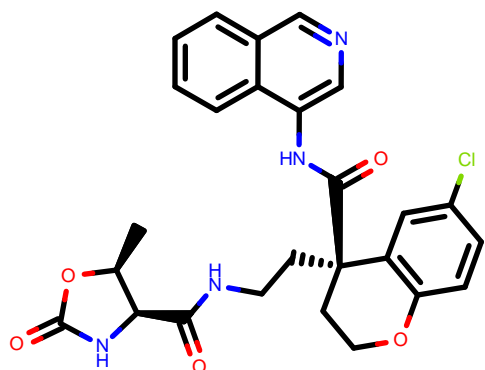
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4c3cc(cc4)C(=O)Nc5c[nH]5

RUN: RUN3371

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.21

EN300-172640_3_4_1



CID: EN300-172640_3_4_1

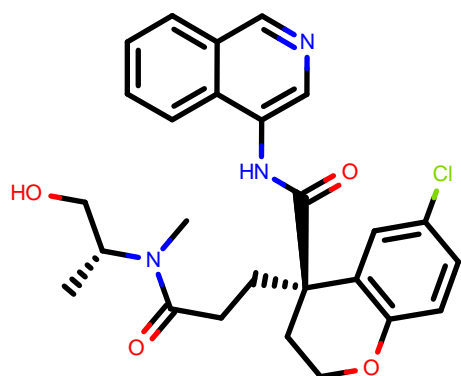
SMILES: C[C@H]1[C@@H](NC(=O)O1)C(=O)NCC[C@]2(C)C(CO)C3c2cc(cc3)C(=O)Nc4cnc5c4ccc5

RUN: RUN5378

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.29

EN300-205110_2_1_1



CID: EN300-205110_2_1_1

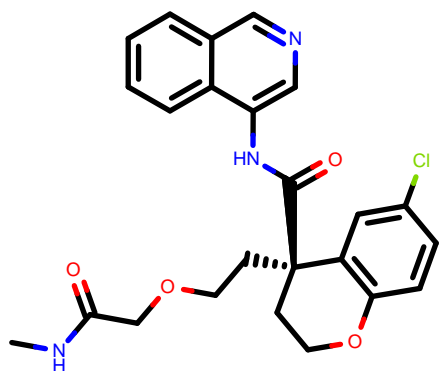
SMILES: C[C@H](CO)N(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2742

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.24

EN300-2977549_3_1_1



CID: EN300-2977549_3_1_1

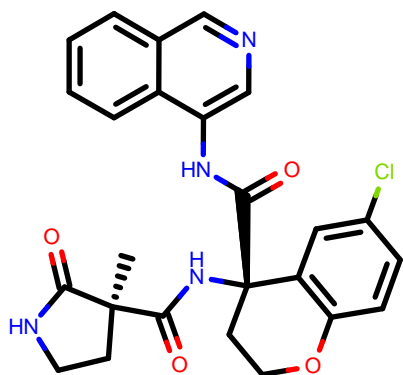
SMILES: CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3986

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.20

EN300-207959_1_1_1



CID: EN300-207959_1_1_1

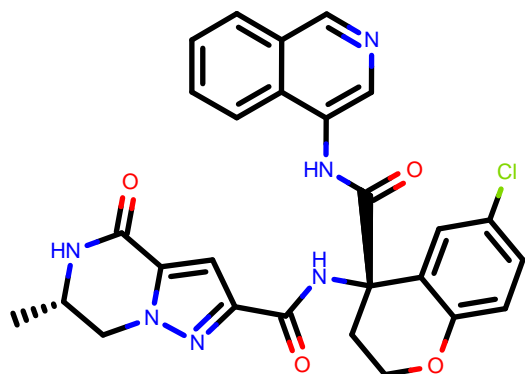
SMILES: C[C@@]1(CCN(C1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3019

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.33

EN300-265285_1_2_1



CID: EN300-265285_1_2_1

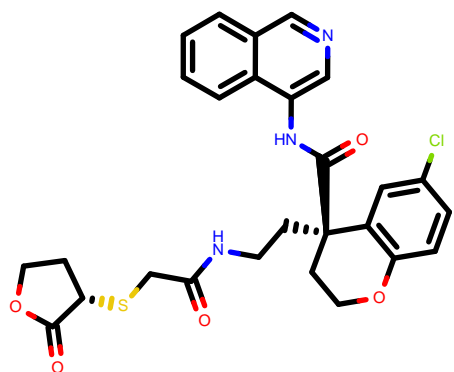
SMILES: C[C@H]1Cn2c(cc(n2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6)C(=O)N1

RUN: RUN4185

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.29

EN300-113218_3_2_1



CID: EN300-113218_3_2_1

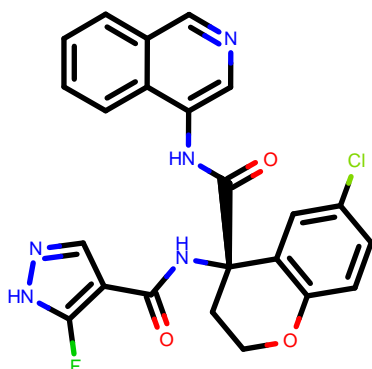
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5CCOC5=O

RUN: RUN5375

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.37

EN300-7121836_1_1_1



CID: EN300-7121836_1_1_1

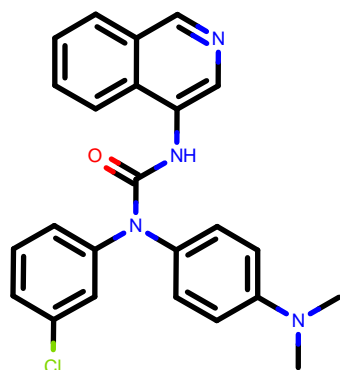
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]c5F

RUN: RUN4213

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.17

MIC-UNK-d36ab305-5_1



CID: MIC-UNK-d36ab305-5_1

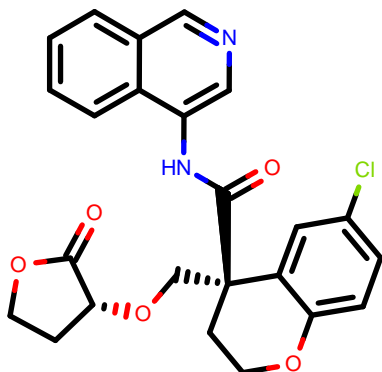
SMILES: CN(C)c1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN173

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.27

EN300-20496_2_1_1



CID: EN300-20496_2_1_1

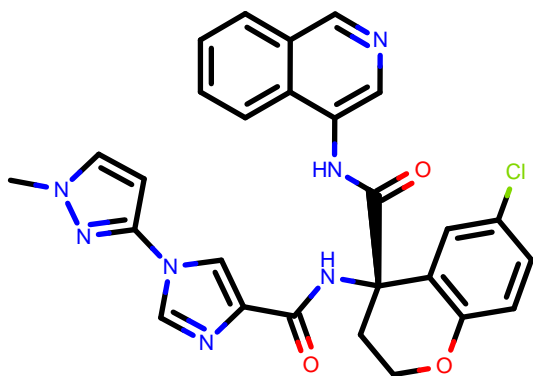
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCOC5=O

RUN: RUN4446

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.21

EN300-1726340_1_1_1



CID: EN300-1726340_1_1_1

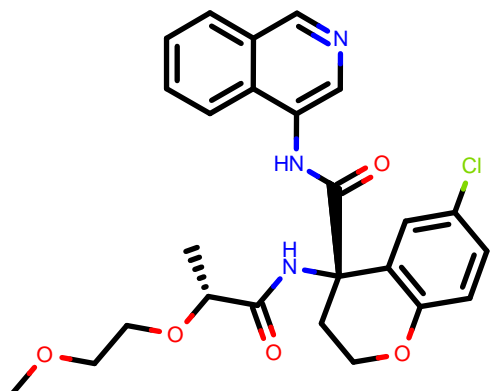
SMILES: Cn1ccc(n1)n2cc(nc2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4294

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.22

EN300-77359_1_2_1



CID: EN300-77359_1_2_1

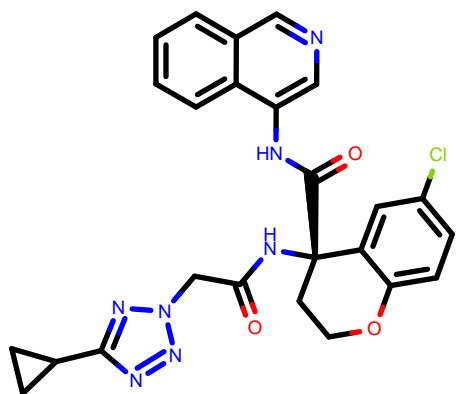
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)OCOC

RUN: RUN4374

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.22

EN300-1719432_1_1_1



CID: EN300-1719432_1_1_1

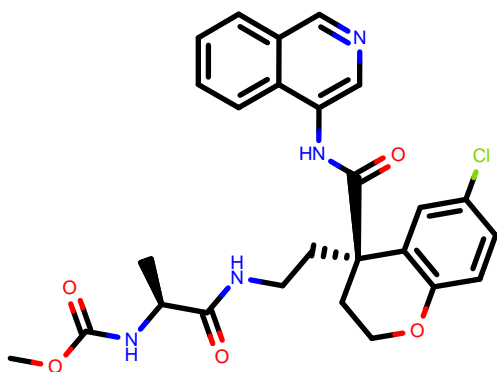
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C(=O)Cn5nc(nc5)C6COC6

RUN: RUN3183

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.26

EN300-120068_3_1_1



CID: EN300-120068_3_1_1

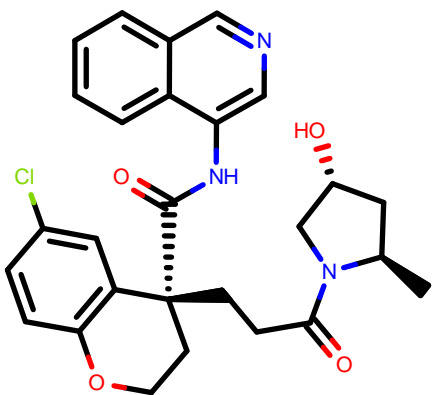
SMILES: C[C@]H(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)OC

RUN: RUN6181

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.28

EN300-173562_2_3_1



CID: EN300-173562_2_3_1

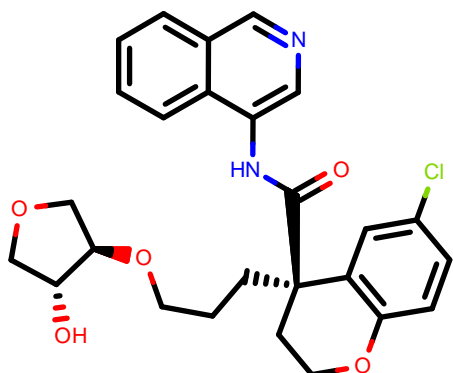
SMILES: C[C@@H]1C[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)O

RUN: RUN6794

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.28

EN300-331828_4_1_1



CID: EN300-331828_4_1_1

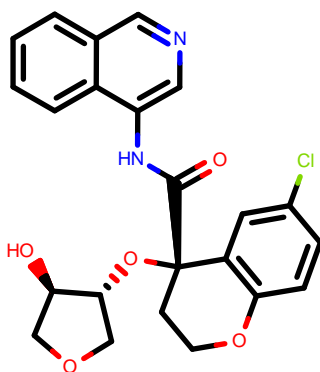
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5OOC[C@H]5O

RUN: RUN3722

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.32

EN300-331828_1_1_1



CID: EN300-331828_1_1_1

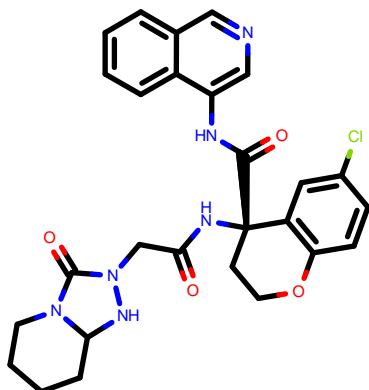
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5OOC[C@H]5O

RUN: RUN7657

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.20

EN300-263346_1_1_1



CID: EN300-263346_1_1_1

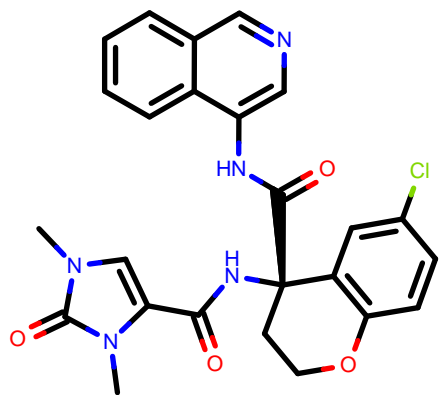
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6c(n5)CCCC6

RUN: RUN6307

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.33

EN300-312618_1_1_1



CID: EN300-312618_1_1_1

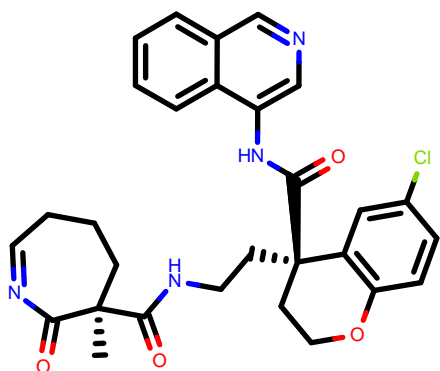
SMILES: Cn1cc(n(c1=O)C(=O)N)C@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN6566

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.22

EN300-6745081_3_2_1



CID: EN300-6745081_3_2_1

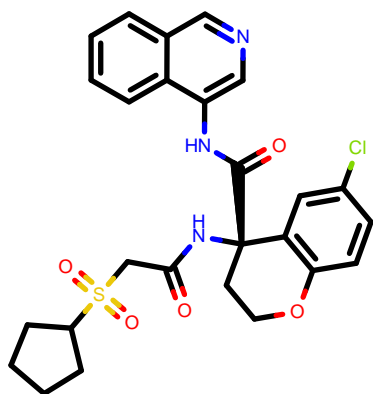
SMILES: C[C@@]1(CCCNC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN3241

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.45

EN300-42154_1_1_1



CID: EN300-42154_1_1_1

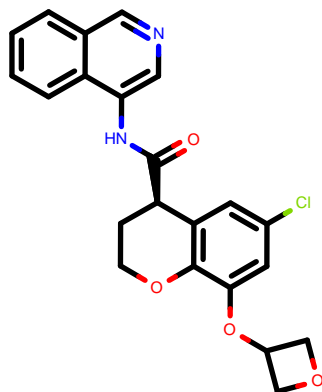
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C5CCCC5

RUN: RUN5792

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.36

EDJ-MED-e4b030d8-4_1



CID: EDJ-MED-e4b030d8-4_1

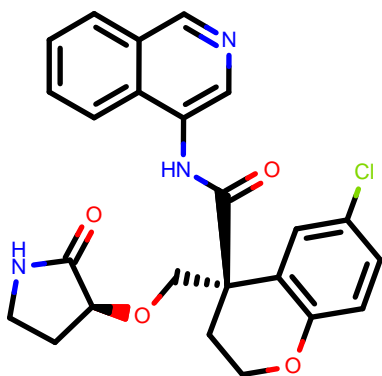
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]H3CCOc4c3cc(cc4OC5COC5)Cl

RUN: RUN278

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.18

EN300-6736413_2_2_1



CID: EN300-6736413_2_2_1

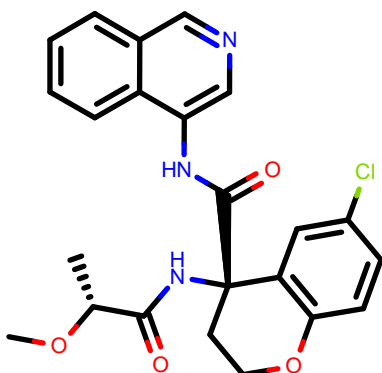
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O

RUN: RUN4117

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.19

EN300-247951_1_1_1



CID: EN300-247951_1_1_1

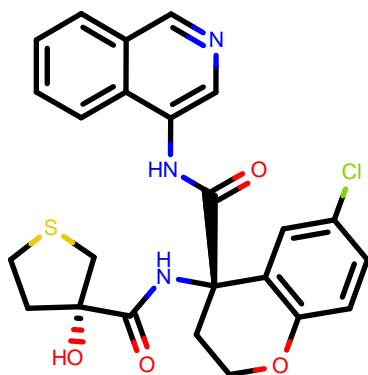
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN3719

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.22

EN300-122656_1_2_1



CID: EN300-122656_1_2_1

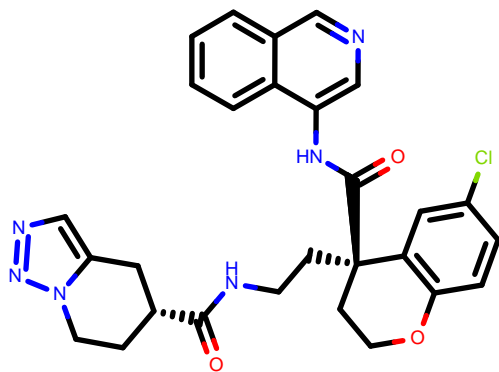
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCSC5)O

RUN: RUN2709

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.42

EN300-7430501_3_1_1



CID: EN300-7430501_3_1_1

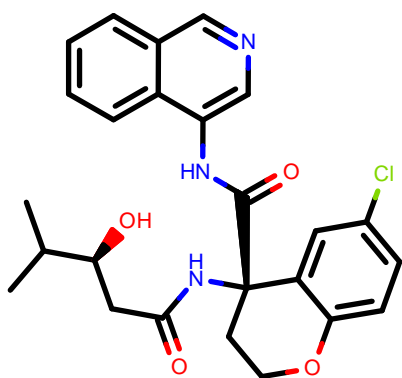
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5CNCn6c(cnn6)C5

RUN: RUN3618

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.36

EN300-155498_1_1_1



CID: EN300-155498_1_1_1

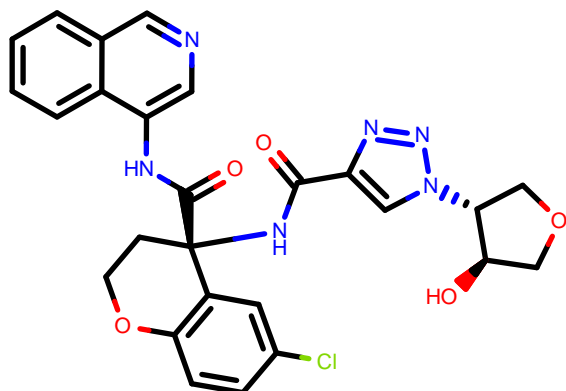
SMILES: CC(C)[C@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6570

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.25

EN300-637424_1_1_1



CID: EN300-637424_1_1_1

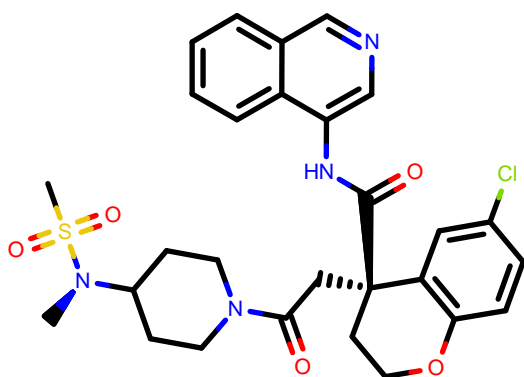
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)N(C(=O)c5cn[nH]5)[C@@H]6OC[C@H]6O

RUN: RUN4870

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.26

ALP-UNI-76695c4f-8_2



CID: ALP-UNI-76695c4f-8_2

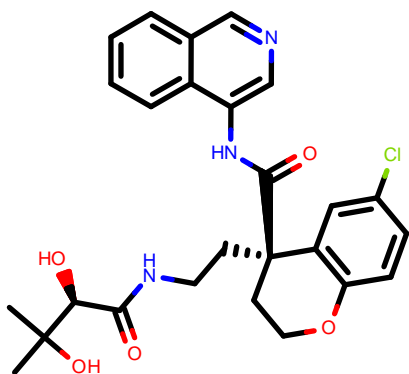
SMILES: CN(C)[C1CCN(CC1)C(=O)C]C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)S(=O)(=O)C

RUN: RUN2047

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.30

EN300-299532_3_2_1



CID: EN300-299532_3_2_1

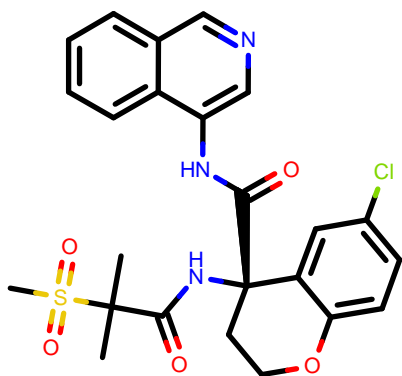
SMILES: CC(C)[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN5628

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.31

EN300-76205_1_1_1



CID: EN300-76205_1_1_1

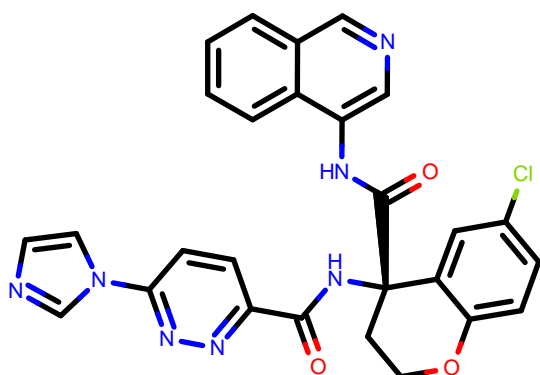
SMILES: CC(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)S(=O)(=O)C

RUN: RUN4748

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.25

EN300-61898_1_1_1



CID: EN300-61898_1_1_1

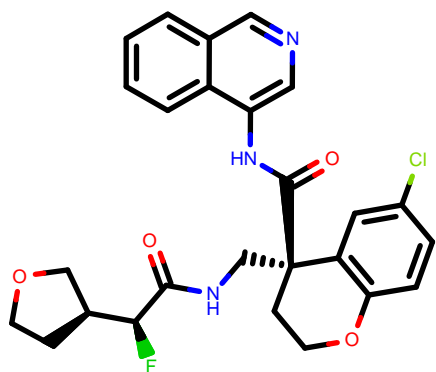
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6n5n6ccn6

RUN: RUN7075

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.25

EN300-783124_2_4_1



CID: EN300-783124_2_4_1

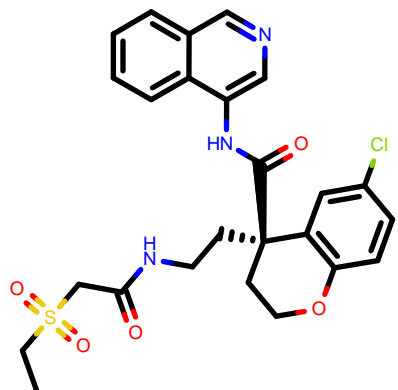
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]([C@@H]5CCOC5)F

RUN: RUN6837

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.23

EN300-53395_3_1_1



CID: EN300-53395_3_1_1

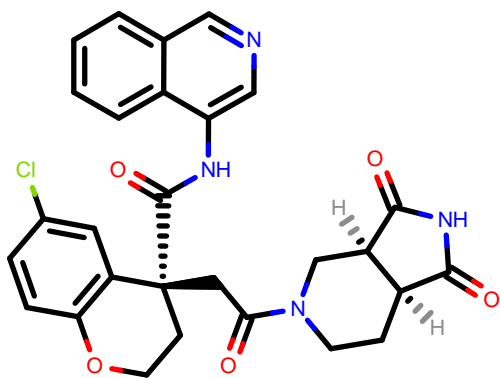
SMILES: CCS(=O)(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN7072

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.35

EN300-104029_1_2_1



CID: EN300-104029_1_2_1

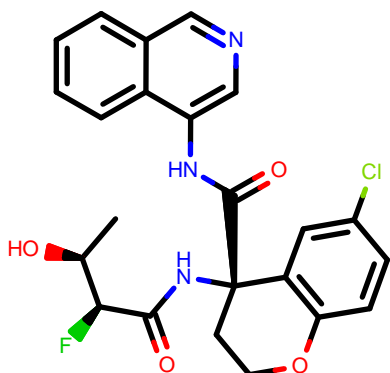
SMILES: c1ccc2c(c1)ncnc2N(C(=O)C[C@@H]3CCOC4C3C(=O)C)C(=O)N5CC[C@H]3C[C@@H]C5(C(=O)N)C6=O

RUN: RUN5033

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.24

EDG-MED-90036822-37_1



CID: EDG-MED-90036822-37_1

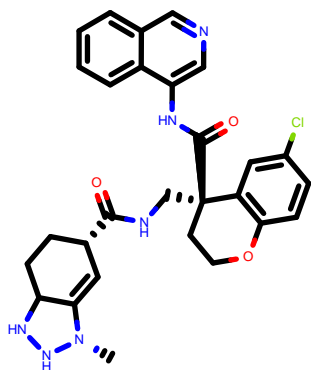
SMILES: C[C@@H]1[C@@H]2C(=O)N[C@@H]1(C(=O)C2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccc4F)O

RUN: RUN1551

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.20

EN300-217343_2_1_1



CID: EN300-217343_2_1_1

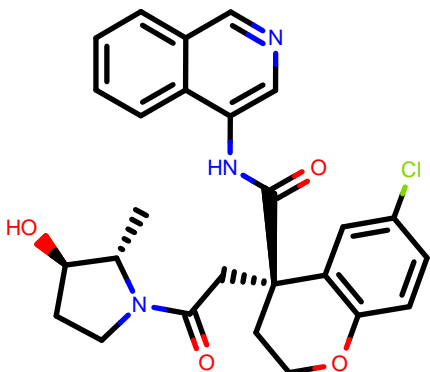
SMILES: Cn1c2c(n1)CC[C@@H]2C(=O)N[C@@H]3(C(=O)C4C3C(=O)C)C(=O)Nc5ncnc6c5ccc6F

RUN: RUN3359

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.37

EN300-245036_1_1_1



CID: EN300-245036_1_1_1

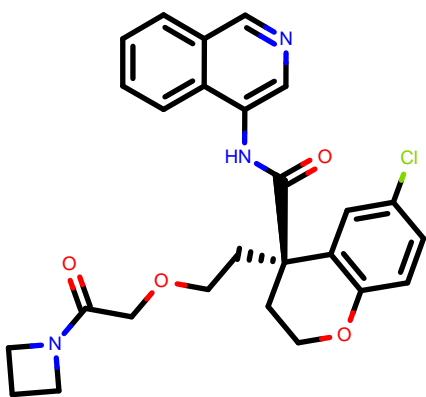
SMILES: C[C@@H]1[C@@H]2C(=O)N[C@@H]1(C(=O)C2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccc4F)O

RUN: RUN6811

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.29

EN300-11195_3_1_1



CID: EN300-11195_3_1_1

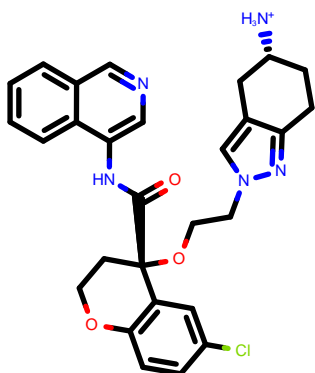
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(C(=O)N5CCCS

RUN: RUN4325

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.24

ED_-GRI-5b13fbe2-60_2



CID: ED_-GRI-5b13fbe2-60_2

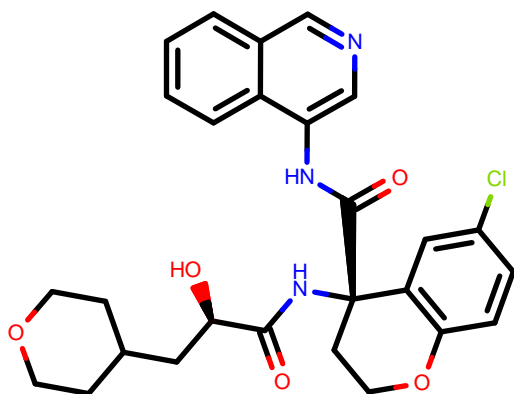
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cc6c(n5)CC[C@H](C6)[NH3+]

RUN: RUN1450

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.35

EN300-1452069_1_1_1



CID: EN300-1452069_1_1_1

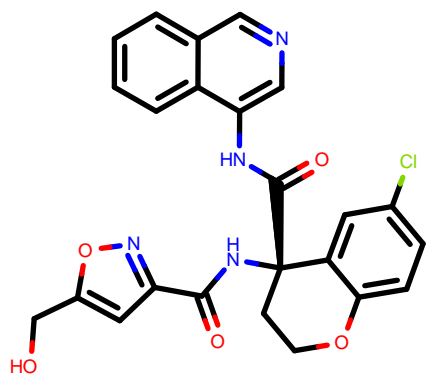
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CC5CCOCC5)O

RUN: RUN4148

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.34

EN300-95507_1_1_1



CID: EN300-95507_1_1_1

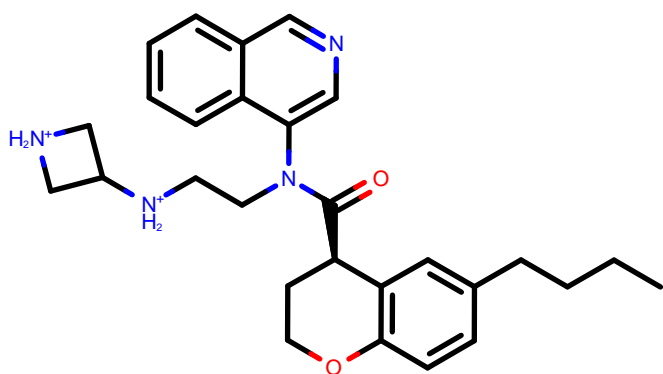
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(cn5)CO

RUN: RUN3557

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.21

MAK-UNK-83e0a0b4-4_1_1



CID: MAK-UNK-83e0a0b4-4_1_1

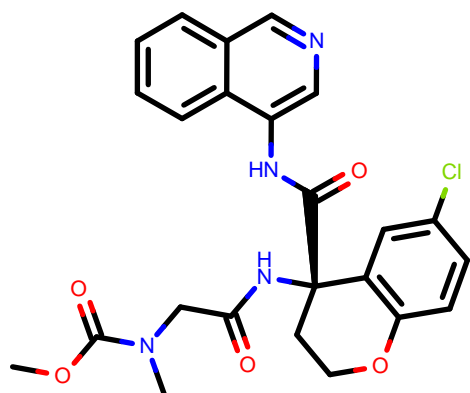
SMILES: CCCCc1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCNC3C[NH2+][C3])c4nccc5c4cccc5

RUN: RUN4271

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.45

EN300-39005_1_1_1



CID: EN300-39005_1_1_1

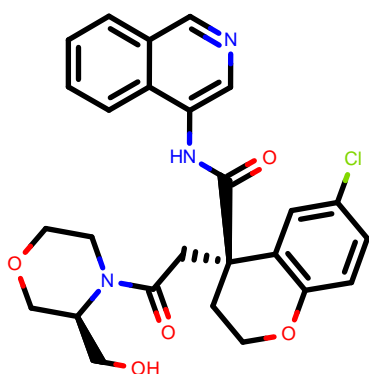
SMILES: CN(CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)C(=O)OC

RUN: RUN7682

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-38_1



CID: EDJ-MED-d203f206-38_1

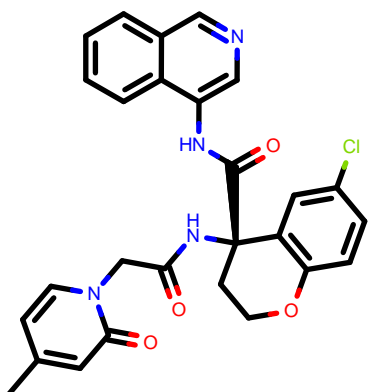
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN2436

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.36

EN300-184446_1_1_1



CID: EN300-184446_1_1_1

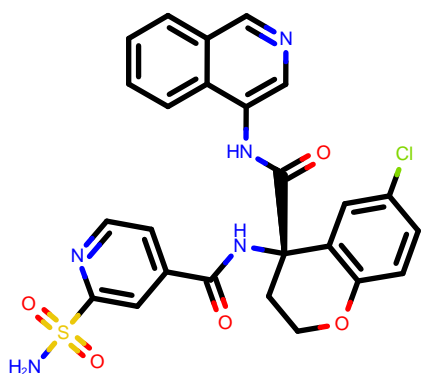
SMILES: Cc1ccn(c(=O)c1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN5213

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.29

EN300-141628_1_1_1



CID: EN300-141628_1_1_1

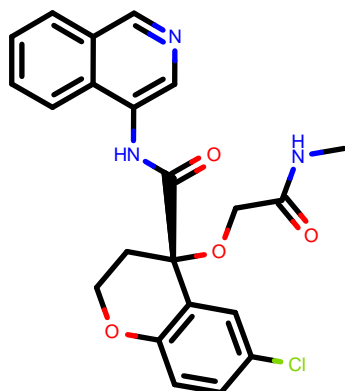
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)S(=O)(=O)N

RUN: RUN4411

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.37

EN300-2977549_1_1_1



CID: EN300-2977549_1_1_1

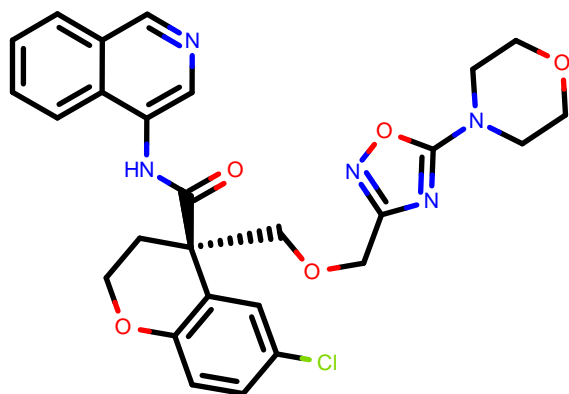
SMILES: CNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5898

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.18

EN300-1608590_2_1_1



CID: EN300-1608590_2_1_1

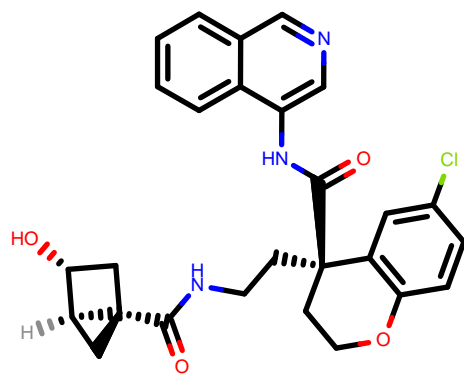
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nc(on5)N6CCOCC6

RUN: RUN7306

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.33

EN300-6493972_3_1_1



CID: EN300-6493972_3_1_1

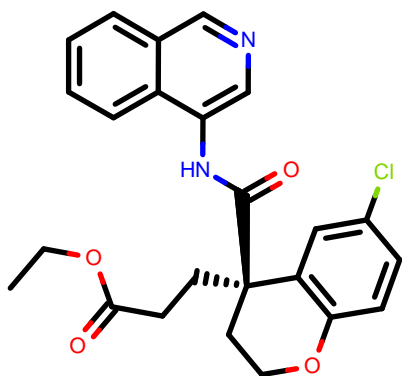
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@]56C[C@@]5(C)C6)O

RUN: RUN6676

DDG (kcal/mol): -1.46

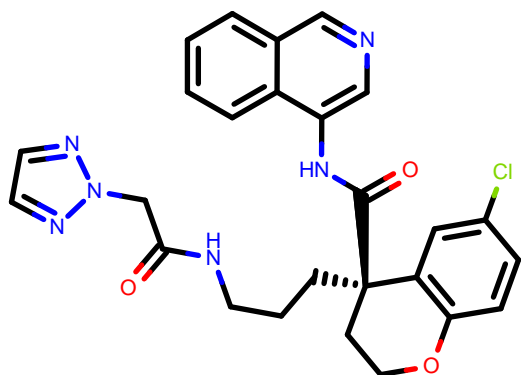
dDDG (kcal/mol): 0.24

JAG-UCB-706446eb-4_1



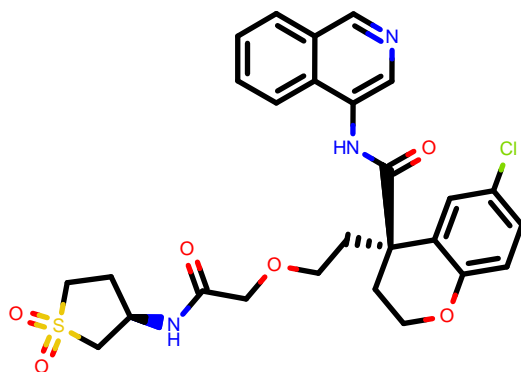
CID:	JAG-UCB-706446eb-4_1
SMILES:	<chem>CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4</chem>
RUN:	RUN620
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.22

EN300-100916_4_1_1



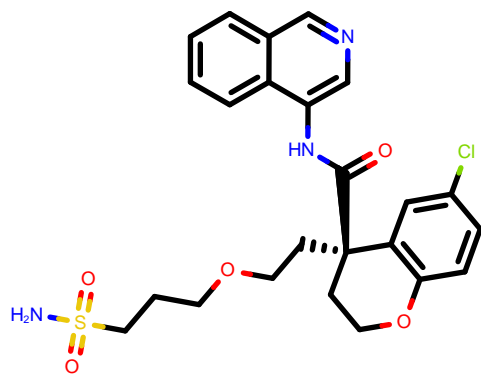
CID:	EN300-100916_4_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)Cn5nccn5</chem>
RUN:	RUN5088
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.34

EN300-05512_3_1_1



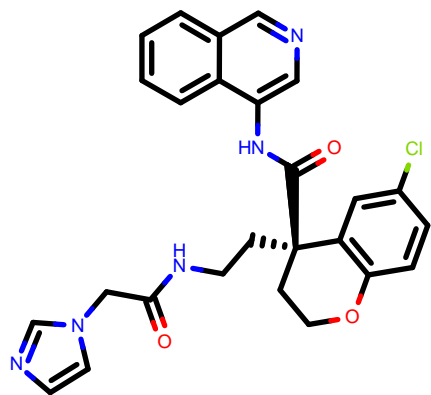
CID:	EN300-05512_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@@]5SCS1=O1=O</chem>
RUN:	RUN4651
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.36

EN300-79588_3_1_1



CID:	EN300-79588_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)N</chem>
RUN:	RUN4079
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.34

EN300-38979_3_1_1



CID: EN300-38979_3_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)C@@3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cnc5

RUN:

RUN5333

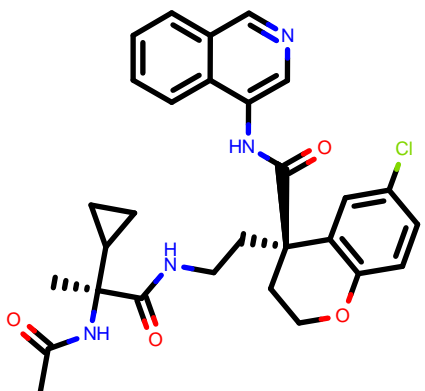
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.27

EN300-67073_3_1_1



CID: EN300-67073_3_1_1

SMILES:

CC(=O)N[C@@]3[C@@]3(C1CC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN:

RUN5875

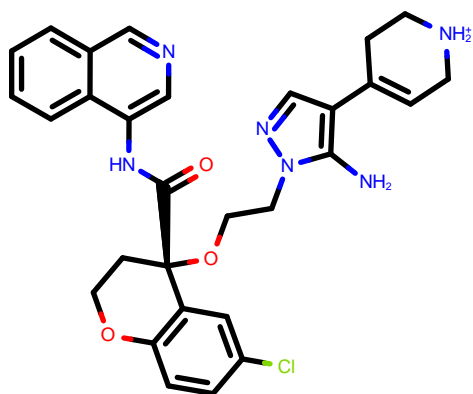
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.36

ED_-GRI-5b13fbe2-35_1



CID: ED_-GRI-5b13fbe2-35_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)C@@3[C@@]3(CCOc4c3cc(cc4)C)OCCn5c(c1n5)C6=CC(N)C=C6N

RUN:

RUN1449

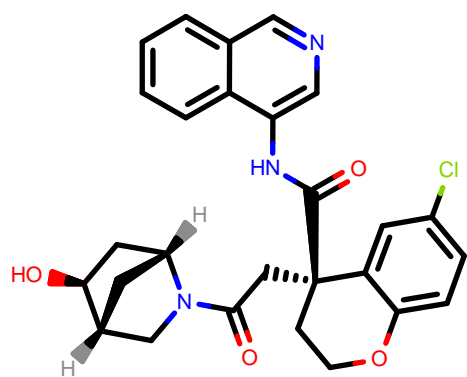
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.29

EN300-307084_1_1_1



CID: EN300-307084_1_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)C@@3[C@@]3(CCOc4c3cc(cc4)C)C[C@@H]5C[C@@H](C)C[C@@H]5O

RUN:

RUN3739

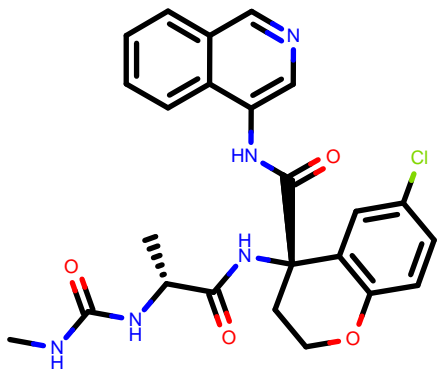
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.29

EN300-2958082_1_1_1



CID: EN300-2958082_1_1_1

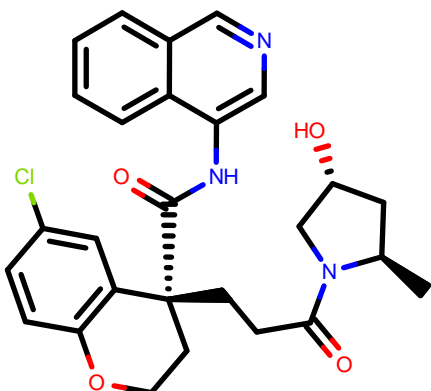
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)NC

RUN: RUN4590

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-173562_2_3_1



CID: EN300-173562_2_3_1

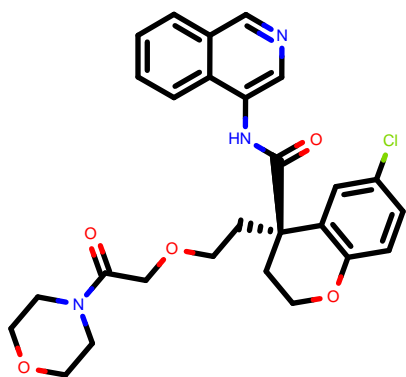
SMILES: C[C@@H]1[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN7576

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.26

EN300-1241327_3_1_1



CID: EN300-1241327_3_1_1

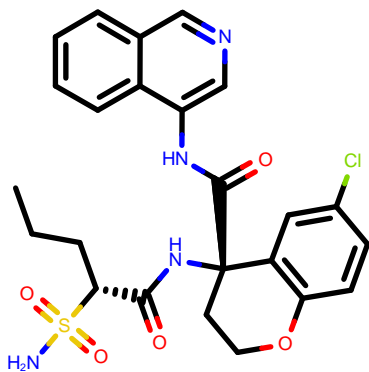
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5

RUN: RUN3717

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.25

EN300-206592_1_2_1



CID: EN300-206592_1_2_1

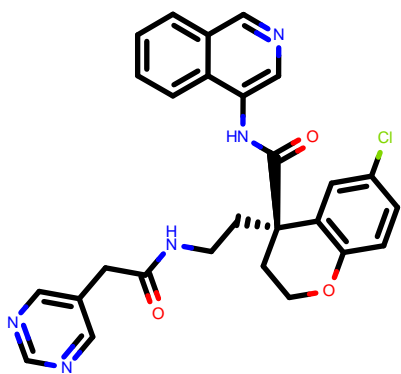
SMILES: CCC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)S(=O)(=O)N

RUN: RUN3748

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.39

EN300-185751_3_1_1



CID: EN300-185751_3_1_1

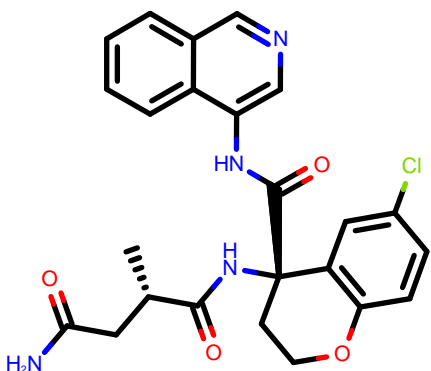
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cncnc5

RUN: RUN5457

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-202757_1_1_1



CID: EN300-202757_1_1_1

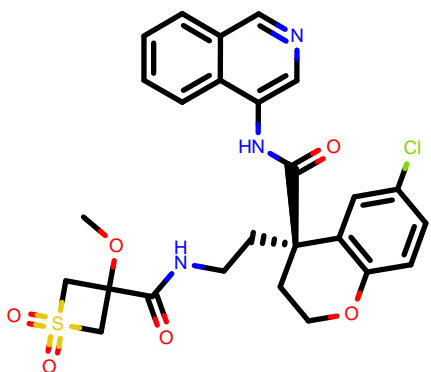
SMILES: C[C@@H](CC(=O)N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN5804

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.29

EN300-704025_3_1_1



CID: EN300-704025_3_1_1

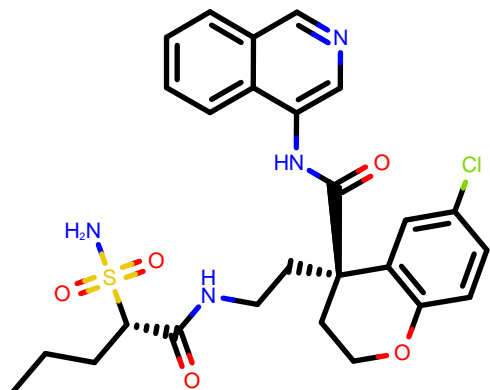
SMILES: COc1(CS(=O)(=O)C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN4932

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.42

EN300-206592_3_1_1



CID: EN300-206592_3_1_1

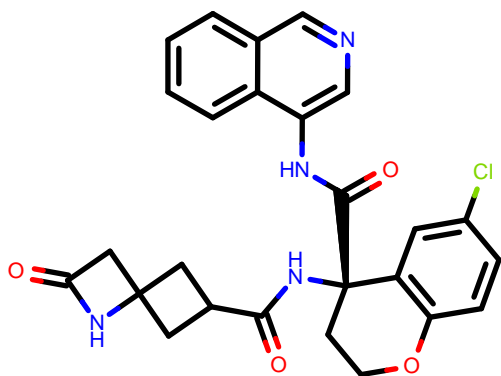
SMILES: CCC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)S(=O)(=O)N

RUN: RUN4094

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.31

EN300-1700760_1_1_1



CID: EN300-1700760_1_1_1

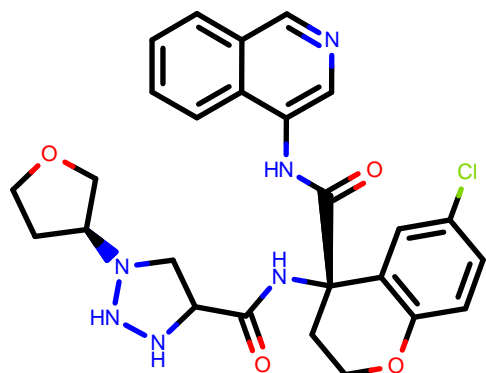
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN3176

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.22

EN300-151461_1_2_1



CID: EN300-151461_1_2_1

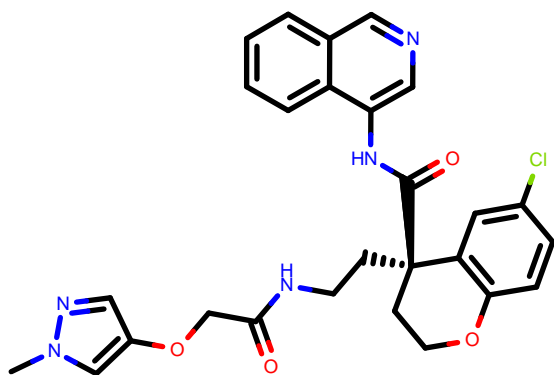
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)[C@H]6CCOC6

RUN: RUN5580

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EN300-201553_3_1_1



CID: EN300-201553_3_1_1

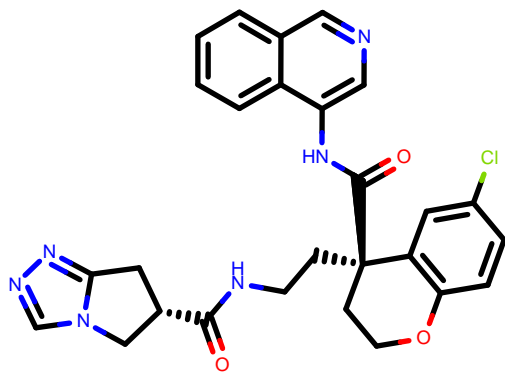
SMILES: Cn1cc(en1)OCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5o4ccoc5

RUN: RUN4577

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.30

EN300-6745453_3_2_1



CID: EN300-6745453_3_2_1

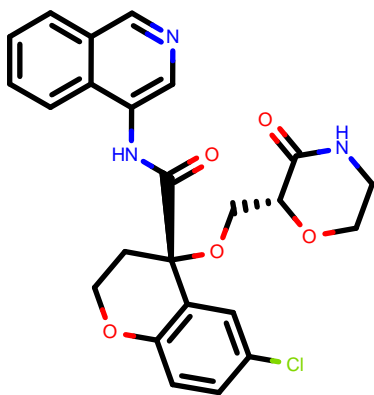
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C6c6nnn6C5

RUN: RUN3047

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.37

EN300-1706036_1_1_1



CID: EN300-1706036_1_1_1

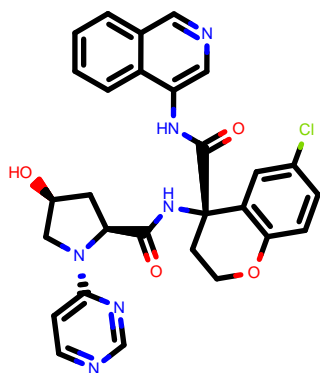
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C(=O)NCCO5

RUN: RUN7796

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.28

EN300-310022_1_1_1



CID: EN300-310022_1_1_1

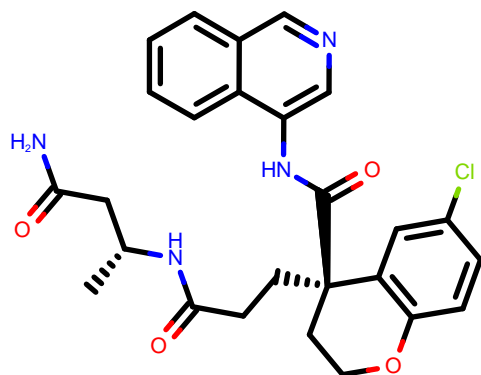
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@H]5C(=O)N5c6ccncc6O

RUN: RUN6196

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.32

EN300-84785_2_2_1



CID: EN300-84785_2_2_1

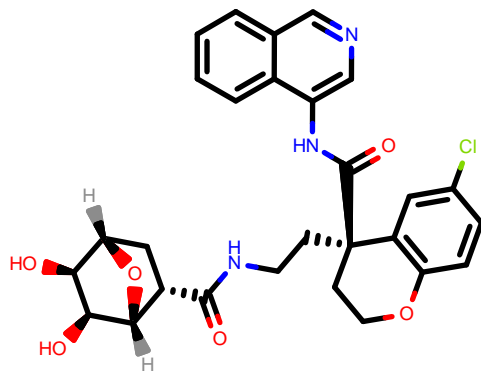
SMILES: C[C@@H](CC(=O)N)NC(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4

RUN: RUN5800

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.27

EN300-6764836_3_2_1



CID: EN300-6764836_3_2_1

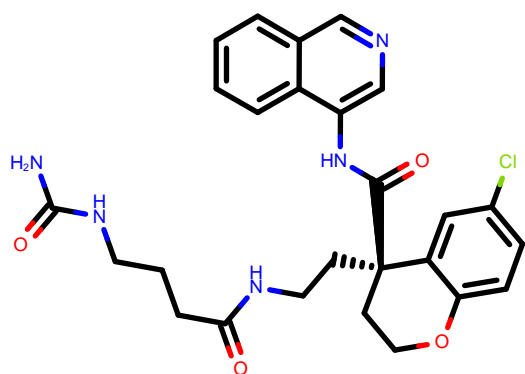
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN[C@@H]5C(=O)N[C@@H]6C(=O)NCCO6

RUN: RUN5964

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.29

EN300-05620_3_1_1



CID: EN300-05620_3_1_1

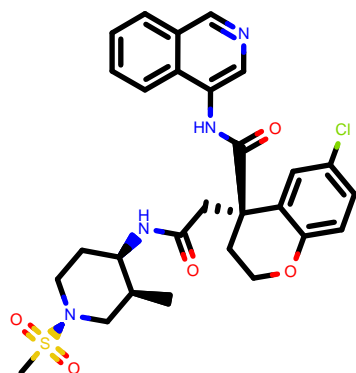
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4O)CCNC(=O)CCNC(=O)N

RUN: RUN3319

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.36

ALP-POS-2da19ca7-7_8



CID: ALP-POS-2da19ca7-7_8

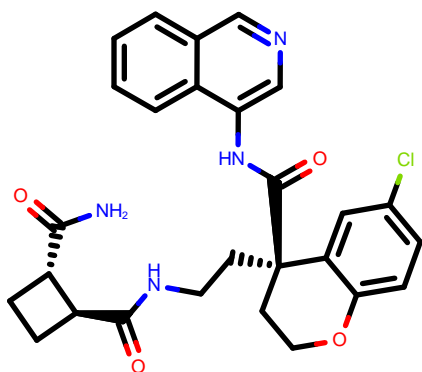
SMILES: C[C@H]1C[N@@]1CC[C@H]1NC(=O)[C@@]2(C)CCOc3c2cc(cc3O)N4Cnc5c4ccccc5S(=O)(=O)C

RUN: RUN2285

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.44

EN300-217107_3_2_1



CID: EN300-217107_3_2_1

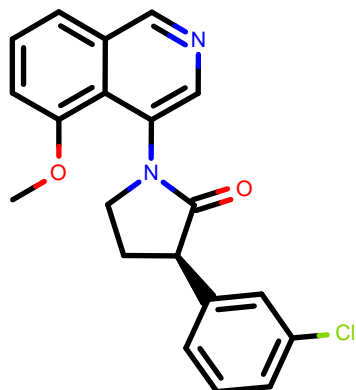
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4O)C@H]5CC[C@@]3H5Cl=O)N

RUN: RUN4285

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.31

MIC-UNK-50cce87d-8_1



CID: MIC-UNK-50cce87d-8_1

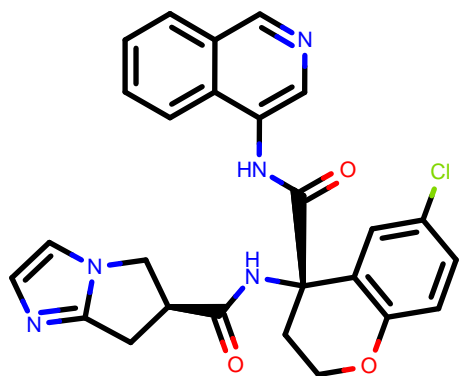
SMILES: COc1cccc2c1c(cnc2)N3CC[C@@]4(C)C(=O)c4ccccc4Cl

RUN: RUN558

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.24

EN300-7385329_1_2_1



CID: EN300-7385329_1_2_1

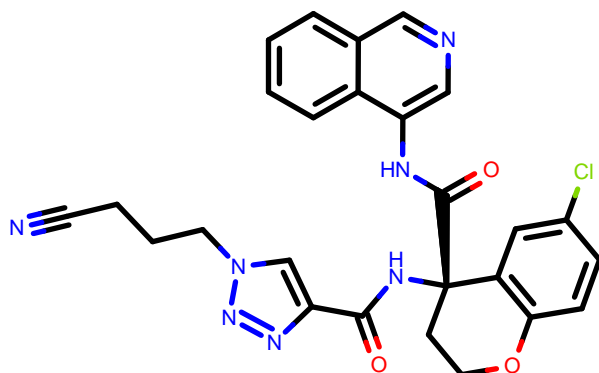
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C6c[nH]cc[n+]6C5

RUN: RUN3573

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.30

EN300-120569_1_1_1



CID: EN300-120569_1_1_1

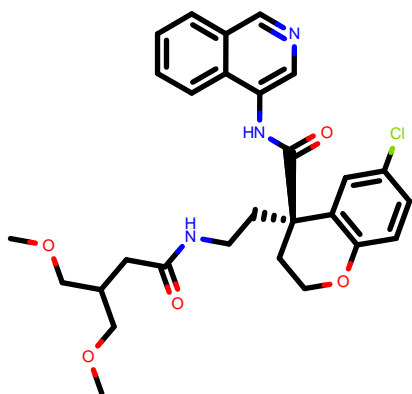
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)CCCC#N

RUN: RUN5834

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.30

EN300-7102031_3_1_1



CID: EN300-7102031_3_1_1

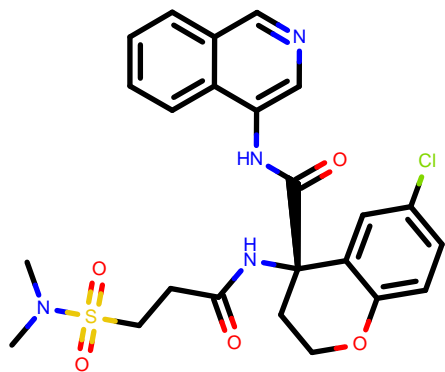
SMILES: COC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4)COC

RUN: RUN6270

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.55

EN300-50631_1_1_1



CID: EN300-50631_1_1_1

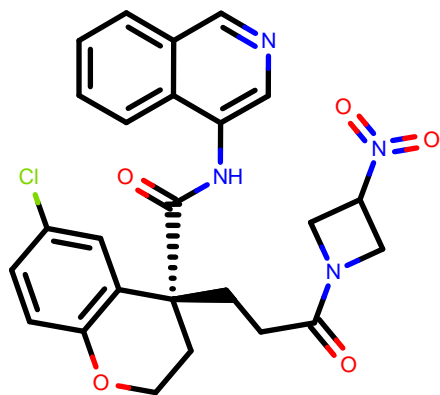
SMILES: CN(C)S(=O)(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN4999

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.32

EN300-7461023_2_1_1



CID: EN300-7461023_2_1_1

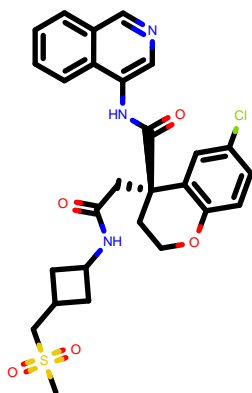
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC(C5)N(=O)=O

RUN: RUN7641

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.26

EN300-7430165_1_1_1



CID: EN300-7430165_1_1_1

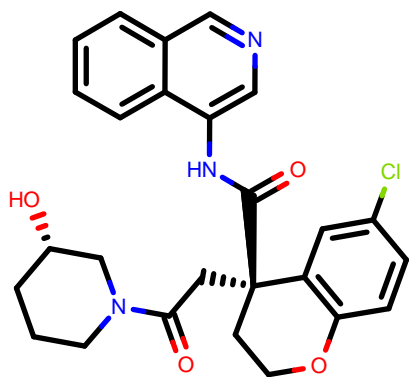
SMILES: CS(=O)(=O)CC1CC(C1)NC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccoc5

RUN: RUN7421

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.32

EN300-20284_1_1_1



CID: EN300-20284_1_1_1

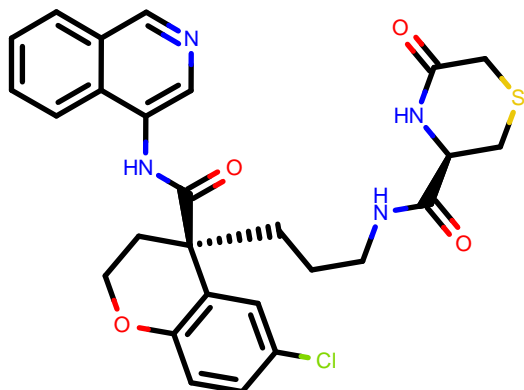
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN4562

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.29

EN300-657320_4_1_1



CID: EN300-657320_4_1_1

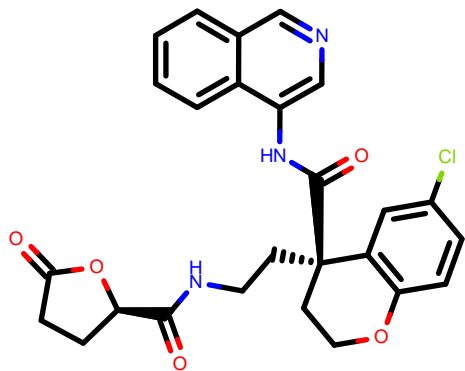
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCN(C(=O)[C@@H]5CSCC(=O)N5)

RUN: RUN6901

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.30

EN300-332606_3_1_1



CID: EN300-332606_3_1_1

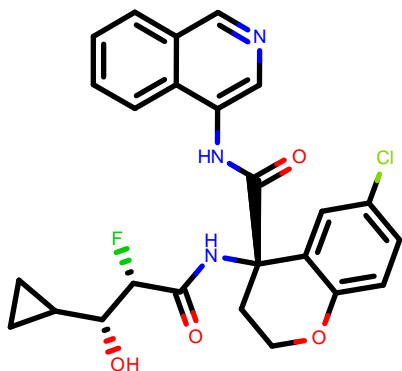
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4C)CCNC(=O)C@H)5CCCC(=O)O5

RUN: RUN5065

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.23

EDG-MED-90036822-78_2



CID: EDG-MED-90036822-78_2

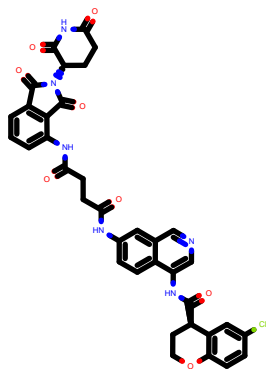
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4C)C)NC(=O)C@H)[C@@H](C5CC5)O[F]

RUN: RUN1673

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.22

DAR-DIA-9e4459de-15_5



CID: DAR-DIA-9e4459de-15_5

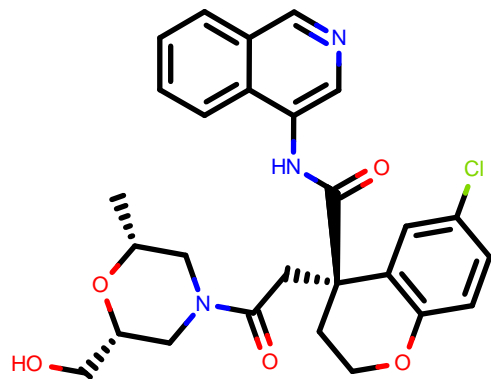
SMILES: c1cc2c(c1)NC(=O)CCCl(=O)Nc3ccc4c(c3)ncoc4NC(=O)C@H)5COC6c8c5cc(c6)C)c7c(c2O)[C@H](7)CCCl(=O)NC7=O)O

RUN: RUN1364

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.28

EN300-157776_1_1_1



CID: EN300-157776_1_1_1

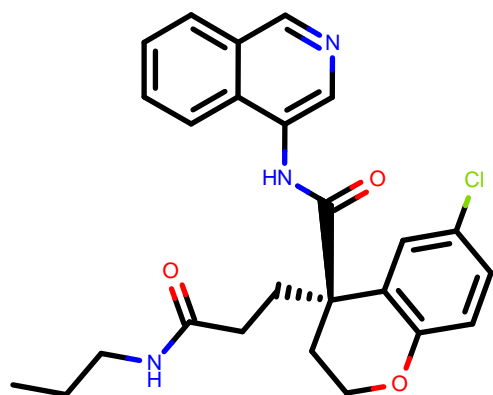
SMILES: C[C@@]H1CN[C@@]H(O1)C(O)C(=O)C[C@@]2(CCOc3c2cc(cc3C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN4101

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.33

JAG-UCB-706446eb-2_1



CID: JAG-UCB-706446eb-2_1

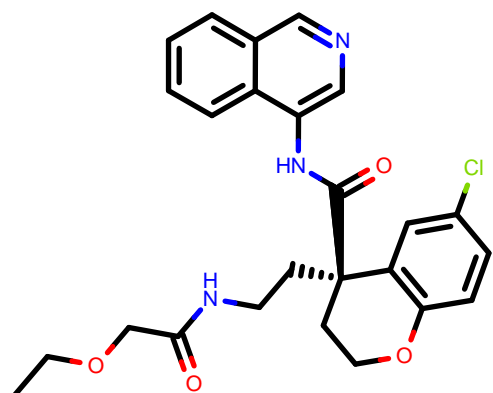
SMILES: CCCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN572

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.20

EN300-21303_3_1_1



CID: EN300-21303_3_1_1

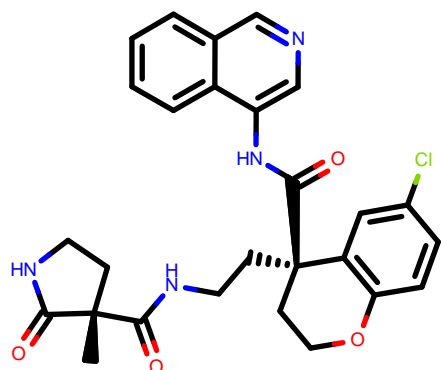
SMILES: CCOCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3691

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.25

EN300-207959_3_1_1



CID: EN300-207959_3_1_1

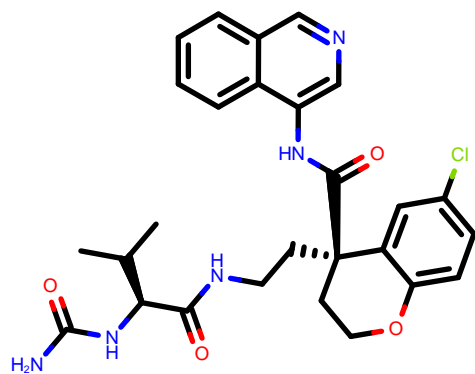
SMILES: C[C@@]1(CCN1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN2968

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.27

EN300-87528_3_1_1



CID: EN300-87528_3_1_1

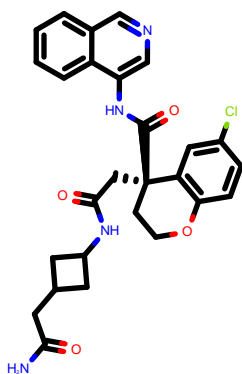
SMILES: CC(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)N

RUN: RUN5401

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.34

EN300-393334_1_1_1



CID: EN300-393334_1_1_1

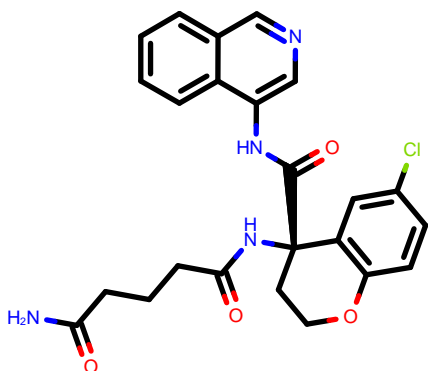
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CC(=O)N

RUN: RUN5474

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.36

EN300-59478_1_1_1



CID: EN300-59478_1_1_1

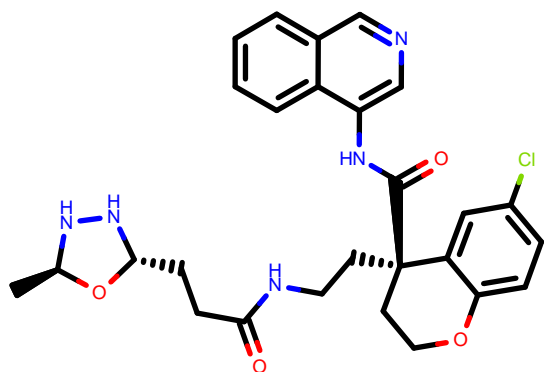
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN4330

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.29

EN300-304662_3_1_2



CID: EN300-304662_3_1_2

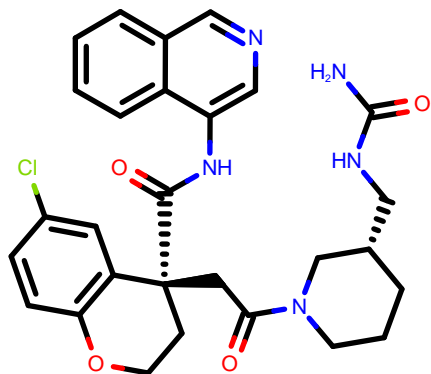
SMILES: C[C@H]1NN[C@@H](O1)CCCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN6972

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.34

EN300-42195_1_2_1



CID: EN300-42195_1_2_1

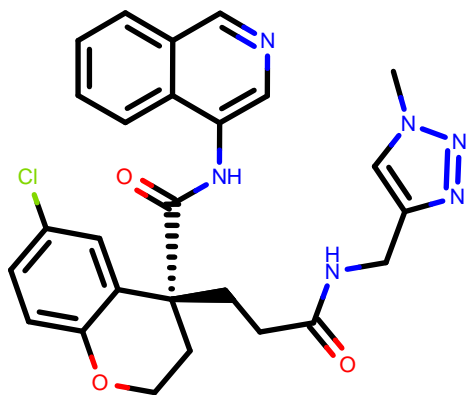
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CNC(=O)N

RUN: RUN6277

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.32

EN300-266023_2_1_1



CID: EN300-266023_2_1_1

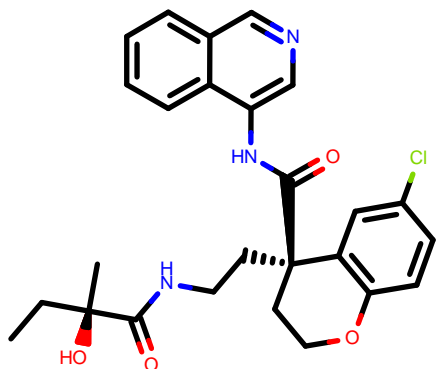
SMILES: Cn1cc(nn1)CNC(=O)CC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7515

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.26

EN300-248888_3_1_1



CID: EN300-248888_3_1_1

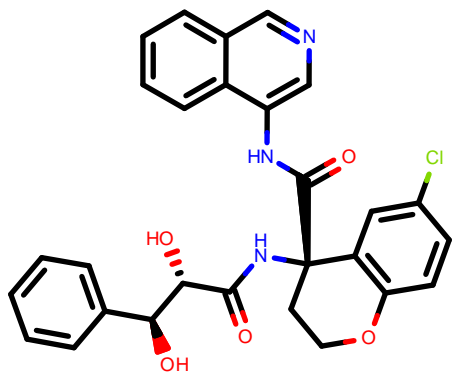
SMILES: C[C@@](C=C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN5887

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.31

EN300-2923949_1_1_1



CID: EN300-2923949_1_1_1

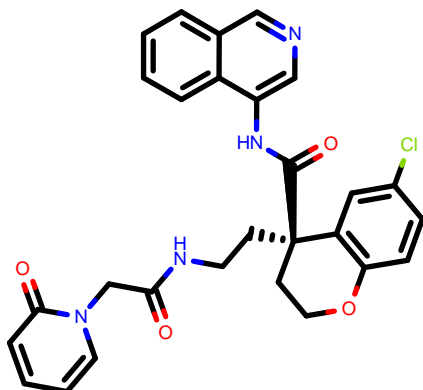
SMILES: c1ccc(cc1)[C@@H]([C@@H](C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O

RUN: RUN3896

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.30

EN300-11714_3_1_1



CID: EN300-11714_3_1_1

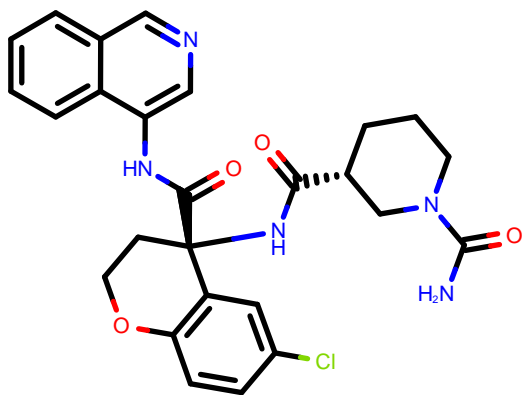
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)Cn5cccc5=O

RUN: RUN5548

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.28

EN300-14767_1_1_1



CID: EN300-14767_1_1_1

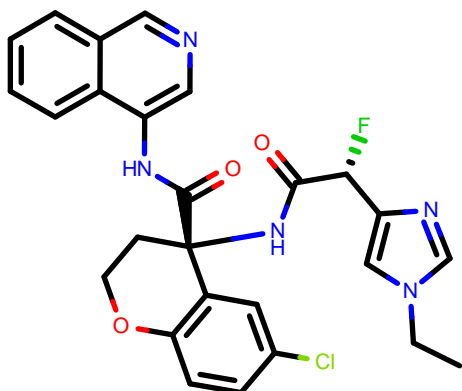
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCN(C5)C(=O)N

RUN: RUN2957

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.29

EDG-MED-90036822-53_2



CID: EDG-MED-90036822-53_2

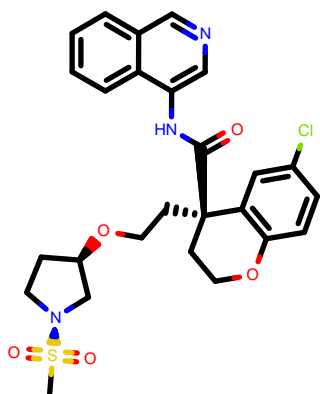
SMILES: CCn1cc(nc1)[C@H](C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5F

RUN: RUN1643

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.24

EN300-301690_3_2_1



CID: EN300-301690_3_2_1

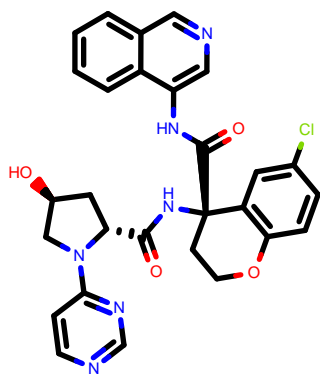
SMILES: CS(=O)(=O)[N@@]1CC[C@H](C1)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN3337

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.28

EN300-310022_1_2_2



CID: EN300-310022_1_2_2

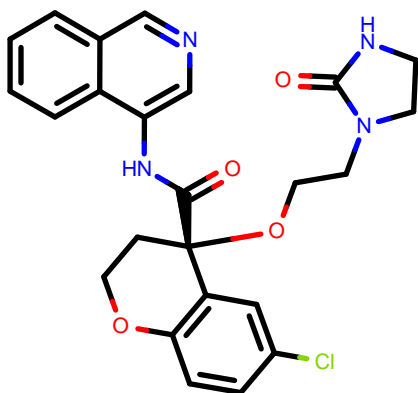
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H](C5)C(=O)O

RUN: RUN3361

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.40

EN300-214800_1_1_1



CID: EN300-214800_1_1_1

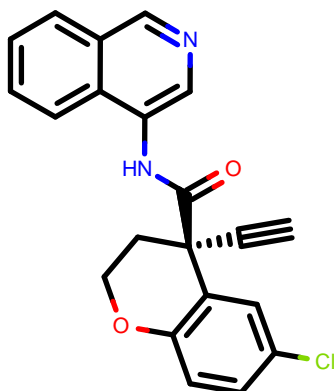
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCNC5=O

RUN: RUN3406

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.23

PET-UNK-29afea89-1_1



CID: PET-UNK-29afea89-1_1

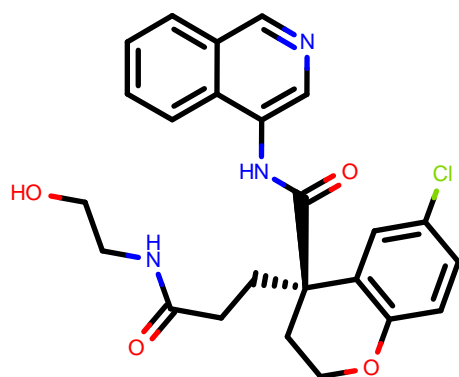
SMILES: C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN583

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.11

EN300-19392_2_1_1



CID: EN300-19392_2_1_1

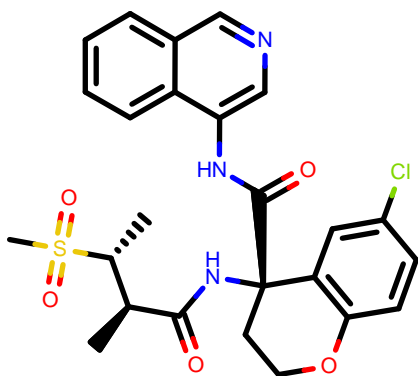
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCO

RUN: RUN6351

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.32

EN300-182725_1_1_1



CID: EN300-182725_1_1_1

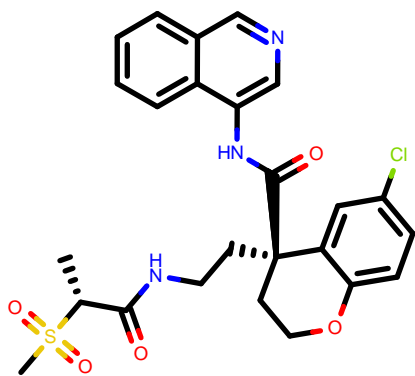
SMILES: CC@@H(Cl)S(=O)(=O)C(=O)N[C@@]3(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6581

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.24

EN300-39405_3_2_1



CID: EN300-39405_3_2_1

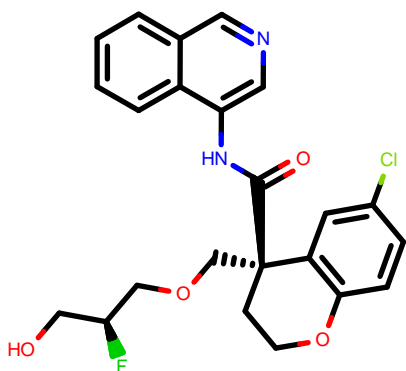
SMILES: C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)S(=O)(=O)C

RUN: RUN3620

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.39

EDJ-MED-fcba3f31-5_1



CID: EDJ-MED-fcba3f31-5_1

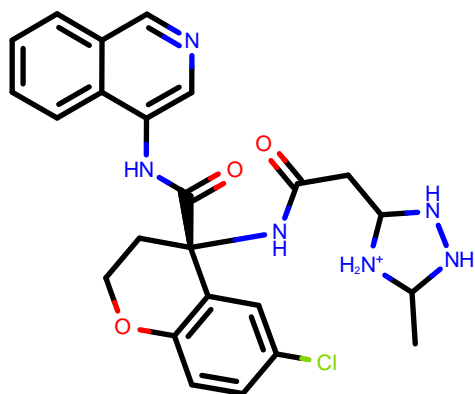
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F

RUN: RUN2402

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.25

EN300-119126_1_1_1



CID: EN300-119126_1_1_1

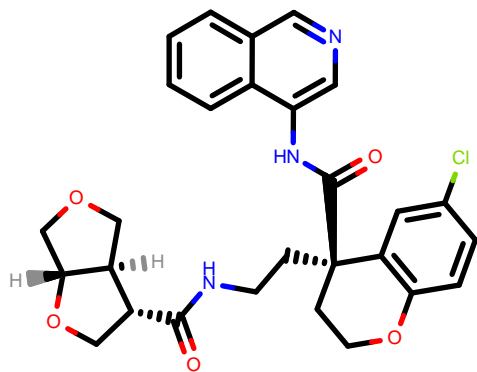
SMILES: Cc1[nH]nc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5276

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.21

EN300-6482296_3_7_1



CID: EN300-6482296_3_7_1

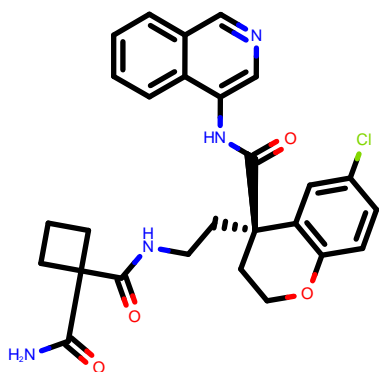
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@H]5COC6

RUN: RUN5845

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.30

EN300-68747_3_1_1



CID: EN300-68747_3_1_1

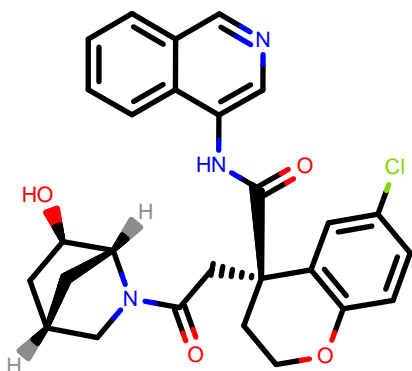
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)C5(CCC5)C(=O)N

RUN: RUN3646

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.35

EN300-2010317_1_1_1



CID: EN300-2010317_1_1_1

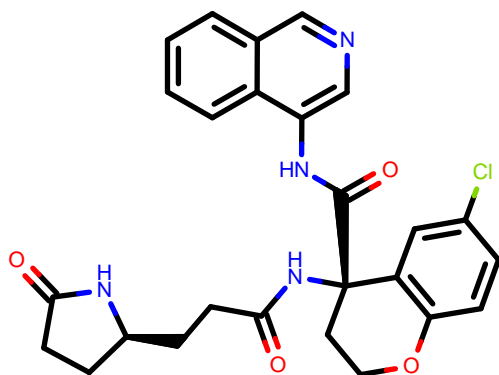
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)C(O)N5C[C@@H]6C[C@@H]5[C@@]3O

RUN: RUN4370

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.26

EN300-104592_1_2_1



CID: EN300-104592_1_2_1

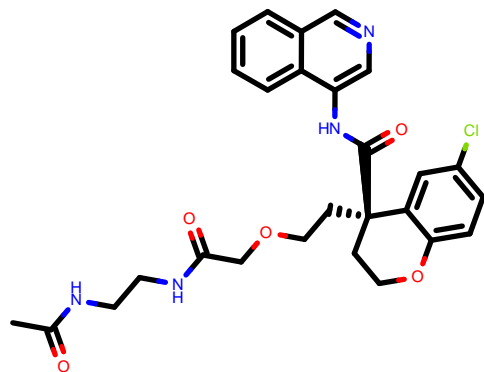
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)CC[C@@H]5CCCC(=O)N5

RUN: RUN6166

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.25

EN300-23129_3_1_1



CID: EN300-23129_3_1_1

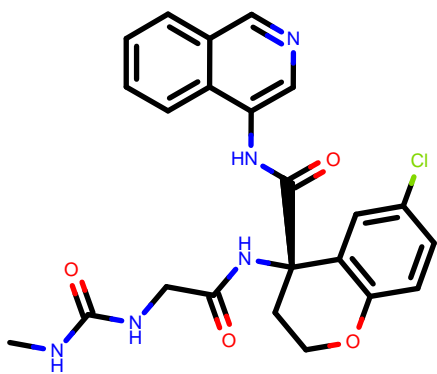
SMILES: CC(=O)NCCNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5680

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.25

EN300-36911_1_1_1



CID: EN300-36911_1_1_1

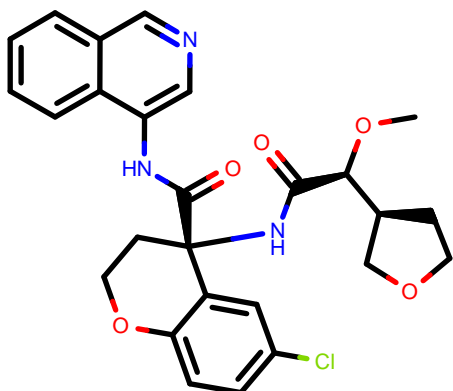
SMILES: CNC(=O)NCC(=O)N[C@]11(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4281

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.20

EN300-298552_1_3_1



CID: EN300-298552_1_3_1

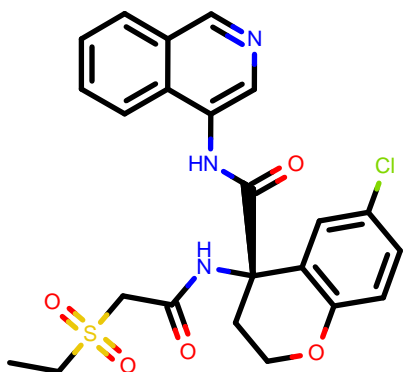
SMILES: CO[C@@H]([C@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3197

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.29

EN300-53395_1_1_1



CID: EN300-53395_1_1_1

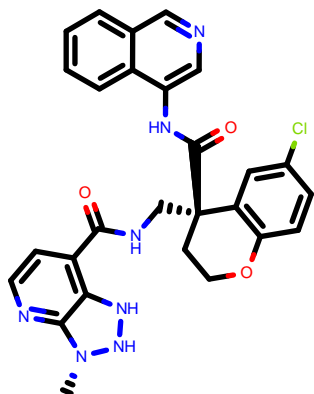
SMILES: CCS(=O)(=O)CC(=O)N[C@]11(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3897

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.23

EN300-202106_2_1_1



CID: EN300-202106_2_1_1

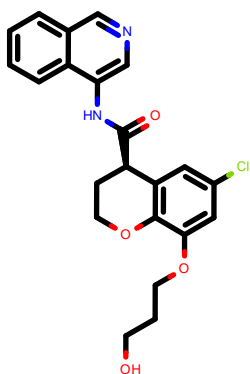
SMILES: Cn1c2c(c(cn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6)n1

RUN: RUN7601

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.27

LAU-MED-88a3970a-3_1



CID: LAU-MED-88a3970a-3_1

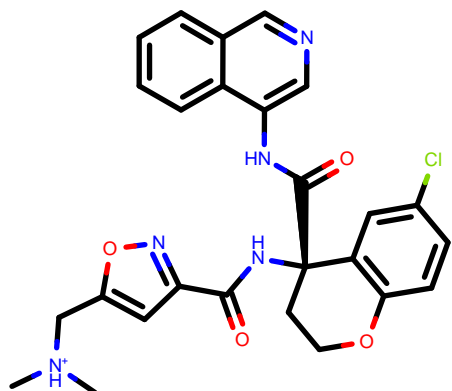
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCCCO)Cl

RUN: RUN1361

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.21

EN300-124457_1_1_1



CID: EN300-124457_1_1_1

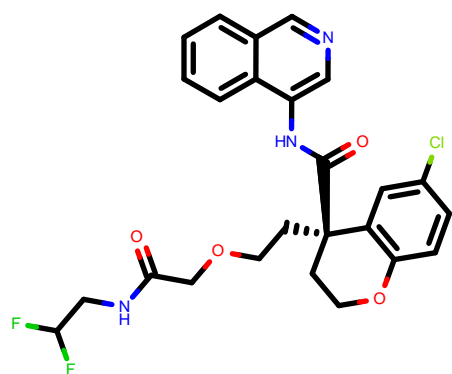
SMILES: C[NH+](C)Cc1cc(nc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6607

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.27

EN300-120586_3_1_1



CID: EN300-120586_3_1_1

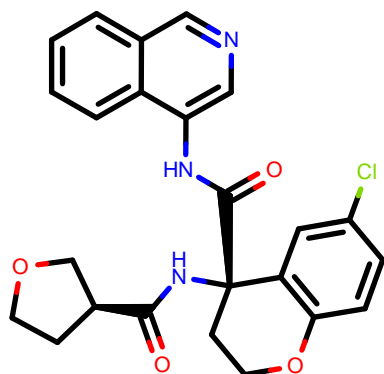
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NCC(F)F

RUN: RUN3565

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.27

EN300-170463_1_1_1



CID: EN300-170463_1_1_1

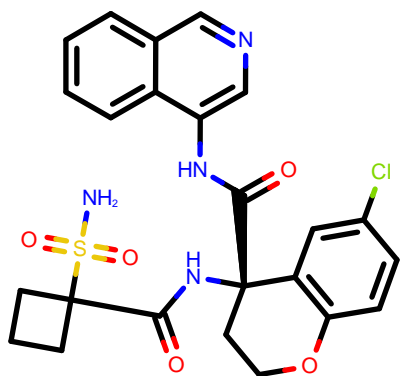
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC5

RUN: RUN2851

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.32

EN300-1440321_1_1_1



CID: EN300-1440321_1_1_1

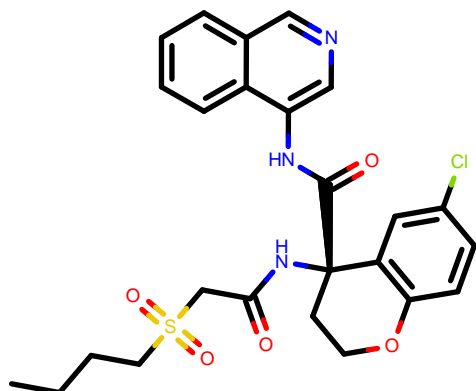
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)S(=O)(=O)N

RUN: RUN4181

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.38

EN300-686903_1_1_1



CID: EN300-686903_1_1_1

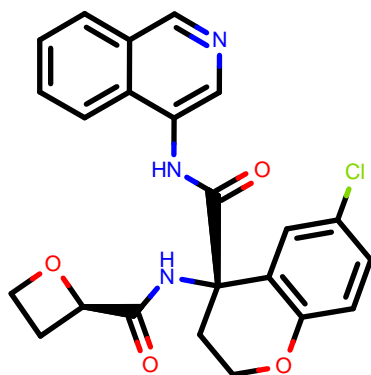
SMILES: CCCCS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN4825

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.34

EN300-85760_1_2_1



CID: EN300-85760_1_2_1

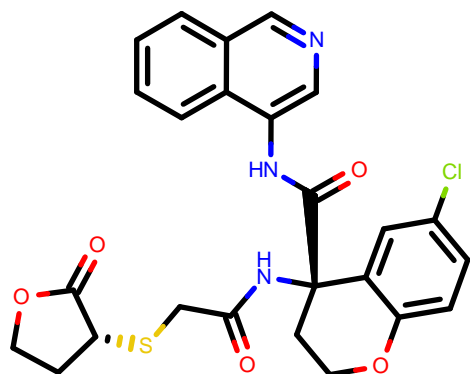
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC5

RUN: RUN4189

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.21

EN300-113218_1_1_1



CID: EN300-113218_1_1_1

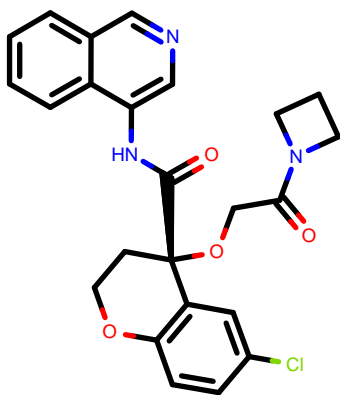
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@@H]5CCOC5=O

RUN: RUN5023

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.28

EN300-11195_1_1_1



CID: EN300-11195_1_1_1

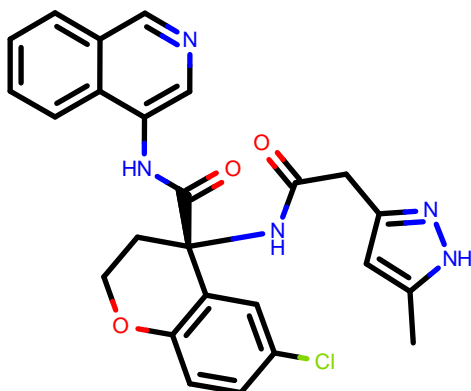
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC5

RUN: RUN3752

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.21

EN300-105110_1_1_1



CID: EN300-105110_1_1_1

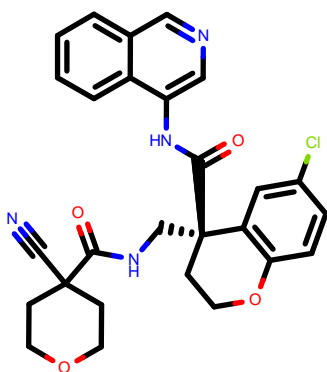
SMILES: Cc1cc(n[nH]1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6202

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.23

EN300-74089_2_1_1



CID: EN300-74089_2_1_1

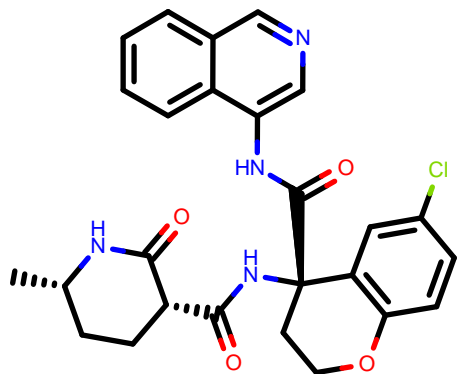
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCOCC5)C#N

RUN: RUN4478

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.32

EN300-6505003_1_4_1



CID: EN300-6505003_1_4_1

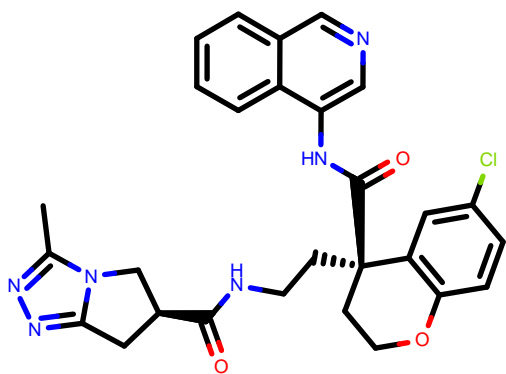
SMILES: C[C@H]1CC[C@H](C(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4640

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.29

EN300-6729747_3_2_1



CID: EN300-6729747_3_2_1

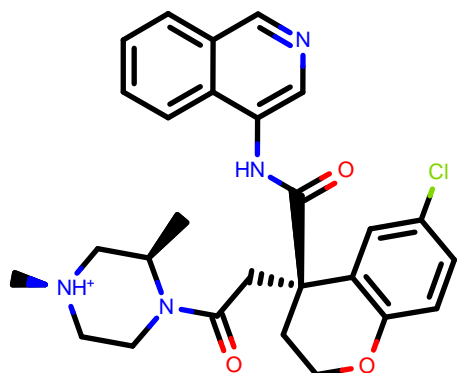
SMILES: Cc1nc2n1C[C@H](C2)C(=O)NCC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4719

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.35

EDG-MED-ba1ac7b9-15_5



CID: EDG-MED-ba1ac7b9-15_5

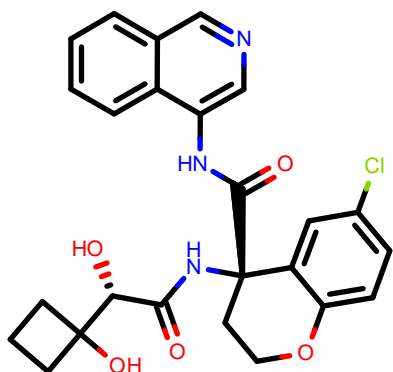
SMILES: C[C@@H]1C[N@@H+](CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C

RUN: RUN2520

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.36

EN300-1073320_1_2_1



CID: EN300-1073320_1_2_1

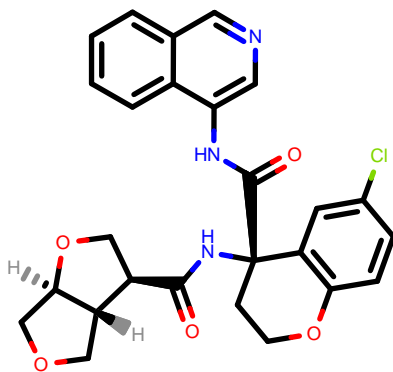
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5(CCC5)O)O

RUN: RUN5890

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.30

EN300-6482296_1_7_1



CID: EN300-6482296_1_7_1

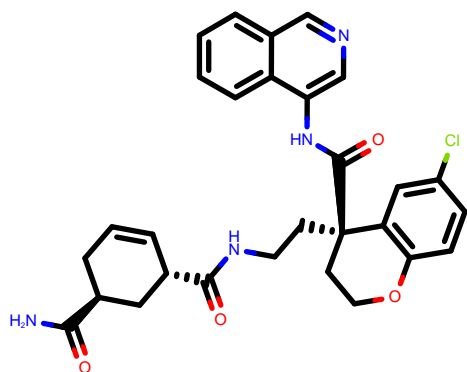
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5COC[C@H]5)CO

RUN: RUN3985

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.27

EN300-90142_3_2_1



CID: EN300-90142_3_2_1

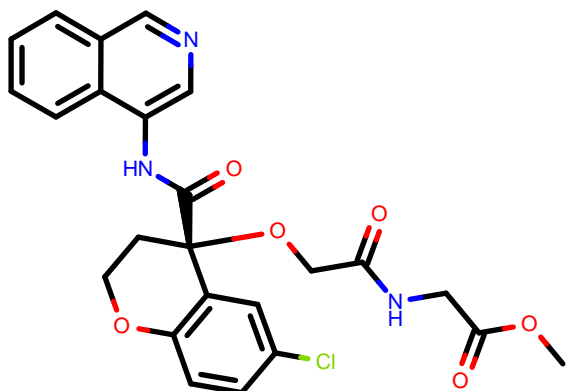
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)CCOC4c3cc(cc4)CNC(=O)[C@@H](C)CCOC5C(=O)N

RUN: RUN5571

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.34

EN300-04409_1_1_1



CID: EN300-04409_1_1_1

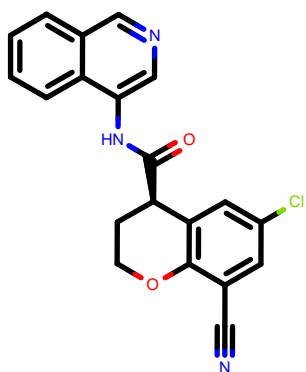
SMILES: COC(=O)CNC(=O)CO[C@@H](C)CCOC2c1cc(cc2)C(=O)Nc3ncc4c3cccc4

RUN: RUN5211

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.23

RAL-THA-05e671eb-20_1



CID: RAL-THA-05e671eb-20_1

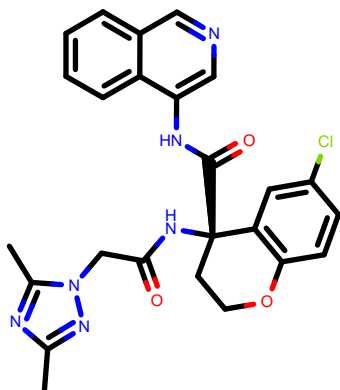
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)CCOC4c3cc(cc4C#N)Cl

RUN: RUN1893

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.09

EN300-7423123_1_1_1



CID: EN300-7423123_1_1_1

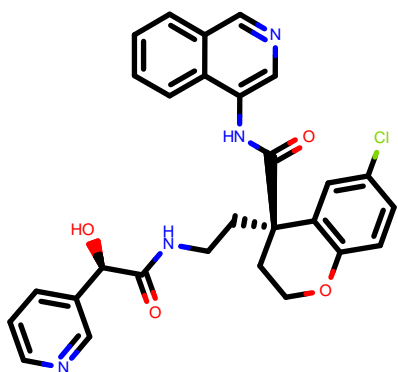
SMILES: Cc1nc(n1)CC(=O)N[C@@H](C)CCOC3c2cc(cc3)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN4587

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.31

EN300-134855_3_1_1



CID: EN300-134855_3_1_1

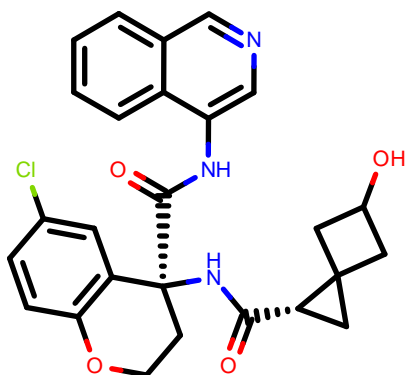
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5HJ(c5ccoc5)O

RUN: RUN5799

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.32

EN300-1717166_1_2_1



CID: EN300-1717166_1_2_1

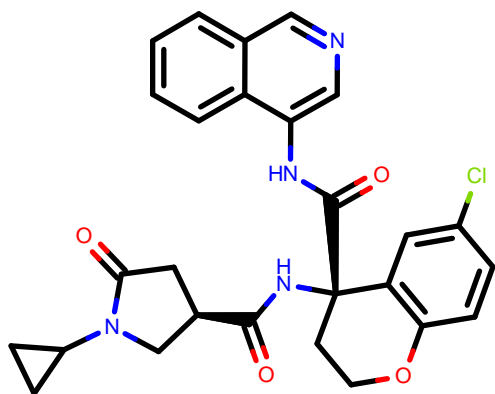
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5HJ5CC56CC(C6)O

RUN: RUN3910

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-12440_1_1_1



CID: EN300-12440_1_1_1

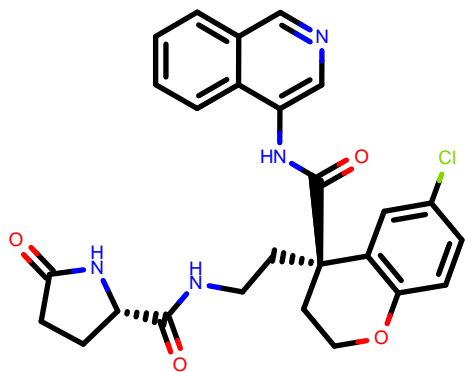
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5HJ5CC(=O)N(C5)C6CC6

RUN: RUN7189

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.25

EN300-19515_3_1_1



CID: EN300-19515_3_1_1

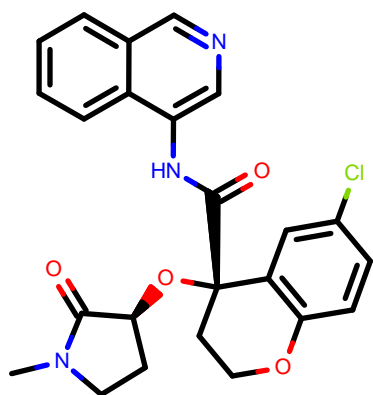
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5HJ5CCCC(=O)N5

RUN: RUN3801

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-98648_1_1_1



CID: EN300-98648_1_1_1

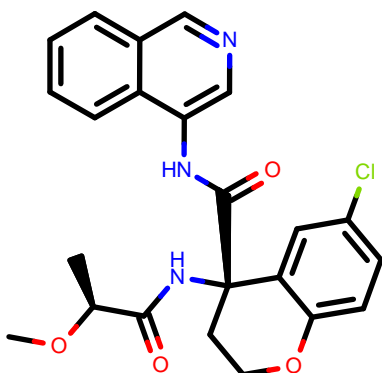
SMILES: CN1CC[C@@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN4162

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.17

EN300-51257_1_1_1



CID: EN300-51257_1_1_1

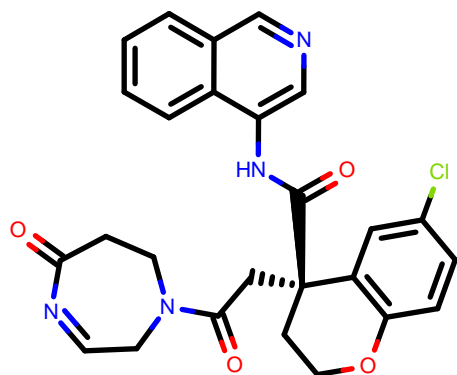
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN4525

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.23

EN300-69107_1_1_1



CID: EN300-69107_1_1_1

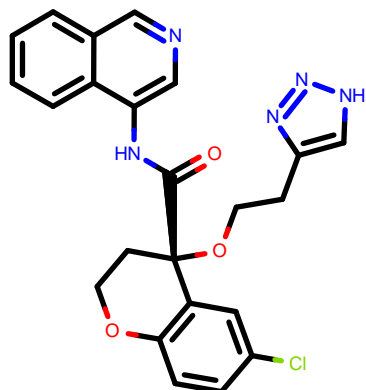
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(=O)NCC5

RUN: RUN3084

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.30

EN300-222357_1_1_1



CID: EN300-222357_1_1_1

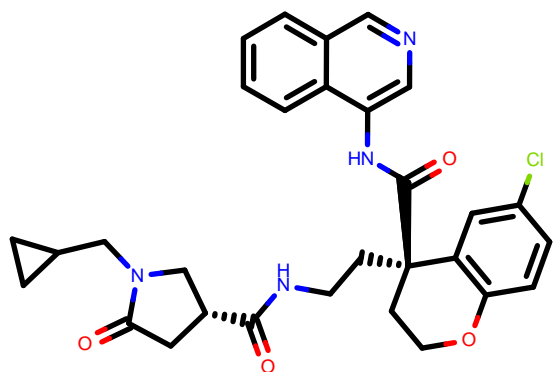
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cn[nH]n5

RUN: RUN4660

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.22

EN300-31969_3_1_1



CID: EN300-31969_3_1_1

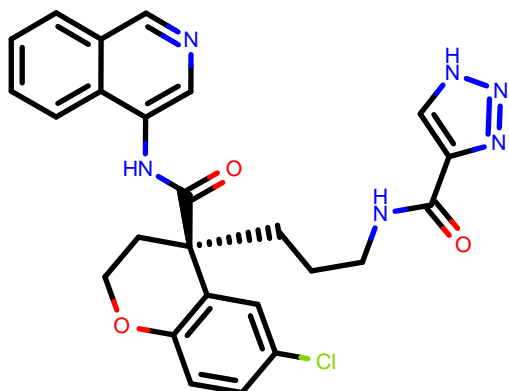
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)O)CCNC(=O)N[C@@H]5COC5

RUN: RUN5074

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.32

EN300-31998_4_1_1



CID: EN300-31998_4_1_1

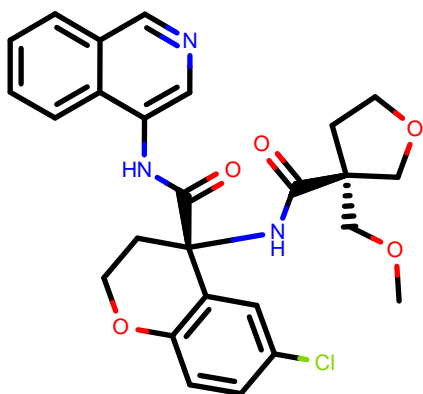
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)O)CCNC(=O)c5cn[nH]n5

RUN: RUN5082

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.29

EN300-248883_1_1_1



CID: EN300-248883_1_1_1

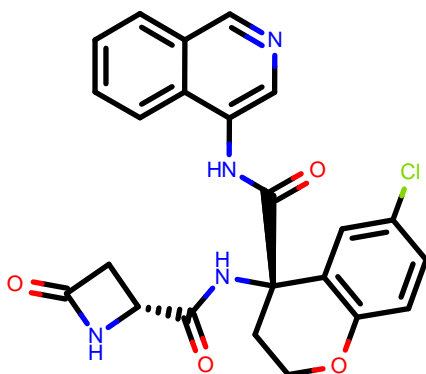
SMILES: COC[C@@1](CCOC1)C(=O)N[C@@2](CCOC3C2CC(C3)O)N[C@@H]4COC5C4COC5

RUN: RUN3150

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.25

EN300-101505_1_2_1



CID: EN300-101505_1_2_1

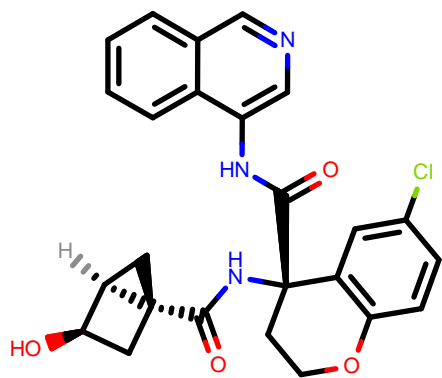
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)O)C(=O)N[C@@H]5C(=O)N5

RUN: RUN5493

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.21

EN300-7433125_1_1_1



CID: EN300-7433125_1_1_1

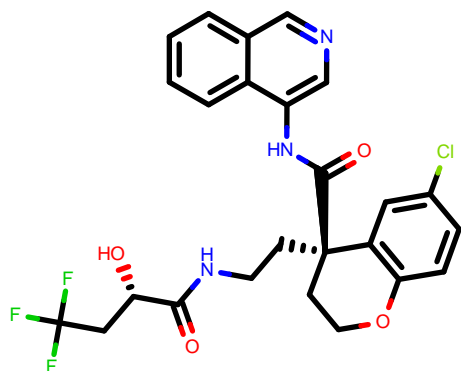
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4ccc(cc4)Cl)N(C)C(=O)C[C@@H]5C[C@@H]5O

RUN: RUN4907

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.23

EN300-1932013_3_2_1



CID: EN300-1932013_3_2_1

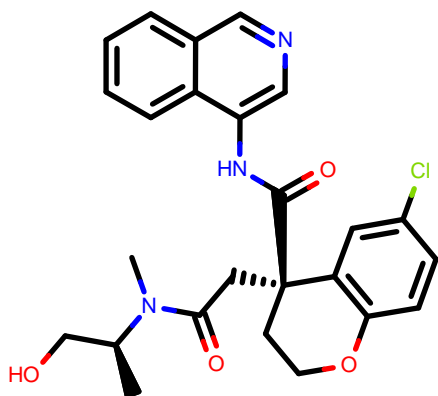
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4ccc(cc4)Cl)CCNC(=O)C[C@@H](C(F)(F)F)O

RUN: RUN3939

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.42

EN300-204419_1_1_1



CID: EN300-204419_1_1_1

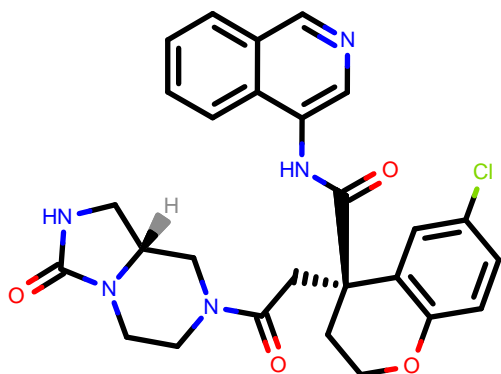
SMILES: C[C@@H](CO)N(C)C(=O)C[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4304

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.33

EN300-100765_1_1_1



CID: EN300-100765_1_1_1

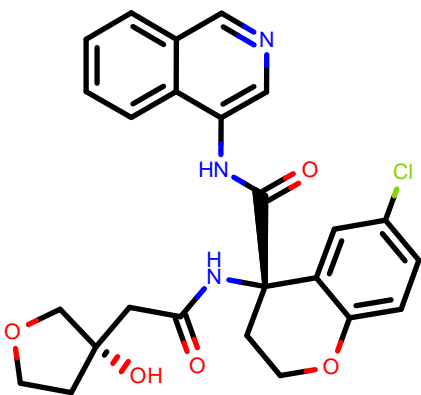
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4ccc(cc4)Cl)CC(=O)N5CCN6[C@@H](C5)CN6=O

RUN: RUN6057

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.28

EN300-360157_1_2_1



CID: EN300-360157_1_2_1

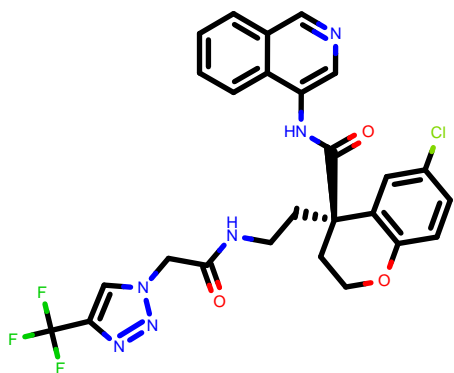
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@]5(C)COC5O

RUN: RUN3702

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.26

EN300-2910941_3_1_1



CID: EN300-2910941_3_1_1

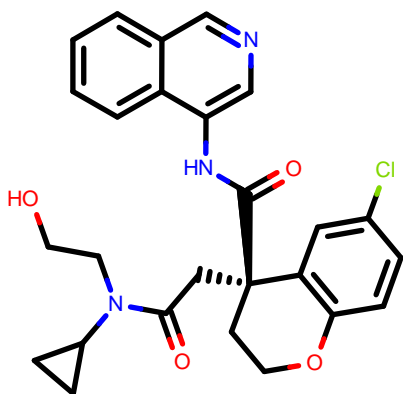
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)Cn5ccn(n5)C(F)(F)F

RUN: RUN4544

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EDG-MED-ba1ac7b9-3_1



CID: EDG-MED-ba1ac7b9-3_1

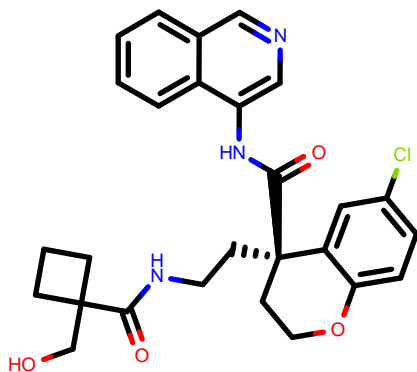
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(CCO)C5CC5

RUN: RUN2472

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.29

EN300-149975_3_1_1



CID: EN300-149975_3_1_1

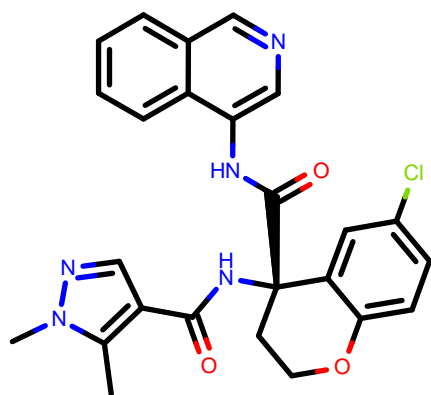
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(C)C5C5O

RUN: RUN2933

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.37

EN300-25866_1_1_1



CID: EN300-25866_1_1_1

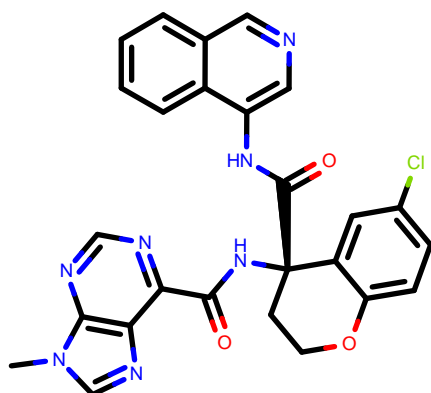
SMILES: Cc1c(cnn1C)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4706

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-7434334_1_1_1



CID: EN300-7434334_1_1_1

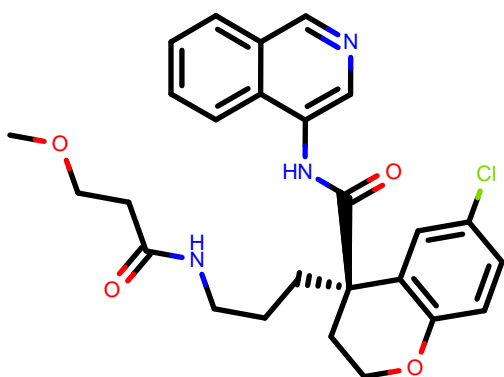
SMILES: C[n+][c][nH]c2c1nnc2C(=O)N[C@]3(CCOC4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6

RUN: RUN4898

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.31

EN300-64536_4_1_1



CID: EN300-64536_4_1_1

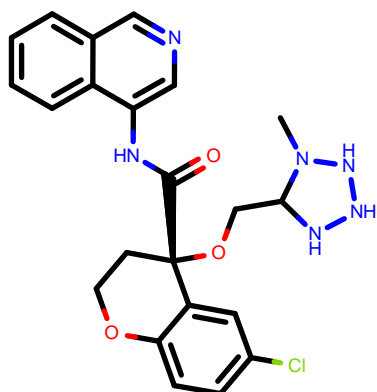
SMILES: COCCOC(=O)NCCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4911

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.36

EN300-62574_1_1_1



CID: EN300-62574_1_1_1

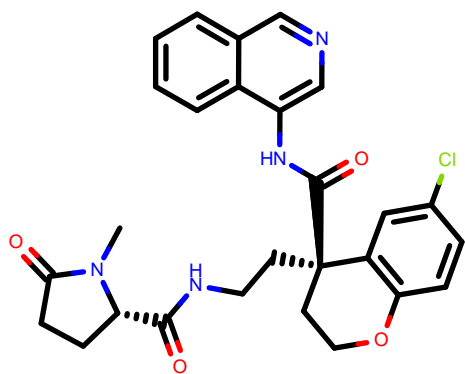
SMILES: Cn1c(nnn1)CO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6689

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.24

EN300-130825_3_1_1



CID: EN300-130825_3_1_1

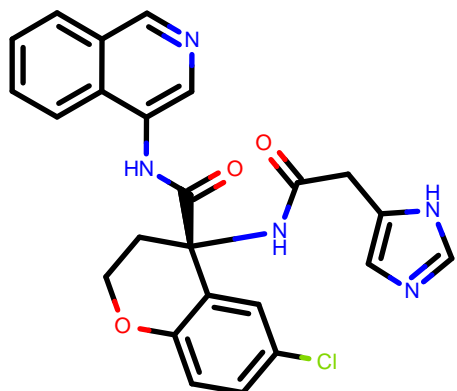
SMILES: CN1[C@@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5429

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.35

EDG-MED-90036822-50_1



CID: EDG-MED-90036822-50_1

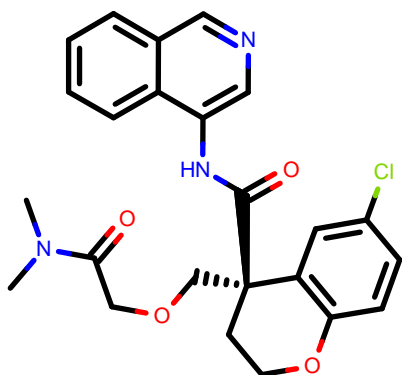
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnc[nH]5

RUN: RUN1600

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.26

EN300-216063_2_1_1



CID: EN300-216063_2_1_1

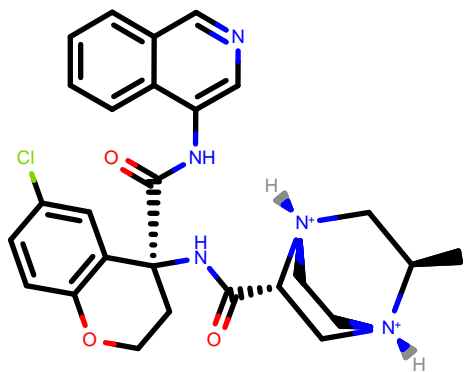
SMILES: CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4890

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.21

EN300-120414_1_1_1



CID: EN300-120414_1_1_1

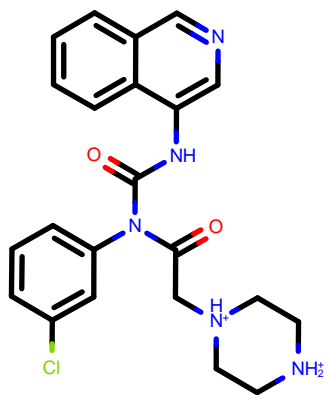
SMILES: ClC1=CN=C2C=CN=C12[C@@H]3C[C@@H]2C1=O)NCC[C@]4(CCOc5c4cc(cc5)Cl)C(=O)Nc6ccc7c6cccc7

RUN: RUN7757

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.34

VLA-UCB-34f3ed0c-7_1



CID: VLA-UCB-34f3ed0c-7_1

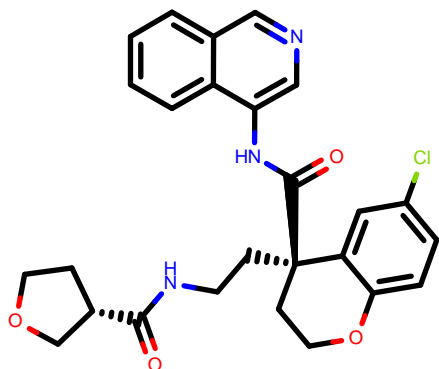
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3ccccc(c3)Cl)C(=O)CN4CC[NH2+]CC4

RUN: RUN616

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.40

EN300-53423_3_2_1



CID: EN300-53423_3_2_1

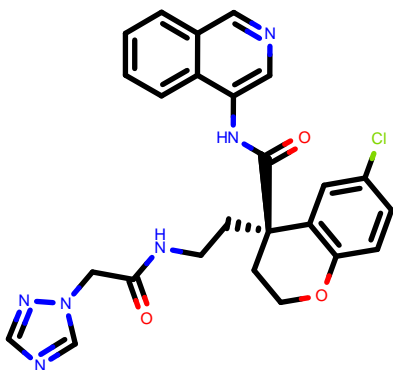
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5

RUN: RUN5779

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.30

EN300-06654_3_1_1



CID: EN300-06654_3_1_1

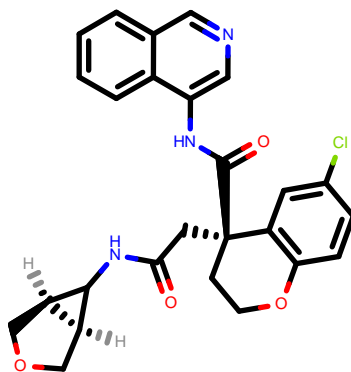
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnfn5

RUN: RUN3390

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.28

EN300-192482_1_1_1



CID: EN300-192482_1_1_1

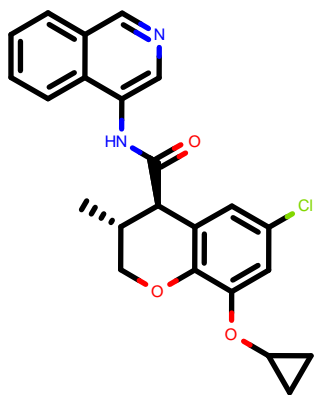
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5[C@H]6[C@@H]5COC6

RUN: RUN6086

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.29

DAR-DIA-0d514e7d-6_1



CID: DAR-DIA-0d514e7d-6_1

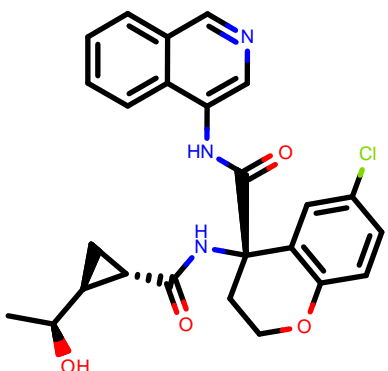
SMILES: C[C@H]1COc2c(cc2OC3CC3)C1[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN782

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.17

EN300-6729572_1_3_1



CID: EN300-6729572_1_3_1

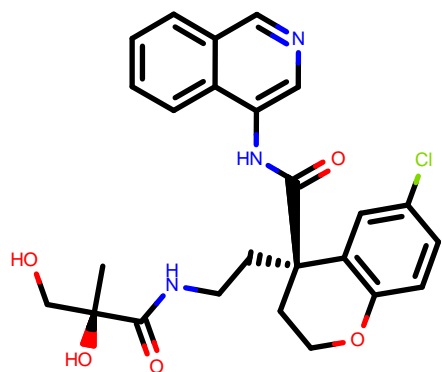
SMILES: C[C@@H]([C@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN3940

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.21

EN300-89418_3_1_1



CID: EN300-89418_3_1_1

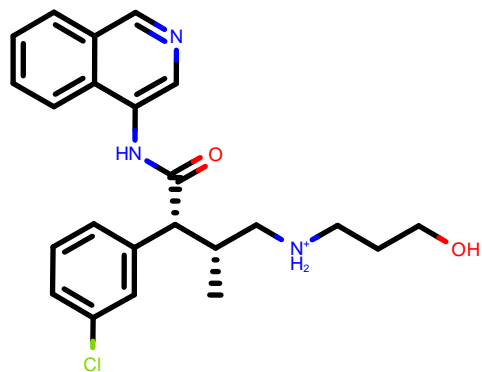
SMILES: C[C@@]([CO])C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN6624

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.46

MAK-UNK-c749d764-6_3



CID: MAK-UNK-c749d764-6_3

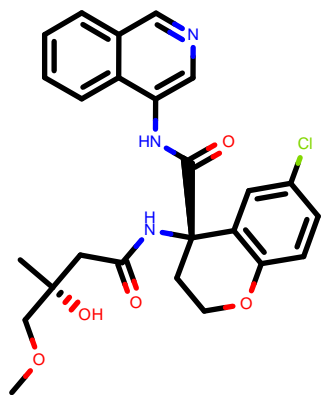
SMILES: C[C@@H]([C(NH2+)CCCO])[C@H]([c1cccc(c1)C]C(=O)Nc2cncc3c2cccc3

RUN: RUN863

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.48

EN300-1296824_1_1_1



CID: EN300-1296824_1_1_1

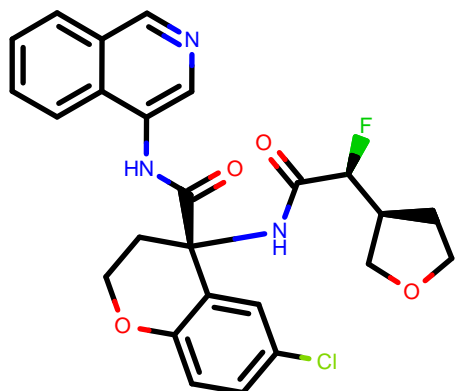
SMILES: C[C@@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)(COC)O

RUN: RUN4498

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.34

EN300-783124_1_4_1



CID: EN300-783124_1_4_1

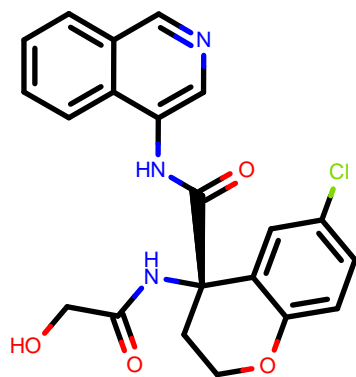
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C)[H]5CCOC5F

RUN: RUN3878

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.22

EN300-19242_1_1_1



CID: EN300-19242_1_1_1

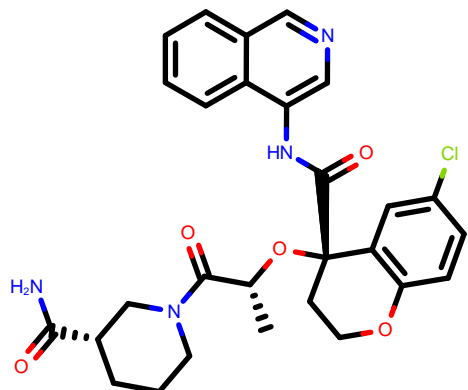
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO

RUN: RUN4963

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.17

EN300-28177_1_2_1



CID: EN300-28177_1_2_1

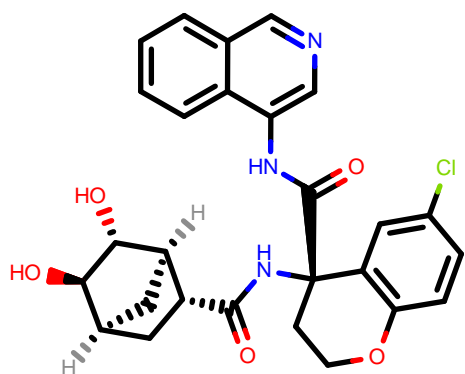
SMILES: C[C@H](C(=O)N1CCCC1C@H)C1(C)C(O)N(C)C2(CCOc3c2cc(cc3)Cl)C1=O)Nc4ccc5c4ccc5

RUN: RUN7194

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.20

EN300-6744028_1_3_1



CID: EN300-6744028_1_3_1

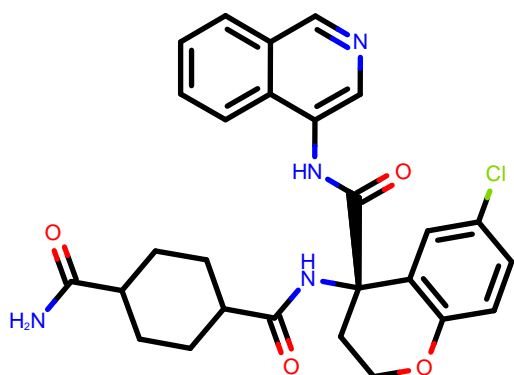
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(NC(=O)C5=CC=C(C=C5)C=C6C=CC(=O)N6)C

RUN: RUN3179

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.28

EN300-35778_1_1_1



CID: EN300-35778_1_1_1

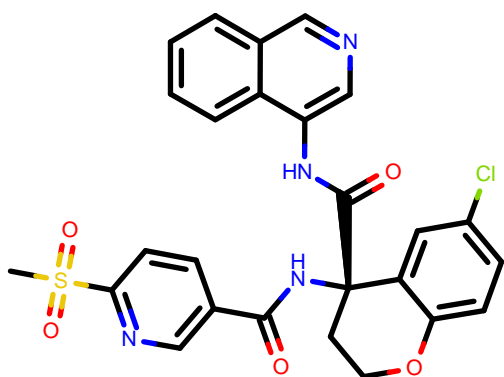
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(NC(=O)C5=CC=C(C=C5)C=C6C=CC(=O)N6)C

RUN: RUN4054

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.26

EN300-206769_1_1_1



CID: EN300-206769_1_1_1

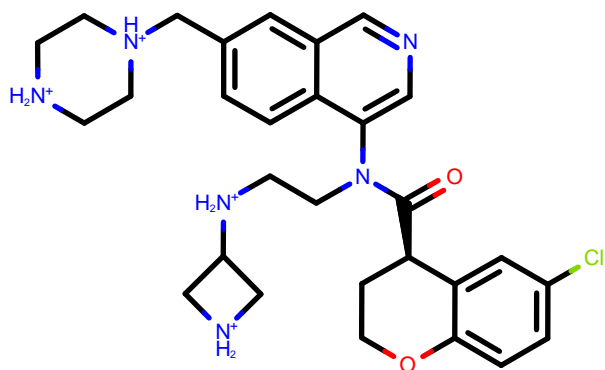
SMILES: CS(=O)(=O)c1ccc(nc1)C(=O)N[C@@]2(C)CCOc3cc2cc(c3)C(NC(=O)C4=CC=CC=C4)C

RUN: RUN5150

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.28

MAK-UNK-83e0a0b4-2_1_1



CID: MAK-UNK-83e0a0b4-2_1_1

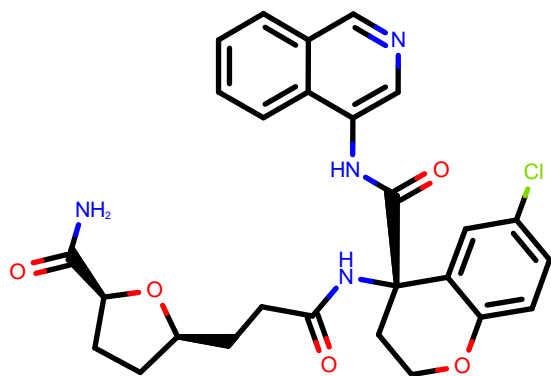
SMILES: c1cc2cc(c1CN3CC[NH2+]JC3)ncnc2N(CCN4C[NH2+]C4)C(=O)[C@@]3(C)CCOc4cc3cc(c4)C

RUN: RUN4936

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.33

EN300-364992_1_1_1



CID: EN300-364992_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOc4ccc(cc4)C)N(C(=O)CC)C@H5CC[C@@H](O5)Cl

RUN:

RUN3718

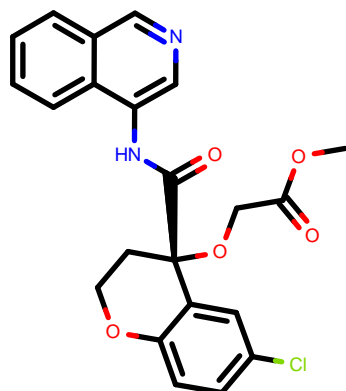
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.36

EN300-19700_1_1_1



CID: EN300-19700_1_1_1

SMILES:

COC(=O)CO[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN:

RUN4435

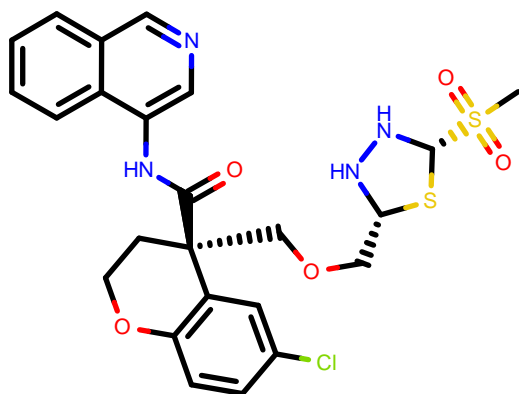
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.16

EN300-160080_2_1_4



CID: EN300-160080_2_1_4

SMILES:

CS(=O)(=O)[C@@H]1N[C@@H]2[C@@H](S1)COC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN:

RUN7172

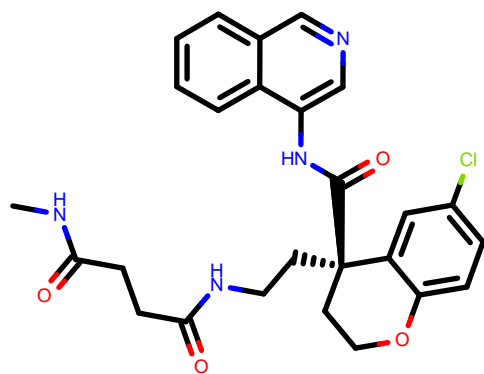
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.45

EN300-1081277_3_1_1



CID: EN300-1081277_3_1_1

SMILES:

CNC(=O)CCC(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN:

RUN7747

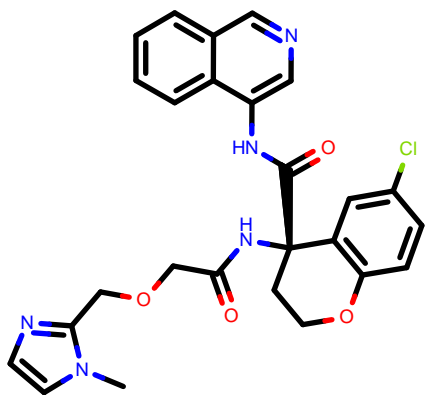
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.30

EN300-212341_1_1_1



CID: EN300-212341_1_1_1

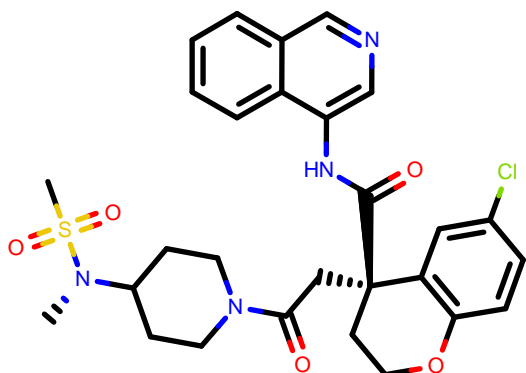
SMILES: Cn1ccnc1COCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7343

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.27

ALP-UNI-3496895b-9_1



CID: ALP-UNI-3496895b-9_1

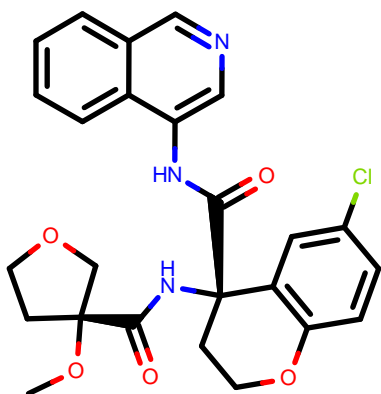
SMILES: CN@]1C1CCN(CC1)C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5S(=O)(=O)C

RUN: RUN2398

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.30

EN300-174668_1_1_1



CID: EN300-174668_1_1_1

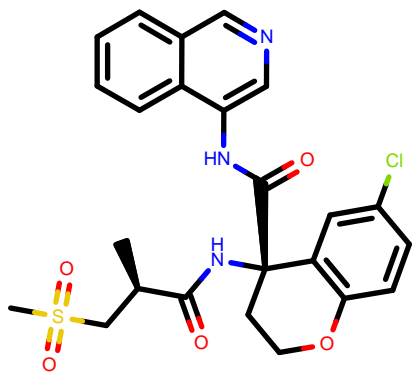
SMILES: CO[C@@]1(CCOC1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3025

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.29

EN300-97699_1_2_1



CID: EN300-97699_1_2_1

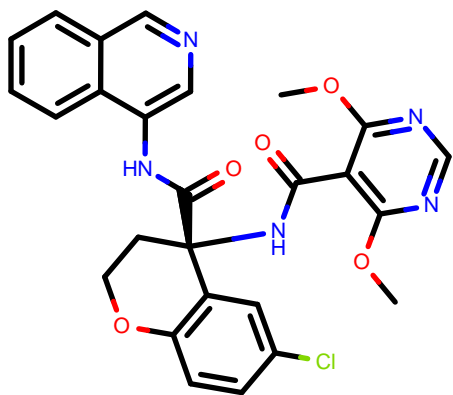
SMILES: C[C@H](CS(=O)(=O)C)C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6135

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.49

EN300-70431_1_1_1



CID: EN300-70431_1_1_1

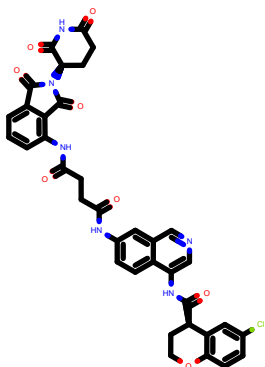
SMILES: COc1c(c(nen1)OC)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccoc5

RUN: RUN3160

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.25

DAR-DIA-9e4459de-15_2



CID: DAR-DIA-9e4459de-15_2

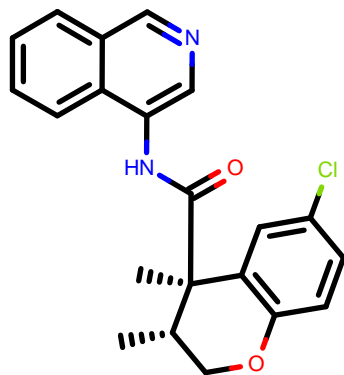
SMILES: c1cc2c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)nc4NC(=O)C[C@@]5(CCOc6c5cc(c6)C)C(=O)Nc7cnc8c7ccoc8

RUN: RUN1385

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.32

DAR-DIA-0d514e7d-28_1



CID: DAR-DIA-0d514e7d-28_1

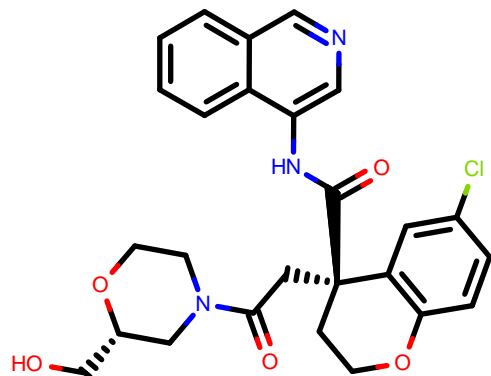
SMILES: C[C@H]1COc2ccc(cc2[C@@]1(C)C)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN724

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.09

EN300-101373_1_2_1



CID: EN300-101373_1_2_1

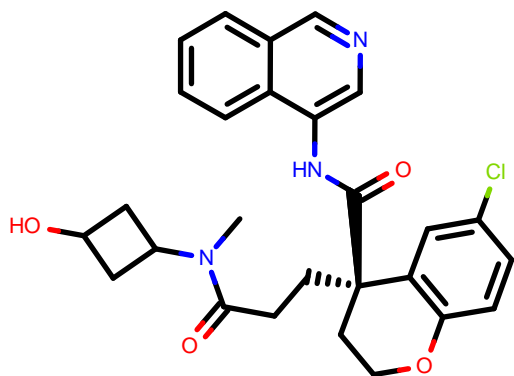
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@@H](C5)CO

RUN: RUN3860

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.41

EN300-97697_2_1_1



CID: EN300-97697_2_1_1

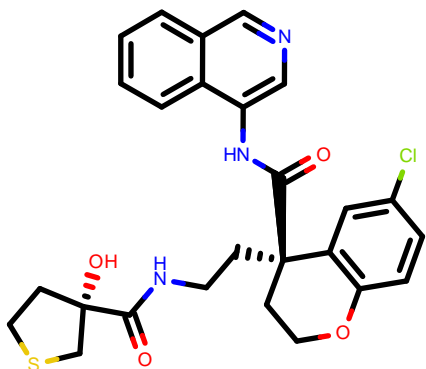
SMILES: CN(C1CC(C1)O)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6919

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.24

EN300-122656_3_1_1



CID: EN300-122656_3_1_1

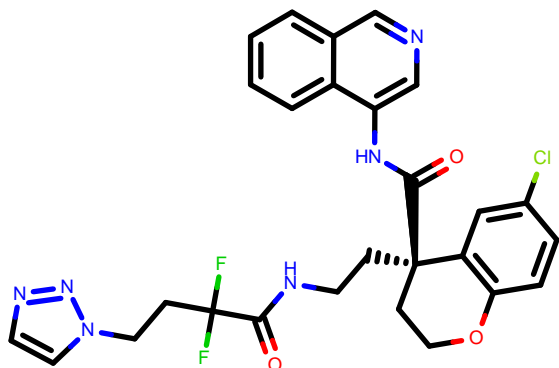
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCSC5)O

RUN: RUN6354

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.36

EN300-6474220_3_1_1



CID: EN300-6474220_3_1_1

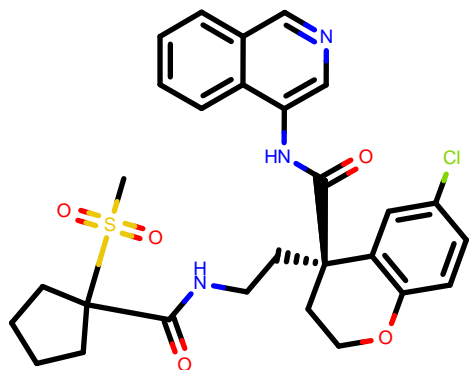
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(Cc5cnnc5)F

RUN: RUN5385

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.47

EN300-60831_3_1_1



CID: EN300-60831_3_1_1

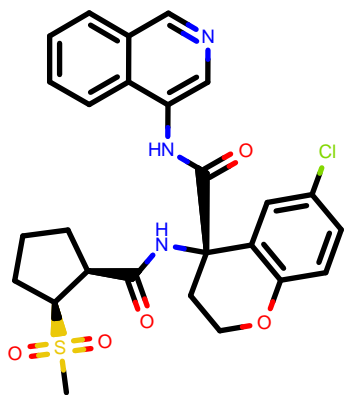
SMILES: CS(=O)(=O)C1(CCCC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3994

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.58

EN300-1387145_1_4_1



CID: EN300-1387145_1_4_1

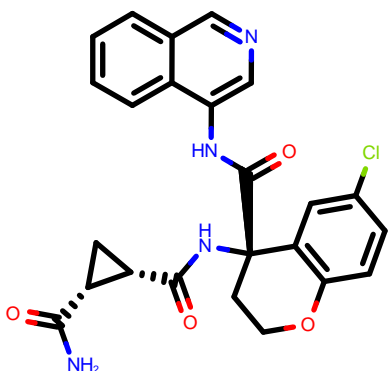
SMILES: CS(=O)(=O)[C@H]1CCC[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5390

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.34

EN300-331941_1_1_1



CID: EN300-331941_1_1_1

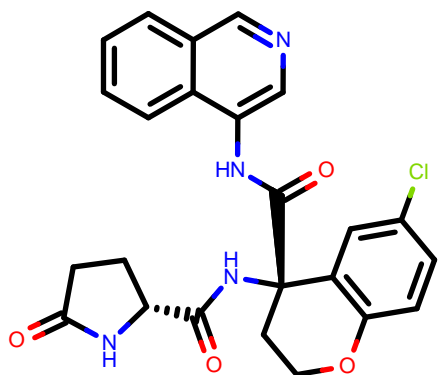
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5C(=O)N

RUN: RUN4393

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.27

EN300-54541_1_1_1



CID: EN300-54541_1_1_1

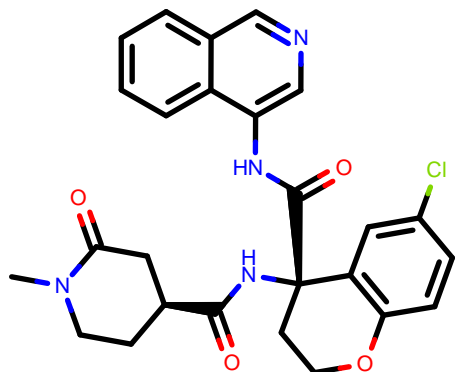
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCNC(=O)N5

RUN: RUN3867

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.20

EN300-30458_1_1_1



CID: EN300-30458_1_1_1

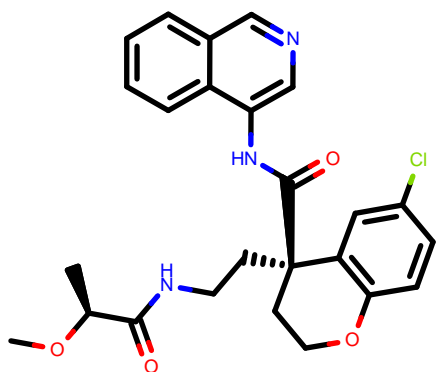
SMILES: CN1CC[C@@]@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5117

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.25

EN300-258477_3_1_1



CID: EN300-258477_3_1_1

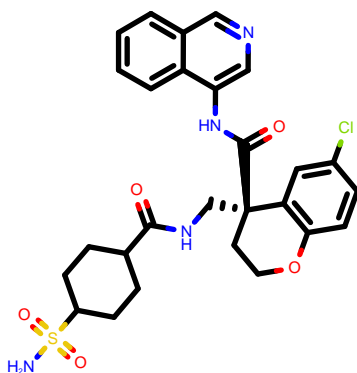
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)OC

RUN: RUN3180

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.29

EN300-83864_2_1_1



CID: EN300-83864_2_1_1

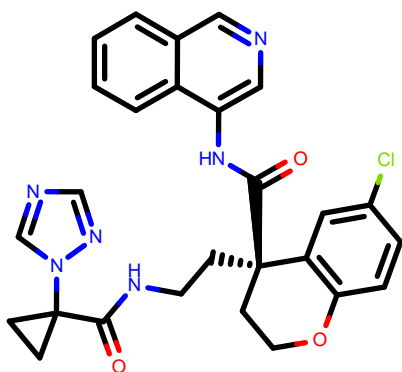
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5CCCC(C5)S(=O)(=O)N

RUN: RUN5301

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.38

EN300-246440_3_1_1



CID: EN300-246440_3_1_1

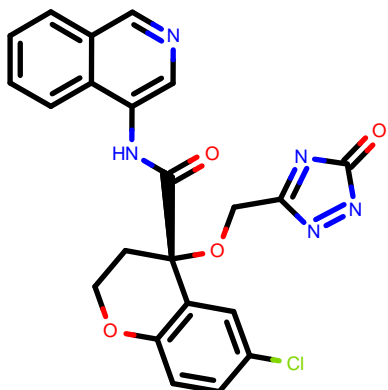
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(CC5)n6cncn6

RUN: RUN3134

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.30

EN300-73772_1_1_1



CID: EN300-73772_1_1_1

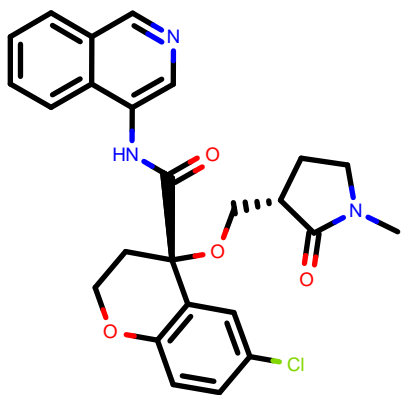
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5[nH]c(=O)[nH]n5

RUN: RUN4711

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.21

EN300-260816_1_2_1



CID: EN300-260816_1_2_1

SMILES:

CN1CC[C@H](C1=O)CO[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccoc5

RUN:

RUN4757

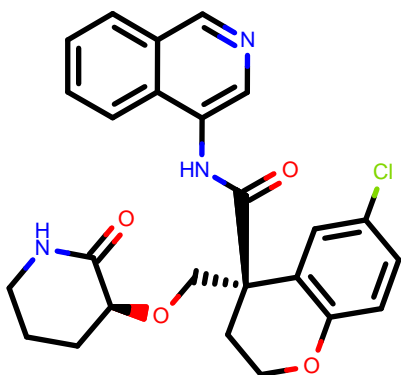
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.27

EN300-107267_2_2_1



CID: EN300-107267_2_2_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CO)C@H]5CCNC5=O

RUN:

RUN6250

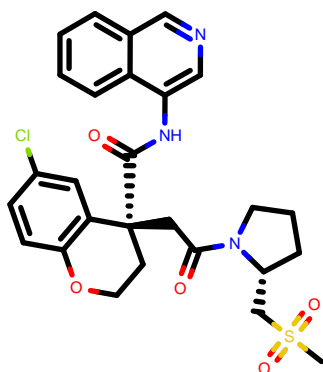
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.20

EN300-300294_1_1_1



CID: EN300-300294_1_1_1

SMILES:

CS(=O)(=O)C[C@H]1CCCN1C(=O)C[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccoc5

RUN:

RUN5060

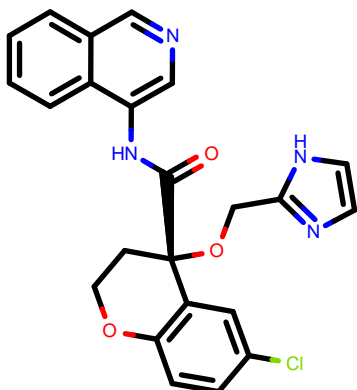
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.30

EDG-MED-4c68219f-17_1



CID: EDG-MED-4c68219f-17_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OC)C5[nH]cnc5

RUN:

RUN1508

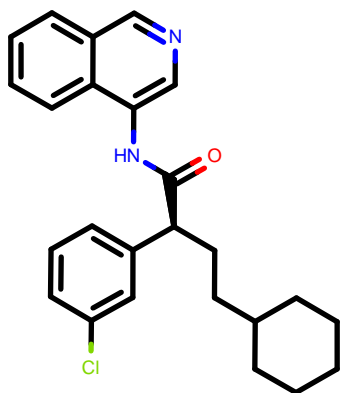
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

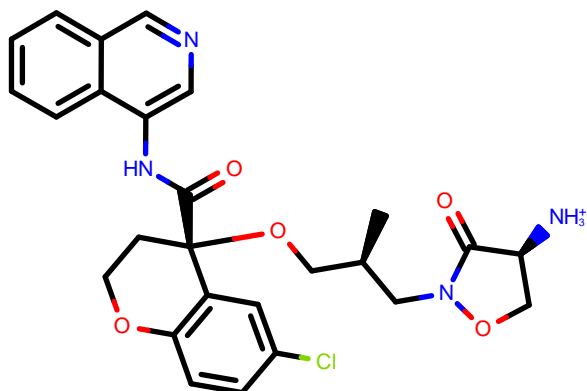
0.20

ALP-POS-3b848b35-4_1



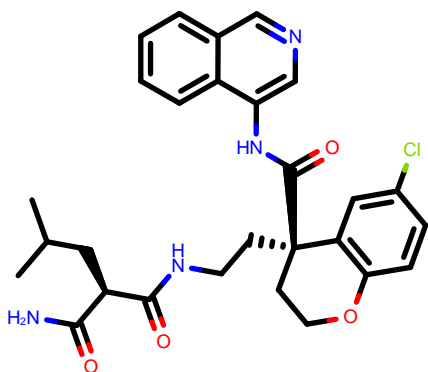
CID:	ALP-POS-3b848b35-4_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)C@@H](CCC3CCCCC3)c4ccccc4)Cl</chem>
RUN:	RUN56
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.35

EDG-MED-4c68219f-1_3



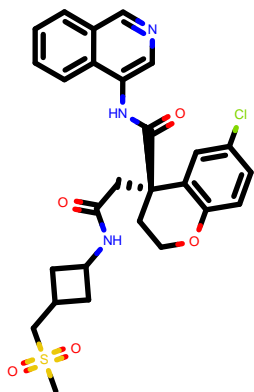
CID:	EDG-MED-4c68219f-1_3
SMILES:	<chem>ClC@@H](CN1C(=O)C@H](CO1)N13+)]CO[C@@2](COC3c2cc(c3)Cl)C(=O)N44nc5c4cccc5</chem>
RUN:	RUN1555
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.41

EN300-250126_3_2_1



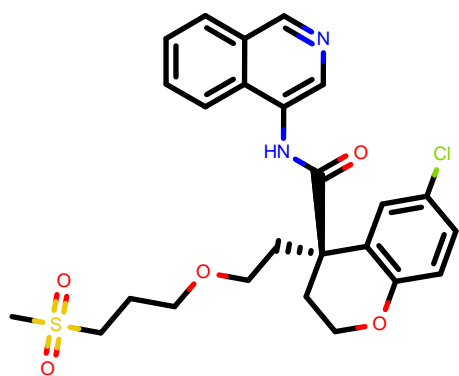
CID:	EN300-250126_3_2_1
SMILES:	<chem>CC(C)C[C@@H](C(=O)N)C(=O)NCC[C@@1](CCOC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN4462
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.36

EN300-7429970_1_1_1



CID:	EN300-7429970_1_1_1
SMILES:	<chem>CS(=O)(=O)CC1CC(C1)NC(=O)C[C@@2](CCOC3c2cc(cc3)Cl)C(=O)N44nc5c4cccc5</chem>
RUN:	RUN4725
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.35

EN300-68794_3_1_1



CID: EN300-68794_3_1_1

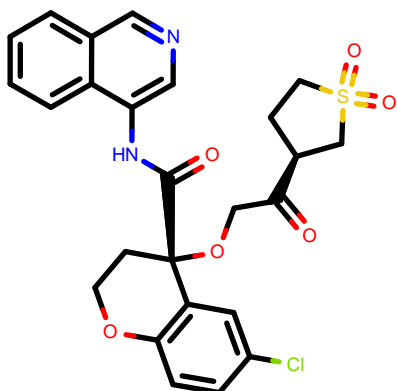
SMILES: CS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6860

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.35

EN300-226314_1_2_1



CID: EN300-226314_1_2_1

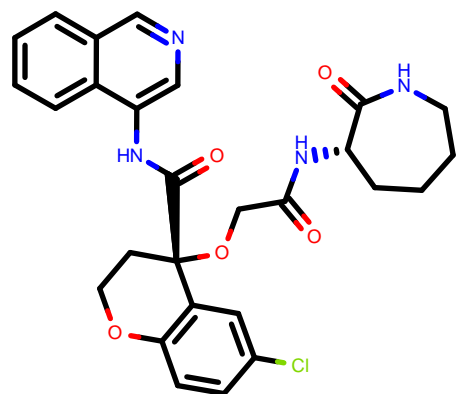
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCS(=O)(=O)C5

RUN: RUN4974

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.27

EN300-37195_1_2_1



CID: EN300-37195_1_2_1

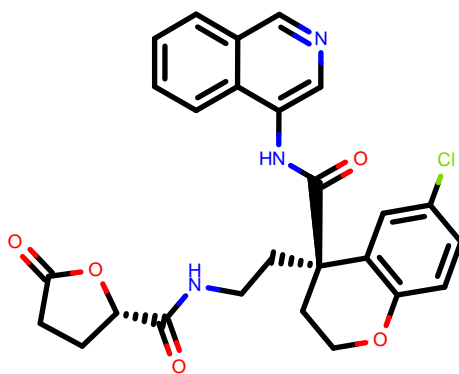
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN7225

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.28

EN300-359750_3_1_1



CID: EN300-359750_3_1_1

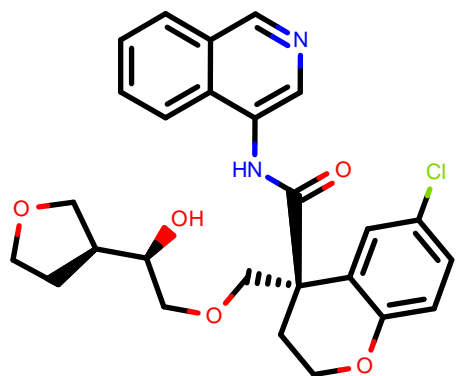
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)N[C@@H]5CCCC(=O)O5

RUN: RUN5514

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-1911992_2_3_1



CID: EN300-1911992_2_3_1

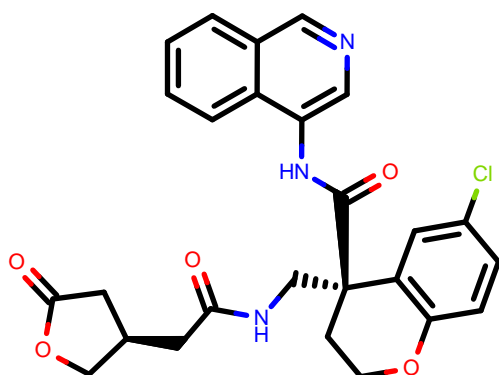
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](C@H)5CCOC5O

RUN: RUN6721

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.32

EN300-109535_2_1_1



CID: EN300-109535_2_1_1

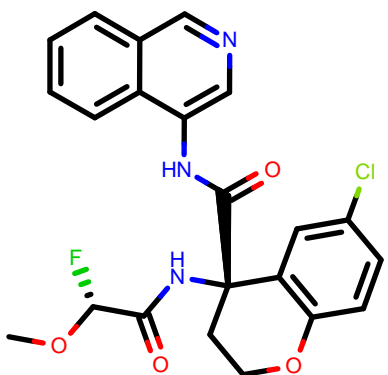
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@@H]5OC(=O)OC5

RUN: RUN7663

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.23

EDG-MED-90036822-33_1



CID: EDG-MED-90036822-33_1

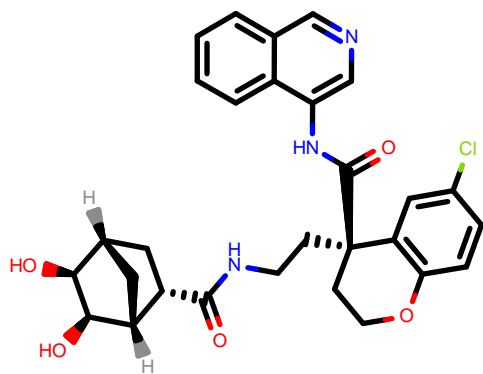
SMILES: CO[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)F

RUN: RUN1537

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.20

EN300-6744028_3_8_1



CID: EN300-6744028_3_8_1

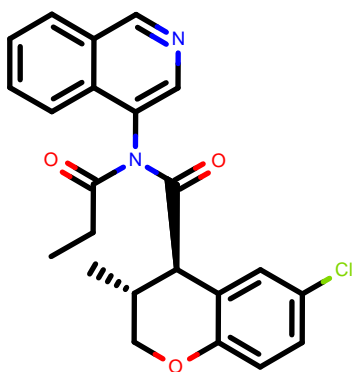
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCN(C=O)[C@@H]5C[C@@H](C@H)6[C@@H]5O6O

RUN: RUN5319

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.34

DAR-DIA-5ff57136-2_1_1



CID: DAR-DIA-5ff57136-2_1_1

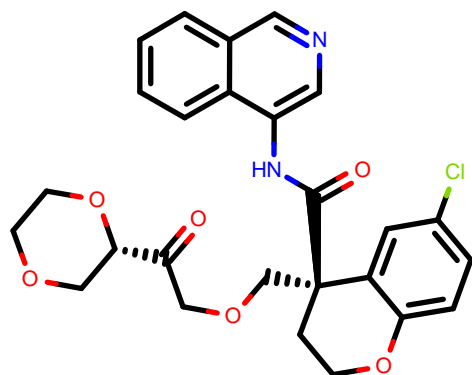
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl

RUN: RUN3807

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.19

EN300-6238494_2_1_1



CID: EN300-6238494_2_1_1

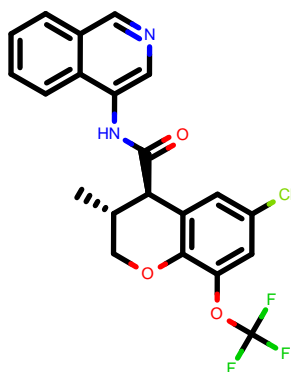
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4O)COC(=O)[C@@H]5COCOC5

RUN: RUN4153

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-18_1



CID: DAR-DIA-0d514e7d-18_1

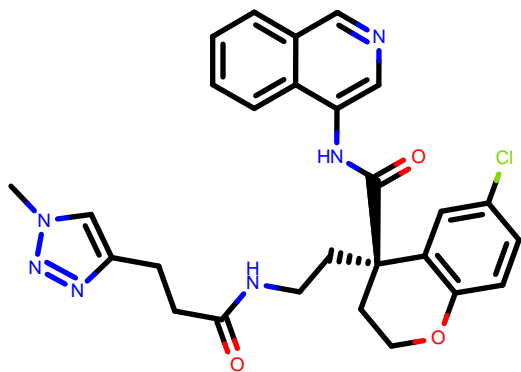
SMILES: C[C@H]1COc2c(cc(cc2OC(F)(F)F)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4

RUN: RUN743

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.15

EN300-306047_3_1_1



CID: EN300-306047_3_1_1

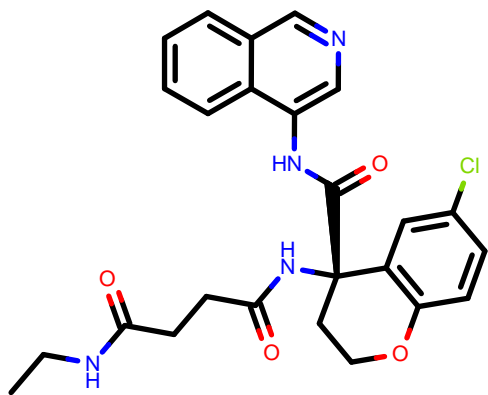
SMILES: Cn1cc(nn1)CCC(=O)NCC[C@@H]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5528

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.24

EN300-68889_1_1_1



CID: EN300-68889_1_1_1

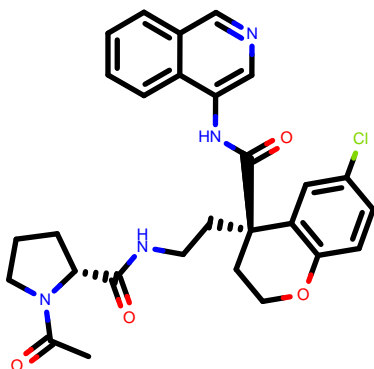
SMILES: CCNC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN5073

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.27

EN300-12587_3_1_1



CID: EN300-12587_3_1_1

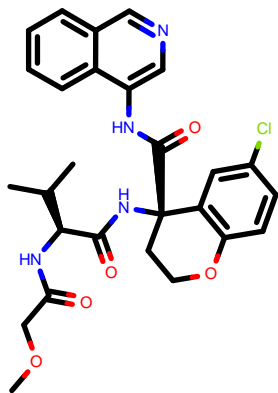
SMILES: CC(=O)N1CCC[C@@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7467

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.46

EN300-83918_1_1_1



CID: EN300-83918_1_1_1

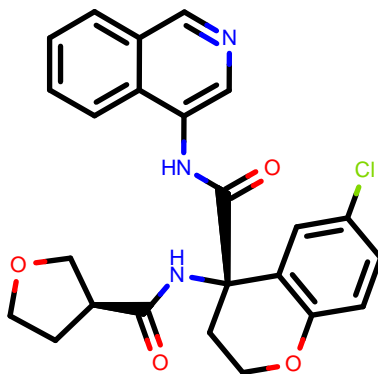
SMILES: CC(C)[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)NC(=O)CO

RUN: RUN5754

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-53423_1_2_1



CID: EN300-53423_1_2_1

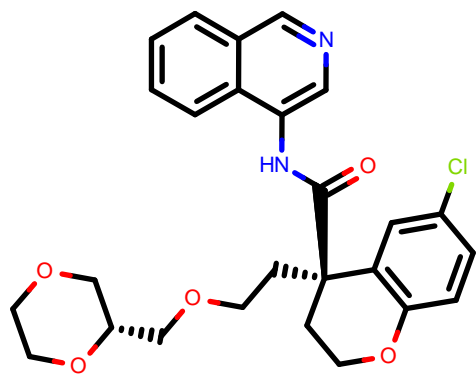
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC5

RUN: RUN3527

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.29

EN300-139167_3_2_1



CID: EN300-139167_3_2_1

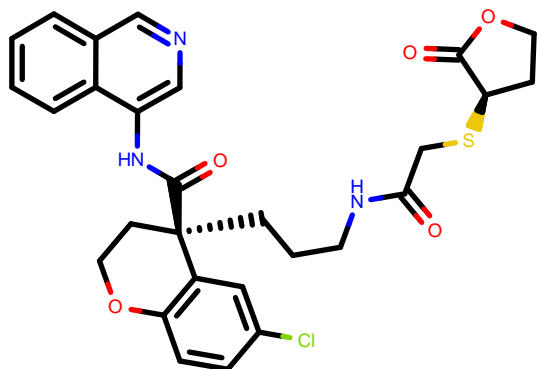
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN3596

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.29

EN300-113218_4_1_1



CID: EN300-113218_4_1_1

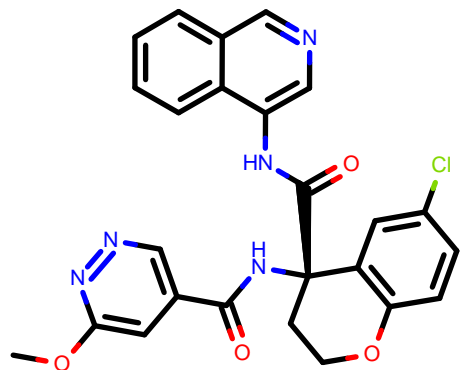
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5COCOC5=O

RUN: RUN5932

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.42

EN300-252260_1_1_1



CID: EN300-252260_1_1_1

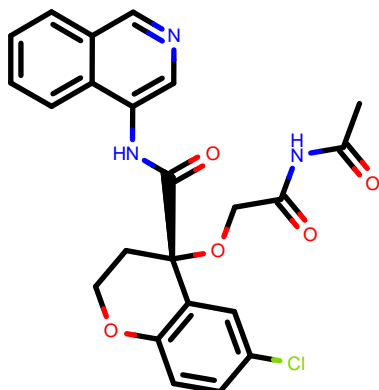
SMILES: COc1cc(cnn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc4c3cccc5

RUN: RUN6341

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.22

EN300-249475_1_1_1



CID: EN300-249475_1_1_1

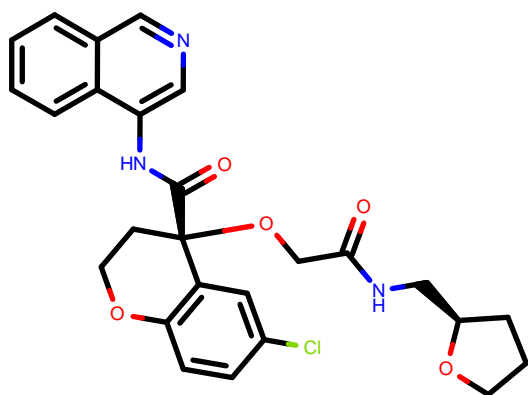
SMILES: CC(=O)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6015

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.23

EN300-01527_1_2_1



CID: EN300-01527_1_2_1

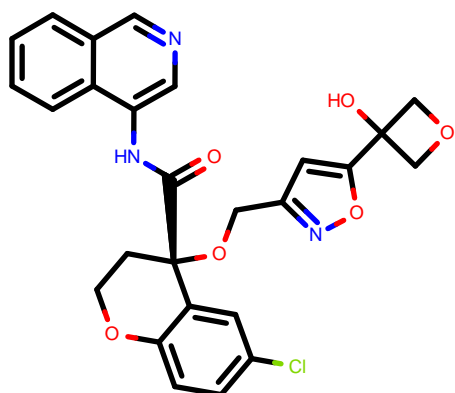
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCCC5

RUN: RUN5606

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.30

EN300-7457159_1_1_1



CID: EN300-7457159_1_1_1

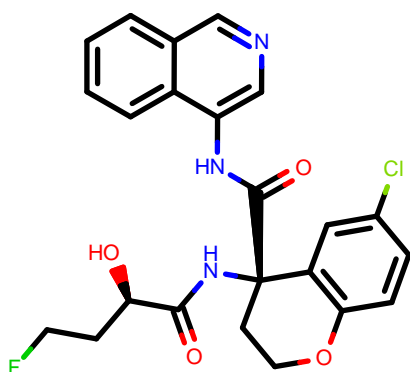
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cc(oc5)O6(COC6)O

RUN: RUN3721

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.28

EDG-MED-90036822-51_1



CID: EDG-MED-90036822-51_1

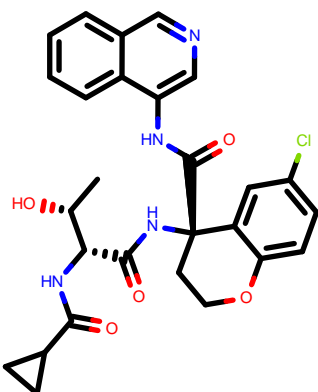
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(CCF)O

RUN: RUN1617

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.24

EN300-96362_1_4_1



CID: EN300-96362_1_4_1

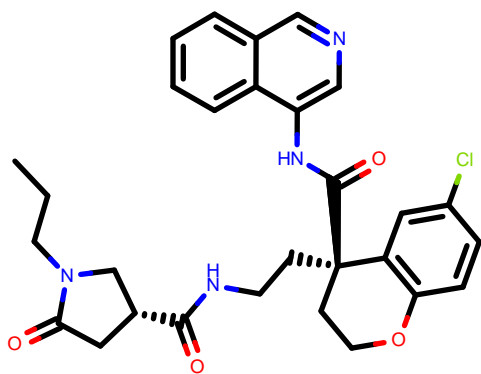
SMILES: C[C@@H]([C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3encc4c3cccc4)NC(=O)C5CC5)O

RUN: RUN4279

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.31

EN300-253443_3_1_1



CID: EN300-253443_3_1_1

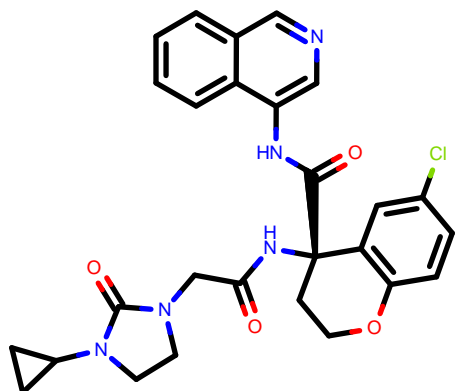
SMILES: CCCN1C[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7142

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.29

EN300-304771_1_1_1



CID: EN300-304771_1_1_1

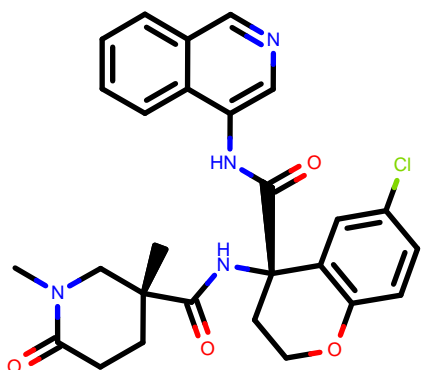
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)N5CCN(C5=O)C6CC6

RUN: RUN4641

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.36

EN300-6734171_1_2_1



CID: EN300-6734171_1_2_1

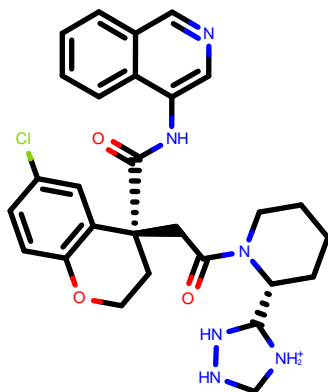
SMILES: C[C@]1(CCC(=O)N(C1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN6035

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.28

EDG-MED-ba1ac7b9-9_1



CID: EDG-MED-ba1ac7b9-9_1

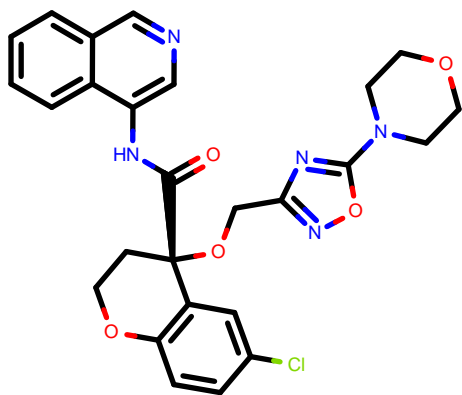
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@]3HJ5c6[nH]n6

RUN: RUN2475

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.27

EN300-1608590_1_1_1



CID: EN300-1608590_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5nc(on5)N6CCOCC6

RUN:

RUN5742

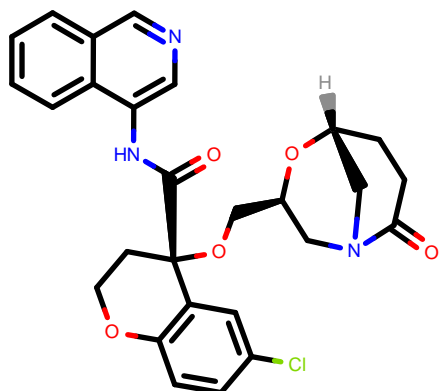
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.29

EN300-2008102_1_1_1



CID: EN300-2008102_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@]5N6C6C[C@H]5)C(=O)O

RUN:

RUN4221

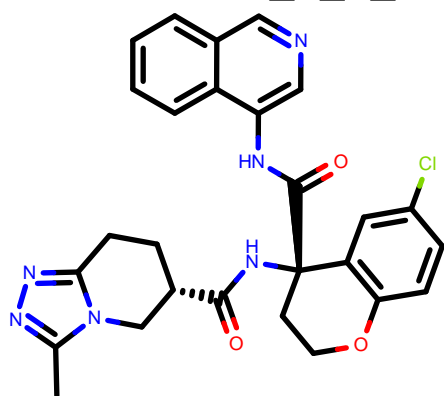
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.26

EN300-50561_1_2_1



CID: EN300-50561_1_2_1

SMILES:

Cc1nnc2n1C[C@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cnc6c5ccc6

RUN:

RUN3542

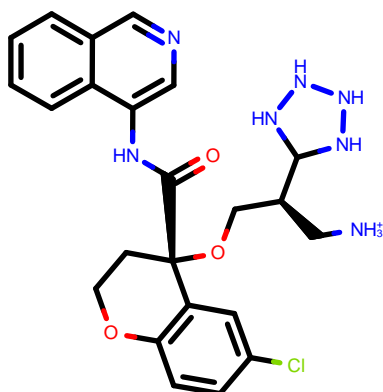
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.23

ED_-GRI-5b13fbe2-9_2



CID: ED_-GRI-5b13fbe2-9_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H](C[NH3+])c5n[n-]nn5

RUN:

RUN1396

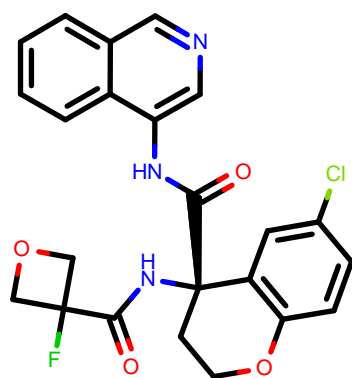
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.34

EDG-MED-90036822-24_1



CID: EDG-MED-90036822-24_1

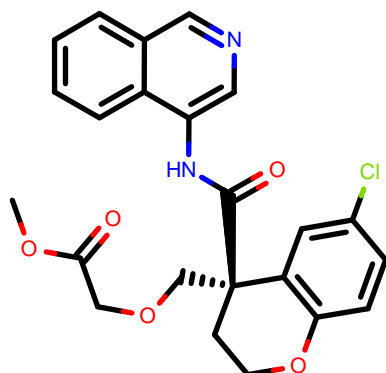
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COC5)F

RUN: RUN1539

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.27

EN300-19700_2_1_1



CID: EN300-19700_2_1_1

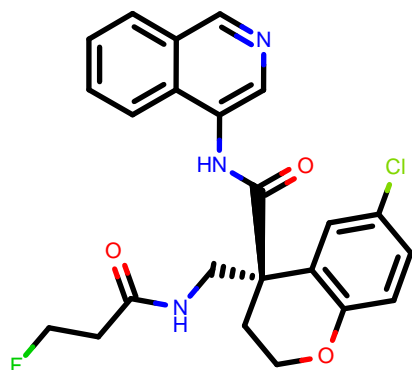
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4743

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.19

EN300-97758_2_1_1



CID: EN300-97758_2_1_1

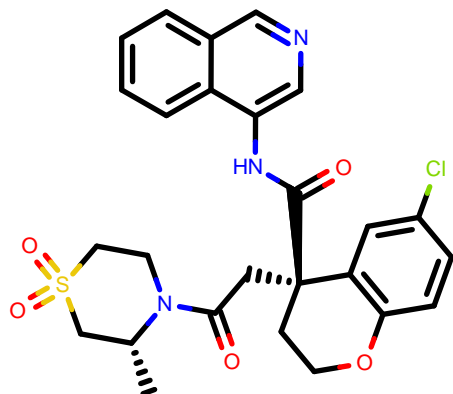
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCF

RUN: RUN5089

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.27

EN300-171215_1_1_1



CID: EN300-171215_1_1_1

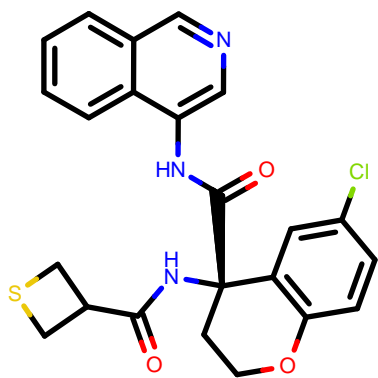
SMILES: C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4792

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.37

EN300-95094_1_1_1



CID: EN300-95094_1_1_1

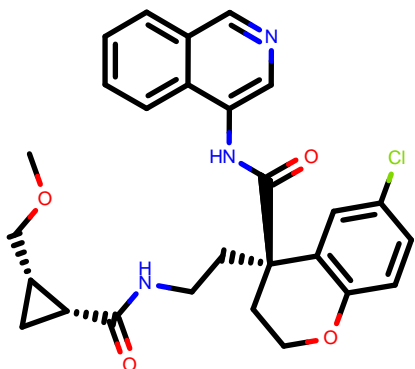
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CSC5

RUN: RUN3362

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.20

EN300-705381_3_1_1



CID: EN300-705381_3_1_1

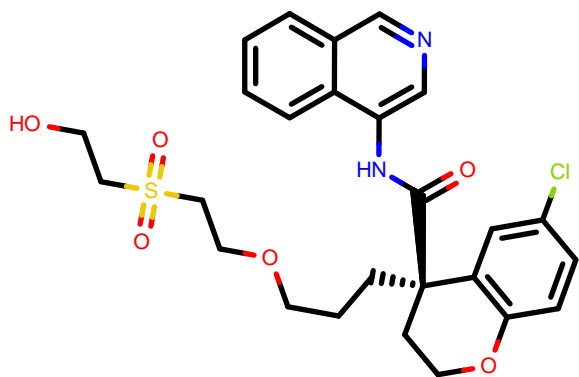
SMILES: COC[C@H]1C[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7237

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.29

EN300-7463171_4_1_1



CID: EN300-7463171_4_1_1

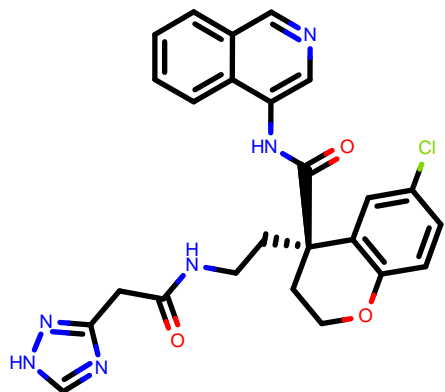
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)CO

RUN: RUN2928

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.68

EN300-96159_3_1_1



CID: EN300-96159_3_1_1

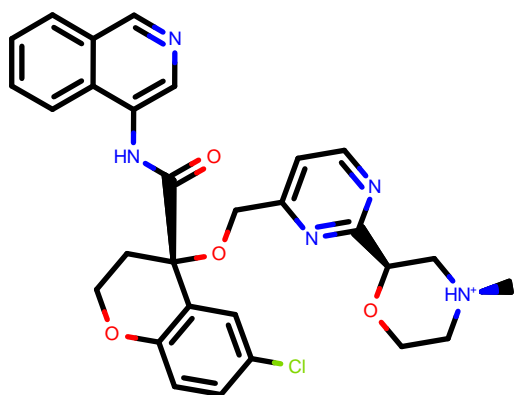
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5[nH]n5

RUN: RUN3364

DDG (kcal/mol): -1.35

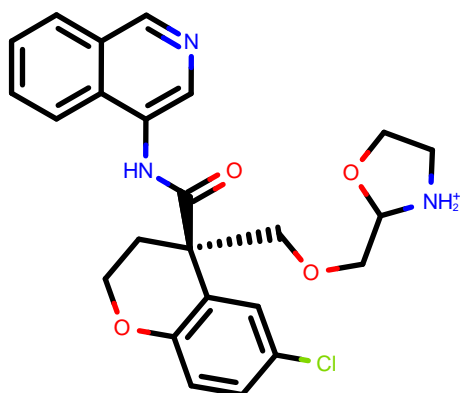
dDDG (kcal/mol): 0.32

ED_-GRI-5b13fbe2-74_4



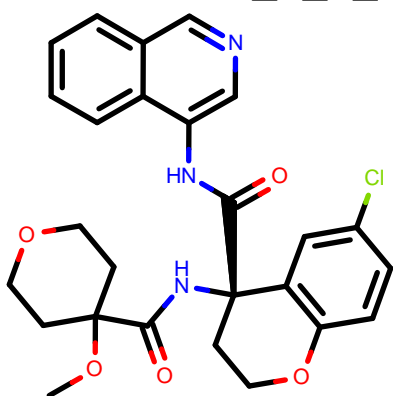
CID:	ED_-GRI-5b13fbe2-74_4
SMILES:	<chem>C[N@H]1CCO[C@H](C1)c2nccc(n2)CO[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nccoc5c6ccoc6</chem>
RUN:	RUN1503
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.43

EDJ-MED-fcba3f31-3_1



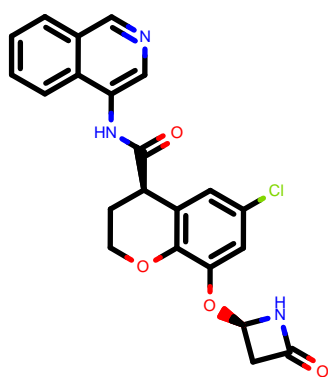
CID:	EDJ-MED-fcba3f31-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5=NCCO5</chem>
RUN:	RUN2382
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.20

EN300-204133_1_1_1



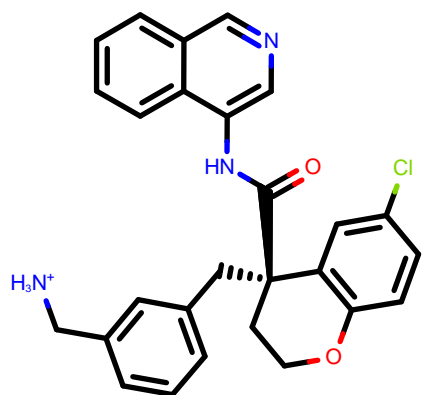
CID:	EN300-204133_1_1_1
SMILES:	<chem>COC1(CCOCC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccoc4c5ccoc5</chem>
RUN:	RUN2974
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.27

VLA-UCB-50c39ae8-8_1_1



CID:	VLA-UCB-50c39ae8-8_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5c[nH]5</chem>
RUN:	RUN3132
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.20

JAG-UCB-706446eb-8_1_1



CID: JAG-UCB-706446eb-8_1_1

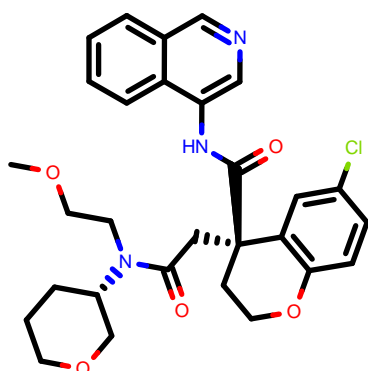
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)Cn5ccoc(c5)[NH3+]

RUN: RUN5393

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.25

JAG-UCB-706446eb-5_2



CID: JAG-UCB-706446eb-5_2

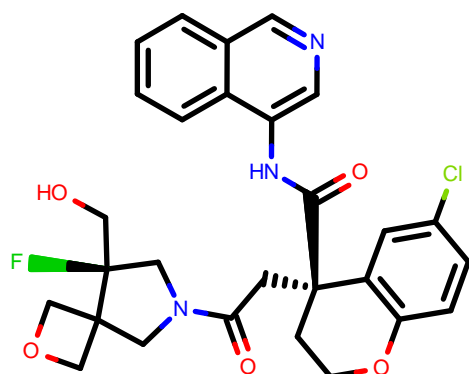
SMILES: COCCN([C@H]1CCCOC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN607

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.37

EN300-1719075_1_1_1



CID: EN300-1719075_1_1_1

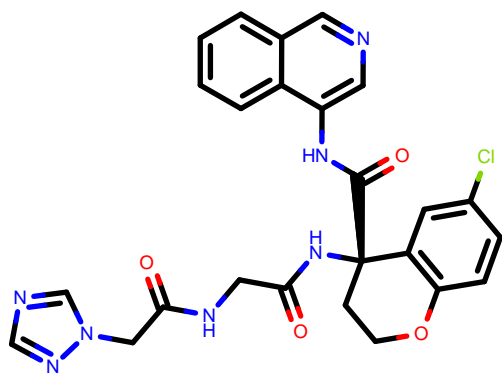
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]([C@]5(C)COC6)C(=O)F

RUN: RUN5903

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.38

EN300-52383_1_1_1



CID: EN300-52383_1_1_1

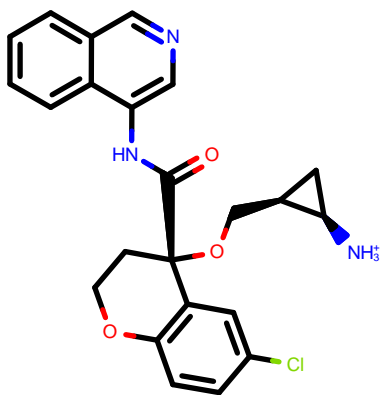
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)Cn5cncn5

RUN: RUN5321

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-69_4



CID: ED_-GRI-5b13fbe2-69_4

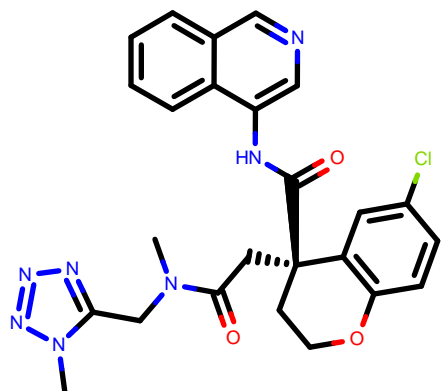
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5[C@@H]5[NH3+]

RUN: RUN1453

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

EN300-148515_1_1_1



CID: EN300-148515_1_1_1

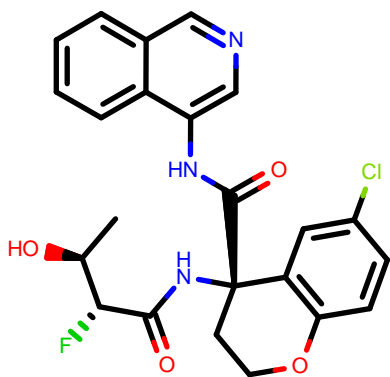
SMILES: Cn1c(nnn1)CN(C)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccc5

RUN: RUN5922

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.28

EDG-MED-90036822-37_3



CID: EDG-MED-90036822-37_3

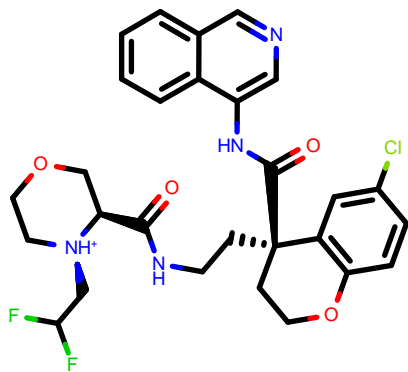
SMILES: C[C@@H]([C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4)F)O

RUN: RUN1558

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.22

EN300-140582_3_1_1



CID: EN300-140582_3_1_1

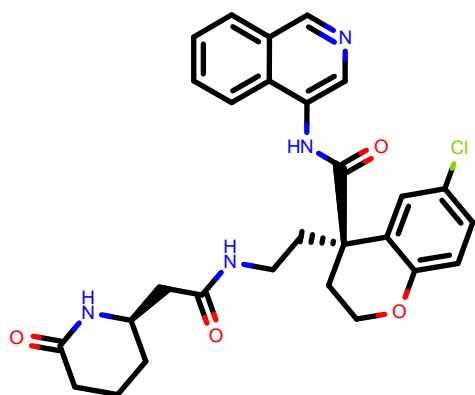
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CN(C=O)[C@@H]5COC[C@@H]5C(F)F

RUN: RUN4029

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.30

EN300-210084_3_2_1



CID: EN300-210084_3_2_1

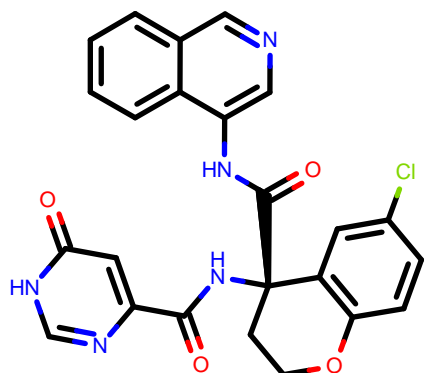
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@H]5CCCC(=O)N5

RUN: RUN5274

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.33

EN300-817811_1_1_1



CID: EN300-817811_1_1_1

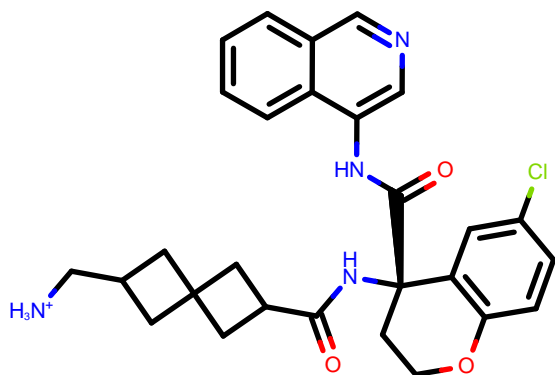
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(=O)[nH]n5

RUN: RUN3884

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

EDG-MED-90036822-103_1



CID: EDG-MED-90036822-103_1

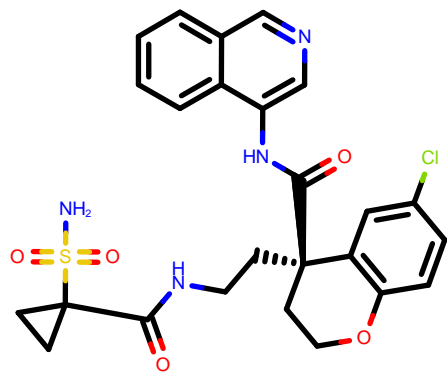
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC6(C5)CC(C6)N[H3+]

RUN: RUN1720

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.38

EN300-223741_3_1_1



CID: EN300-223741_3_1_1

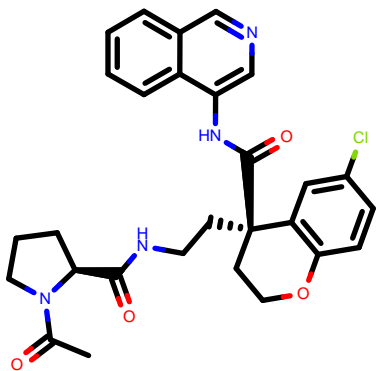
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CS(=O)S(=O)=O)N

RUN: RUN5121

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.33

EN300-211779_3_1_1



CID: EN300-211779_3_1_1

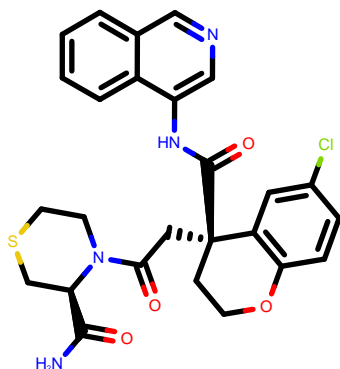
SMILES: CC(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3734

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.35

EN300-122866_1_1_1



CID: EN300-122866_1_1_1

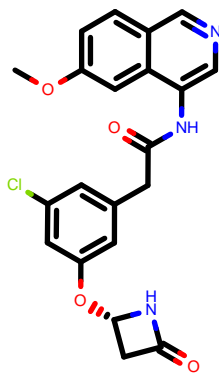
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCSC[C@@]H5C(=O)N

RUN: RUN5372

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.30

ALF-EVA-0b412456-2_2



CID: ALF-EVA-0b412456-2_2

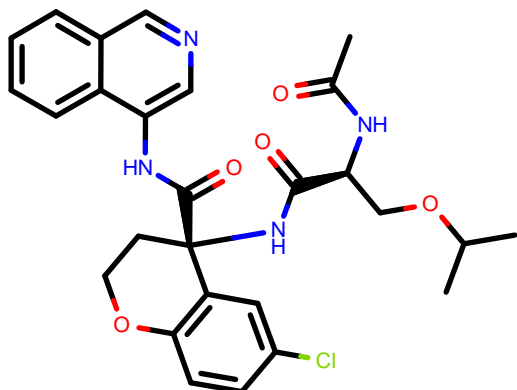
SMILES: COc1ccc2nccc(c2c1)NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4

RUN: RUN2542

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.36

EN300-1299691_1_1_1



CID: EN300-1299691_1_1_1

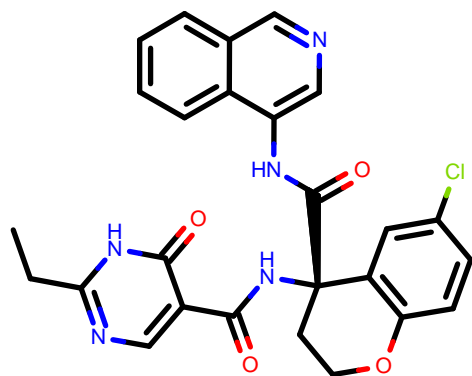
SMILES: CC(C)OC[C@@]H[C@@]1(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)NC(=O)C

RUN: RUN6471

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.29

EN300-1273019_1_1_1



CID: EN300-1273019_1_1_1

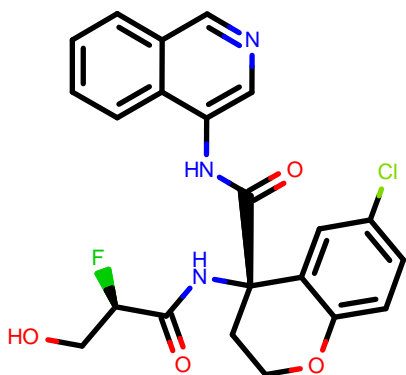
SMILES: CCc1[nH]c(=O)c(en1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5506

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.29

EDG-MED-90036822-15_1



CID: EDG-MED-90036822-15_1

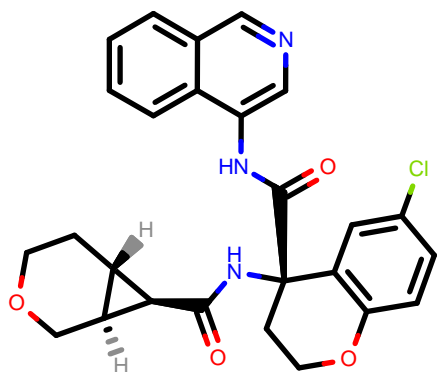
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CO)F

RUN: RUN1520

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.22

EN300-1644723_1_1_1



CID: EN300-1644723_1_1_1

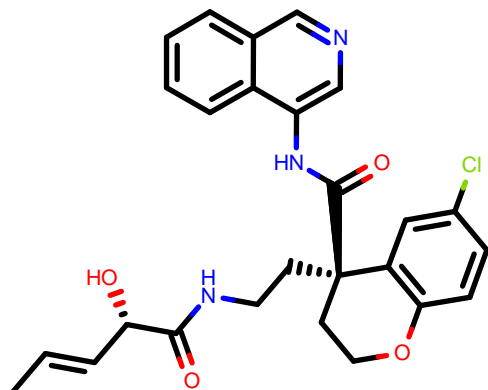
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@H]5COC6

RUN: RUN3269

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.25

EN300-300217_3_2_1



CID: EN300-300217_3_2_1

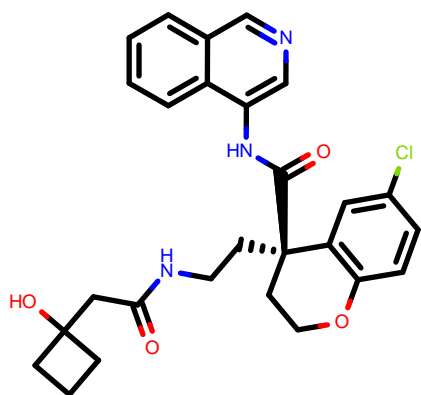
SMILES: C/C=C/[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN6522

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.32

EN300-246423_3_1_1



CID: EN300-246423_3_1_1

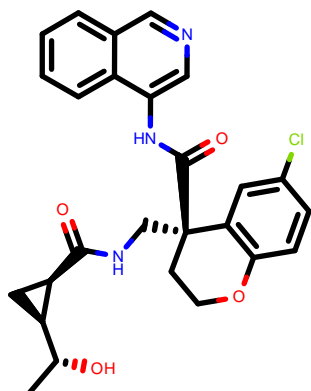
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC5(CCC5)O

RUN: RUN5773

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.25

EN300-6729572_2_8_1



CID: EN300-6729572_2_8_1

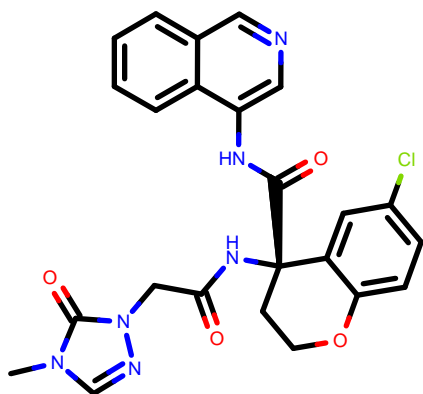
SMILES: C[C@H]([C@H]1[C@H]1C(=O)NC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5)O

RUN: RUN6728

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.22

EN300-120436_1_1_1



CID: EN300-120436_1_1_1

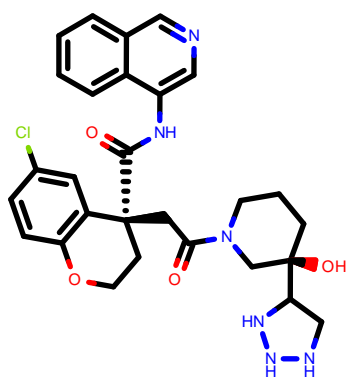
SMILES: Cn1cnn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5

RUN: RUN4359

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.30

EN300-222120_1_1_1



CID: EN300-222120_1_1_1

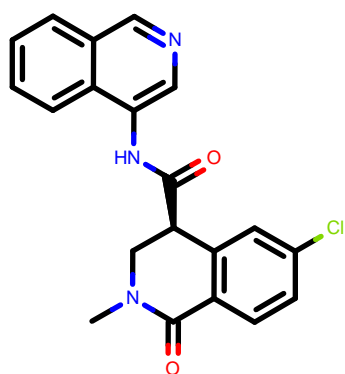
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]6(C)C5c6nc(=N)N6

RUN: RUN2842

DDG (kcal/mol): -1.33

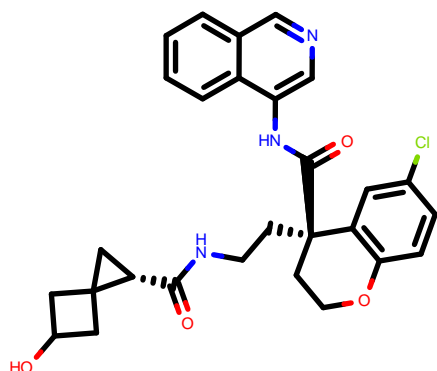
dDDG (kcal/mol): 0.37

MIC-UNK-91acba05-2_2



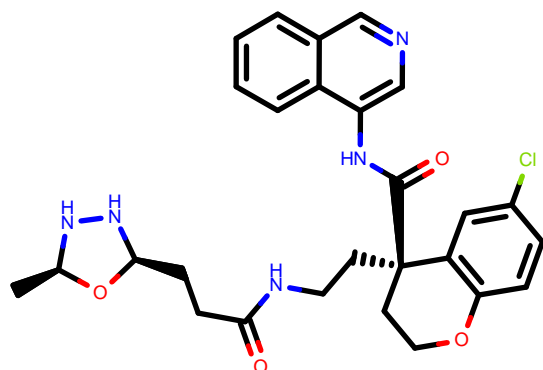
CID:	MIC-UNK-91acba05-2_2
SMILES:	<chem>CN1C[C@H](c2cc(ccc2C1=O)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN364
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.24

KAD-UNI-8a629cb0-35_1



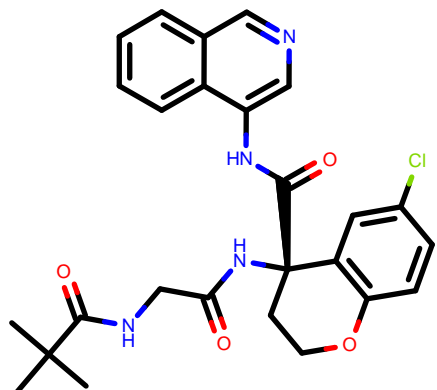
CID:	KAD-UNI-8a629cb0-35_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC56C(C)O</chem>
RUN:	RUN2018
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.33

EN300-304662_3_1_4



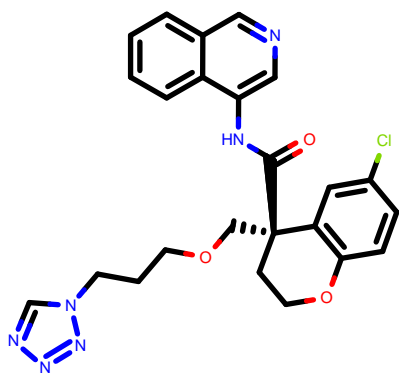
CID:	EN300-304662_3_1_4
SMILES:	<chem>C[C@H]1NN[C@H](O1)CCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN7002
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.27

EN300-12247_1_1_1



CID:	EN300-12247_1_1_1
SMILES:	<chem>CC(C)C(C(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN4482
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.27

EN300-1696962_2_1_1



CID: EN300-1696962_2_1_1

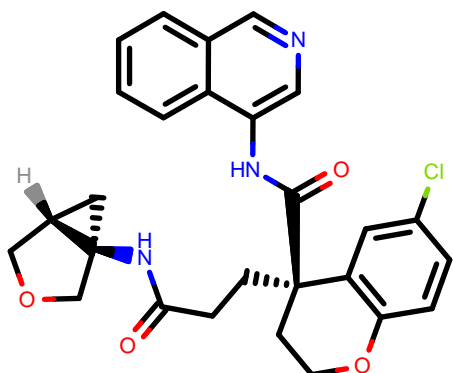
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCN5cnnn5

RUN: RUN4445

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.29

EN300-367383_2_1_1



CID: EN300-367383_2_1_1

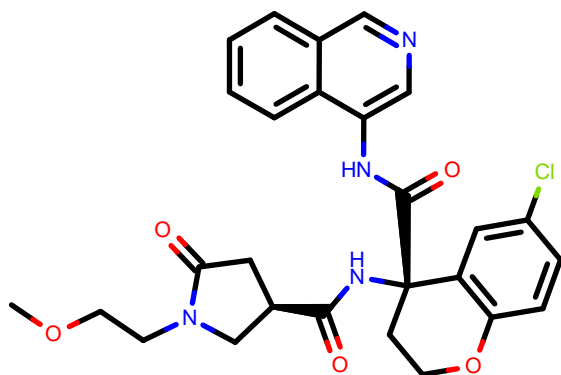
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]56C[C@H]5CO6

RUN: RUN5382

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.27

EN300-31845_1_1_1



CID: EN300-31845_1_1_1

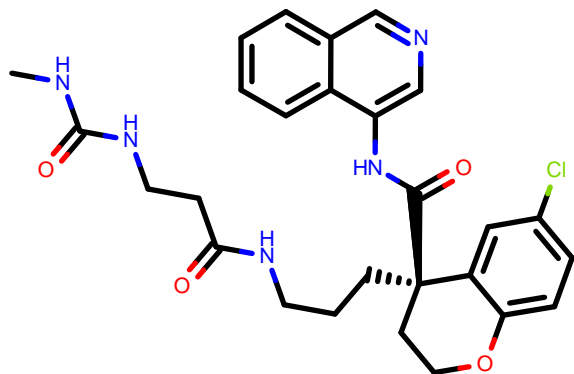
SMILES: COCCN1C[C@@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN5832

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.34

EN300-66494_4_1_1



CID: EN300-66494_4_1_1

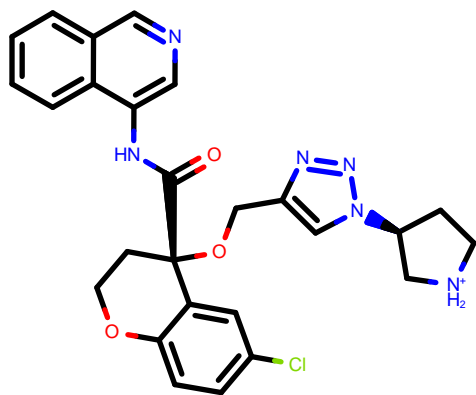
SMILES: CNC(=O)NCCC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4

RUN: RUN6131

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-61_2



CID: ED_-GRI-5b13fbe2-61_2

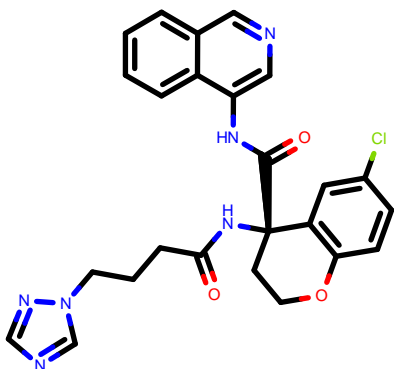
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn[nH5][C@H]6CC[NH2+]C6

RUN: RUN1465

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.28

EN300-316216_1_1_1



CID: EN300-316216_1_1_1

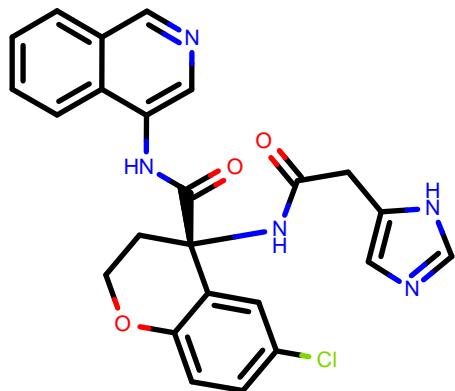
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cn[nH5]

RUN: RUN3507

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.23

EDG-MED-90036822-49_1



CID: EDG-MED-90036822-49_1

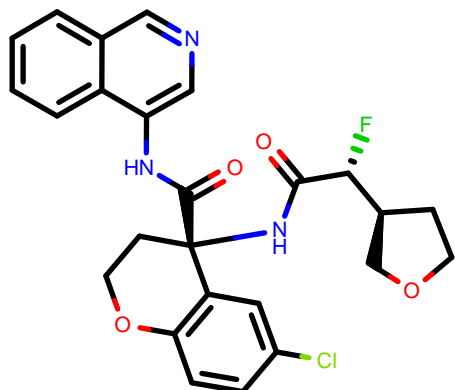
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]5

RUN: RUN1574

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.21

EN300-783124_1_3_1



CID: EN300-783124_1_3_1

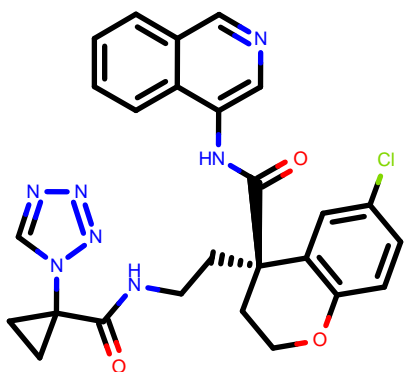
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@H]5COCOC5)F

RUN: RUN2825

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.18

EN300-263085_3_1_1



CID: EN300-263085_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@3(C)C(CO)C(=O)C(C)CCNC(=O)C5(C)C5n6cnn6

RUN:

RUN2802

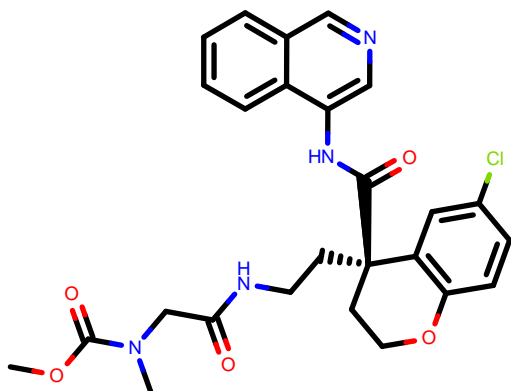
DDG (kcal/mol):

-1.32

dDDG (kcal/mol):

0.34

EN300-39005_3_1_1



CID: EN300-39005_3_1_1

SMILES:

CN(CC(=O)NCC[C@]1(C)C(CO)C(=O)Nc3ccc4c3ccc4)C(=O)OC

RUN:

RUN5764

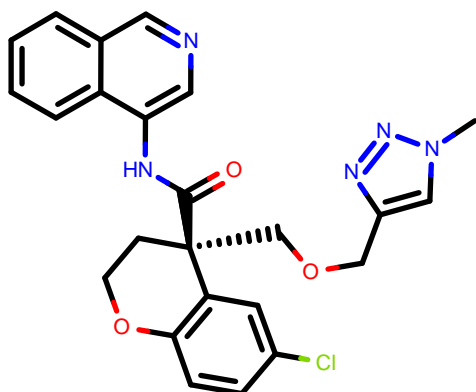
DDG (kcal/mol):

-1.32

dDDG (kcal/mol):

0.31

EN300-120282_2_1_1



CID: EN300-120282_2_1_1

SMILES:

Cn1cc(nn1)COC[C@]2(C)C(CO)C(=O)Nc4ccc5c4ccc5

RUN:

RUN5593

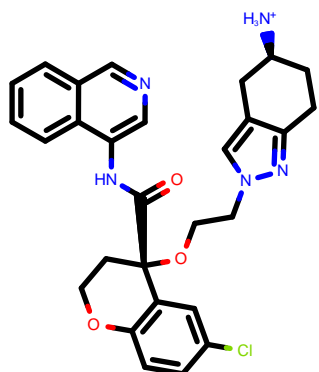
DDG (kcal/mol):

-1.32

dDDG (kcal/mol):

0.23

ED_-GRI-5b13fbe2-60_1



CID: ED_-GRI-5b13fbe2-60_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@3(C)C(CO)C(=O)Nc4ccc5c4ccc5[NH3+]

RUN:

RUN1469

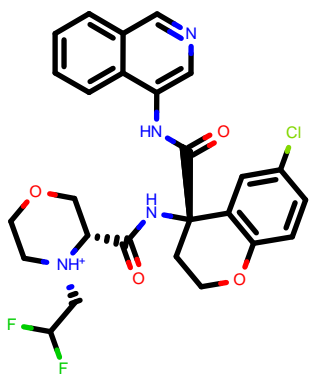
DDG (kcal/mol):

-1.32

dDDG (kcal/mol):

0.45

EN300-140582_1_2_1



CID: EN300-140582_1_2_1

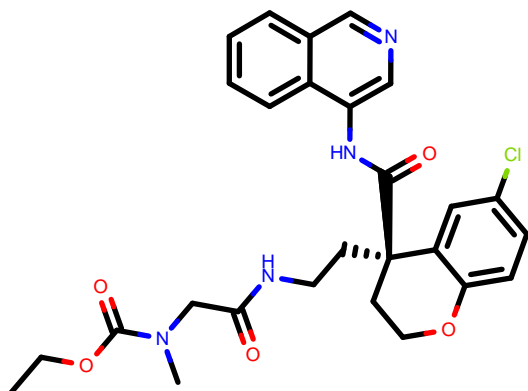
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)I|NC(=O)[C@H]5COCC[N@]5CC(F)F

RUN: RUN3724

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.33

EN300-39101_3_1_1



CID: EN300-39101_3_1_1

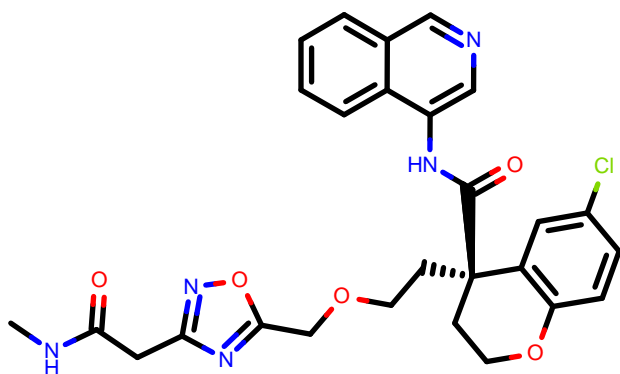
SMILES: CCOC(=O)N(C)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccoc4

RUN: RUN3920

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.35

EN300-99983_3_1_1



CID: EN300-99983_3_1_1

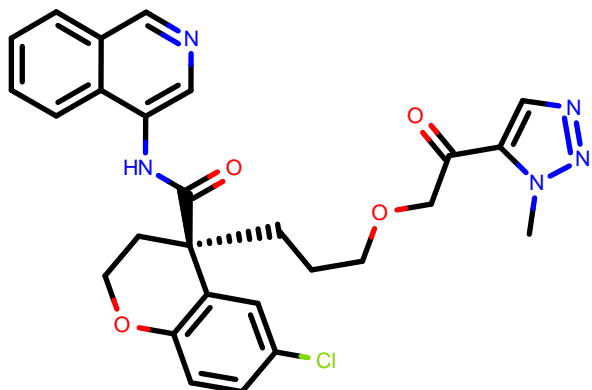
SMILES: CNC(=O)CC1nc(on1)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccoc5

RUN: RUN4254

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.46

EN300-204936_4_1_1



CID: EN300-204936_4_1_1

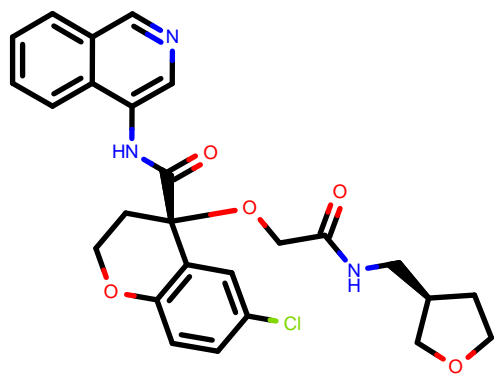
SMILES: Cn1c(cnn1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccoc5

RUN: RUN6592

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.35

EN300-46832_1_2_1



CID: EN300-46832_1_2_1

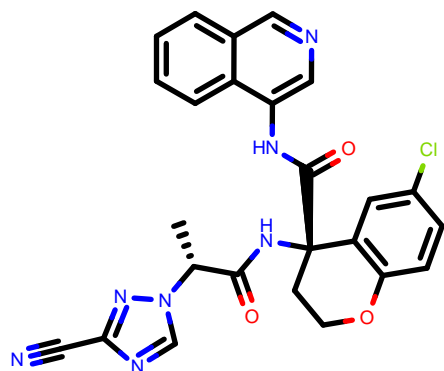
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCOC5

RUN: RUN7726

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.29

EN300-198515_1_2_1



CID: EN300-198515_1_2_1

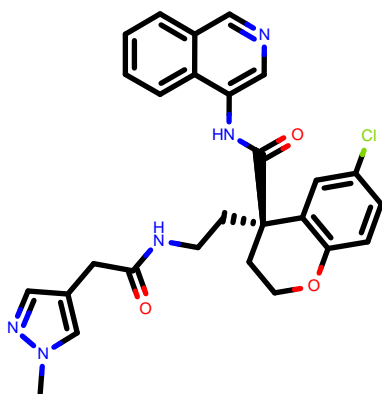
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)n5nc(n5)C#N

RUN: RUN3006

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.30

EN300-63872_3_1_1



CID: EN300-63872_3_1_1

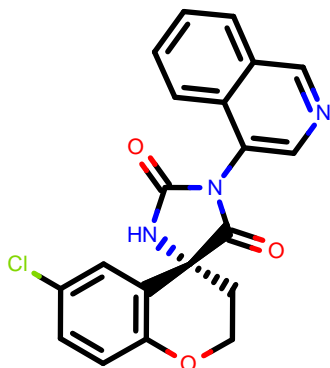
SMILES: Cn1cc(cn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4776

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.27

VLA-UCB-29506327-1_1



CID: VLA-UCB-29506327-1_1

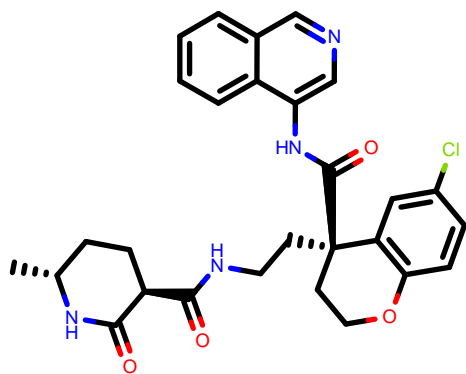
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O

RUN: RUN1219

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.25

EN300-6505003_3_3_1



CID: EN300-6505003_3_3_1

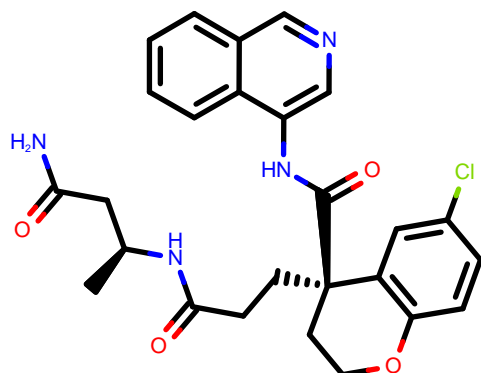
SMILES: C[C@@H]1CC[C@H](C(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN6286

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.32

EN300-84785_2_1_1



CID: EN300-84785_2_1_1

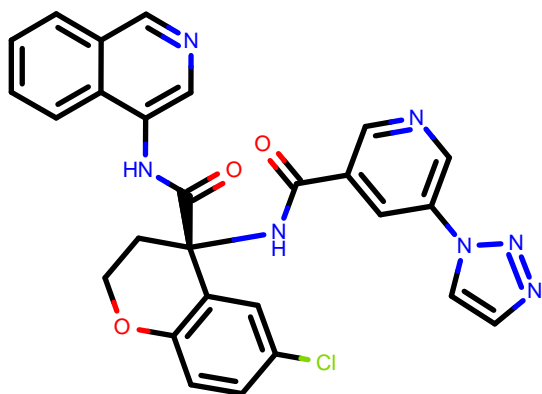
SMILES: C[C@@H](CC(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN5619

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.23

EN300-151298_1_1_1



CID: EN300-151298_1_1_1

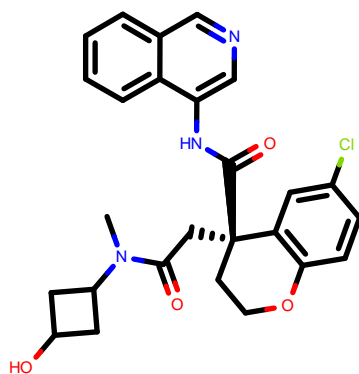
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(cnc5)n6cnm6

RUN: RUN3373

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-93074_1_1_1



CID: EN300-93074_1_1_1

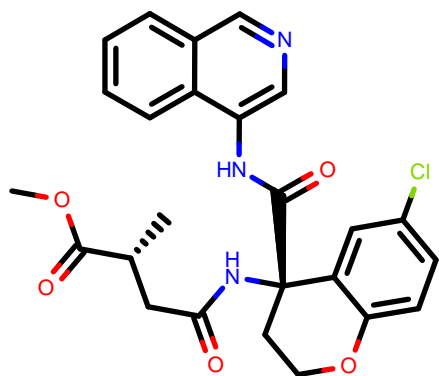
SMILES: CN(C1CC(C1)O)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN6945

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-108413_1_2_1



CID: EN300-108413_1_2_1

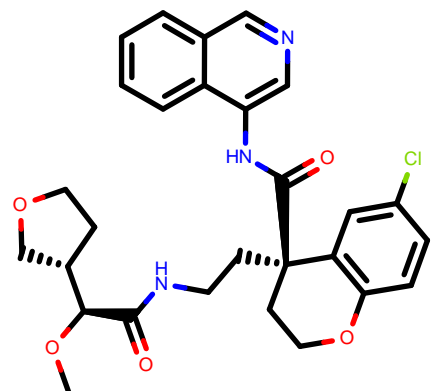
SMILES: C[C@@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)C(=O)OC

RUN: RUN3140

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-298552_3_3_1



CID: EN300-298552_3_3_1

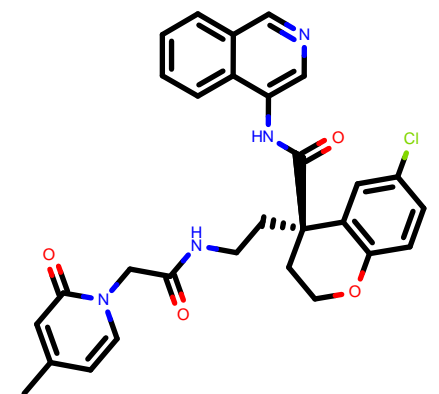
SMILES: CO[C@@H](C[C@@H]1CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN5291

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.30

EN300-184446_3_1_1



CID: EN300-184446_3_1_1

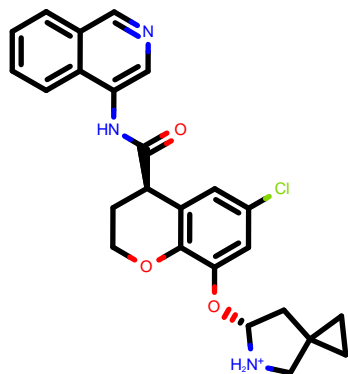
SMILES: Cc1ccn(c(=O)c1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN5756

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.33

DAR-DIA-23e5a6a0-4_1_1



CID: DAR-DIA-23e5a6a0-4_1_1

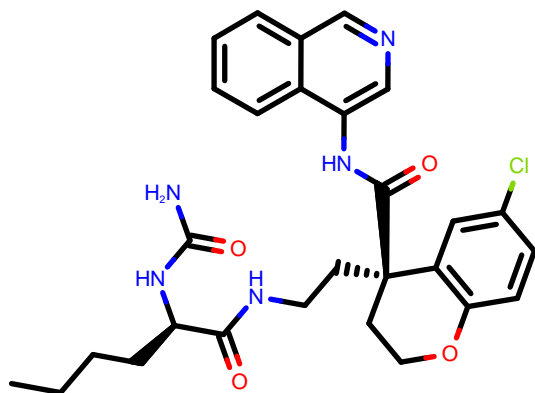
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@@H]5CC6(CC6)[NH2+][5]Cl

RUN: RUN6198

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.32

EN300-55744_3_2_1



CID: EN300-55744_3_2_1

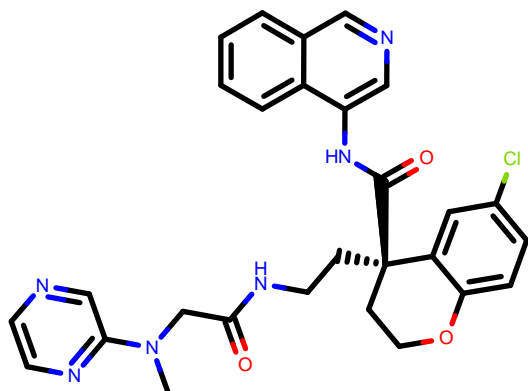
SMILES: CCCC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)NC(=O)N

RUN: RUN6503

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.51

EN300-36855_3_1_2



CID: EN300-36855_3_1_2

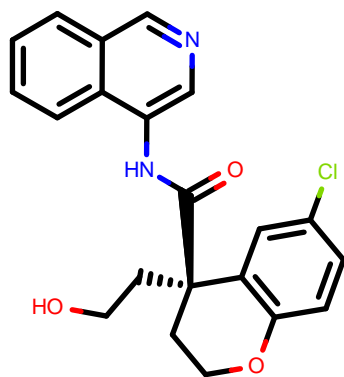
SMILES: CN(CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)c5cnccn5

RUN: RUN3998

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.34

EDG-MED-971238d3-3_1



CID: EDG-MED-971238d3-3_1

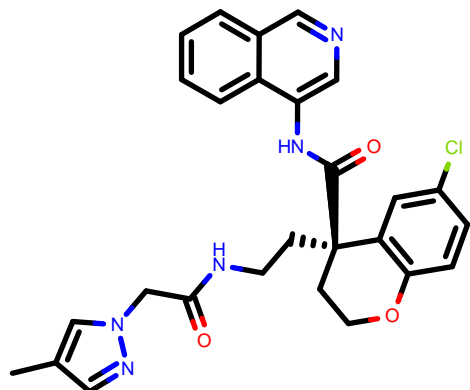
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO

RUN: RUN1302

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.13

EN300-51832_3_1_1



CID: EN300-51832_3_1_1

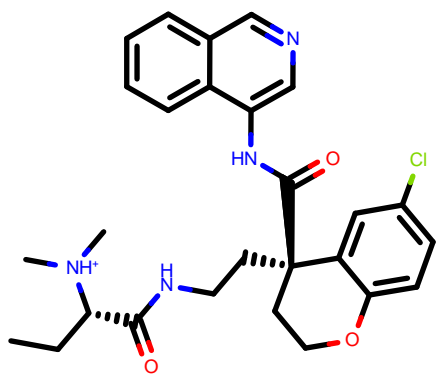
SMILES: Cc1cnn(c1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4113

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

EN300-110012_3_1_1



CID: EN300-110012_3_1_1

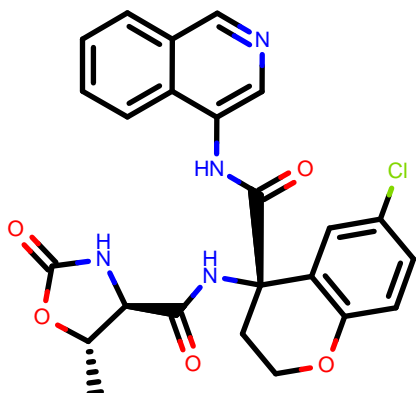
SMILES: CC[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)[NH+](C)C

RUN: RUN7124

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.40

EN300-172640_1_2_1



CID: EN300-172640_1_2_1

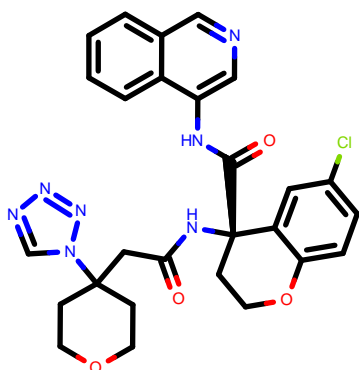
SMILES: C[C@H]1[C@@H](NC(=O)O1)C(=O)N[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4326

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.23

EN300-306097_1_1_1



CID: EN300-306097_1_1_1

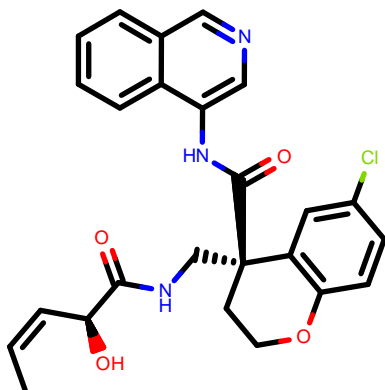
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCOCC5)n6cnnn6

RUN: RUN4263

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

EN300-300217_2_1_1



CID: EN300-300217_2_1_1

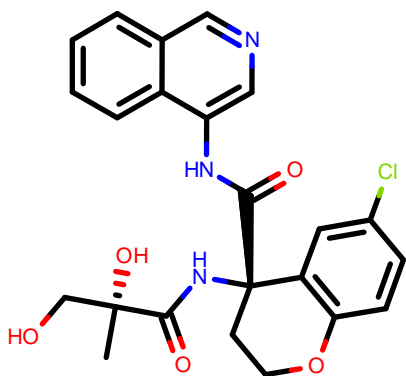
SMILES: C/C=C/[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O

RUN: RUN4245

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.37

EN300-89418_1_1_1



CID: EN300-89418_1_1_1

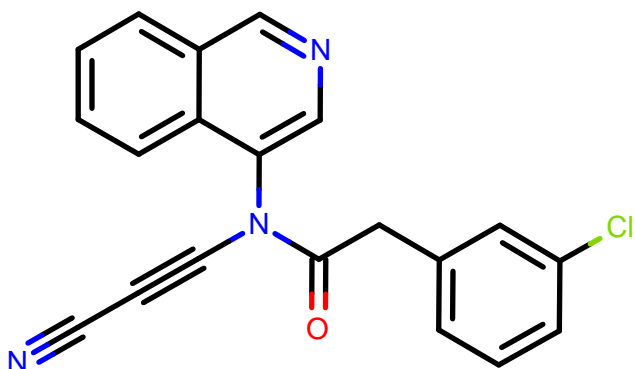
SMILES: C[C@@](C)(CO)N(C=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4O

RUN: RUN5271

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.35

DAR-DIA-076fb6ea-5_1



CID: DAR-DIA-076fb6ea-5_1

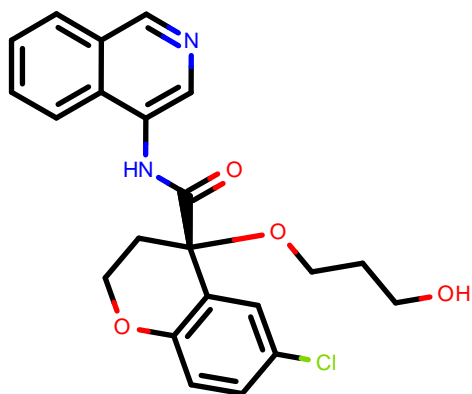
SMILES: c1ccc2c(c1)cncc2N(C#CC#N)C(=O)Cc3ccccc(c3)Cl

RUN: RUN1238

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.35

EN300-221518_1_1_1



CID: EN300-221518_1_1_1

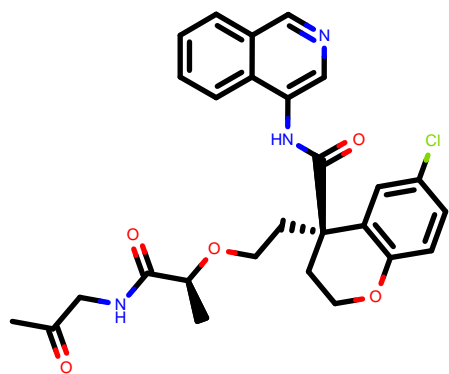
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO

RUN: RUN5850

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.19

EN300-131093_3_1_1



CID: EN300-131093_3_1_1

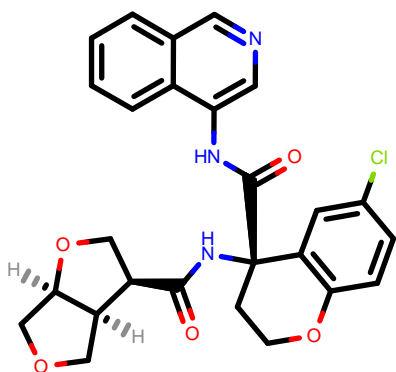
SMILES: C[C@@]([H])(C(=O)NCC(=O)C)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4790

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.39

EN300-6482296_1_3_1



CID: EN300-6482296_1_3_1

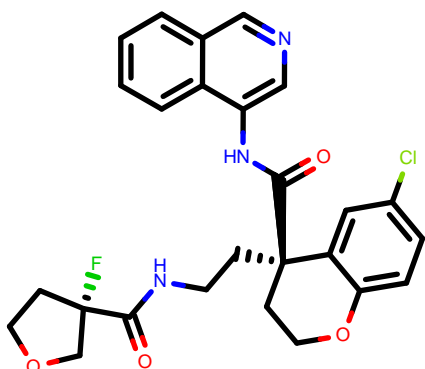
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C=O)[C@@H]5CO[C@H]6C@H5COO6

RUN: RUN4219

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.33

EN300-188356_3_1_1



CID: EN300-188356_3_1_1

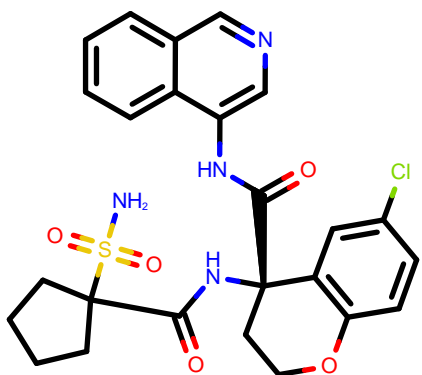
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCOOC5)F

RUN: RUN4723

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.34

EN300-6486793_1_1_1



CID: EN300-6486793_1_1_1

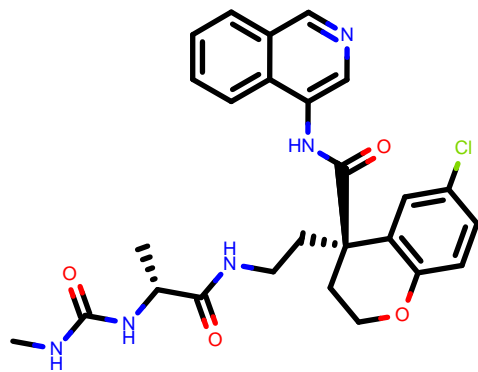
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCCC5)S(=O)(=O)N

RUN: RUN4095

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.40

EN300-2958082_3_1_1



CID: EN300-2958082_3_1_1

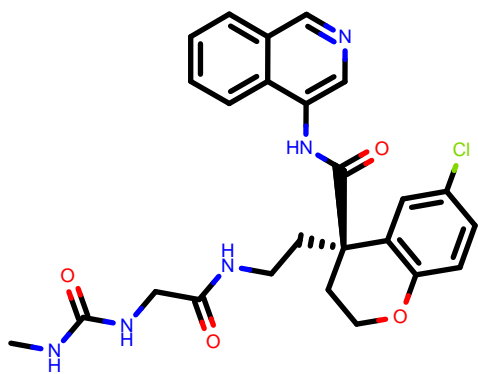
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)NC(=O)NC

RUN: RUN4892

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.29

EN300-36911_3_1_1



CID: EN300-36911_3_1_1

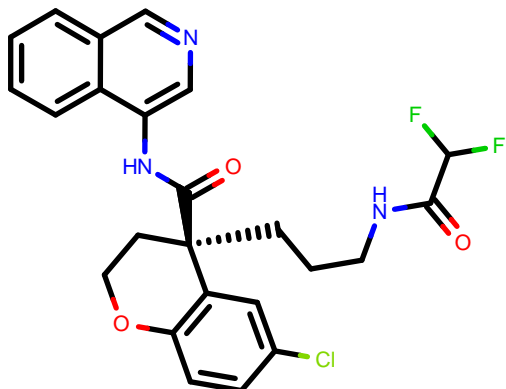
SMILES: CNC(=O)NCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN7021

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.30

EN300-19507_4_1_1



CID: EN300-19507_4_1_1

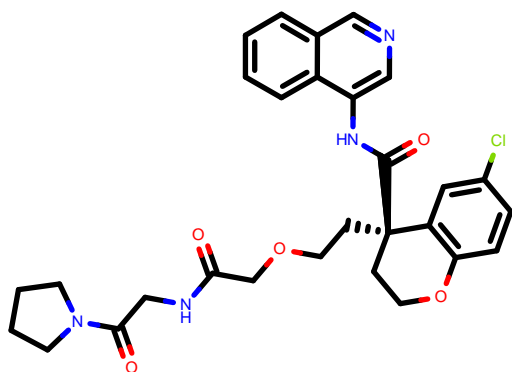
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C(F)F

RUN: RUN3855

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.25

EN300-28340_3_1_1



CID: EN300-28340_3_1_1

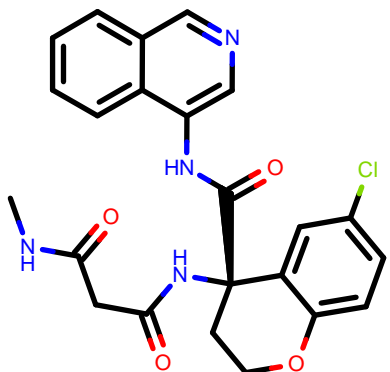
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCC(=O)N5CCCC5

RUN: RUN5594

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.32

EN300-128463_1_1_1



CID: EN300-128463_1_1_1

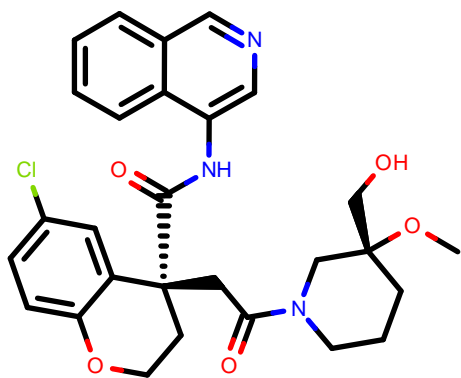
SMILES: CNC(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3735

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.21

EN300-299806_1_1_1



CID: EN300-299806_1_1_1

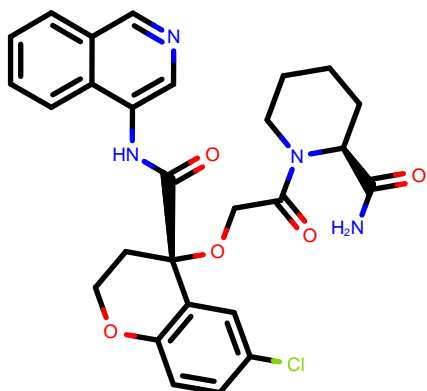
SMILES: CO[C@@]1(CCCN(C1)C(=O)C[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5)CO

RUN: RUN4441

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.37

EN300-22879_1_2_1



CID: EN300-22879_1_2_1

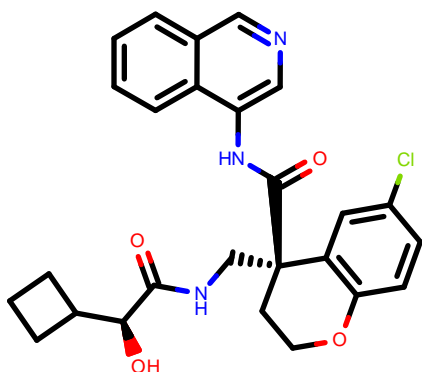
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN5967

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.28

EN300-249764_2_2_1



CID: EN300-249764_2_2_1

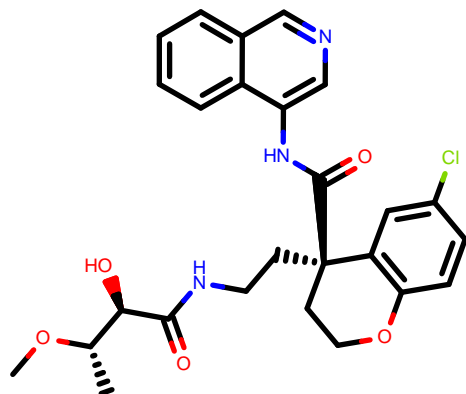
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H](C5CCC5)O

RUN: RUN4968

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.26

EN300-220194_3_3_1



CID: EN300-220194_3_3_1

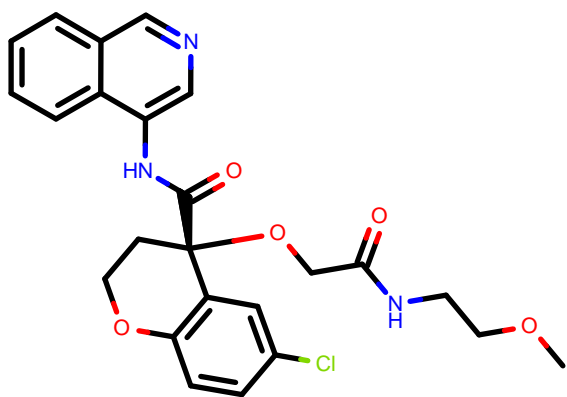
SMILES: C[C@@]H([C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O)O

RUN: RUN4521

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.30

EN300-02015_1_1_1



CID: EN300-02015_1_1_1

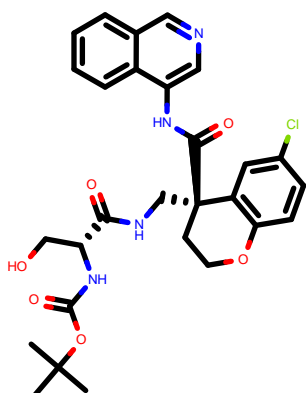
SMILES: COCCNC(=O)CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN: RUN7334

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.26

EN300-72109_2_2_1



CID: EN300-72109_2_2_1

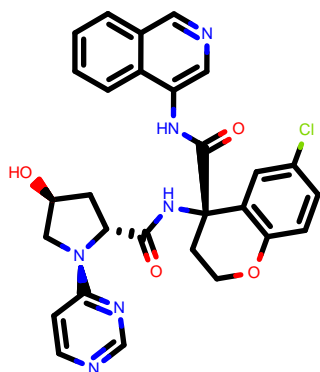
SMILES: CC(C)(C)OC(=O)N[C@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN: RUN6912

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.49

EN300-310022_1_2_1



CID: EN300-310022_1_2_1

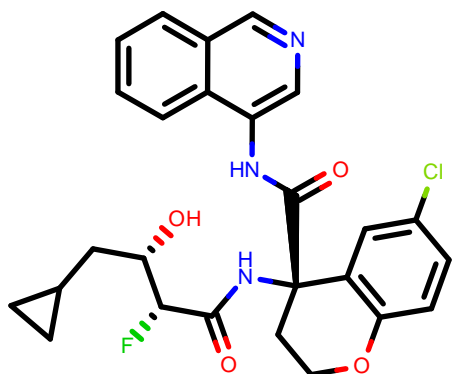
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N[C@]1(C)C(=O)Nc5ncc6c5ccc6O

RUN: RUN3355

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.37

EDG-MED-90036822-108_3



CID: EDG-MED-90036822-108_3

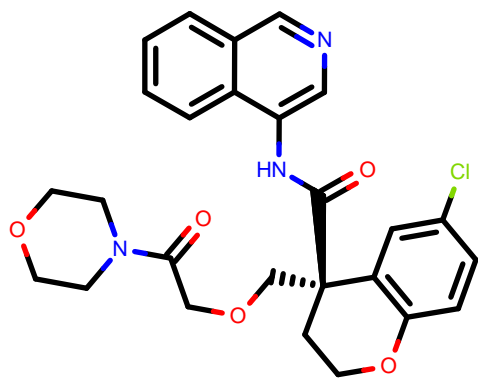
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N[C@]1(C)C(=O)Nc5ncc6c5ccc6O

RUN: RUN1752

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.23

EN300-1241327_2_1_1



CID: EN300-1241327_2_1_1

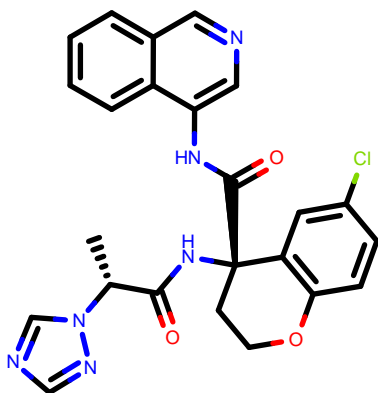
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)N5CCOCC5

RUN: RUN5191

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.29

EN300-30397_1_2_1



CID: EN300-30397_1_2_1

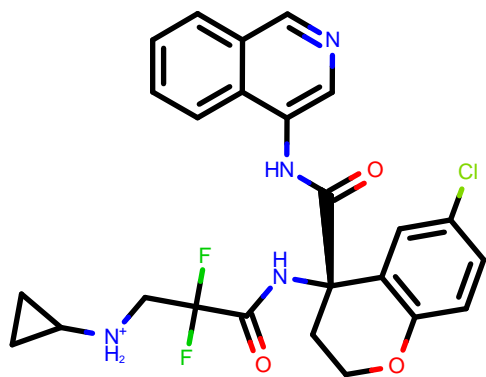
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)n5cncn5

RUN: RUN3376

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EDG-MED-90036822-105_1



CID: EDG-MED-90036822-105_1

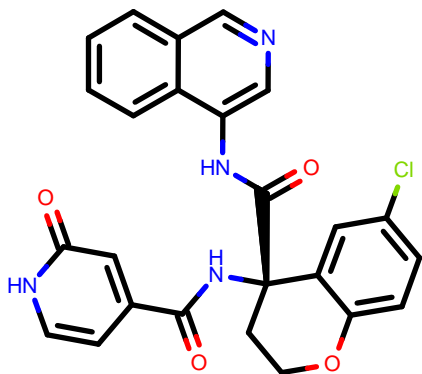
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(CNC5CC5)F(F)F

RUN: RUN1813

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.29

EN300-97661_1_1_1



CID: EN300-97661_1_1_1

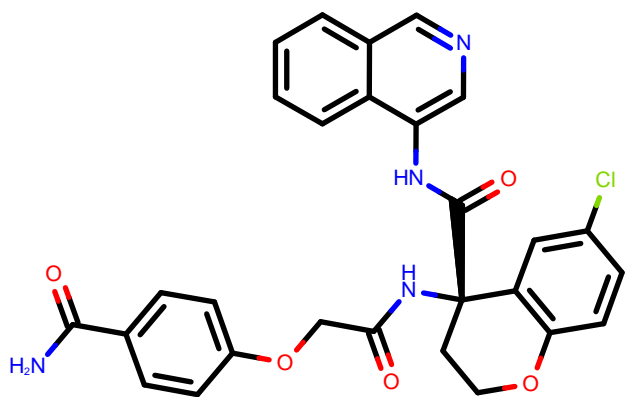
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc[nH]c(=O)c5

RUN: RUN3868

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EN300-55498_1_1_1



CID: EN300-55498_1_1_1

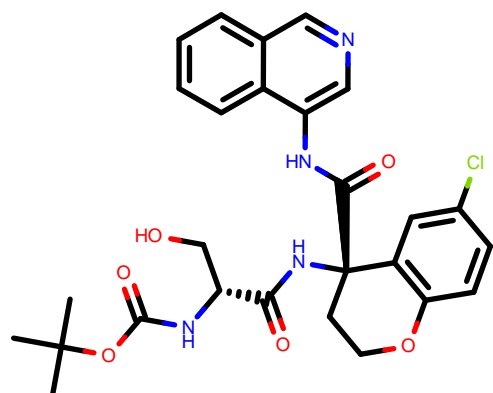
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COc5ccc(cc5)C(=O)N

RUN: RUN5836

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.28

EN300-72109_1_2_1



CID: EN300-72109_1_2_1

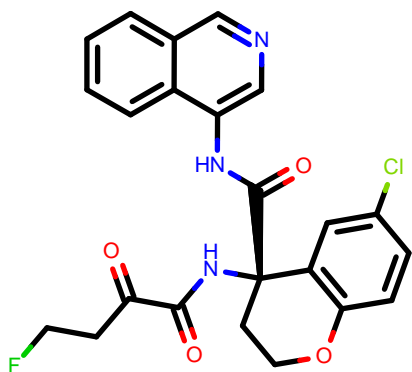
SMILES: CC(C)(C)OC(=O)N[C@@H](CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN7208

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.28

EDG-MED-90036822-44_1



CID: EDG-MED-90036822-44_1

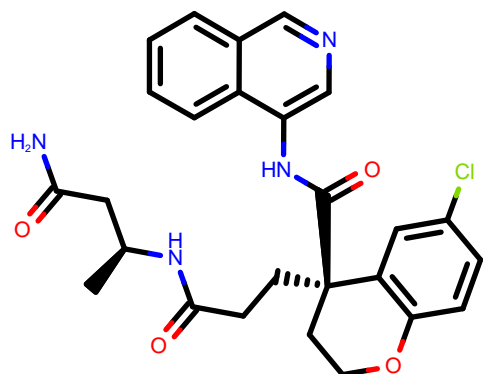
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)CCF

RUN: RUN1599

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.19

EN300-84785_2_1_1



CID: EN300-84785_2_1_1

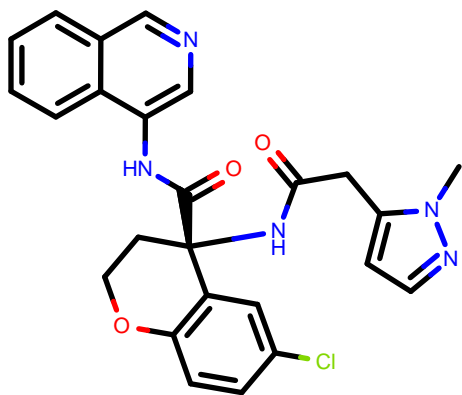
SMILES: C[C@@H](CC(=O)N)NC(=O)CC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5857

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.22

EN300-114805_1_1_1



CID: EN300-114805_1_1_1

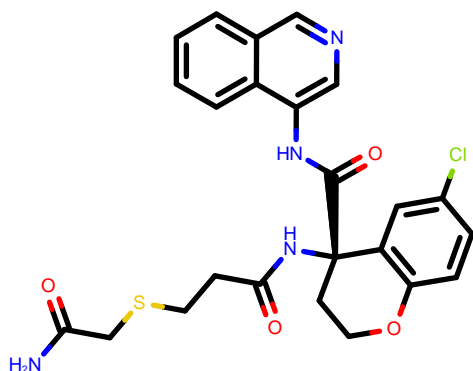
SMILES: Cn1c(ccn1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4529

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.24

EN300-31015_1_1_1



CID: EN300-31015_1_1_1

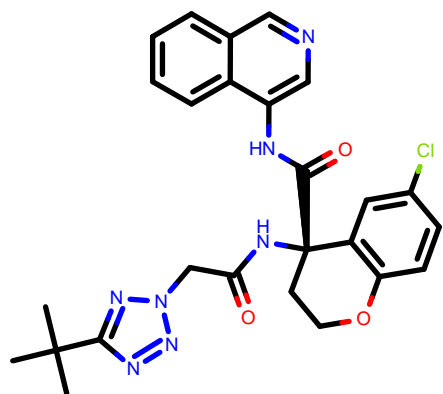
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC4c3cc(cc4)Cl)NC(=O)CCSCC(=O)N

RUN: RUN6178

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.24

EN300-1703143_1_1_1



CID: EN300-1703143_1_1_1

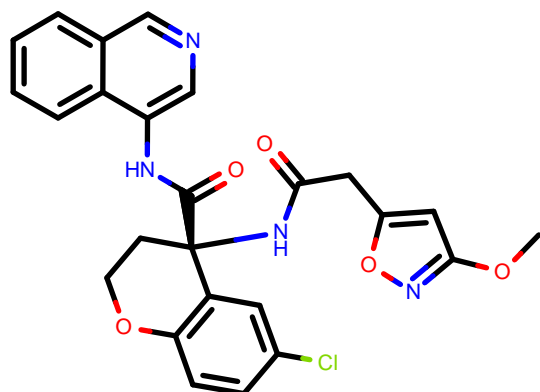
SMILES: CC(C)(C)c1nnn(n1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4053

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.35

EN300-127197_1_1_1



CID: EN300-127197_1_1_1

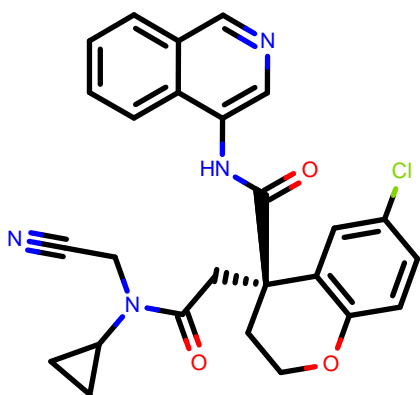
SMILES: COc1cc(on1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3342

DDG (kcal/mol): -1.29

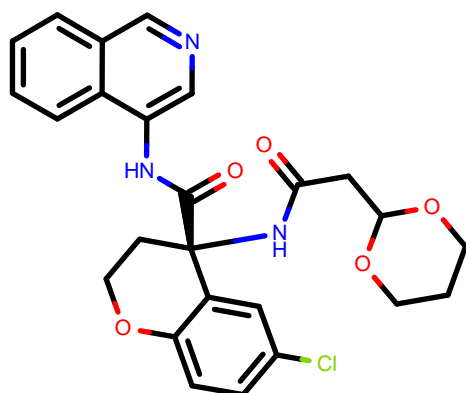
dDDG (kcal/mol): 0.30

EDG-MED-ba1ac7b9-8_1



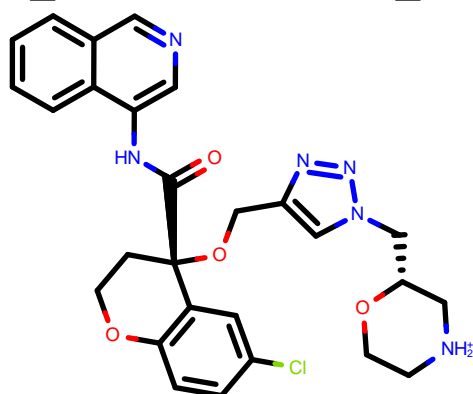
CID:	EDG-MED-ba1ac7b9-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(CC#N)C5CC5</chem>
RUN:	RUN2508
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.25

EN300-157502_1_1_1



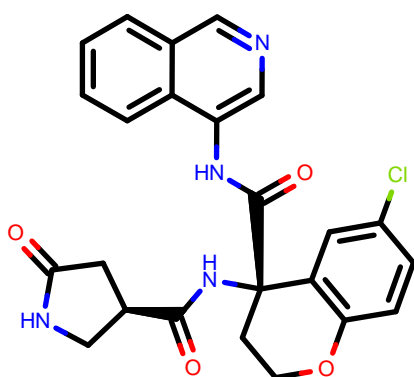
CID:	EN300-157502_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5OCCO5</chem>
RUN:	RUN4431
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.26

ED_-GRI-5b13fbe2-7_1



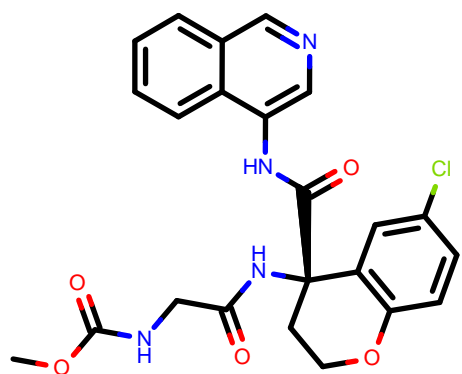
CID:	ED_-GRI-5b13fbe2-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5n(m5)C[C@@]6CNC(=O)N6</chem>
RUN:	RUN1433
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.34

EN300-59487_1_1_1



CID:	EN300-59487_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4CNC(=O)N4</chem>
RUN:	RUN3271
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.21

EN300-50009_1_1_1



CID: EN300-50009_1_1_1

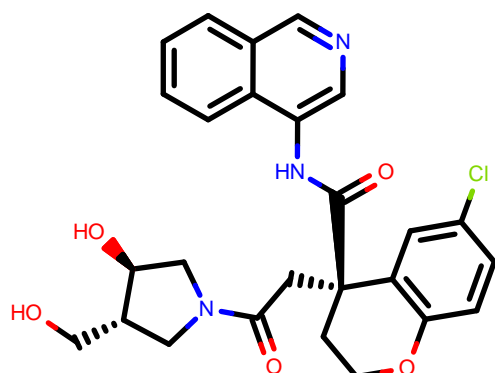
SMILES: COC(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4406

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EN300-248521_1_3_1



CID: EN300-248521_1_3_1

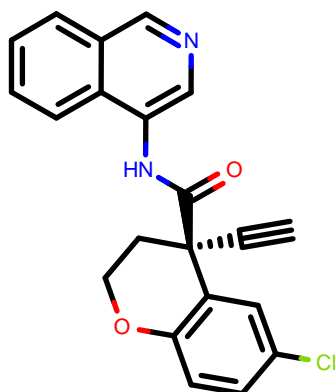
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)O)CO

RUN: RUN4655

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

PET-UNK-29afea89-1_1_1



CID: PET-UNK-29afea89-1_1_1

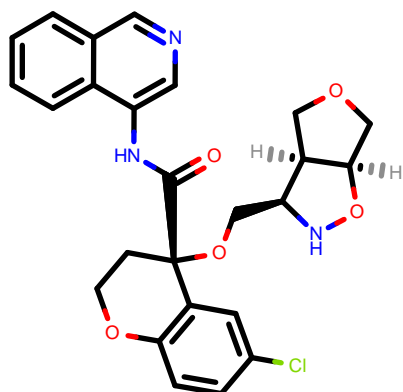
SMILES: C#C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5057

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.11

EN300-7436306_1_1_2



CID: EN300-7436306_1_1_2

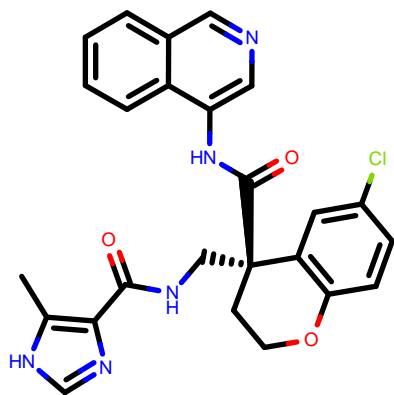
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5[C@@H]6COC[C@H]6ON5

RUN: RUN5302

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.23

EN300-266736_2_1_1



CID: EN300-266736_2_1_1

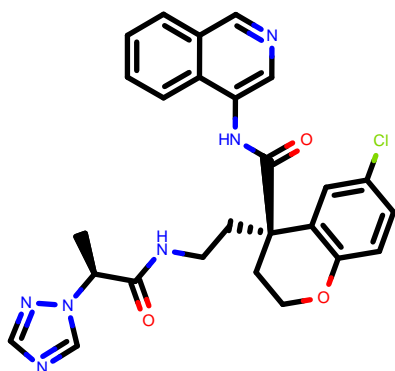
SMILES: Cc1c[nH]1C(=O)NC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4491

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.25

EN300-30397_3_1_1



CID: EN300-30397_3_1_1

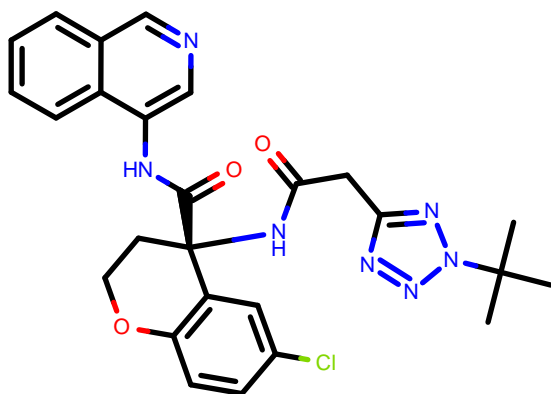
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5nnn5

RUN: RUN3564

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.30

EN300-297927_1_1_1



CID: EN300-297927_1_1_1

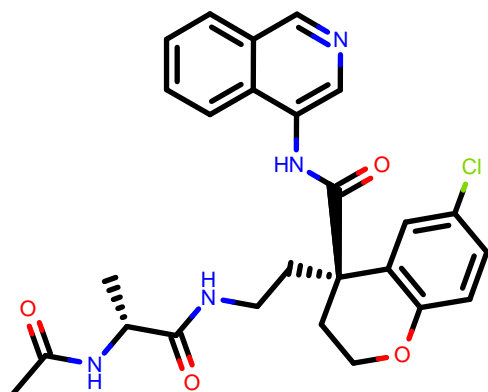
SMILES: CC(C)(C)n1nc(n1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4264

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.28

EN300-18569_3_2_1



CID: EN300-18569_3_2_1

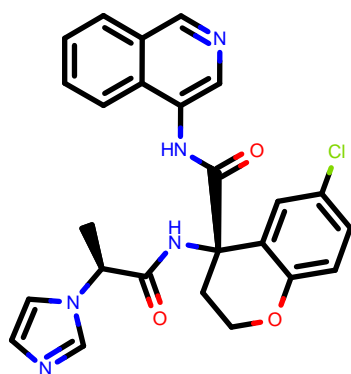
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C

RUN: RUN6361

DDG (kcal/mol): -1.28

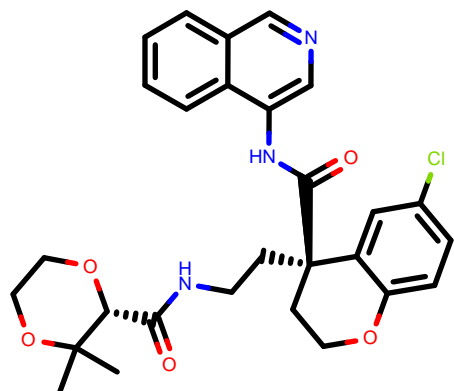
dDDG (kcal/mol): 0.30

EDG-MED-90036822-60_1



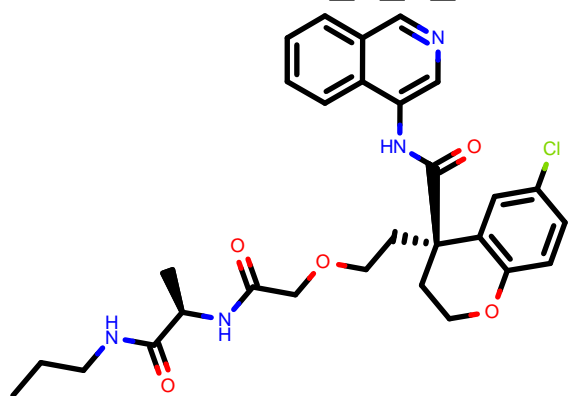
CID:	EDG-MED-90036822-60_1
SMILES:	<chem>C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)n5ccn5</chem>
RUN:	RUN1596
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.23

EN300-1601684_3_2_1



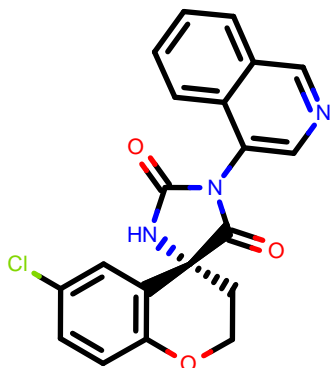
CID:	EN300-1601684_3_2_1
SMILES:	<chem>CC1([C@H](OCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)C</chem>
RUN:	RUN4810
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.32

EN300-23214_3_1_1



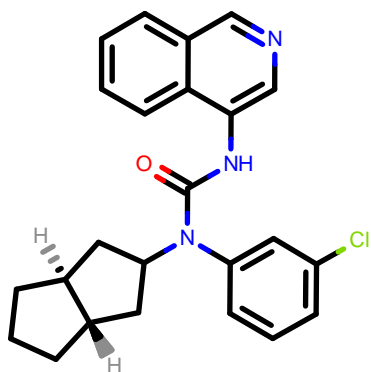
CID:	EN300-23214_3_1_1
SMILES:	<chem>CCCNC(=O)[C@@H](C)NC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4</chem>
RUN:	RUN4449
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.49

VLA-UNK-cf7facf1-1_1



CID:	VLA-UNK-cf7facf1-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN2164
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.24

MIC-UNK-cdc2493e-4_3



CID: MIC-UNK-cdc2493e-4_3

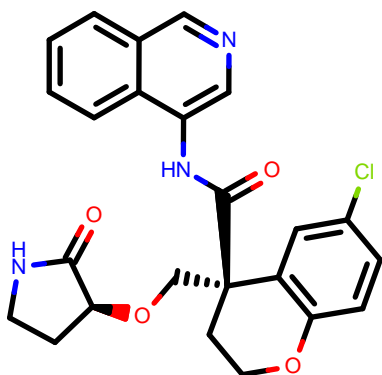
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C4C[C@@H]5CCCC[C@H]5C4

RUN: RUN448

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.29

EN300-6736413_2_2_1



CID: EN300-6736413_2_2_1

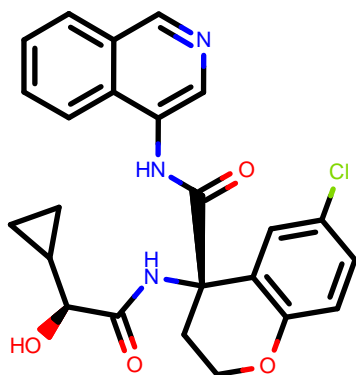
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O

RUN: RUN3572

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.21

EN300-72211_1_2_1



CID: EN300-72211_1_2_1

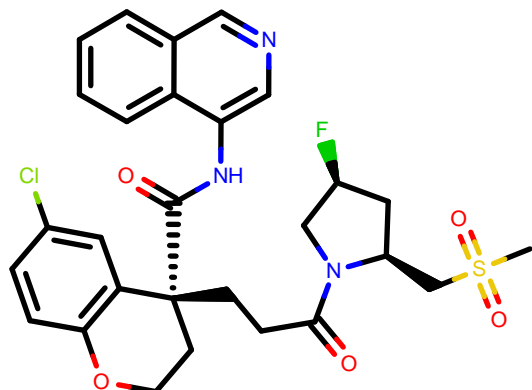
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCS5=O

RUN: RUN4252

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.27

EN300-1702864_2_1_1



CID: EN300-1702864_2_1_1

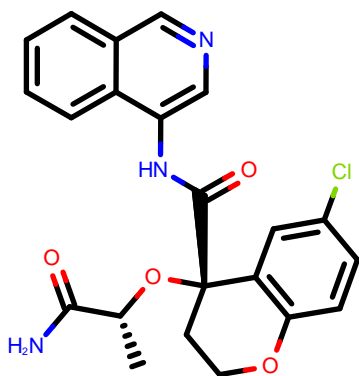
SMILES: CS(=O)(=O)C[C@H]1CC(F)N1C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C1=O)Nc4ncnc5ccc45F

RUN: RUN7479

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.31

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

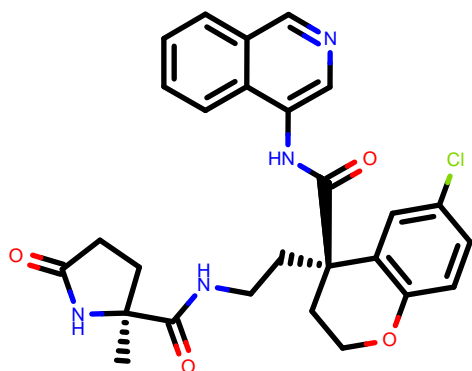
SMILES: C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN6234

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.19

EN300-177118_3_2_1



CID: EN300-177118_3_2_1

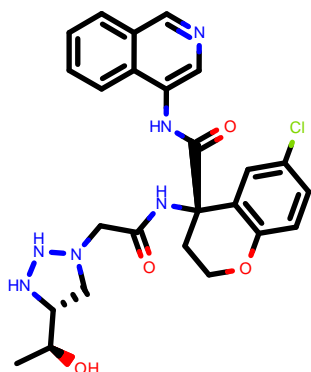
SMILES: C[C@]1(CCC(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3391

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.31

EN300-109540_1_1_1



CID: EN300-109540_1_1_1

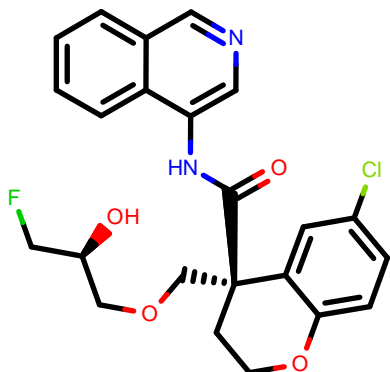
SMILES: C[C@H](c1cn(nn1)CC(=O)N)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5O

RUN: RUN4098

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.28

EN300-1968342_2_1_1



CID: EN300-1968342_2_1_1

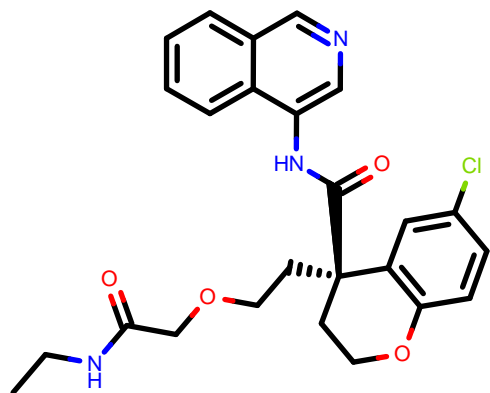
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O

RUN: RUN6326

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.29

EN300-7003350_3_1_1



CID: EN300-7003350_3_1_1

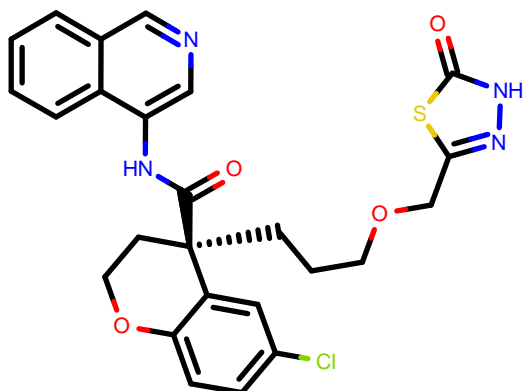
SMILES: CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4249

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.22

EN300-171766_4_1_1



CID: EN300-171766_4_1_1

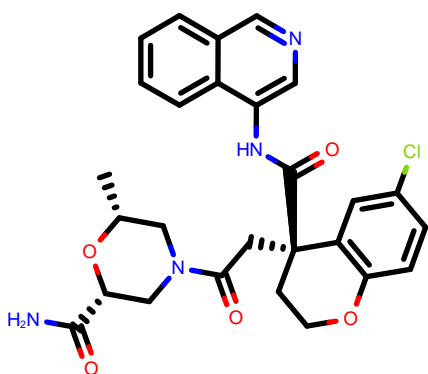
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5n[nH]c(=O)s5

RUN: RUN3798

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.36

EN300-295905_1_1_1



CID: EN300-295905_1_1_1

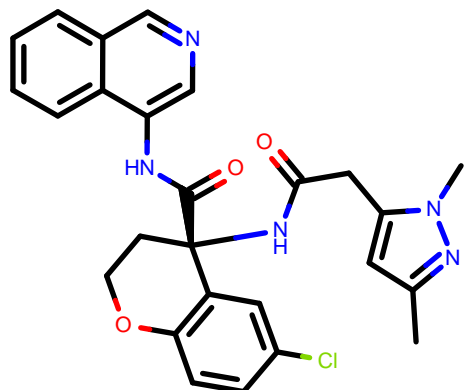
SMILES: C[C@@H]1CN[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3061

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.31

EN300-6499639_1_1_1



CID: EN300-6499639_1_1_1

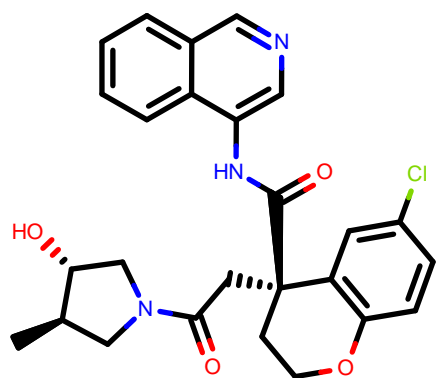
SMILES: CC1=N[N@]1[C@@H](C1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5C

RUN: RUN5343

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.26

EN300-124052_1_3_1



CID: EN300-124052_1_3_1

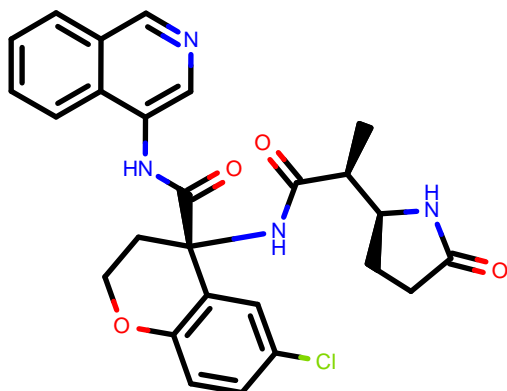
SMILES: C[C@@H]1CN(C[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN5608

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.26

EN300-249421_1_1_1



CID: EN300-249421_1_1_1

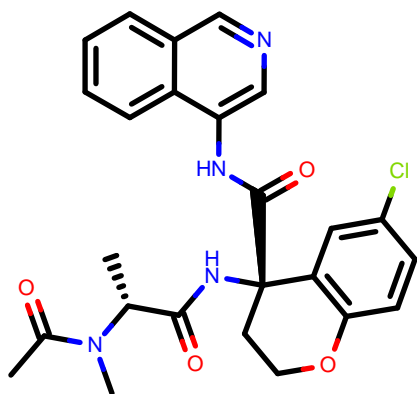
SMILES: C[C@@H]1[C@@H]1CCC(=O)N1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN4788

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.27

EN300-863933_1_2_1



CID: EN300-863933_1_2_1

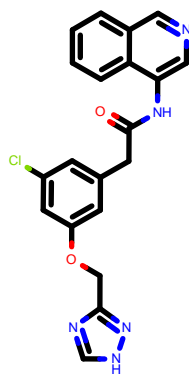
SMILES: C[C@H]1C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4N(C)C(=O)C

RUN: RUN3534

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.30

RAL-THA-1d44ff04-2_1



CID: RAL-THA-1d44ff04-2_1

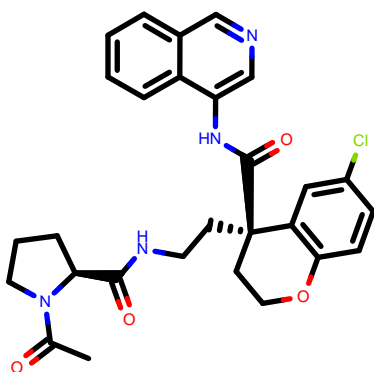
SMILES: c1ccc2c(c1)cnc2NC(=O)CC3cc(cc(c3)Cl)OCc4[nH]n4

RUN: RUN394

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.33

EN300-12587_3_2_1



CID: EN300-12587_3_2_1

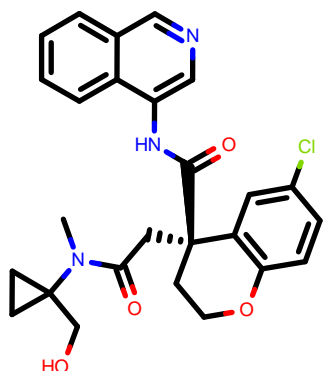
SMILES: CC(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5589

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.31

EN300-211403_1_1_1



CID: EN300-211403_1_1_1

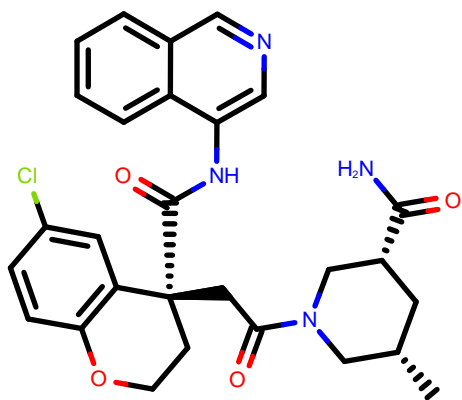
SMILES: CN(C(=O)C[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncoc4c3ccoc4)C5(C)C5)CO

RUN: RUN7698

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.34

EN300-1724086_1_4_1



CID: EN300-1724086_1_4_1

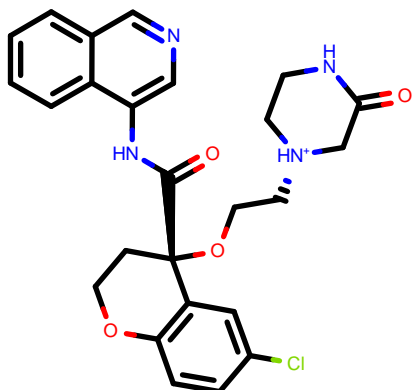
SMILES: C[C@H]1C[C@H](CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5)C(=O)N

RUN: RUN3731

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.29

ED_-GRI-5b13fbe2-31_1



CID: ED_-GRI-5b13fbe2-31_1

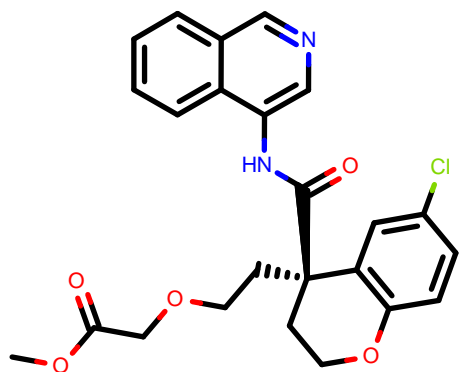
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCC[N@@H]5CCNC(=O)C5

RUN: RUN1424

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.40

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

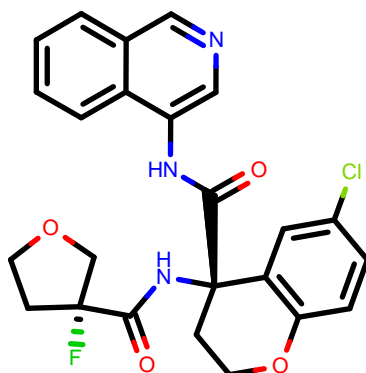
SMILES: COC(=O)COCC[C@@]1(COC(=O)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN3957

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.21

EN300-188356_1_2_1



CID: EN300-188356_1_2_1

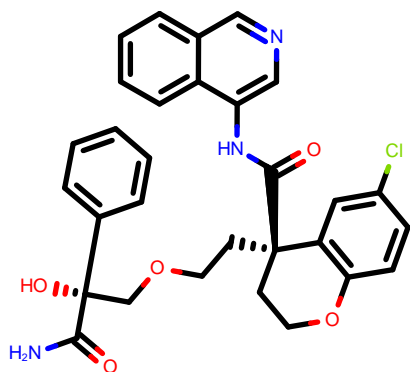
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)F

RUN: RUN3811

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.31

EN300-248526_3_1_1



CID: EN300-248526_3_1_1

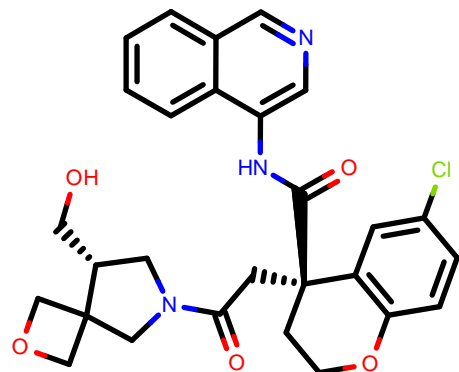
SMILES: c1ccc(cc1)[C@@]1(COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N

RUN: RUN3881

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.39

EN300-395654_1_2_1



CID: EN300-395654_1_2_1

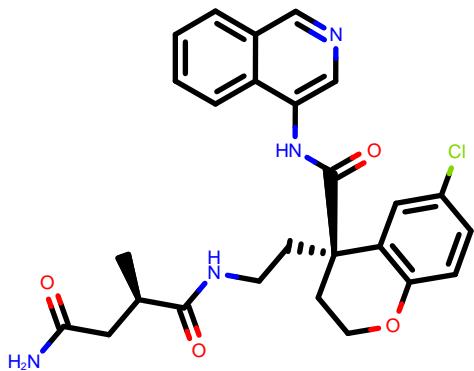
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C6(C5)COC6)CO

RUN: RUN4869

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.28

EN300-202757_3_2_1



CID: EN300-202757_3_2_1

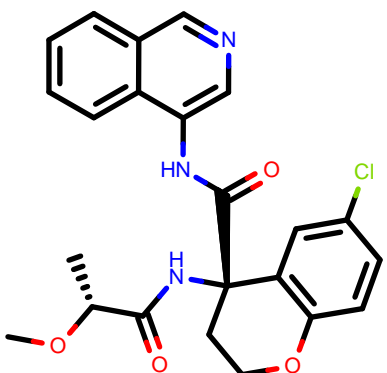
SMILES: C[C@H](CC(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5501

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.32

EN300-51257_1_2_1



CID: EN300-51257_1_2_1

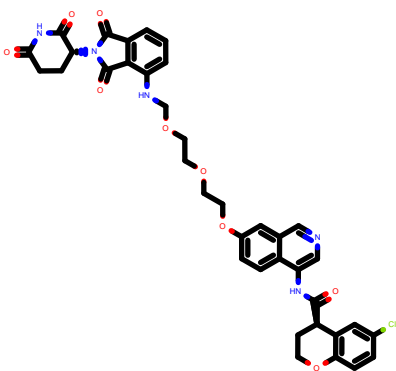
SMILES: C[C@H](C(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4OC

RUN: RUN3539

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.19

DAR-DIA-9e4459de-11_3



CID: DAR-DIA-9e4459de-11_3

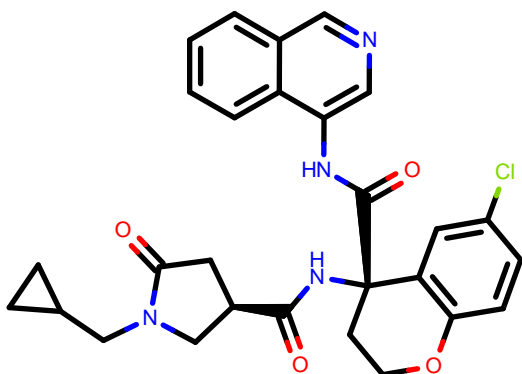
SMILES: c1cc2c(c1)NCOCCCCO3cc4c(c3)cmc4N[C@@](C@@H5COC6cc(cc6)Cl)c7c(c2O)C@@H7C(C)N(C7-O)O

RUN: RUN1375

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.39

EN300-31969_1_1_1



CID: EN300-31969_1_1_1

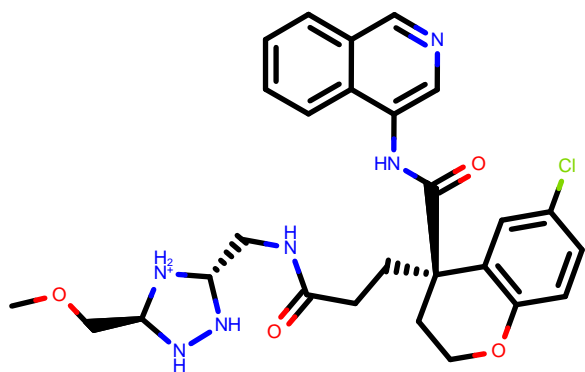
SMILES: c1cc2c(c1)cmc2N[C@@](C@@H3)C(CO4c4cc(cc4)N)N(C1=O)C@@H5C(C)N(C5)COC6C6

RUN: RUN7007

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.28

EN300-299390_2_1_2



CID: EN300-299390_2_1_2

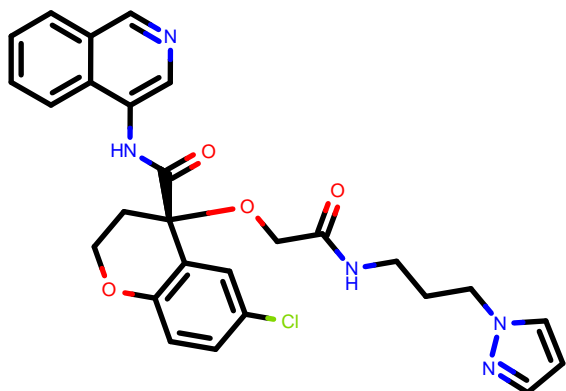
SMILES: COC[C@H]1[NH2]NHC(=O)[C@H](N1)CNC(=O)CC[C@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5273

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.71

EN300-47500_1_1_1



CID: EN300-47500_1_1_1

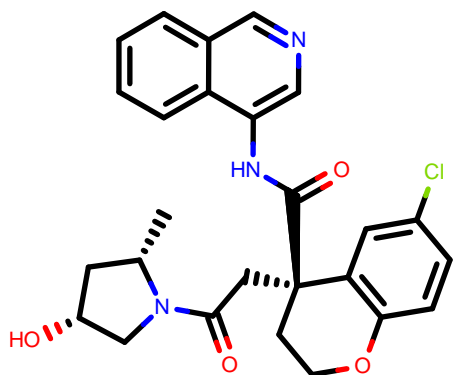
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]([C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N)CNC5ccn5

RUN: RUN4877

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.28

EN300-173562_1_4_1



CID: EN300-173562_1_4_1

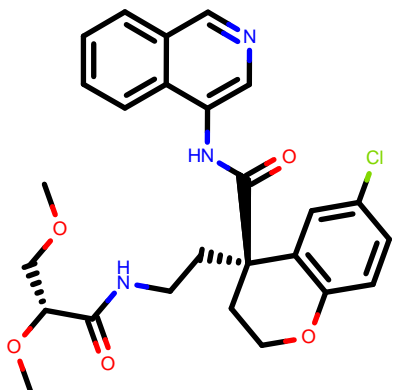
SMILES: C[C@H]1C[C@H](CN1C(=O)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN5677

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.27

EN300-305282_3_2_1



CID: EN300-305282_3_2_1

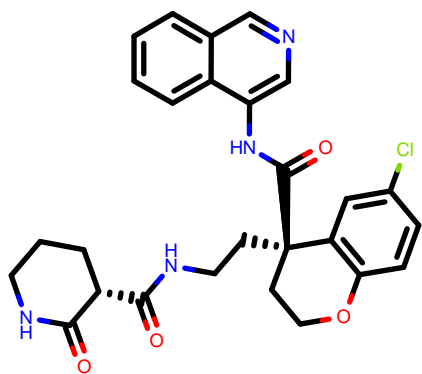
SMILES: COC[C@H](Cl(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)OC

RUN: RUN4541

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.42

EN300-82616_3_2_1



CID: EN300-82616_3_2_1

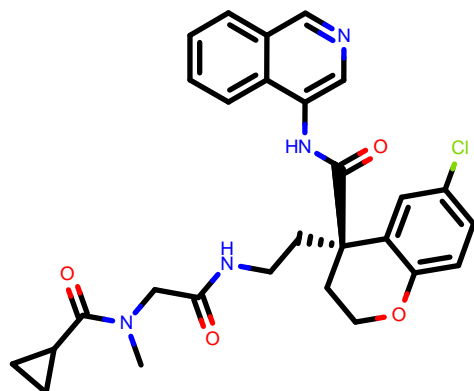
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H]5CCNC5=O

RUN: RUN4766

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.24

EN300-31146_3_1_1



CID: EN300-31146_3_1_1

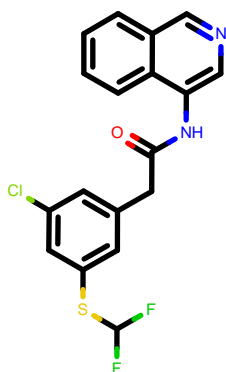
SMILES: CN(CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)C(=O)C5CC5

RUN: RUN5950

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.36

MIC-UNK-16ccb665-2_1



CID: MIC-UNK-16ccb665-2_1

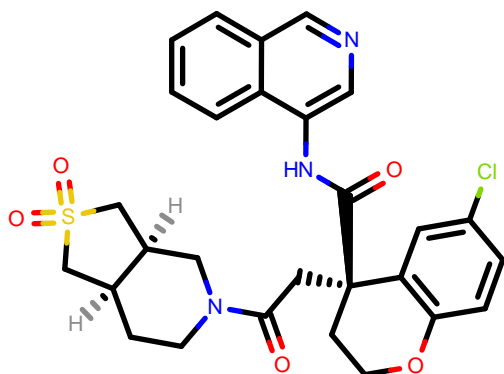
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)SC(F)F

RUN: RUN2183

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.32

ALP-UNI-76695c4f-4_4



CID: ALP-UNI-76695c4f-4_4

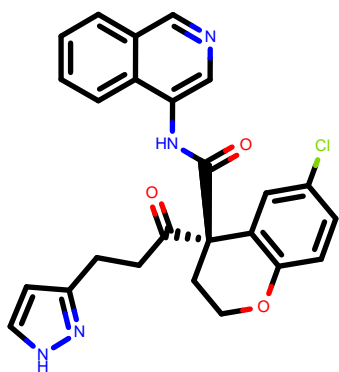
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSCC[C@@H]6CS(=O)(=O)C@H]6C

RUN: RUN2025

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.37

VLA-UCB-34f3ed0c-8_1



CID: VLA-UCB-34f3ed0c-8_1

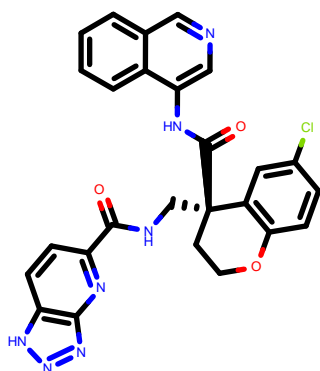
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]5

RUN: RUN584

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.28

EN300-133058_2_1_1



CID: EN300-133058_2_1_1

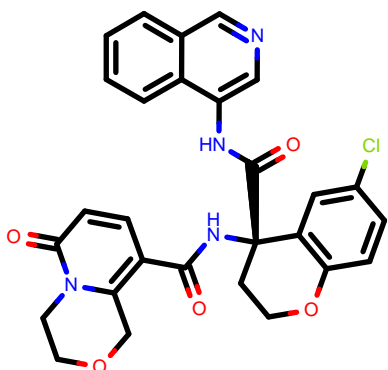
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CNC(=O)c5ccc6c(n5)[nH]6

RUN: RUN4716

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-7538678_1_1_1



CID: EN300-7538678_1_1_1

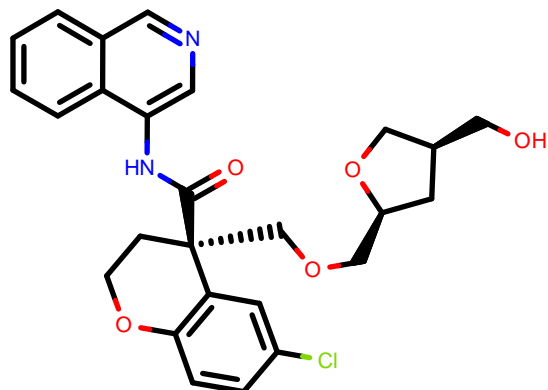
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)c5ccc(=O)n6c5COCC6

RUN: RUN5436

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-11_1



CID: EDJ-MED-fcba3f31-11_1

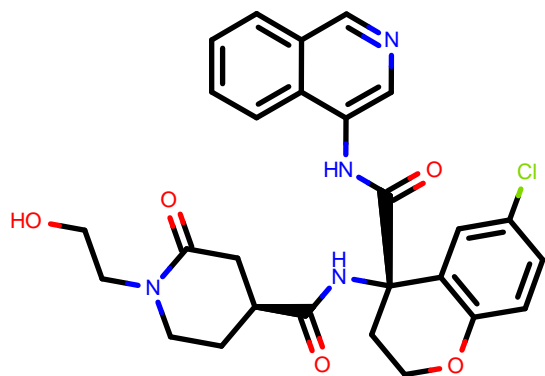
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C[C@@H](CO)CO

RUN: RUN2366

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.31

EN300-1723663_1_2_1



CID: EN300-1723663_1_2_1

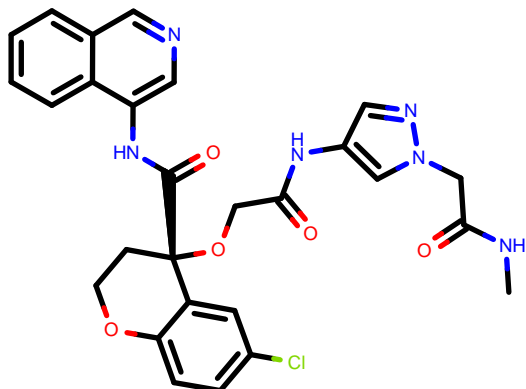
SMILES: c1ccc2c(c1)nc(=O)nc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCN(C(=O)C5)C5CO

RUN: RUN4753

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.33

EN300-48861_1_1_1



CID: EN300-48861_1_1_1

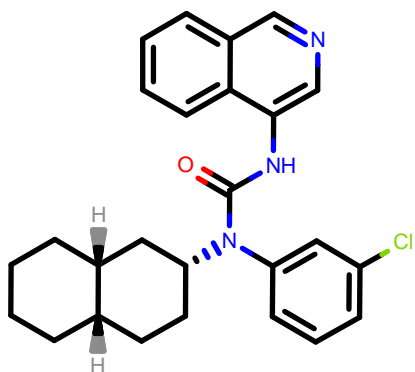
SMILES: CNC(=O)C[C@H]1cc(c[nH]1)NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5705

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

MIC-UNK-cdc2493e-8_1



CID: MIC-UNK-cdc2493e-8_1

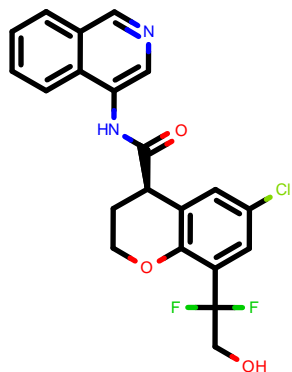
SMILES: c1ccc2c(c1)nc(=O)nc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@H]5CC[C@@]6(C)[C@H]5C4

RUN: RUN477

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.36

MIC-UNK-08fa0751-1_1



CID: MIC-UNK-08fa0751-1_1

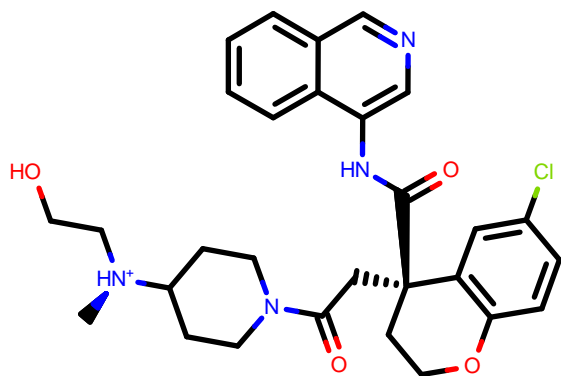
SMILES: c1ccc2c(c1)nc(=O)nc2NC(=O)[C@@H]3CCOC4c3cc(cc4C(CO)(F)F)Cl

RUN: RUN1368

DDG (kcal/mol): -1.26

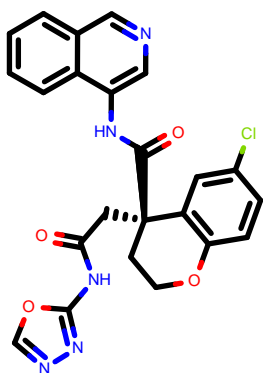
dDDG (kcal/mol): 0.18

EDG-MED-ba1ac7b9-28_3



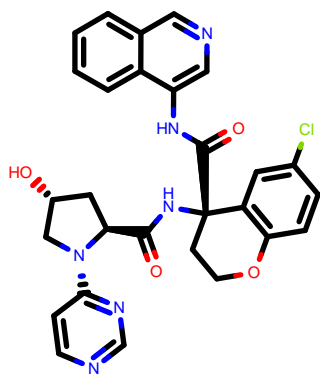
CID:	EDG-MED-ba1ac7b9-28_3
SMILES:	<chem>C[N+](H)(CCO)C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5</chem>
RUN:	RUN2570
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.66

CHO-MSK-a31cca77-1_1



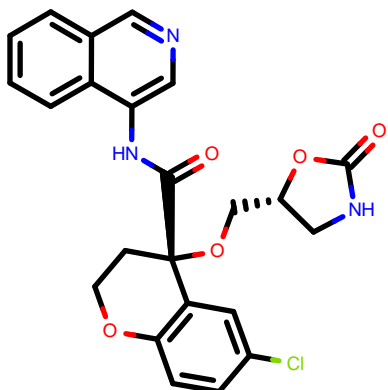
CID:	CHO-MSK-a31cca77-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnc5</chem>
RUN:	RUN2031
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.21

EN300-310022_1_3_1



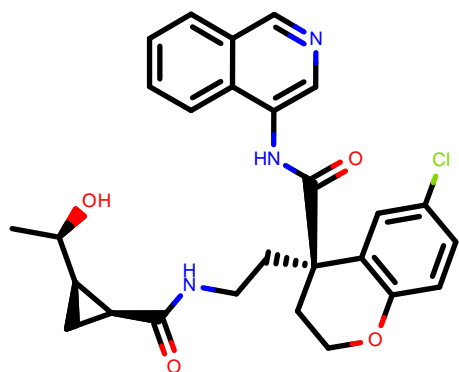
CID:	EN300-310022_1_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5C[C@@H](CN5c6ccccc6)O</chem>
RUN:	RUN4275
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.38

EN300-203293_1_2_1



CID:	EN300-203293_1_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CNC(=O)O5</chem>
RUN:	RUN6620
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.29

EN300-6729572_3_2_1



CID: EN300-6729572_3_2_1

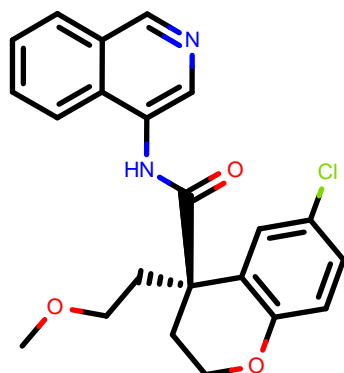
SMILES: C[C@@H](C@@[H]1C[C@@[H]1C(=O)NCC)C(=O)Nc2ccc3c2c(cc3)C(C)C(=O)Nc4nc5c4ccc5O

RUN: RUN5048

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EDJ-MED-28ec730d-2_1_1



CID: EDJ-MED-28ec730d-2_1_1

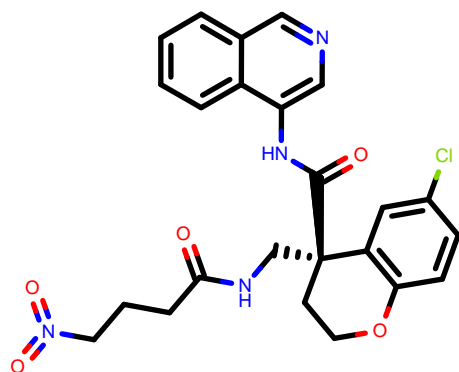
SMILES: COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN4133

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.16

EN300-143449_2_1_1



CID: EN300-143449_2_1_1

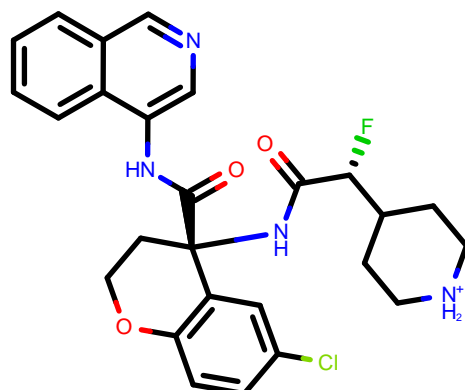
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6=O

RUN: RUN5160

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EDG-MED-90036822-95_1



CID: EDG-MED-90036822-95_1

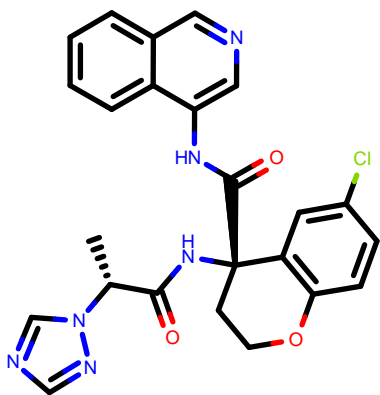
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6[nH+]c5c6F

RUN: RUN1669

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.30

EN300-30397_1_2_1



CID: EN300-30397_1_2_1

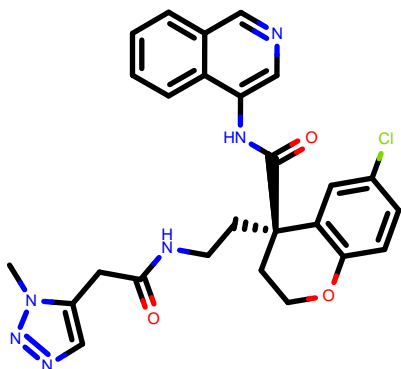
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)n5cncn5

RUN: RUN4615

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-6486855_3_1_1



CID: EN300-6486855_3_1_1

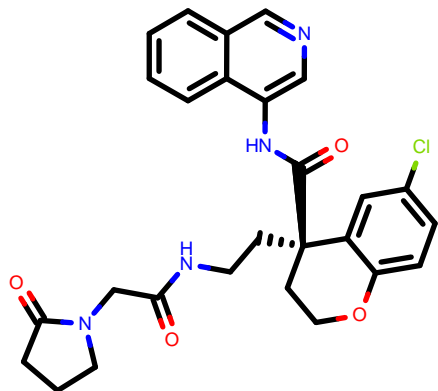
SMILES: Cn1c(cnn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN5021

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EN300-11934_3_1_1



CID: EN300-11934_3_1_1

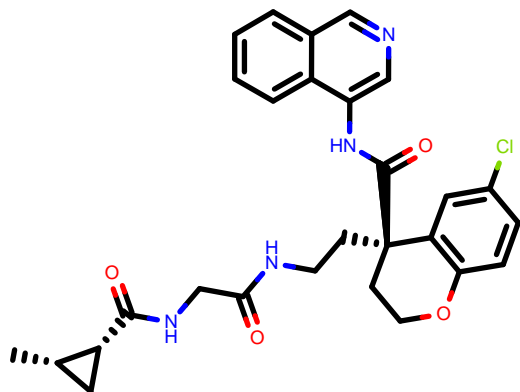
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)N5CCCC5=O

RUN: RUN4770

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.28

EN300-30768_3_4_1



CID: EN300-30768_3_4_1

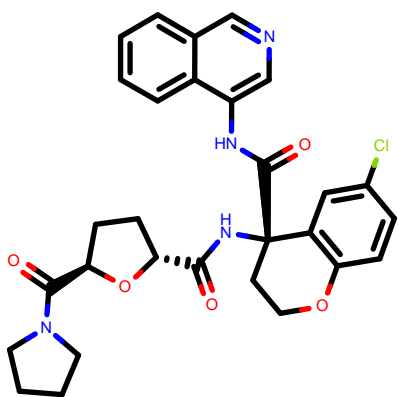
SMILES: C[C@H]1C[C@H]1C(=O)NCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN6496

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

ALP-UNI-dbbfd3db-6_2



CID: ALP-UNI-dbbfd3db-6_2

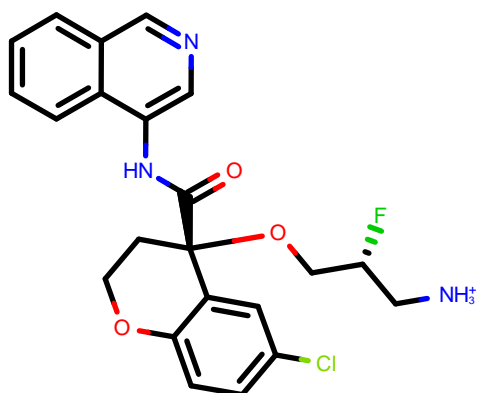
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)N)C(=O)C@H5CC(C@@H)O5C1=O

RUN: RUN2641

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.34

ED_-GRI-5b13fbe2-41_1



CID: ED_-GRI-5b13fbe2-41_1

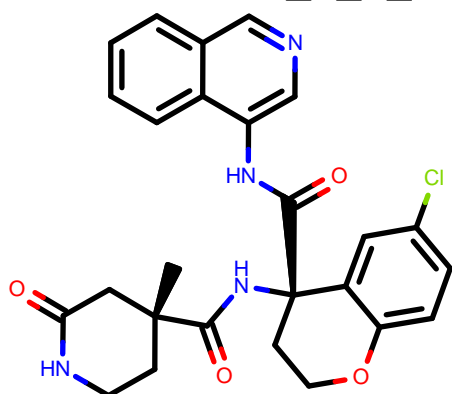
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)N)C(=O)C@H5C(NH3+)F

RUN: RUN1435

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.45

EN300-315854_1_2_1



CID: EN300-315854_1_2_1

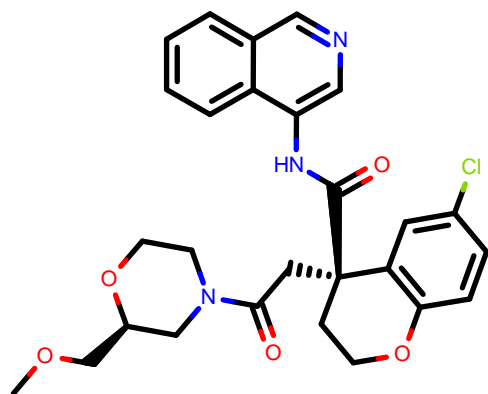
SMILES: C[C@]1(C)CNC(=O)C1C(=O)N[C@@H]2[C@@H](COC3=CC=C(C=C3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN5066

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-6742996_1_1_1



CID: EN300-6742996_1_1_1

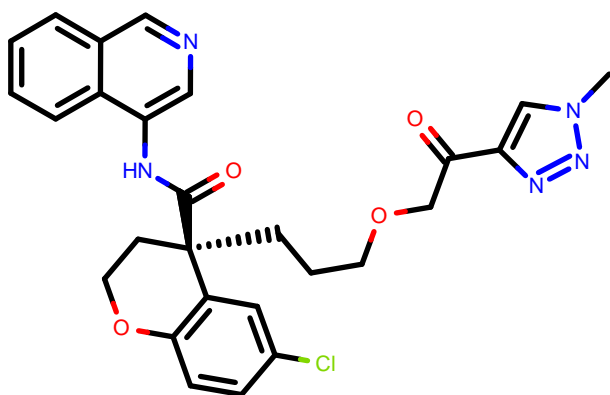
SMILES: COC[C@@H]1CN(CCO1)C(=O)C[C@@H]2[C@@H](COC3=CC=C(C=C3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN4738

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.33

EN300-263153_4_1_1



CID: EN300-263153_4_1_1

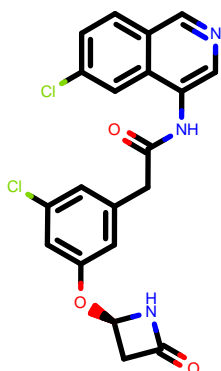
SMILES: Cn1cc(nn1)C(=O)COC(C)C@2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN6507

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.33

ALF-EVA-0b412456-1_1



CID: ALF-EVA-0b412456-1_1

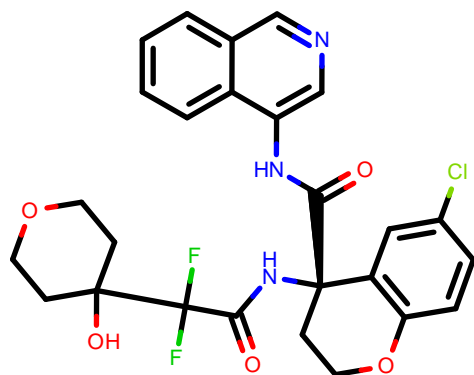
SMILES: c1cc2nccc(c2cc1Cl)NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN2535

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.34

EN300-706065_1_1_1



CID: EN300-706065_1_1_1

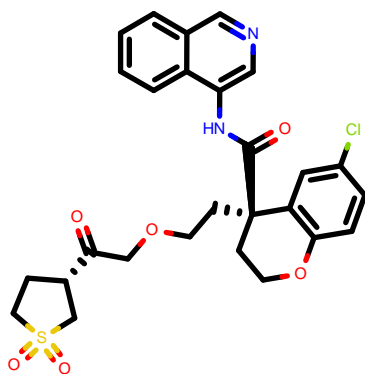
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(C5(COCC5)O)(F)F

RUN: RUN4503

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-226314_3_2_1



CID: EN300-226314_3_2_1

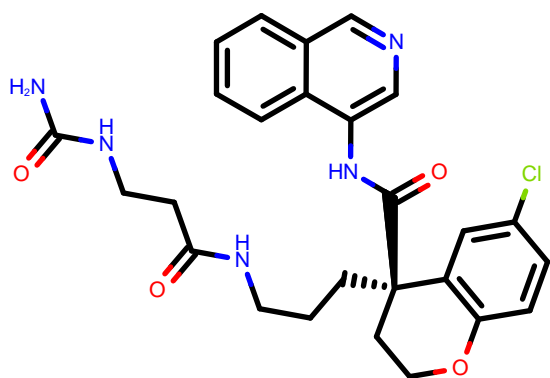
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@@H]5SCCS(=O)(=O)C5

RUN: RUN3142

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-10729_4_1_1



CID: EN300-10729_4_1_1

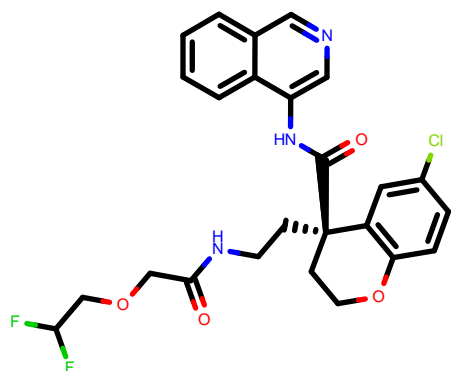
SMILES: c1ccc2c(e1)ncoc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCNC(=O)N

RUN: RUN7051

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-315792_3_1_1



CID: EN300-315792_3_1_1

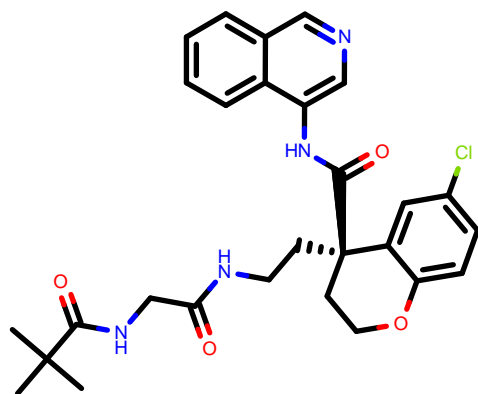
SMILES: c1ccc2c(e1)ncoc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COCC(F)F

RUN: RUN4646

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-12247_3_1_1



CID: EN300-12247_3_1_1

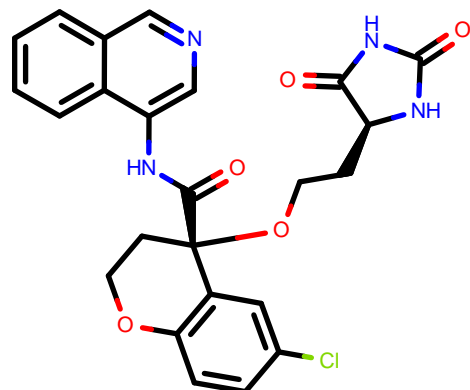
SMILES: CC(C)(C)C(=O)NCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN6994

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.27

EN300-6498856_1_2_1



CID: EN300-6498856_1_2_1

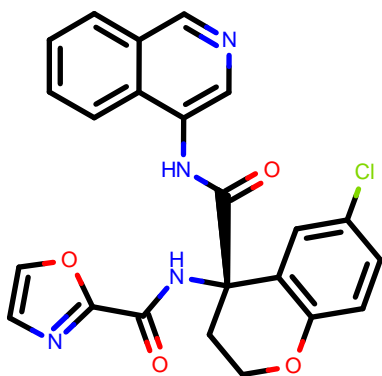
SMILES: c1ccc2c(e1)ncoc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OCC[C@H]5C(=O)NC(=O)N5

RUN: RUN4350

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.26

EN300-318344_1_1_1



CID: EN300-318344_1_1_1

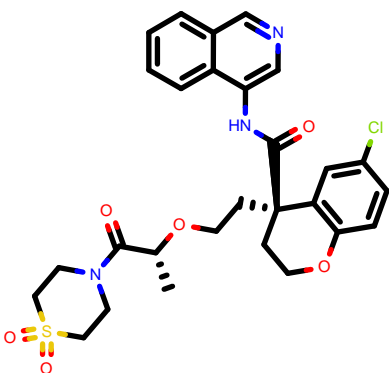
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nccc5

RUN: RUN5197

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.20

EN300-1265949_3_2_1



CID: EN300-1265949_3_2_1

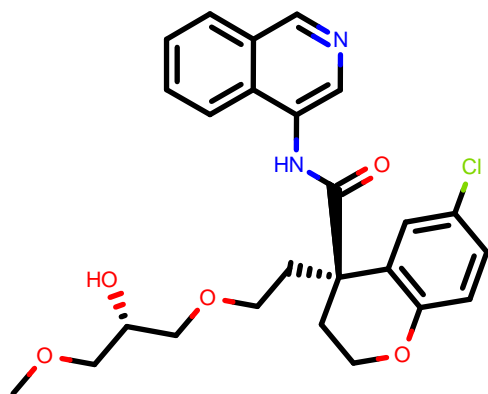
SMILES: C[C@H](C(=O)N1CCS(=O)(=O)CC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN5504

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.34

EN300-1915260_3_1_1



CID: EN300-1915260_3_1_1

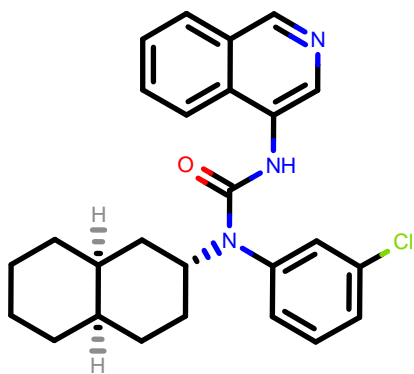
SMILES: COC[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN4908

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.43

MIC-UNK-cdc2493e-8_7



CID: MIC-UNK-cdc2493e-8_7

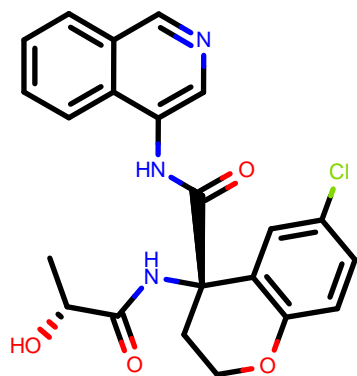
SMILES: c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@H]5CCCC[C@H]5C4

RUN: RUN506

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.39

EN300-19542_1_2_1



CID: EN300-19542_1_2_1

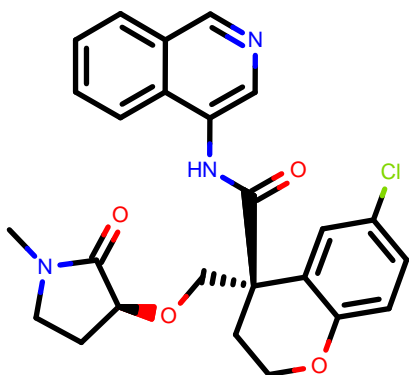
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN5118

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.19

EN300-98648_2_1_1



CID: EN300-98648_2_1_1

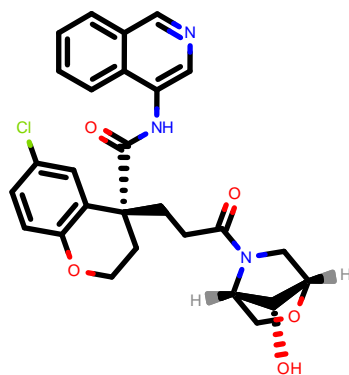
SMILES: CN1CC[C@@H](C1=O)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3693

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.21

EN300-6493060_2_1_1



CID: EN300-6493060_2_1_1

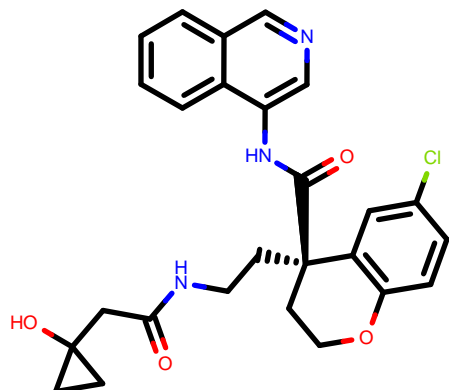
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H](C)C[C@@H]5O6

RUN: RUN6809

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-207873_3_1_1



CID: EN300-207873_3_1_1

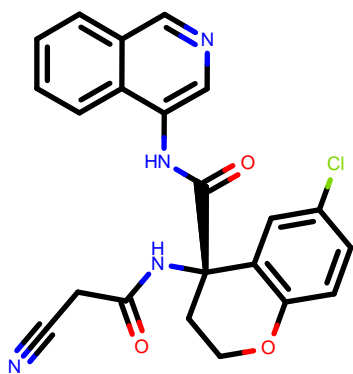
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CCNC(=O)CC5(C)CC5)O

RUN: RUN6695

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.26

EDG-MED-90036822-56_1



CID: EDG-MED-90036822-56_1

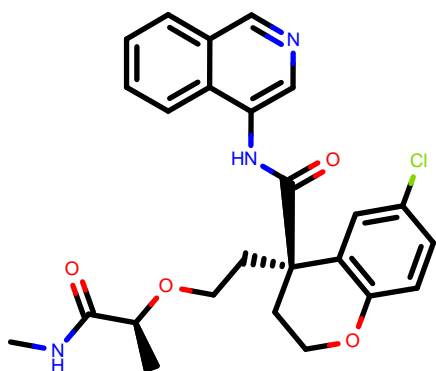
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC#N

RUN: RUN1571

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.15

EN300-211482_3_1_1



CID: EN300-211482_3_1_1

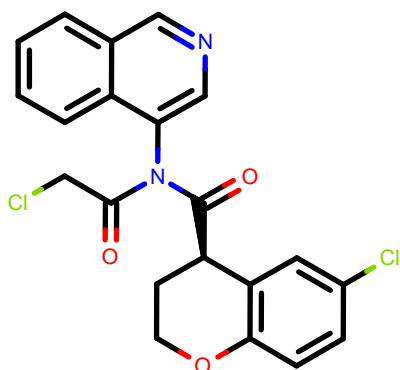
SMILES: C[C@@H](C(=O)NC)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN5042

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.26

VLA-UCB-50c39ae8-6_1_1



CID: VLA-UCB-50c39ae8-6_1_1

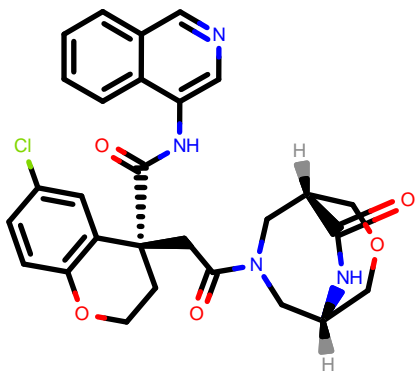
SMILES: c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN3495

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.23

EN300-6477207_1_1_1



CID: EN300-6477207_1_1_1

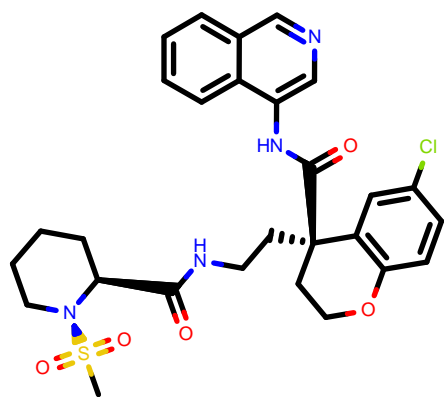
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@@H]6COCC[C@H]5NOC6=O

RUN: RUN5312

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.45

EN300-24014_3_2_1



CID: EN300-24014_3_2_1

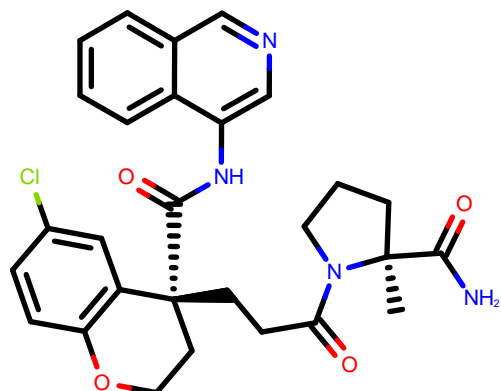
SMILES: CS(=O)(=O)N@1CCCCC@H1C(=O)NC(C)@2(COC3C2cc(c3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN5144

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.50

EN300-1697763_2_1_1



CID: EN300-1697763_2_1_1

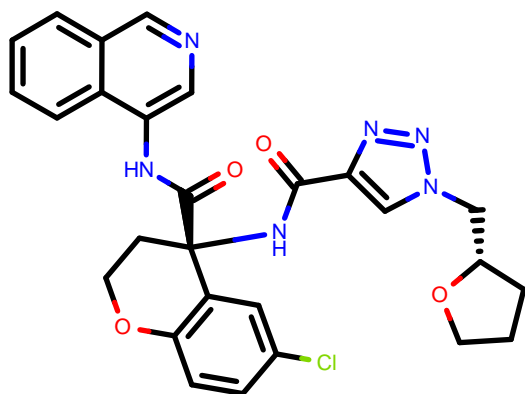
SMILES: ClC@1(CCCN1C(=O)CC(C)@2(CCOc3c2cc(c3)Cl)C(=O)Nc4nc5c4ccc5)C(=O)N

RUN: RUN7127

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.34

EN300-368758_1_1_1



CID: EN300-368758_1_1_1

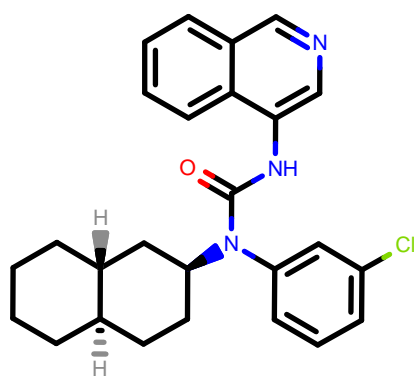
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3(CCOc4c3cc(c4)Cl)NC(=O)c5cn(n5)C(C)@H]6CCCC6

RUN: RUN7110

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.26

MIC-UNK-cdc2493e-8_4



CID: MIC-UNK-cdc2493e-8_4

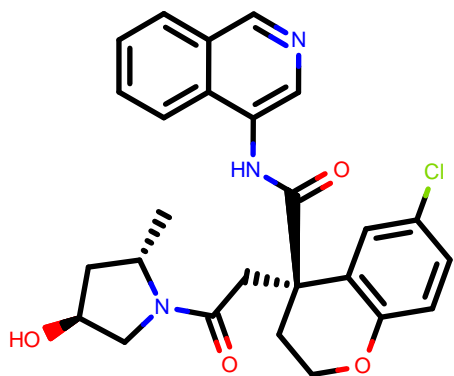
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C@H4CC(C)@H5CCCC(C)@H]5C4

RUN: RUN458

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.53

EN300-173562_1_2_1



CID: EN300-173562_1_2_1

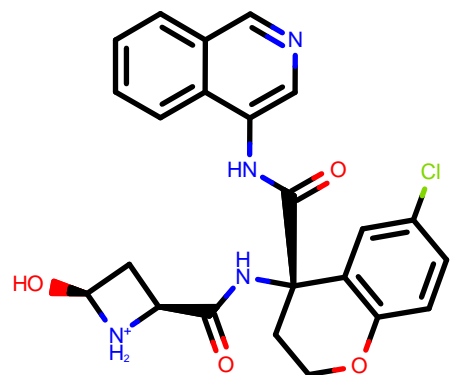
SMILES: C[C@H]1C[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN6846

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.24

EN300-103219_1_1_1



CID: EN300-103219_1_1_1

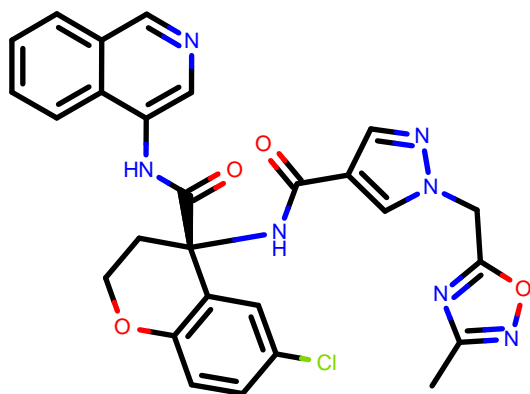
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC(=O)N5

RUN: RUN4934

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.24

EN300-135310_1_1_1



CID: EN300-135310_1_1_1

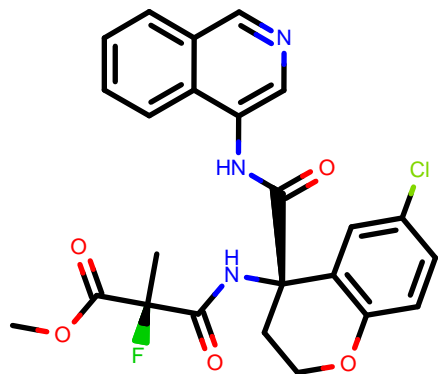
SMILES: Cc1nc(nc1)Cn2cc(nc2)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cnc6c5cnc6

RUN: RUN4308

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.29

EN300-7464289_1_2_1



CID: EN300-7464289_1_2_1

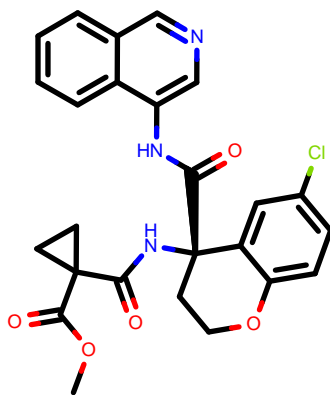
SMILES: C[C@@](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4)C(=O)OC)F

RUN: RUN3541

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.24

EN300-138787_1_1_1



CID: EN300-138787_1_1_1

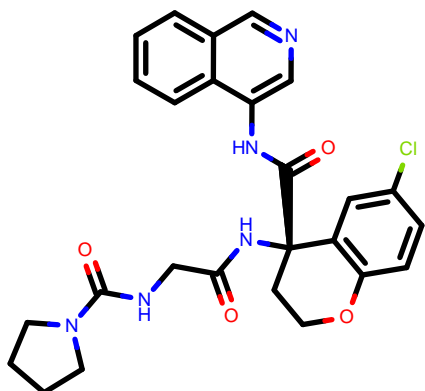
SMILES: COC(=O)C1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN4165

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.21

EN300-383906_1_1_1



CID: EN300-383906_1_1_1

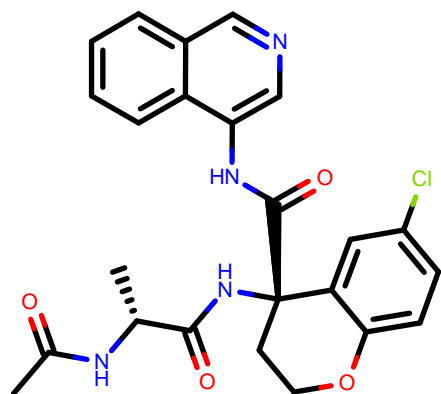
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Nc5ccccc5

RUN: RUN7375

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.30

EN300-18569_1_2_1



CID: EN300-18569_1_2_1

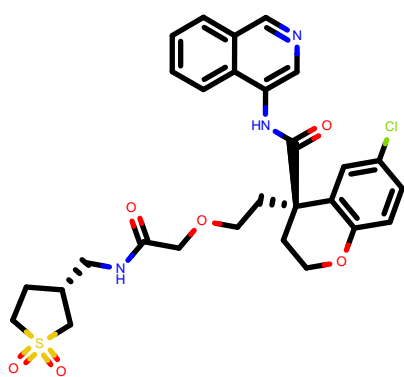
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccccc4)NC(=O)C

RUN: RUN3843

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.22

EN300-47606_3_2_1



CID: EN300-47606_3_2_1

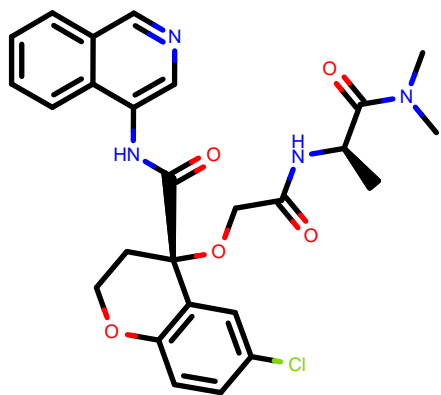
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N[C@@]5(CCS(=O)(=O)C)C5

RUN: RUN5974

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.35

EN300-47657_1_2_1



CID: EN300-47657_1_2_1

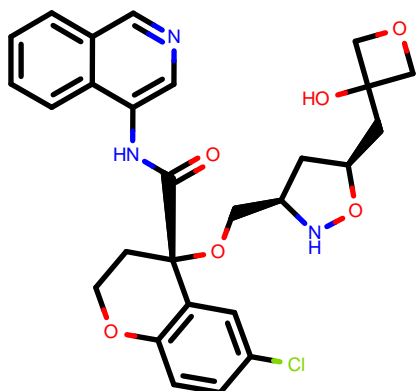
SMILES: C[C@H](C(=O)N(C)C)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4

RUN: RUN4367

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.33

EN300-7457160_1_1_2



CID: EN300-7457160_1_1_2

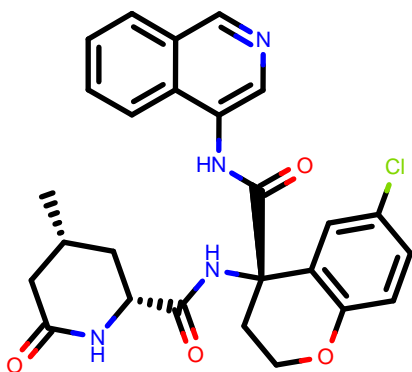
SMILES: c1ccc2c(c1)ncn2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5[C@@H]ON5C6(COC6)O

RUN: RUN6457

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.34

EN300-345656_1_1_1



CID: EN300-345656_1_1_1

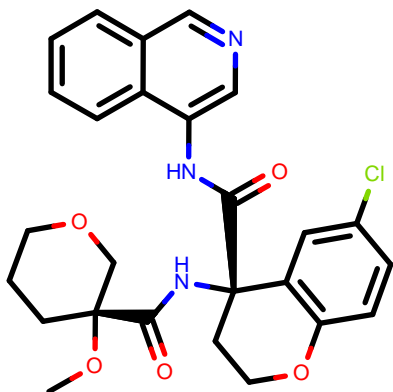
SMILES: C[C@@H]1C[C@@H](NC(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN5566

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.27

EN300-1072199_1_1_1



CID: EN300-1072199_1_1_1

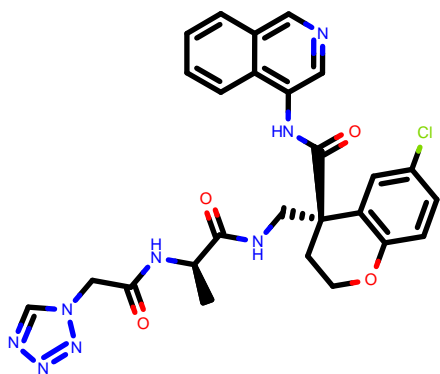
SMILES: CO[C@@]1(CCCOC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN3077

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.27

EN300-649743_2_1_1



CID: EN300-649743_2_1_1

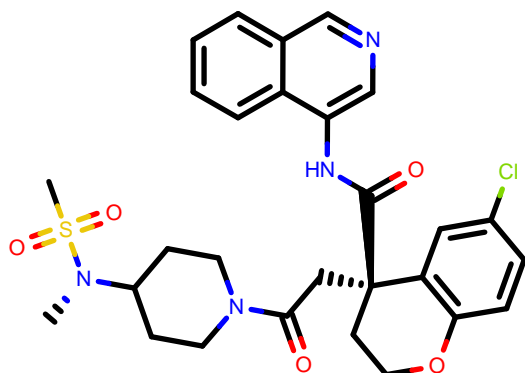
SMILES: C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4)NC(=O)Cn5nnn5

RUN: RUN4107

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.41

ALP-UNI-76695c4f-8_1



CID: ALP-UNI-76695c4f-8_1

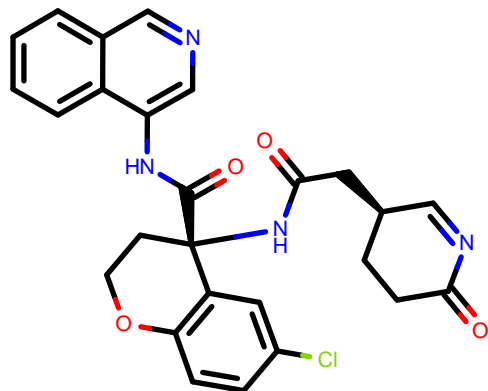
SMILES: C[N@]1(C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5)S(=O)(=O)C

RUN: RUN2049

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.25

EN300-246992_1_1_1



CID: EN300-246992_1_1_1

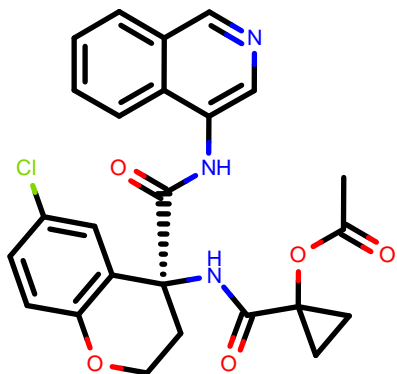
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5H5CCC(=O)NC5

RUN: RUN6915

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.31

EN300-173023_1_1_1



CID: EN300-173023_1_1_1

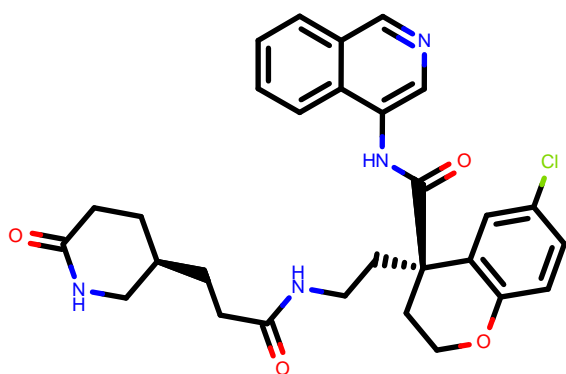
SMILES: CC(=O)OC1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN5028

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.33

EN300-1215738_3_1_1



CID: EN300-1215738_3_1_1

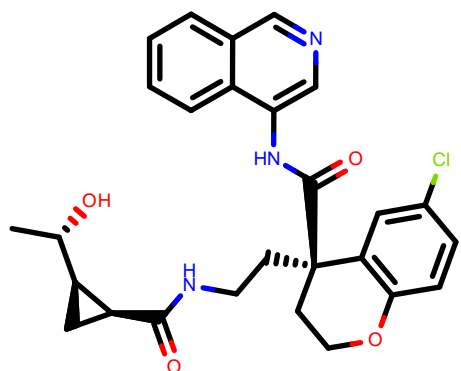
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4C=CC=C(C=C4)C)CCNC(=O)CC[C@@H]5CCCC(=O)NCS

RUN: RUN7058

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.33

EN300-6729572_3_1_1



CID: EN300-6729572_3_1_1

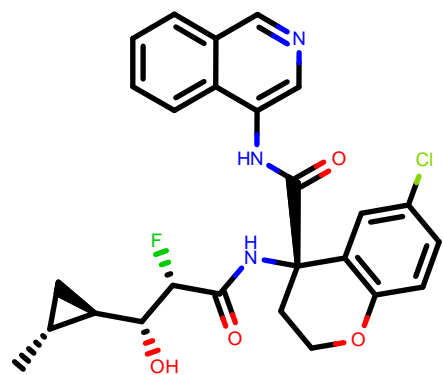
SMILES: C[C@@H]1[C@@H]2[C@@H]1[C@@]3[C@@H]2[C@@H]3C(=O)N[C@@]4[C@@]5C=CC=C(C=C5)C)C(=O)N4cnc5c4ccc5O

RUN: RUN4509

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.30

EDG-MED-90036822-94_7



CID: EDG-MED-90036822-94_7

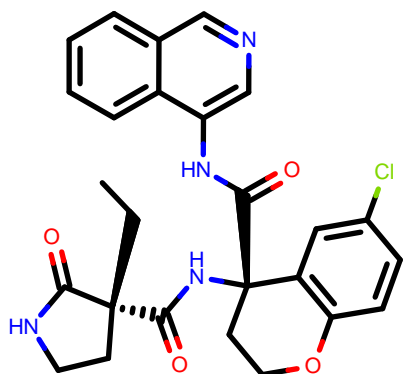
SMILES: C[C@@H]1[C@@H]2[C@@H]1[C@@]3[C@@H]2[C@@H]3C(=O)N[C@@]4[C@@]5C=CC=C(C=C5)C)C(=O)N4cnc5c4ccc5F

RUN: RUN1714

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.29

EN300-304135_1_2_1



CID: EN300-304135_1_2_1

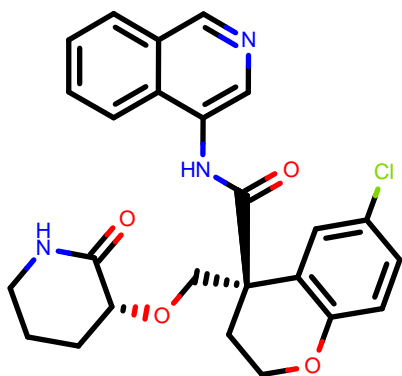
SMILES: CC[C@@]1(C)CNC1=O[C@@]2[C@@]3C=CC=C(C=C3)C)C(=O)N4cnc5c4ccc5S

RUN: RUN3708

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.29

EN300-107267_2_1_1



CID: EN300-107267_2_1_1

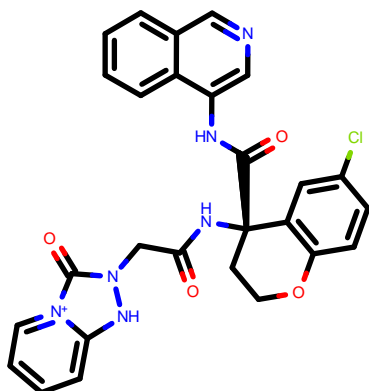
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC@H5CCCCN5=O

RUN: RUN3989

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.22

EN300-27476_1_1_1



CID: EN300-27476_1_1_1

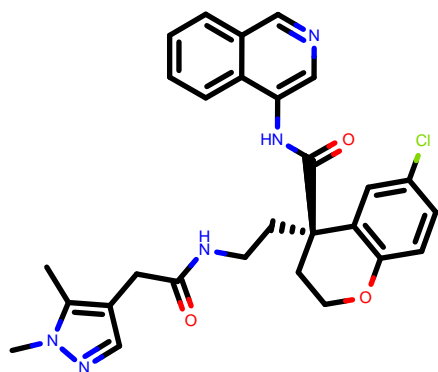
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6ccccc6n5

RUN: RUN5044

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.34

EN300-219437_3_1_1



CID: EN300-219437_3_1_1

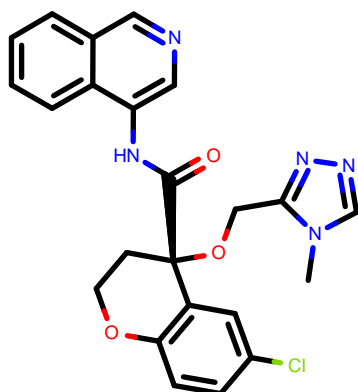
SMILES: Cc1c(cnn1C)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5806

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.29

EN300-113112_1_1_1



CID: EN300-113112_1_1_1

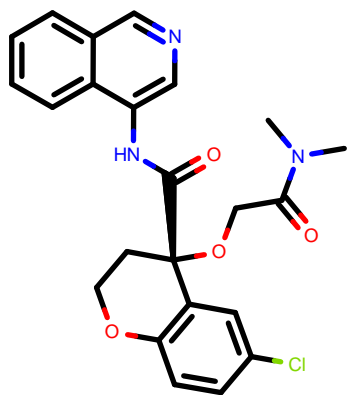
SMILES: Cn1cnnc1CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6428

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.20

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

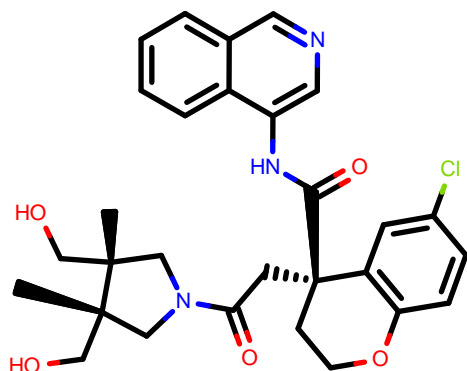
SMILES: CN(C)C(=O)CO[C@]1(C)COC2c1cc(cc2Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4210

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.21

EN300-318058_1_1_1



CID: EN300-318058_1_1_1

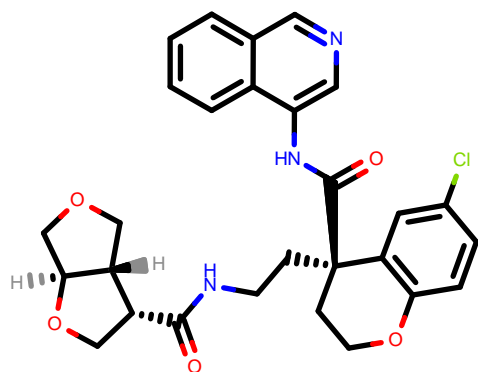
SMILES: C[C@@]1(CN(C)C@]1)COC(C=O)[C@]2(C)COC3c2cc(c3Cl)C(=O)Nc4ncc5c4ccc5CO

RUN: RUN5258

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.32

EN300-6482296_3_1_1



CID: EN300-6482296_3_1_1

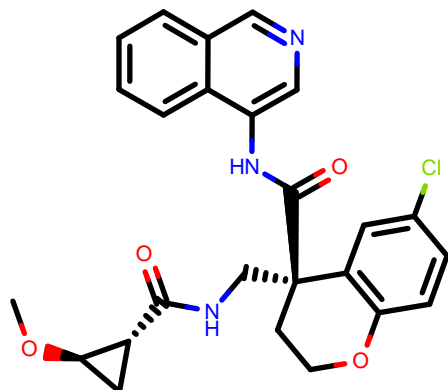
SMILES: C1cc2c(c1)ccc2N(C=O)C@]1(C)COC3c3ccc4c3)C(=O)Nc5c6c5c4ccc6

RUN: RUN4742

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.28

EN300-650518_2_1_1



CID: EN300-650518_2_1_1

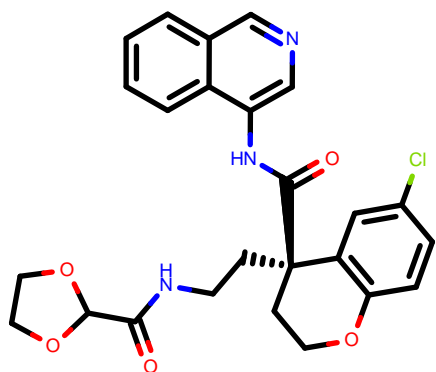
SMILES: CO[C@@]1(C)C@H]1C(=O)NC[C@]2(C)COC3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN7003

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.21

EN300-154942_3_1_1



CID: EN300-154942_3_1_1

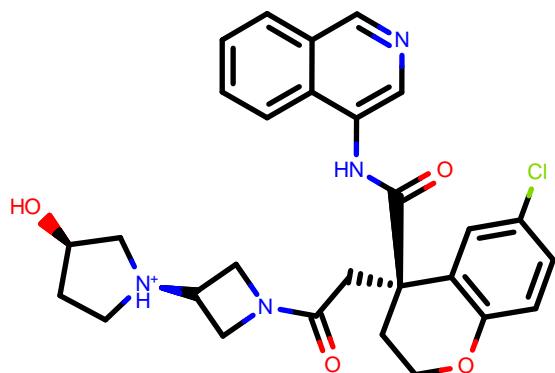
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5OCCO5

RUN: RUN5124

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.28

EDG-MED-ba1ac7b9-4_7



CID: EDG-MED-ba1ac7b9-4_7

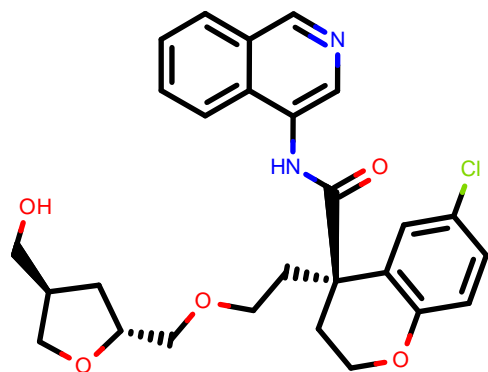
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)(N)H6CC(=O)H7(C)O

RUN: RUN2495

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.28

EN300-6494158_3_2_1



CID: EN300-6494158_3_2_1

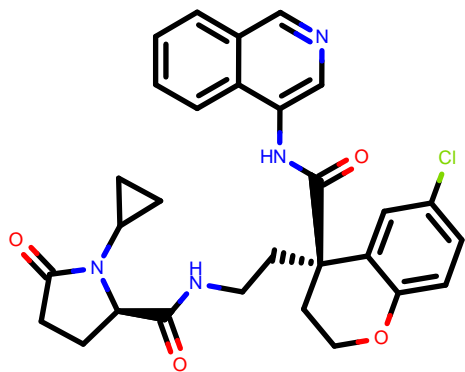
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5C[C@@H](CO)C5O

RUN: RUN4290

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.31

EN300-3044054_3_2_1



CID: EN300-3044054_3_2_1

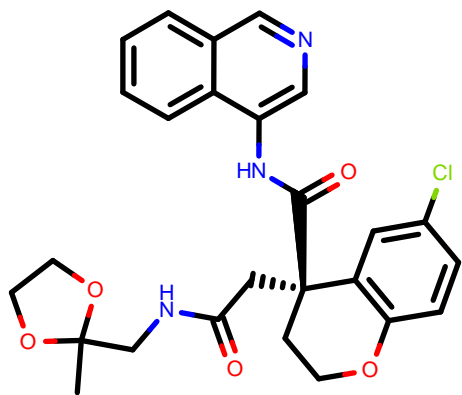
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCC(=O)N5C6CC6

RUN: RUN6308

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.36

EN300-114894_1_1_1



CID: EN300-114894_1_1_1

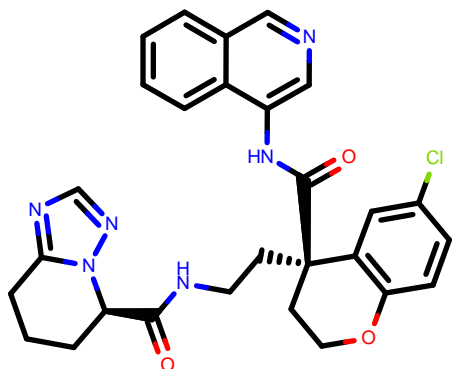
SMILES: CC1(OCCO1)CNC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN7087

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.31

EN300-1273016_3_2_1



CID: EN300-1273016_3_2_1

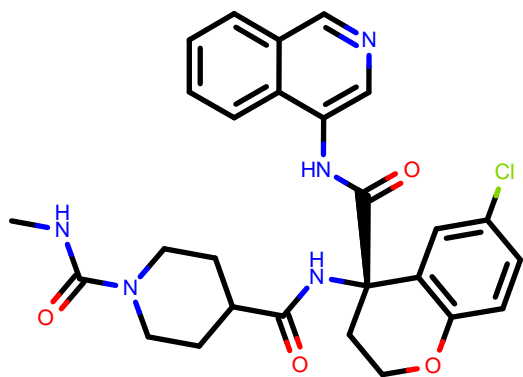
SMILES: c1ccc2c(c1)ncoc2N[C@@]3(C)C(COc4c3cc(cc4)Cl)CCN[C@@]3(C)C@H5CCc6c5n6

RUN: RUN4303

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.32

EN300-6478526_1_1_1



CID: EN300-6478526_1_1_1

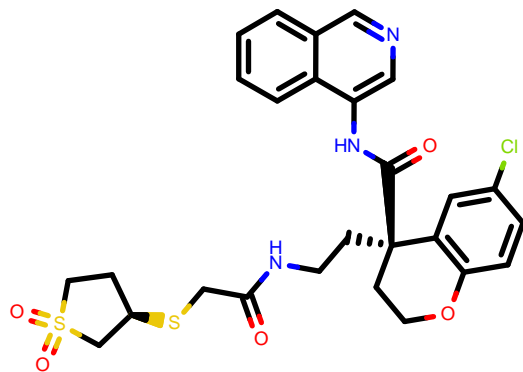
SMILES: CNC(=O)N1CCC(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5078

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.27

EN300-13890_3_1_1



CID: EN300-13890_3_1_1

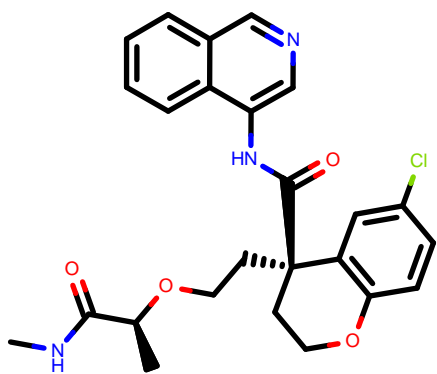
SMILES: c1ccc2c(c1)ncoc2N[C@@]3(C)C(COc4c3cc(cc4)Cl)CCN[C@@]3(C)C@H5CS6S(=O)(=O)6

RUN: RUN3588

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.36

EN300-211482_3_1_1



CID: EN300-211482_3_1_1

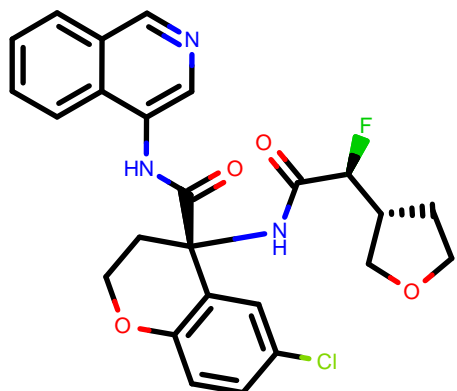
SMILES: C[C@@H](C(=O)NC)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN4447

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-783124_1_2_1



CID: EN300-783124_1_2_1

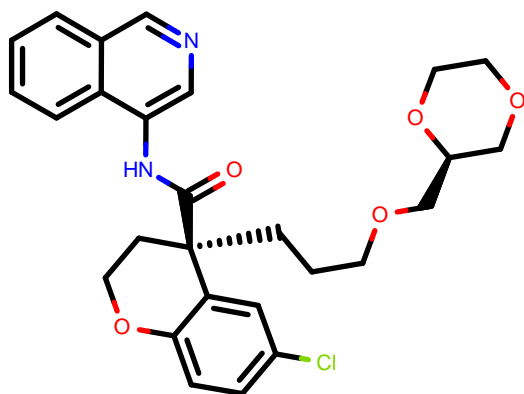
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@@H]5CCOC5)F

RUN: RUN3074

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.18

EN300-139167_4_1_1



CID: EN300-139167_4_1_1

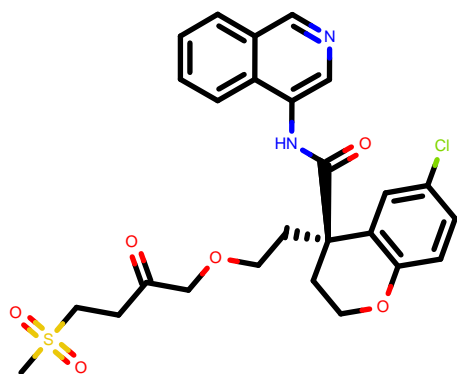
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCOC5

RUN: RUN7311

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.30

EN300-1988306_3_1_1



CID: EN300-1988306_3_1_1

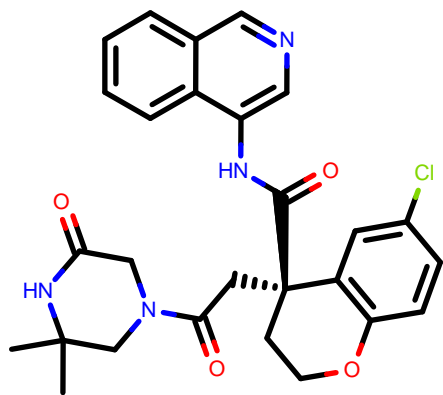
SMILES: CS(=O)(=O)CCC(=O)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN4644

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.43

EN300-7493939_1_1_1



CID: EN300-7493939_1_1_1

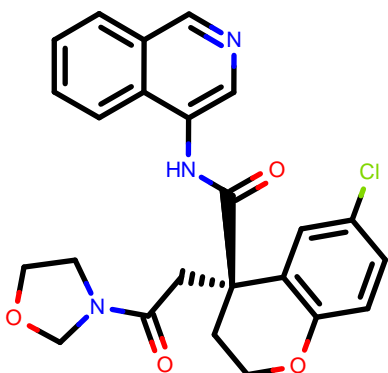
SMILES: CC1(CN(CC(=O)N1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C

RUN: RUN4726

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.24

EN300-211422_1_1_1



CID: EN300-211422_1_1_1

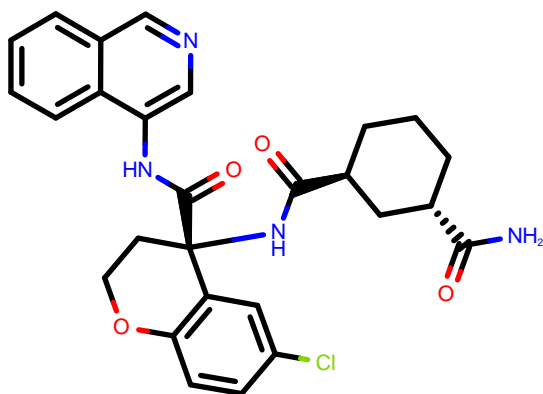
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC5

RUN: RUN6076

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.23

EN300-90142_1_2_1



CID: EN300-90142_1_2_1

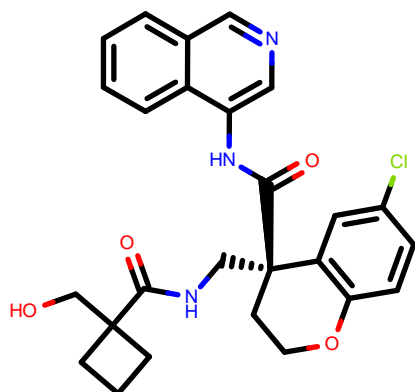
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C1=O)[C@@H]5CC[C@@]3(H)C5)Cl=O

RUN: RUN3508

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.39

EDJ-MED-40433386-4_1



CID: EDJ-MED-40433386-4_1

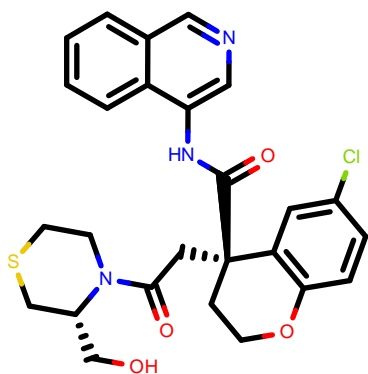
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C1=O)C5(CCC5)CO

RUN: RUN2357

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.28

EN300-122579_1_2_1



CID: EN300-122579_1_2_1

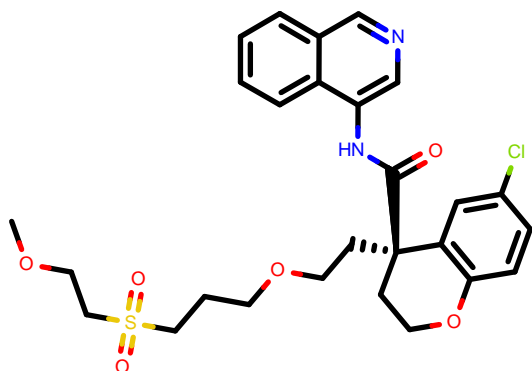
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CC(=O)N5CCSC[C@H]5CO

RUN: RUN3894

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.29

EN300-62857_3_1_1



CID: EN300-62857_3_1_1

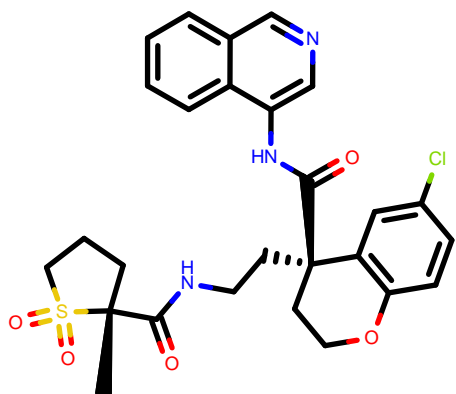
SMILES: COCCS(=O)(=O)CCOCOC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4

RUN: RUN4002

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.56

EN300-373476_3_1_1



CID: EN300-373476_3_1_1

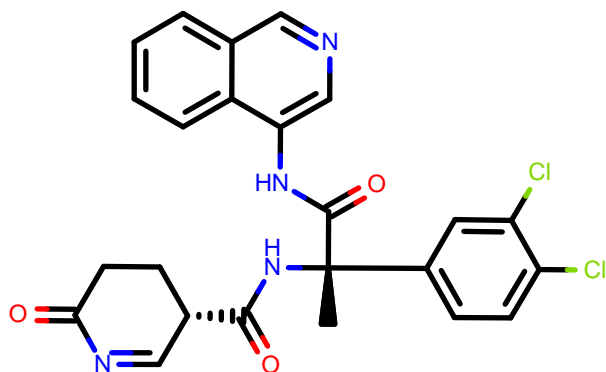
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5

RUN: RUN4571

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.37

MAT-POS-e9e99895-3_4



CID: MAT-POS-e9e99895-3_4

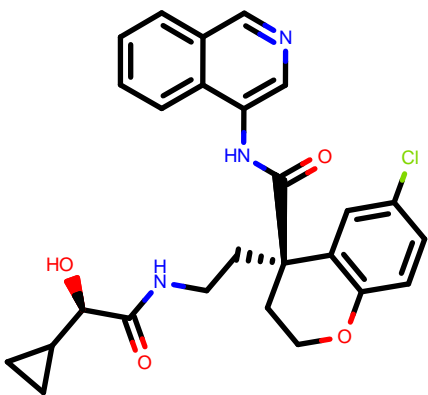
SMILES: C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2nccc3c2ccc3)NC(=O)[C@H]4CCC(=O)NC4

RUN: RUN2099

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.28

EN300-72211_3_1_1



CID: EN300-72211_3_1_1

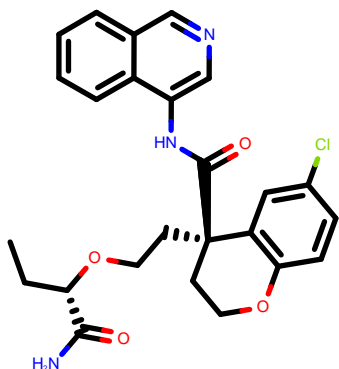
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C5CC5)O

RUN: RUN7017

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

EN300-65839_3_1_1



CID: EN300-65839_3_1_1

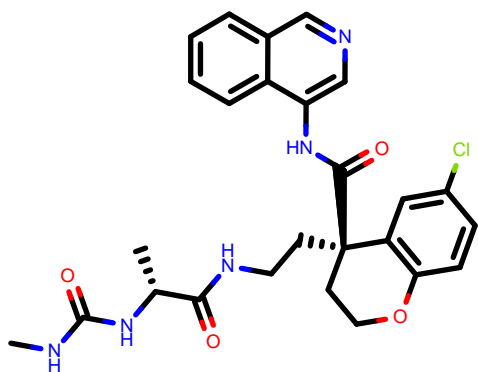
SMILES: CC[C@@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4

RUN: RUN3007

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.31

EN300-1258964_3_2_1



CID: EN300-1258964_3_2_1

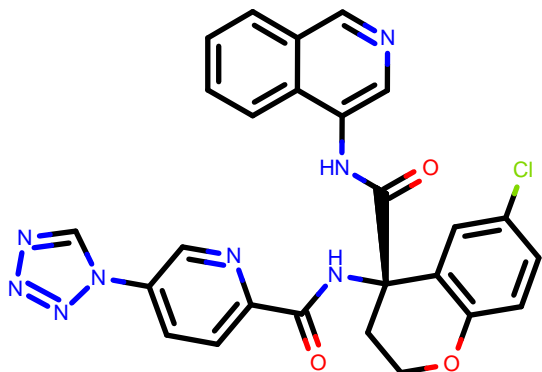
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4)NC(=O)NC

RUN: RUN3706

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

EN300-262409_1_1_1



CID: EN300-262409_1_1_1

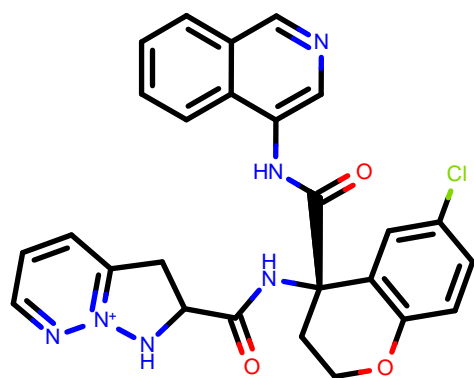
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccoc(n5)n6cnm6

RUN: RUN4695

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.22

EN300-6473108_1_1_1



CID: EN300-6473108_1_1_1

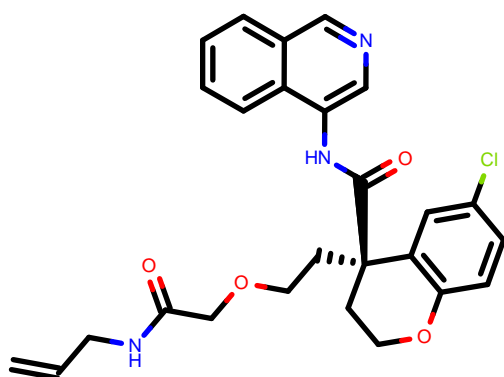
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)c5cc6ccnnc6n5

RUN: RUN3550

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.24

EN300-17184_3_1_1



CID: EN300-17184_3_1_1

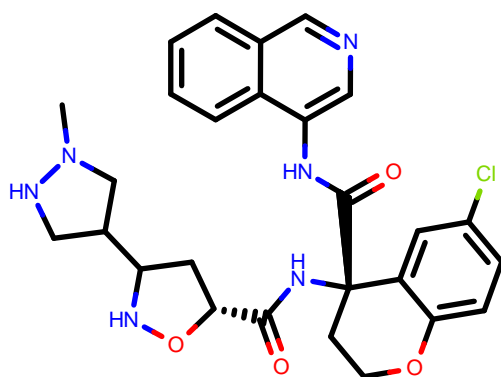
SMILES: C=CCNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4

RUN: RUN4268

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

ALP-UNI-dbbfd3db-13_2



CID: ALP-UNI-dbbfd3db-13_2

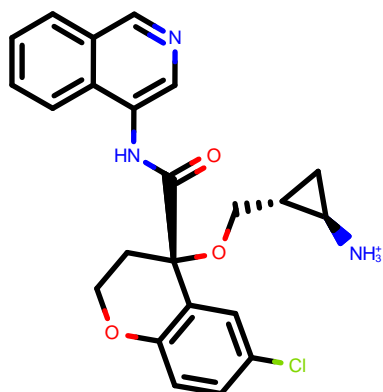
SMILES: Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cnc6c5cccc6

RUN: RUN2626

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.33

ED_-GRI-5b13fbe2-71_1



CID: ED_-GRI-5b13fbe2-71_1

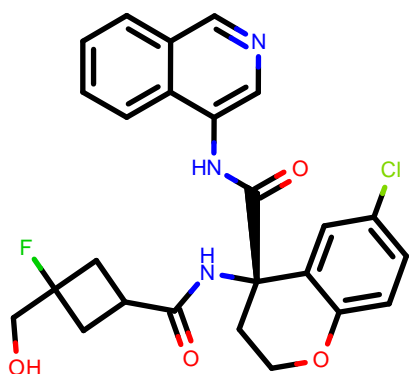
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)OC[C@@]5[H]5C[C@H]5[NH3+]

RUN: RUN1485

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.27

EN300-6746890_1_1_1



CID: EN300-6746890_1_1_1

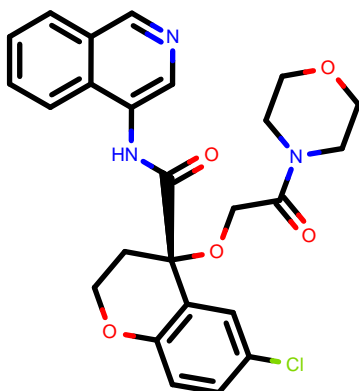
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC(C5)COF

RUN: RUN6408

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.23

EN300-1241327_1_1_1



CID: EN300-1241327_1_1_1

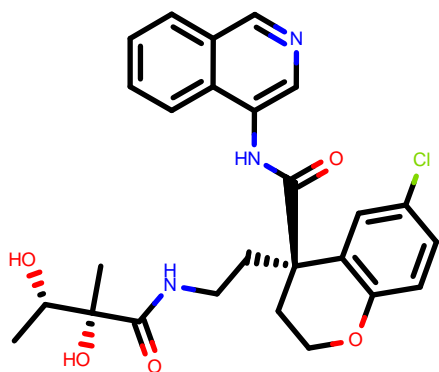
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCOCC5

RUN: RUN4841

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.22

EN300-202922_3_1_1



CID: EN300-202922_3_1_1

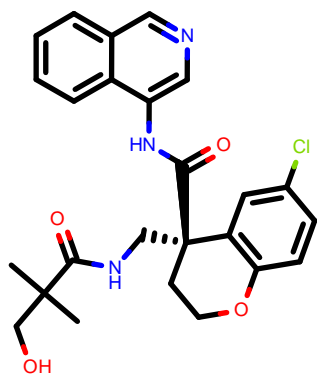
SMILES: C[C@@H](C@@)(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5178

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.36

EN300-65050_2_1_1



CID: EN300-65050_2_1_1

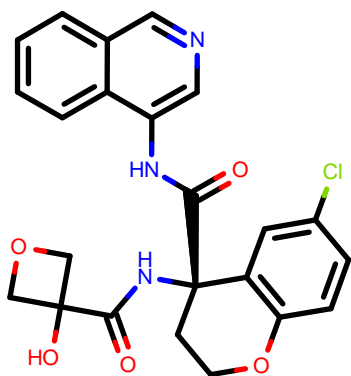
SMILES: CC(C)(CO)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3918

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.27

EN300-101443_1_1_1



CID: EN300-101443_1_1_1

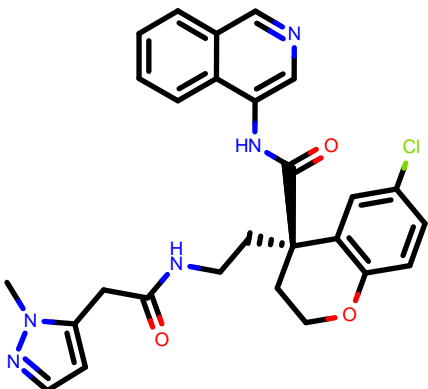
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COC5)O

RUN: RUN3823

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.21

EN300-114805_3_1_1



CID: EN300-114805_3_1_1

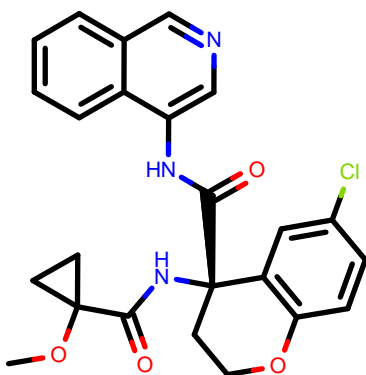
SMILES: Cn1c(ccn1)CC(=O)NCC[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3331

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.22

EN300-182124_1_1_1



CID: EN300-182124_1_1_1

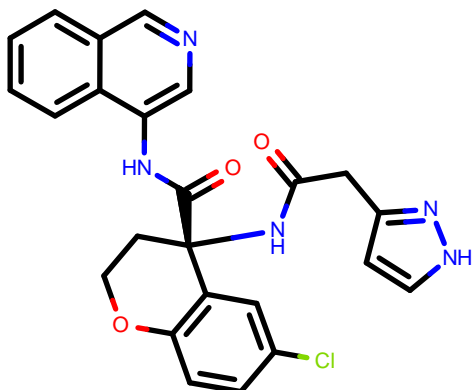
SMILES: COC1(CC1)C(=O)N[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5348

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-4_1



CID: VLA-UCB-34f3ed0c-4_1

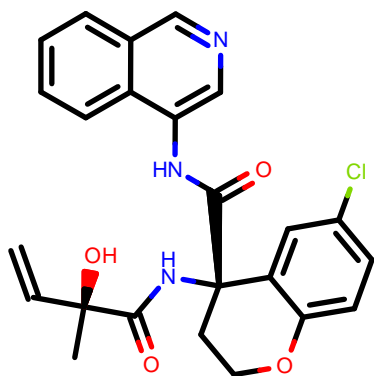
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cn[nH]5

RUN: RUN595

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.19

EN300-248888_1_2_1



CID: EN300-248888_1_2_1

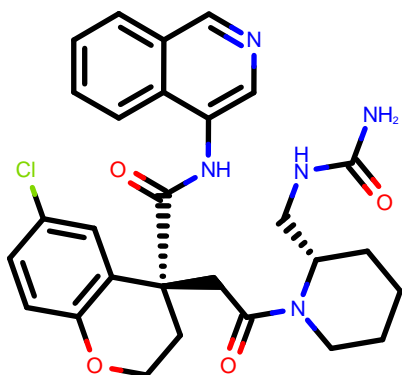
SMILES: C[C@](C=C)(C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN7383

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.29

EN300-62166_1_2_1



CID: EN300-62166_1_2_1

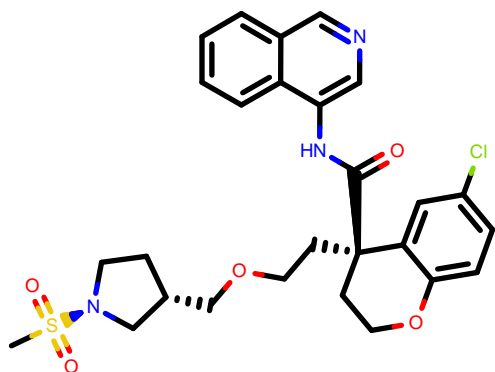
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5CNC(=O)N

RUN: RUN5981

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

EN300-261986_3_1_1



CID: EN300-261986_3_1_1

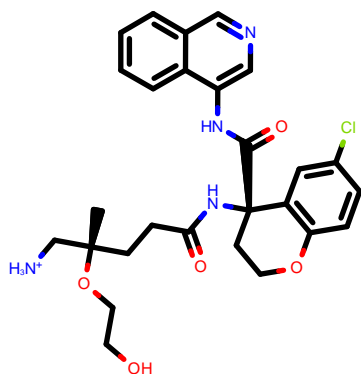
SMILES: CS(=O)(=O)N@1CC[C@@H](C1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5902

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.43

EDG-MED-90036822-22_2



CID: EDG-MED-90036822-22_2

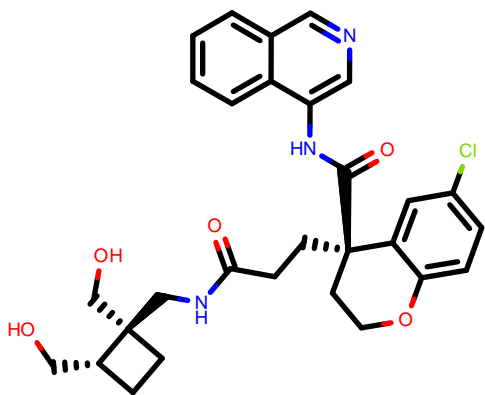
SMILES: C[C@](CCC(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C[NH3+])OCCO

RUN: RUN1625

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.50

EN300-1692359_2_2_1



CID: EN300-1692359_2_2_1

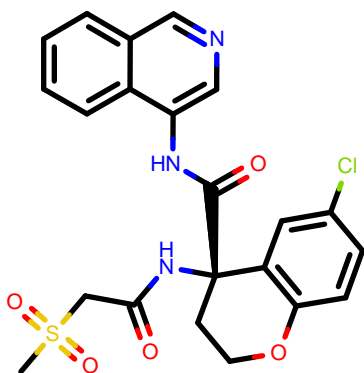
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(CCC(=O)N)C(=O)N[C@@]5(C)CC[C@@]6H5COc6

RUN: RUN7509

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

EN300-53677_1_1_1



CID: EN300-53677_1_1_1

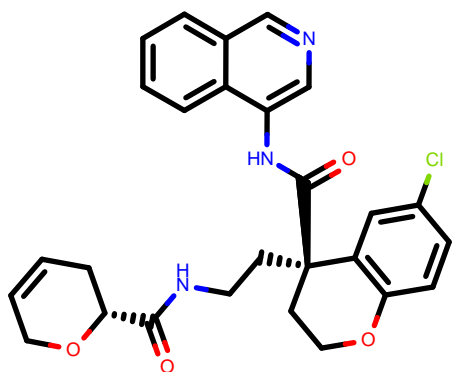
SMILES: CS(=O)(=O)CC(=O)N[C@@]1(C)CCOc2c1cc(cc2)C(C(=O)N)C3cnc4c3cccc4

RUN: RUN4337

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.24

EN300-378044_3_2_1



CID: EN300-378044_3_2_1

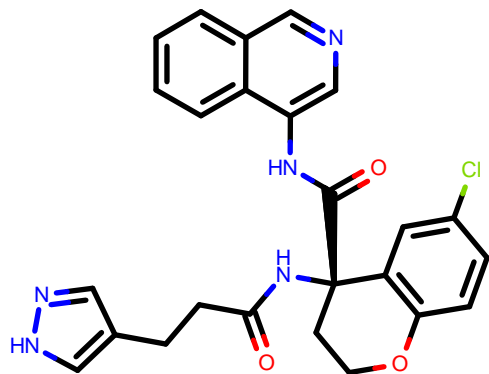
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(C)CNC(=O)[C@@]5(C)COC=CCO5

RUN: RUN4363

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.25

EN300-250836_1_1_1



CID: EN300-250836_1_1_1

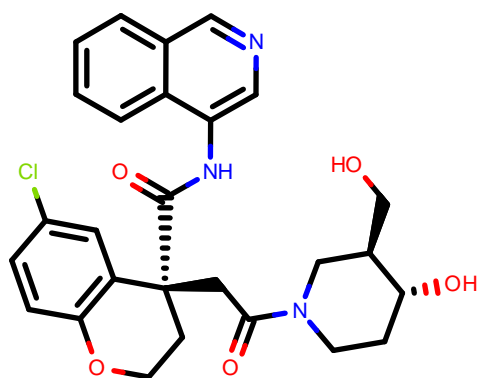
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(C)NC(=O)CC5c[nH]ne5

RUN: RUN5988

DDG (kcal/mol): -1.20

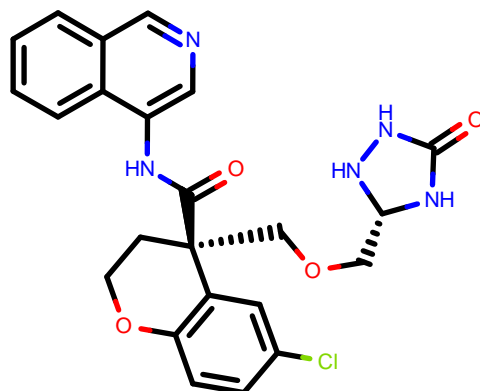
dDDG (kcal/mol): 0.23

EDJ-MED-d203f206-40_1



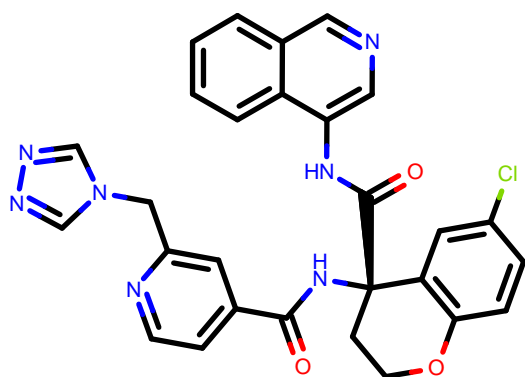
CID:	EDJ-MED-d203f206-40_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)C(=O)N5CC[C@H](C5)O</chem>
RUN:	RUN2450
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.29

EN300-73772_2_1_2



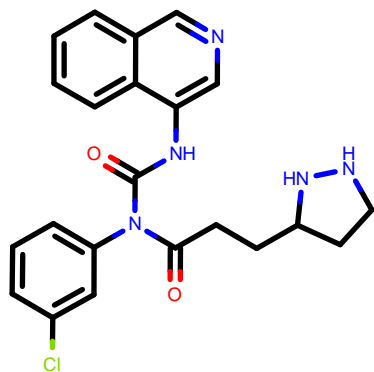
CID:	EN300-73772_2_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)C(=O)N5CC[C@H](C5)O</chem>
RUN:	RUN5152
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.30

EN300-5309123_1_1_1



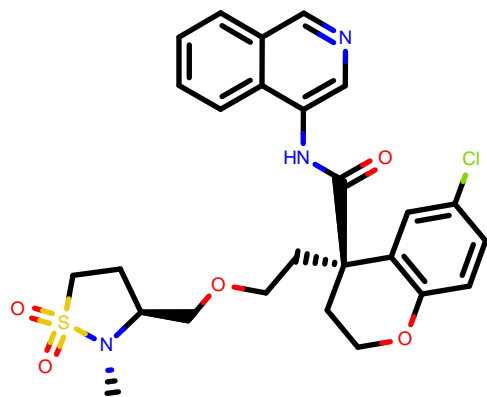
CID:	EN300-5309123_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)C(=O)N5CC[C@H](C5)O</chem>
RUN:	RUN3898
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.32

VLA-UCB-34f3ed0c-5_1



CID:	VLA-UCB-34f3ed0c-5_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)C(=O)N5CC[C@H](C5)O</chem>
RUN:	RUN630
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.38

KAD-UNI-8a629cb0-38_2



CID: KAD-UNI-8a629cb0-38_2

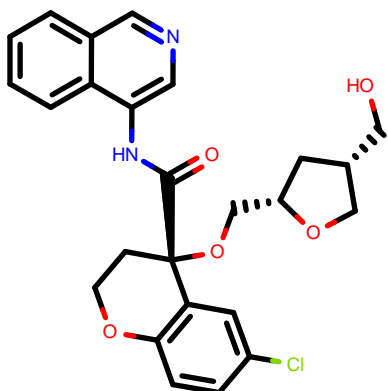
SMILES: C[N@]1[C@@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2048

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-6494158_1_1_1



CID: EN300-6494158_1_1_1

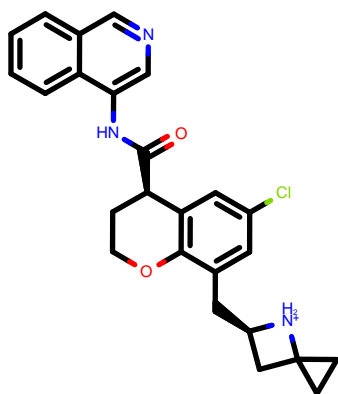
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5C[C@@H](CO)C5

RUN: RUN4621

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.33

DAR-DIA-23e5a6a0-10_1



CID: DAR-DIA-23e5a6a0-10_1

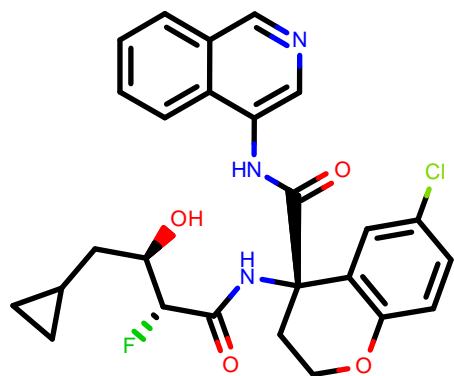
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C[C@@H]5CC6([NH2]H5)CC6)Cl

RUN: RUN346

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.25

EDG-MED-90036822-108_1



CID: EDG-MED-90036822-108_1

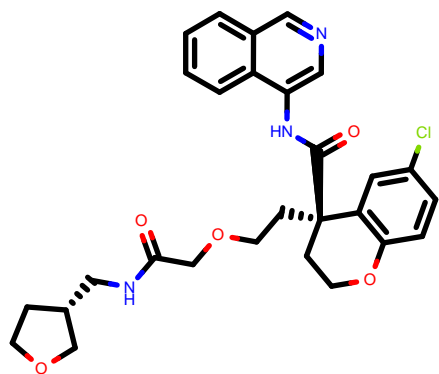
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H](C)C5)O)F

RUN: RUN1791

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.32

EN300-46832_3_2_1



CID: EN300-46832_3_2_1

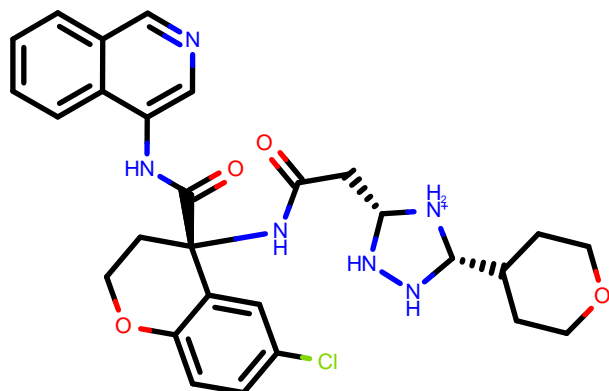
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)NC[C@@H]5CCOC5

RUN: RUN5398

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.35

EN300-385132_1_1_1



CID: EN300-385132_1_1_1

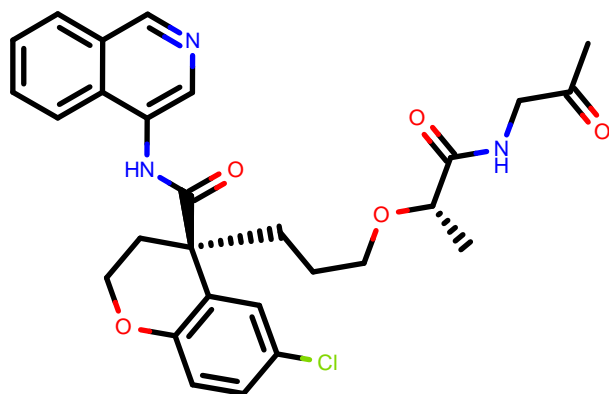
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5[NH2+][NH2+][C@@H]6N5C6CCCC6

RUN: RUN6954

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.92

EN300-131093_4_1_1



CID: EN300-131093_4_1_1

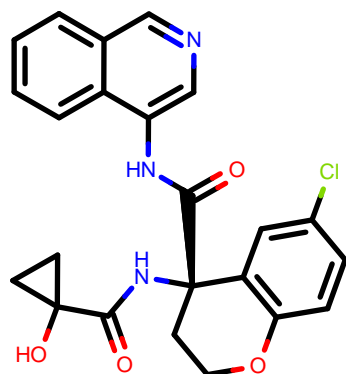
SMILES: C[C@@H](C(=O)NCC(=O)O)OCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5281

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.42

EN300-25702_1_1_1



CID: EN300-25702_1_1_1

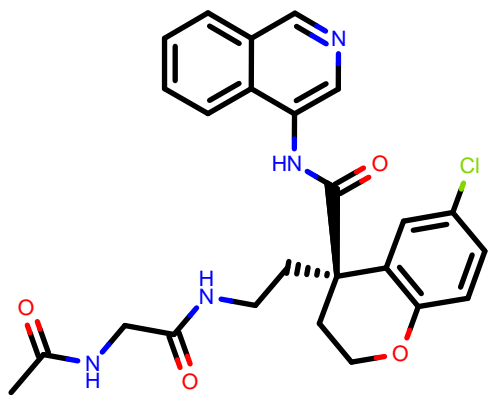
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CC5)O

RUN: RUN4448

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.21

EN300-18561_3_1_1



CID: EN300-18561_3_1_1

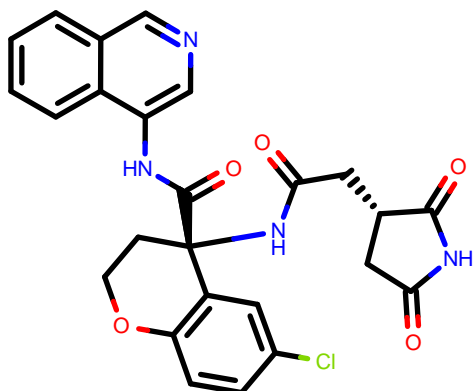
SMILES: CC(=O)NCC(=O)NCC[C@]1(C)C(CO)C2=C1C(=O)Nc3ccc4c3ccc4

RUN: RUN4947

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-227055_1_2_1



CID: EN300-227055_1_2_1

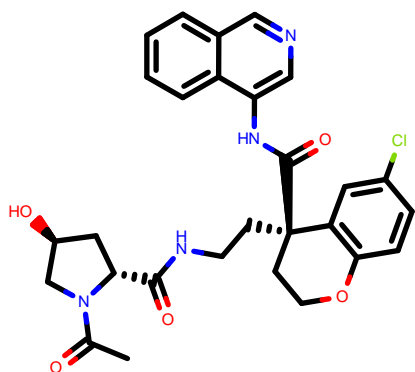
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CO)C4=CC(=O)N(C)C5=O

RUN: RUN5189

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.21

EN300-158274_3_1_1



CID: EN300-158274_3_1_1

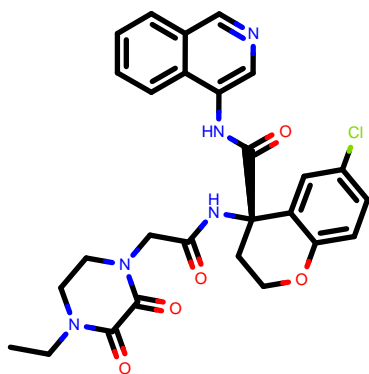
SMILES: CC(=O)N1C[C@@H](C)C(=O)N(C)C2=CC(=O)N(C)C3=CC(=O)N(C)C3=O

RUN: RUN6226

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.41

EN300-39961_1_1_1



CID: EN300-39961_1_1_1

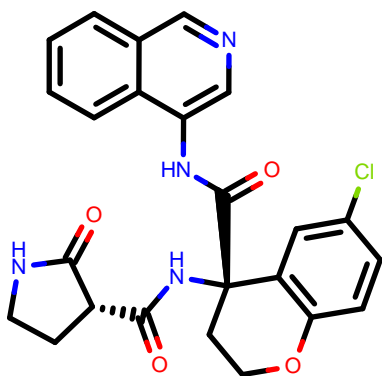
SMILES: CCN1CCN(C(=O)C1=O)CC(=O)N(C)C2=CC(=O)N(C)C3=CC(=O)N(C)C3=O

RUN: RUN6004

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.38

EN300-94945_1_1_1



CID: EN300-94945_1_1_1

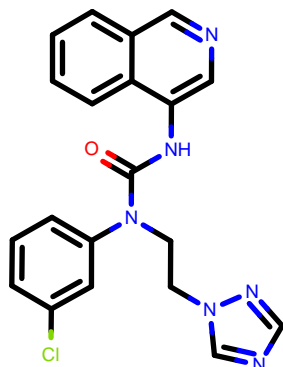
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCNC5=O

RUN: RUN3052

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.22

MIC-UNK-cdc2493e-24_1



CID: MIC-UNK-cdc2493e-24_1

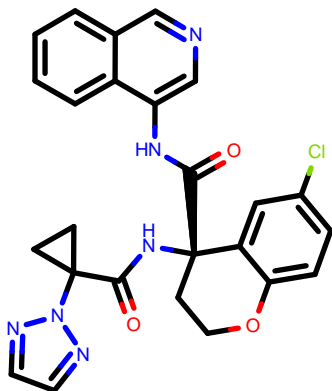
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CCn3cncn3)c4cccc(c4)Cl

RUN: RUN488

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.35

EN300-1722017_1_1_1



CID: EN300-1722017_1_1_1

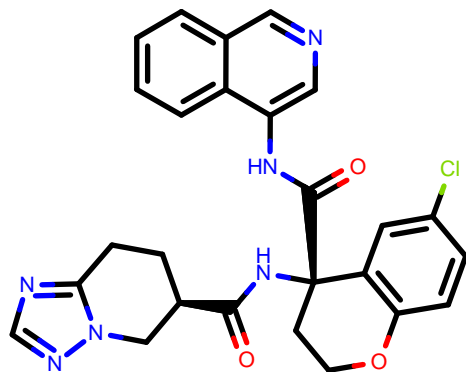
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(C)C5n6nncn6

RUN: RUN4087

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.28

EN300-1662365_1_1_1



CID: EN300-1662365_1_1_1

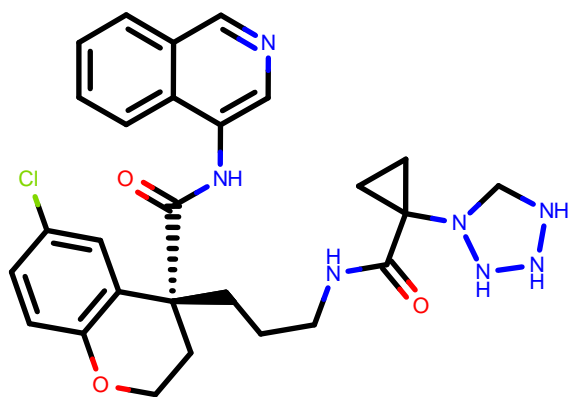
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6c6nncn6C5

RUN: RUN4854

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.27

EN300-263085_4_1_1



CID: EN300-263085_4_1_1

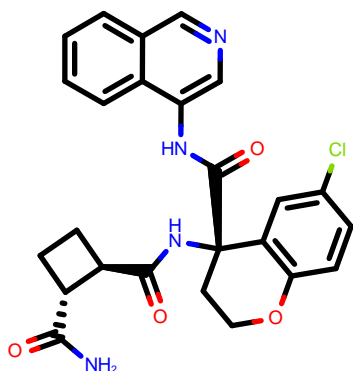
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCCN(C=O)C5(CCS)n6cnm6

RUN: RUN7091

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.33

EN300-217107_1_3_1



CID: EN300-217107_1_3_1

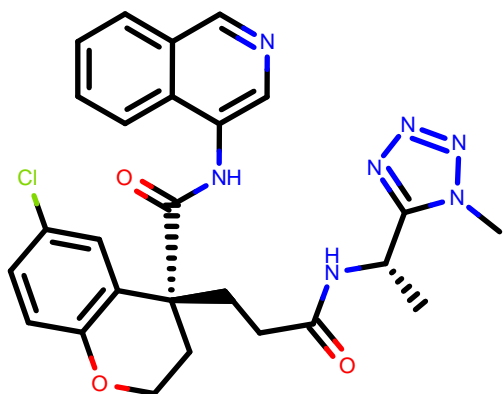
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@@@H5OC[C@@H]5C(=O)N

RUN: RUN3206

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.22

EN300-173020_2_1_1



CID: EN300-173020_2_1_1

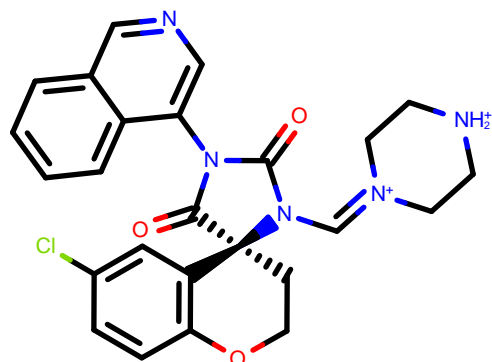
SMILES: C[C@@@H](c1nmmn1C)NC(=O)CC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5o4ccccc5

RUN: RUN6168

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.32

VLA-UCB-34f3ed0c-15_1



CID: VLA-UCB-34f3ed0c-15_1

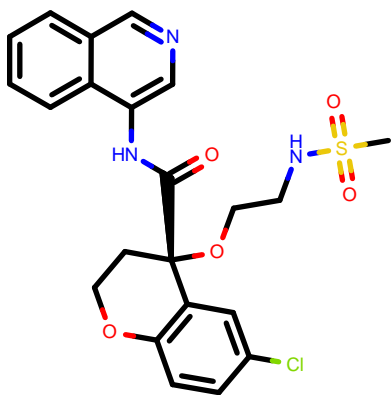
SMILES: c1ccc2c(c1)ncnc2N3C(=O)C@@@4(CCOc5c4cc(cc5)C)N(C3=O)CN6CC[NH2+][C]6

RUN: RUN543

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.46

EN300-1238839_1_1_1



CID: EN300-1238839_1_1_1

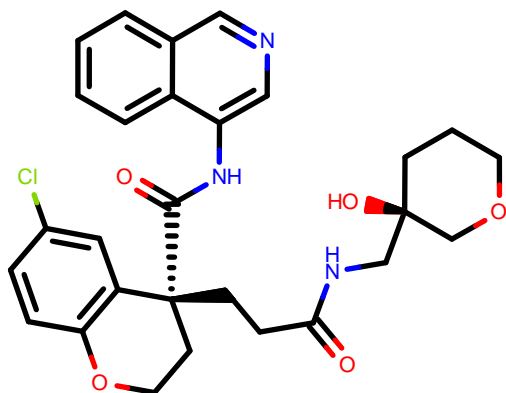
SMILES: CS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4987

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.28

EN300-193679_2_1_1



CID: EN300-193679_2_1_1

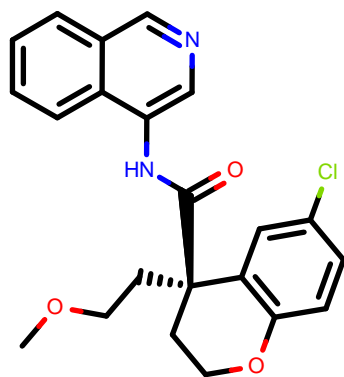
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@]5(CCCOC5)O

RUN: RUN5218

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.31

EDJ-MED-28ec730d-2_1



CID: EDJ-MED-28ec730d-2_1

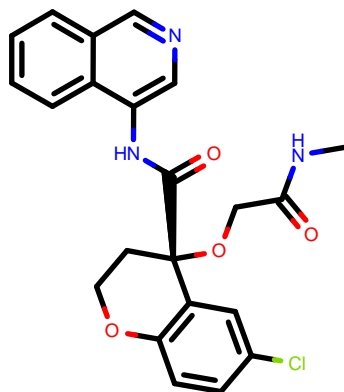
SMILES: COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN587

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.14

EN300-2977549_1_1_1



CID: EN300-2977549_1_1_1

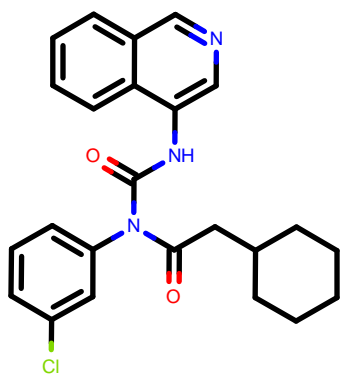
SMILES: CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4712

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.17

VLA-UCB-34f3ed0c-6_1



CID: VLA-UCB-34f3ed0c-6_1

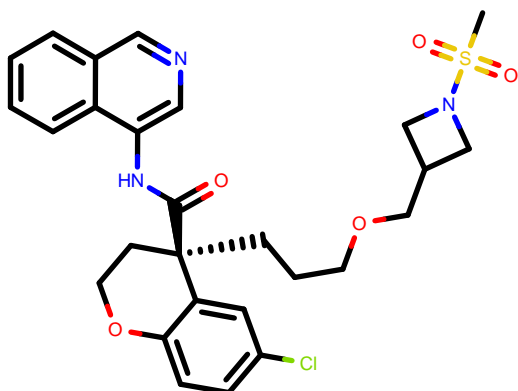
SMILES: c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C(=O)CC4CCCC4

RUN: RUN599

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.45

EN300-302290_4_1_1



CID: EN300-302290_4_1_1

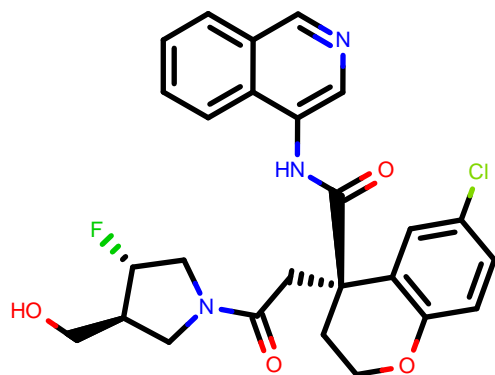
SMILES: CS(=O)(=O)N1CC(C1)COC(C@)2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5o4cccc5

RUN: RUN5672

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.36

EN300-1693852_1_1_1



CID: EN300-1693852_1_1_1

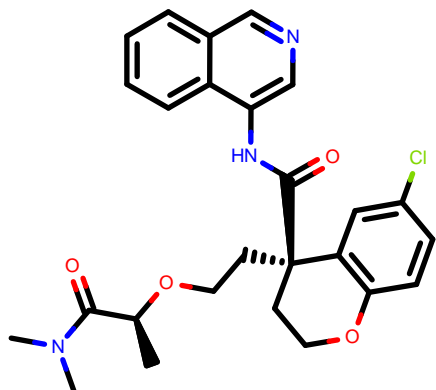
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)F)CO

RUN: RUN4741

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.25

EN300-14458_3_1_1



CID: EN300-14458_3_1_1

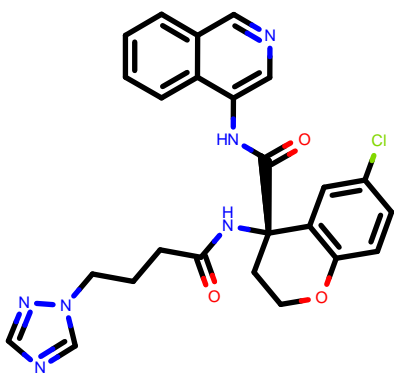
SMILES: C[C@@H](C(=O)N(C)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5565

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.25

EN300-316216_1_1_1



CID: EN300-316216_1_1_1

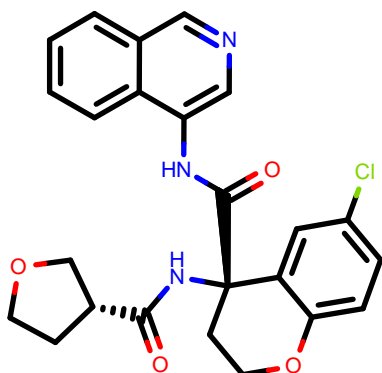
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5cnns5

RUN: RUN6729

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.24

EN300-53423_1_1_1



CID: EN300-53423_1_1_1

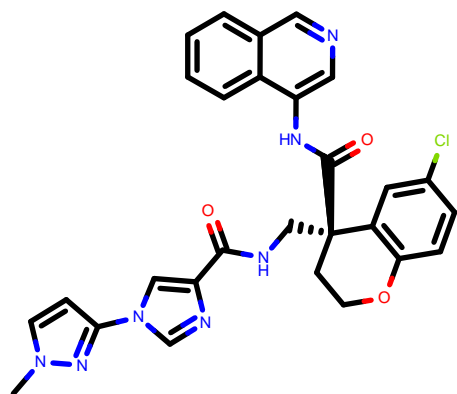
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC5

RUN: RUN4933

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.31

EN300-1726340_2_1_1



CID: EN300-1726340_2_1_1

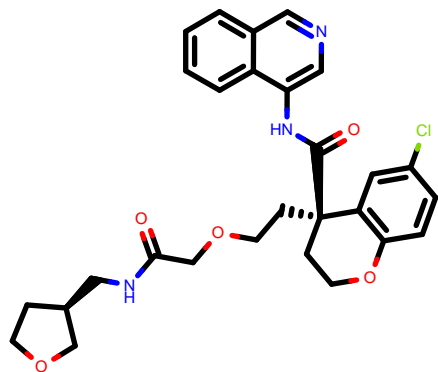
SMILES: Cn1ccc(n1)n2cc(nc2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cncc6c5ccc6

RUN: RUN3999

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.36

EN300-46832_3_1_1



CID: EN300-46832_3_1_1

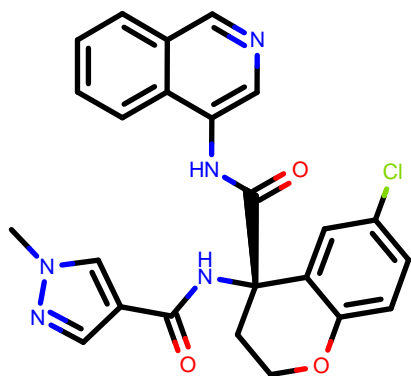
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)NC[C@@H]5CCOC5

RUN: RUN3925

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.29

EN300-14395_1_1_1



CID: EN300-14395_1_1_1

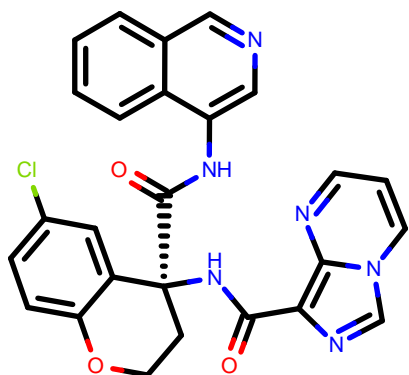
SMILES: Cn1cc(en1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6257

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.21

EN300-249899_1_1_1



CID: EN300-249899_1_1_1

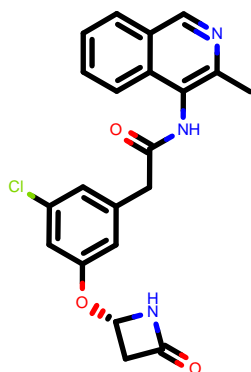
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)c5c6ncccn6cn5

RUN: RUN3202

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.19

RAL-THA-065e0743-2_2



CID: RAL-THA-065e0743-2_2

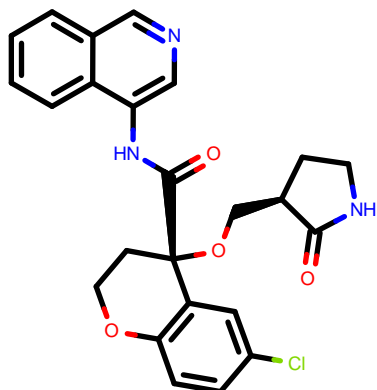
SMILES: Cc1c(c2cccc2cn1)NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4

RUN: RUN411

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.40

EN300-246248_1_2_1



CID: EN300-246248_1_2_1

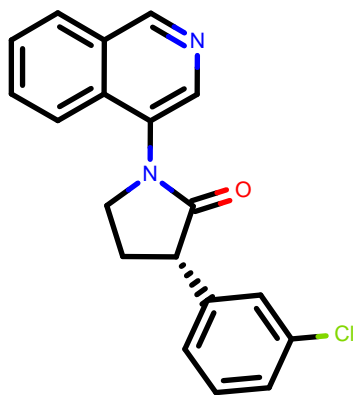
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC[C@H]5CCNC5=O

RUN: RUN3766

DDG (kcal/mol): -1.18

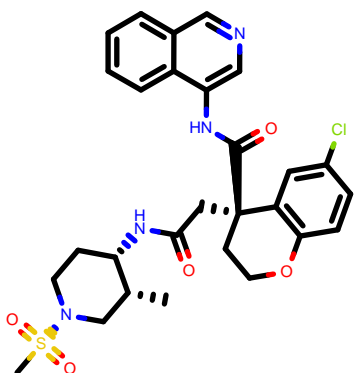
dDDG (kcal/mol): 0.22

PET-UNK-c9c1e0d8-4_2



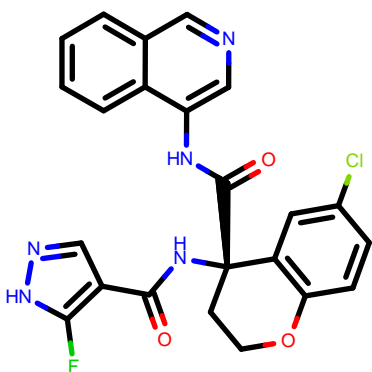
CID:	PET-UNK-c9c1e0d8-4_2
SMILES:	<chem>c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl</chem>
RUN:	RUN36
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.26

ALP-POS-2da19ca7-7_1



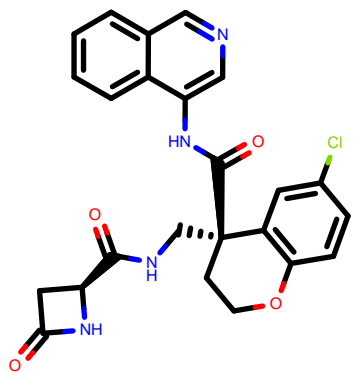
CID:	ALP-POS-2da19ca7-7_1
SMILES:	<chem>C[C@@H]1CN[C@@H](C[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4nc5c4cccc5S(=O)(=O)C</chem>
RUN:	RUN2272
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.34

EDG-MED-90036822-66_1



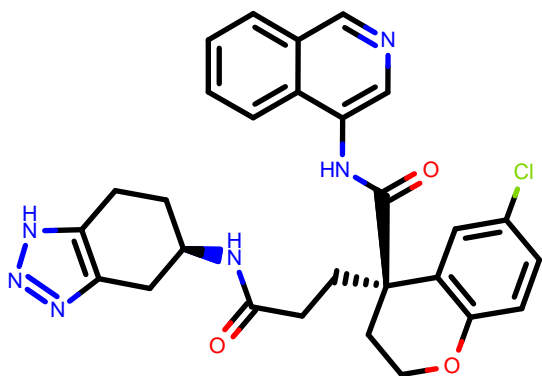
CID:	EDG-MED-90036822-66_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]c5F</chem>
RUN:	RUN1605
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.16

EN300-101505_2_1_1



CID:	EN300-101505_2_1_1
SMILES:	<chem>c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC(=O)N5</chem>
RUN:	RUN5997
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.20

EN300-6491682_2_1_1



CID: EN300-6491682_2_1_1

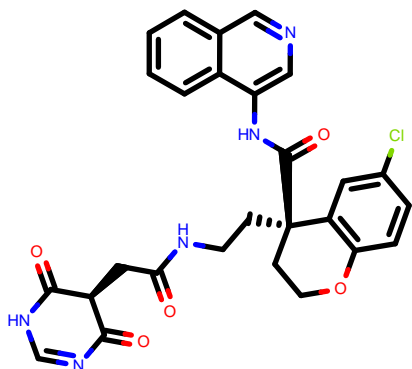
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C(C)C(=O)N[C@@]3(H)C5C6=C(N)N=CN=C5

RUN: RUN7620

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.28

EN300-86205_3_1_2



CID: EN300-86205_3_1_2

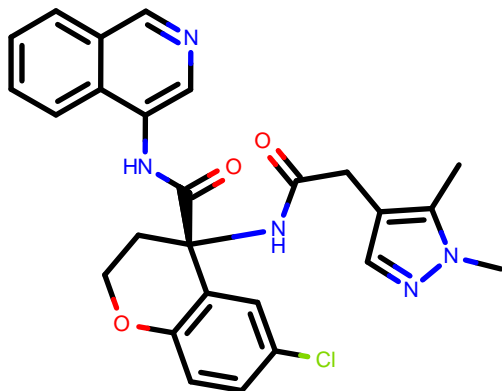
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C(C)C(=O)N[C@@]3(H)C5C6=C(N)N=CN=C5=O

RUN: RUN5615

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.33

EN300-219437_1_1_1



CID: EN300-219437_1_1_1

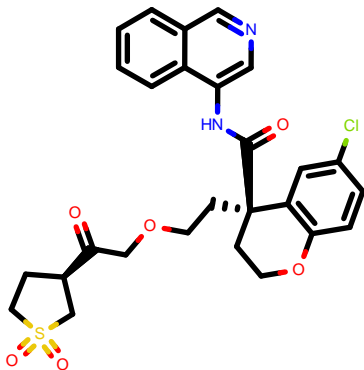
SMILES: Cc1c(cnn1C)CC(=O)N[C@@]2(C)CCOC3C2C(=O)C(C)C(=O)Nc4cnc5c4cccc5

RUN: RUN6867

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.31

EN300-226314_3_1_1



CID: EN300-226314_3_1_1

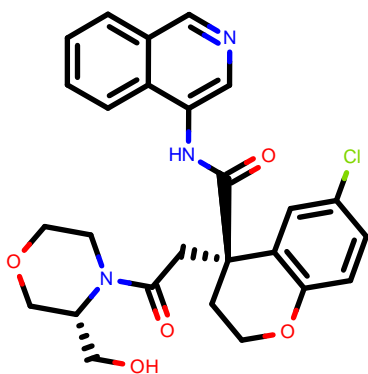
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C(C)C(=O)N[C@@]3(H)S5C6C(=O)C(=O)C5

RUN: RUN7598

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.35

EN300-173903_1_1_1



CID: EN300-173903_1_1_1

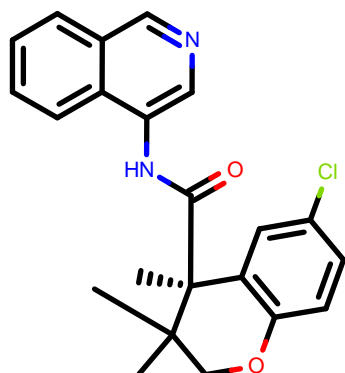
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4ccc(cc4)C(=O)N5CCOC[C@H]5CO

RUN: RUN4317

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.35

DAR-DIA-0d514e7d-30_1



CID: DAR-DIA-0d514e7d-30_1

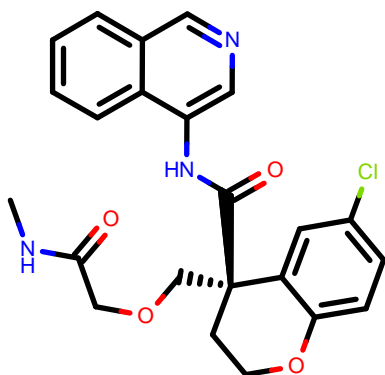
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN727

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.23

EN300-2977549_2_1_1



CID: EN300-2977549_2_1_1

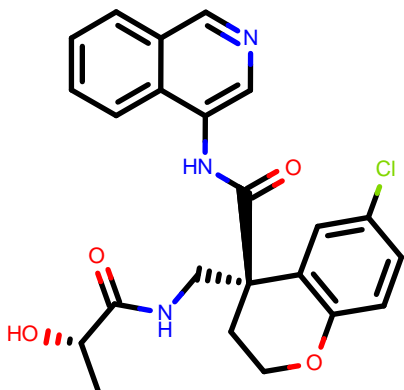
SMILES: CNC(=O)COC[C@@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4591

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.20

EN300-19542_2_1_1



CID: EN300-19542_2_1_1

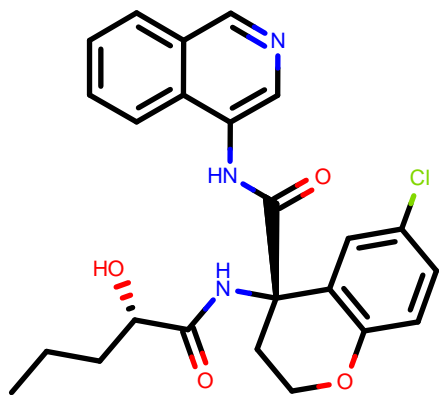
SMILES: C[C@@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4O

RUN: RUN5551

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.26

EN300-316679_1_1_1



CID: EN300-316679_1_1_1

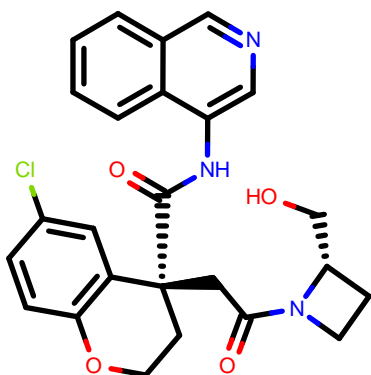
SMILES: CCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5607

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.31

EN300-154332_1_2_1



CID: EN300-154332_1_2_1

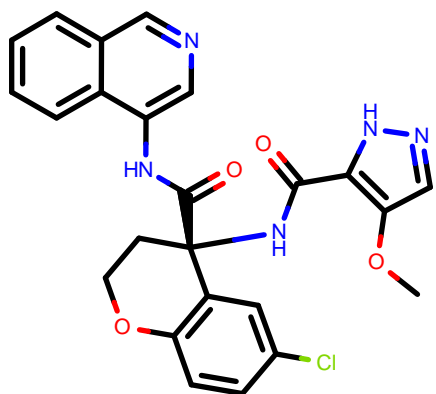
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO

RUN: RUN6552

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.29

EN300-7439284_1_1_1



CID: EN300-7439284_1_1_1

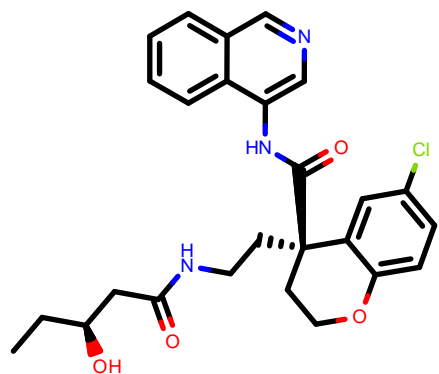
SMILES: COc1cn[nH]c1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4069

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.28

EN300-224741_3_1_1



CID: EN300-224741_3_1_1

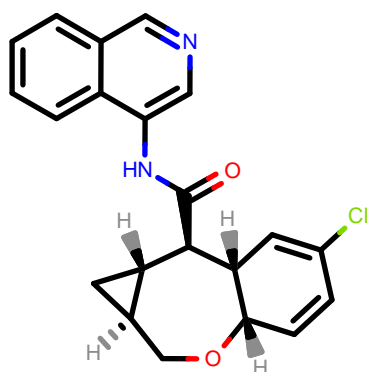
SMILES: CC[C@@H](CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5384

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.30

DAR-DIA-0d514e7d-32_19



CID: DAR-DIA-0d514e7d-32_19

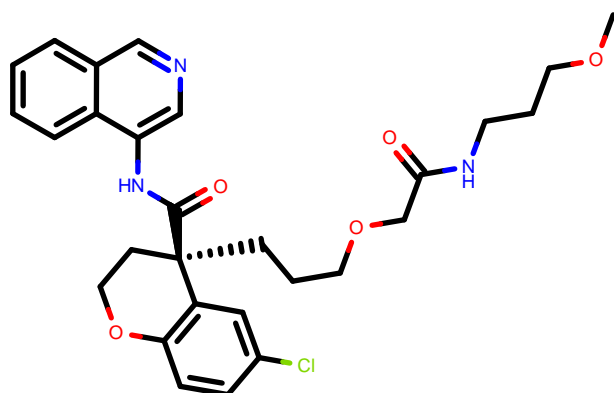
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@H]4C[C@@H]4CO[C@@H]5[C@H]3C=C(C=C5)Cl

RUN: RUN773

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.25

EN300-04492_4_1_1



CID: EN300-04492_4_1_1

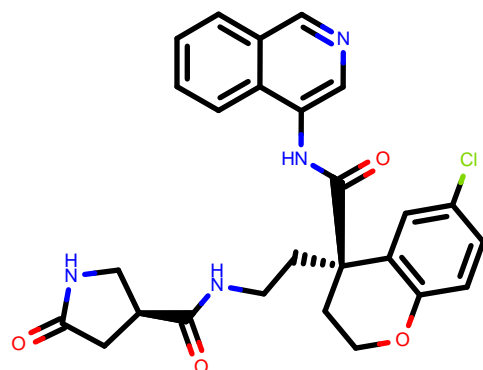
SMILES: COC(C)CNC(=O)COC(C)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6474

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.34

EN300-59487_3_2_1



CID: EN300-59487_3_2_1

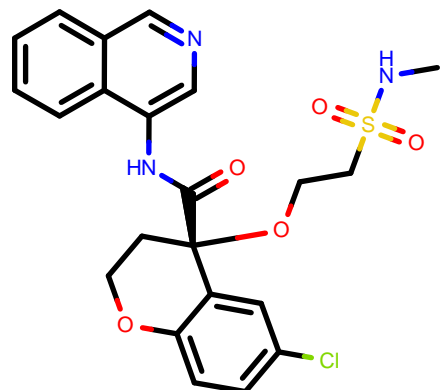
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)NC5

RUN: RUN4116

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.25

EN300-6482967_1_1_1



CID: EN300-6482967_1_1_1

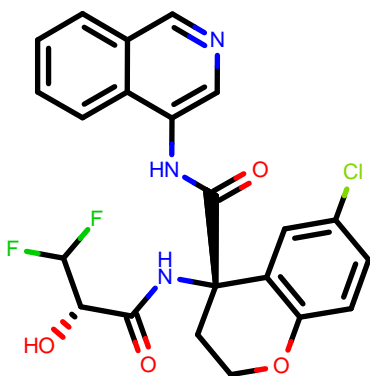
SMILES: CNS(=O)(=O)CCO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6618

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.26

EN300-1932780_1_1_1



CID: EN300-1932780_1_1_1

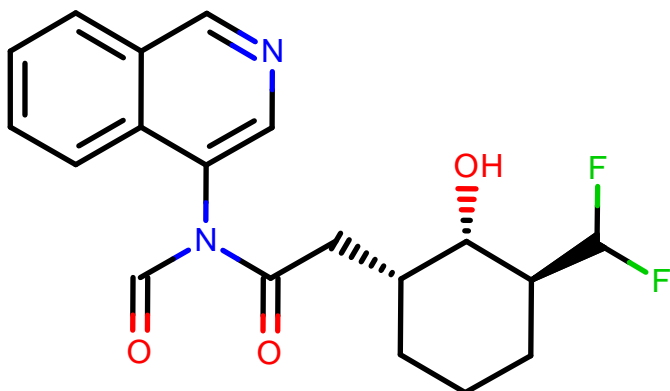
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](C(F)F)O

RUN: RUN3698

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.19

MAK-UNK-c749d764-28_6



CID: MAK-UNK-c749d764-28_6

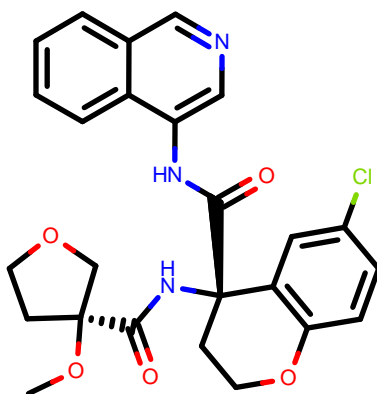
SMILES: c1ccc2c(c1)cncc2N(C=O)C(=O)[C@H]3CCCC[C@@H]([C@H]3O)C(F)F

RUN: RUN1033

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.29

EN300-174668_1_2_1



CID: EN300-174668_1_2_1

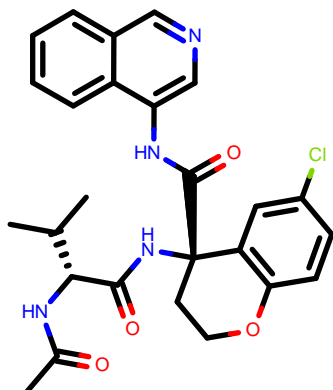
SMILES: CO[C@@]1(CCOC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5o4ccccc5

RUN: RUN3002

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.38

EN300-16582_1_2_1



CID: EN300-16582_1_2_1

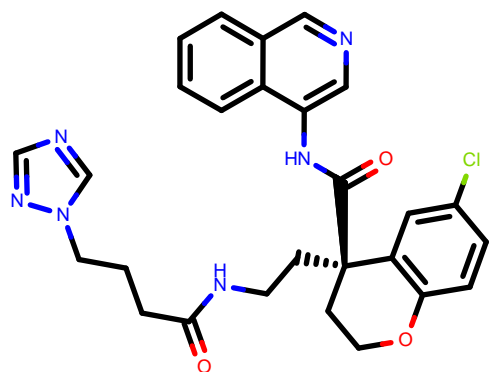
SMILES: CC(C)[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4)NC(=O)C

RUN: RUN3980

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.26

EN300-316216_3_1_1



CID: EN300-316216_3_1_1

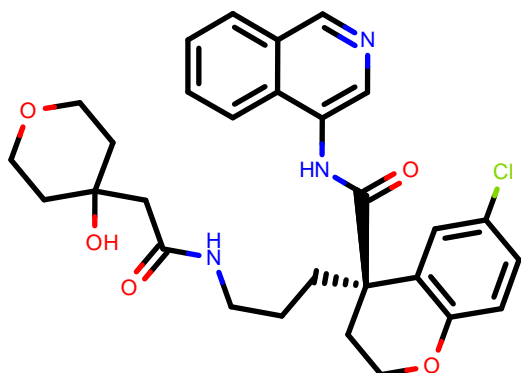
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CCCN5enon5

RUN: RUN5503

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.30

EN300-151423_4_1_1



CID: EN300-151423_4_1_1

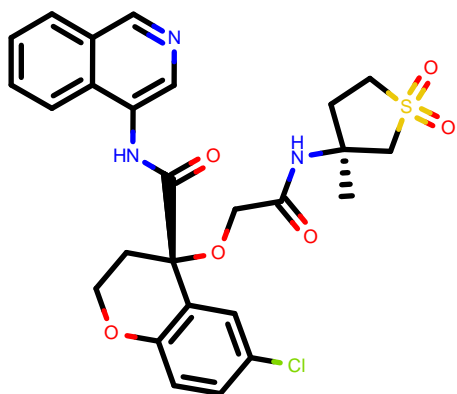
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CC5(COCCO5)O

RUN: RUN7766

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.27

EN300-10414_1_1_1



CID: EN300-10414_1_1_1

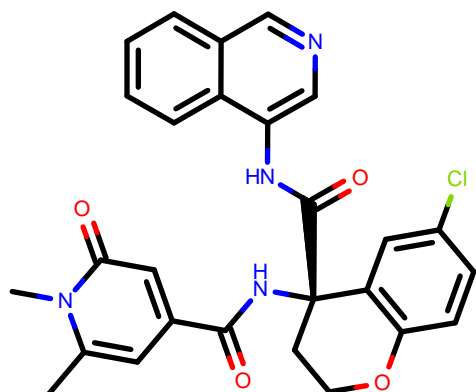
SMILES: C[C@@]1(CCS(=O)(=O)C1)NC(=O)CO[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nnc5c4cccc5

RUN: RUN3856

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.38

EN300-4287199_1_1_1



CID: EN300-4287199_1_1_1

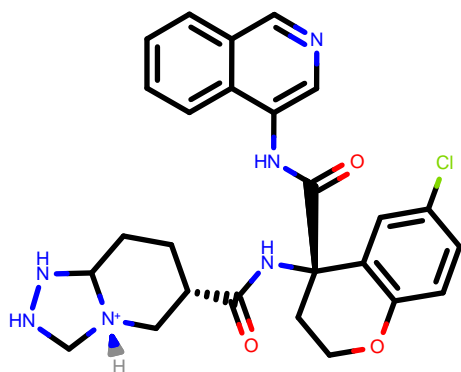
SMILES: Cc1ccc(=O)n1C(C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nnc5c4cccc5

RUN: RUN4868

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.26

EN300-51350_1_2_1



CID: EN300-51350_1_2_1

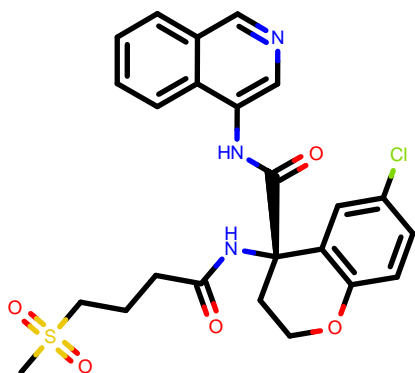
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCc6nnnc6C5

RUN: RUN3451

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.23

EN300-70522_1_1_1



CID: EN300-70522_1_1_1

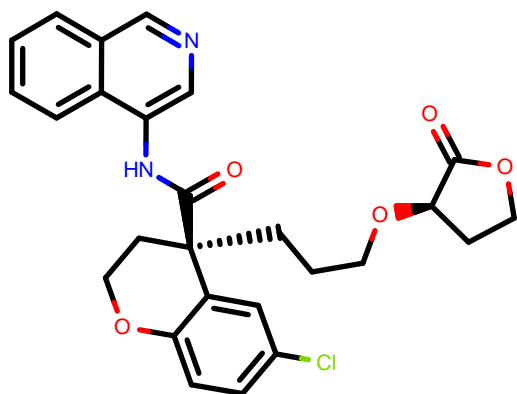
SMILES: CS(=O)(=O)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN6246

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.36

EN300-20496_4_1_1



CID: EN300-20496_4_1_1

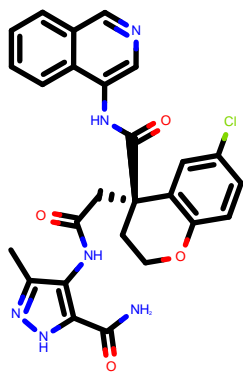
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCCCO[C@@]5(O)CCOC5=O

RUN: RUN4273

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.30

EN300-67302_1_1_1



CID: EN300-67302_1_1_1

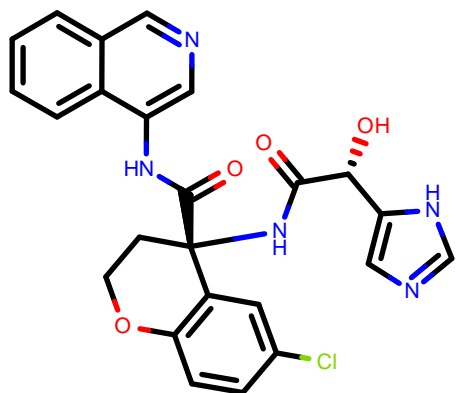
SMILES: Cc1c(c(n[nH]1)C(=O)N)NC(=O)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccoc5

RUN: RUN6532

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.30

EN300-254121_1_1_1



CID: EN300-254121_1_1_1

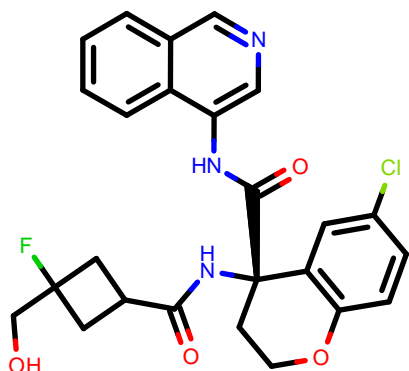
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]3[C@@]3(c5nc[nH]5)O

RUN: RUN3781

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.31

EDG-MED-90036822-77_1



CID: EDG-MED-90036822-77_1

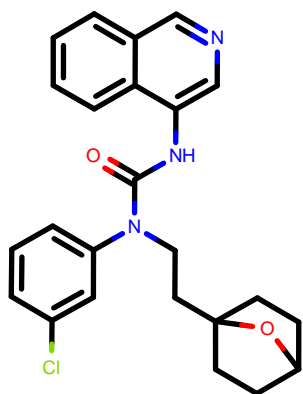
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@@]3[C@@]3(C(F)CO)O

RUN: RUN1633

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.26

ADA-UCB-dc2b944c-6_1



CID: ADA-UCB-dc2b944c-6_1

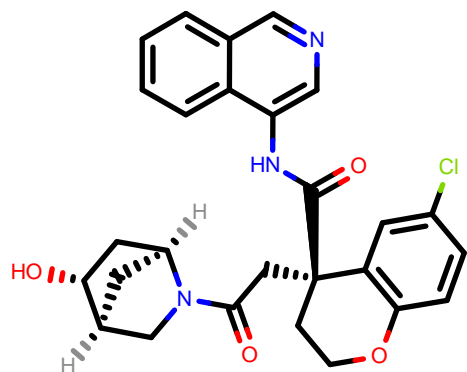
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(CCC34CCC(O3)CC4)c5ccccc(c5)Cl

RUN: RUN573

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.40

EN300-307084_1_2_1



CID: EN300-307084_1_2_1

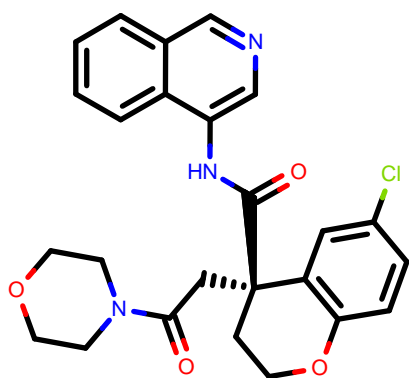
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)O)C[C@@]3[C@@]3(c5nc[nH]5)O

RUN: RUN3785

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.30

EN300-18064_1_1_1



CID: EN300-18064_1_1_1

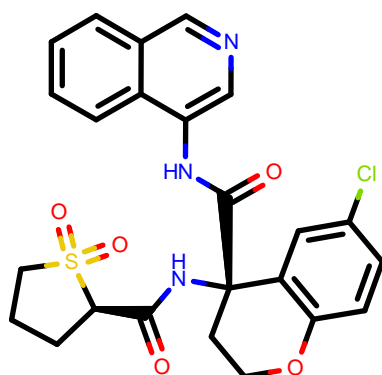
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOCC5

RUN: RUN6971

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.22

EN300-88656_1_2_1



CID: EN300-88656_1_2_1

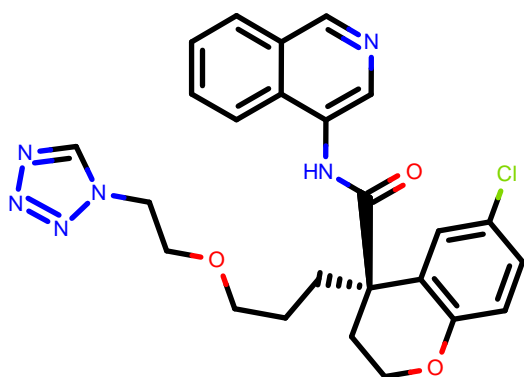
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCS5(=O)=O

RUN: RUN3357

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-364679_4_1_1



CID: EN300-364679_4_1_1

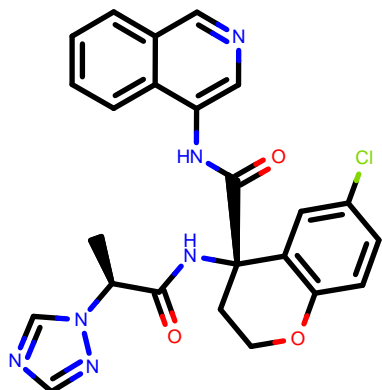
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCn5cnm5

RUN: RUN4246

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-30397_1_1_1



CID: EN300-30397_1_1_1

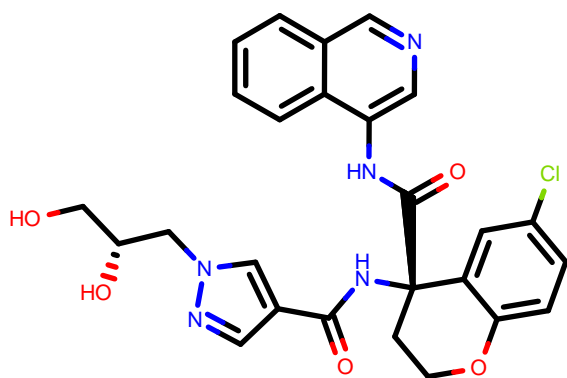
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)n5enm5

RUN: RUN3086

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.30

EN300-246178_1_1_1



CID: EN300-246178_1_1_1

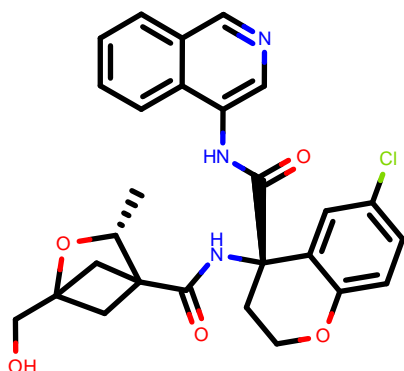
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn(c5)C[C@@H](CO)O

RUN: RUN7465

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.34

EN300-6491795_1_1_1



CID: EN300-6491795_1_1_1

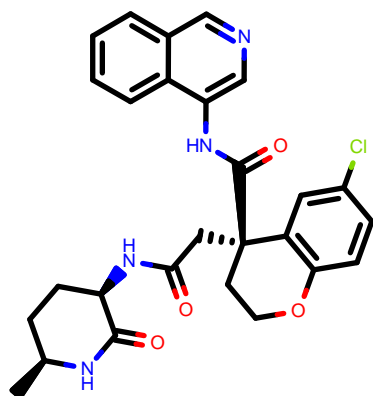
SMILES: C[C@@H]1C2(CC(C2)O1)CO)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ccc6c5ccc6

RUN: RUN5043

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-201180_1_4_1



CID: EN300-201180_1_4_1

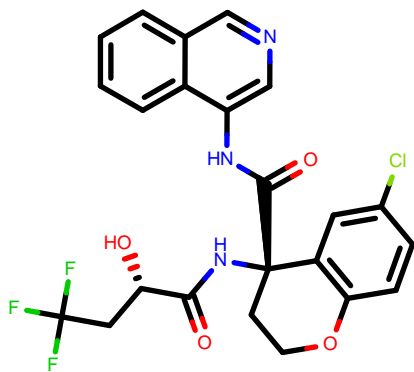
SMILES: C[C@@H]1CC[C@@H](C(=O)N1)NC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5317

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.30

EN300-1932013_1_2_1



CID: EN300-1932013_1_2_1

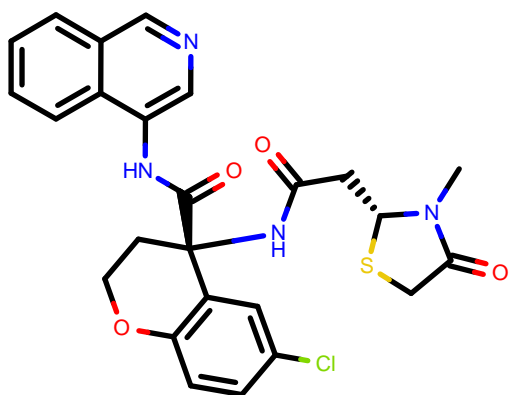
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](CC(F)F)O

RUN: RUN7470

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.30

EN300-143564_1_2_2



CID: EN300-143564_1_2_2

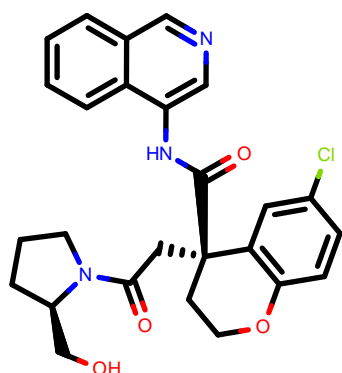
SMILES: CN1[C@@H](SCC1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2977

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.22

EN300-55109_1_1_1



CID: EN300-55109_1_1_1

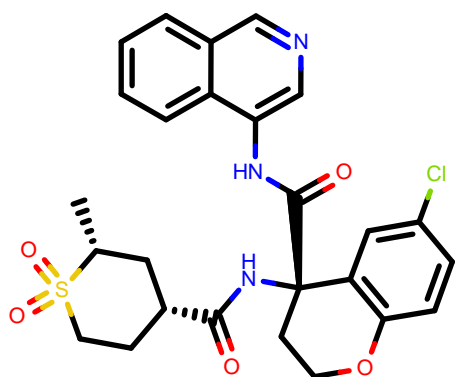
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5CO

RUN: RUN5293

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.24

EN300-6082676_1_1_1



CID: EN300-6082676_1_1_1

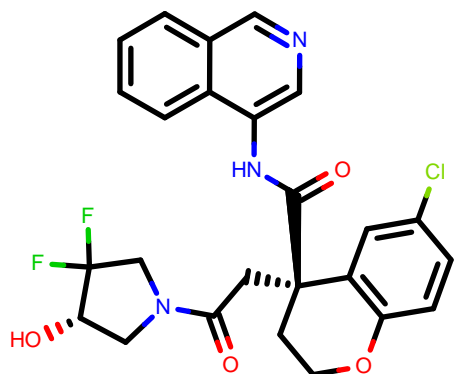
SMILES: C[C@@H]1[C@@H](CSC1=O)O[C@@]2(CO)N[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc4ncc5c4ccccc5

RUN: RUN4465

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.28

EN300-1710153_1_1_1



CID: EN300-1710153_1_1_1

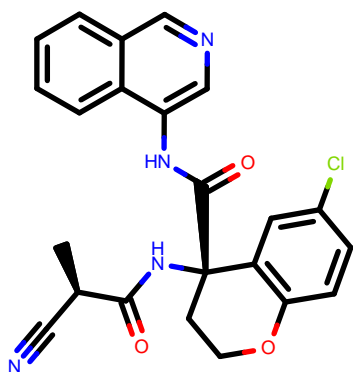
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C(F)F)O

RUN: RUN4077

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.23

EN300-72730_1_2_1



CID: EN300-72730_1_2_1

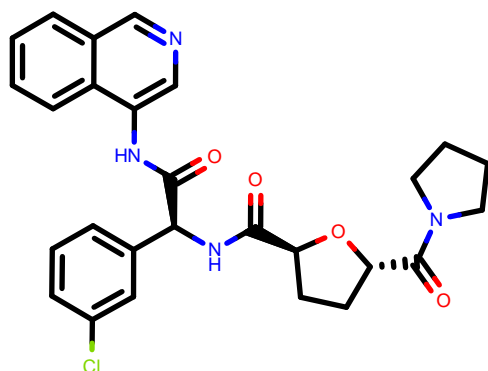
SMILES: C[C@H](C#N)C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5481

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.17

EDJ-MED-ee07cf00-11_6



CID: EDJ-MED-ee07cf00-11_6

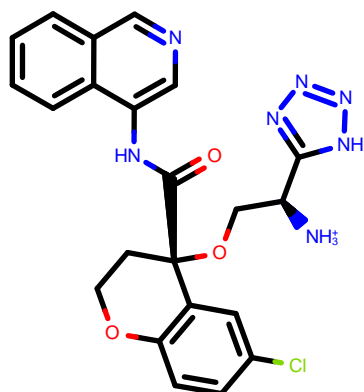
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](Cl)C(=O)N[C@@H](O)C1=CNCC1

RUN: RUN2657

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.48

ED_-GRI-5b13fbe2-3_1



CID: ED_-GRI-5b13fbe2-3_1

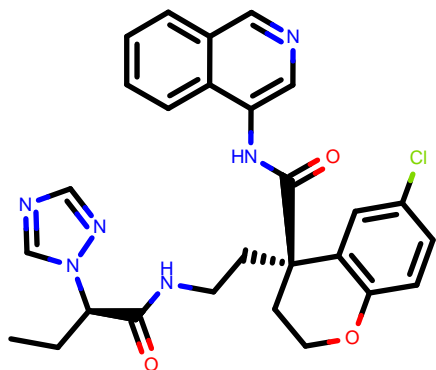
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC[C@@H](c5[nH]n5)N

RUN: RUN1404

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.32

EN300-651307_3_2_1



CID: EN300-651307_3_2_1

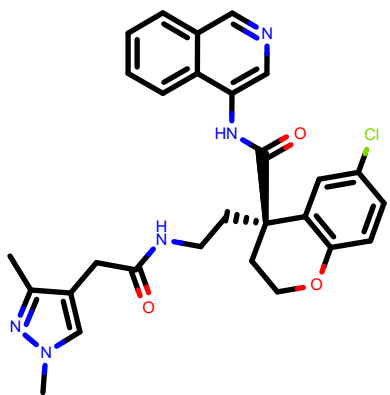
SMILES: CC[C@H](C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cn5

RUN: RUN4004

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.39

EN300-245061_3_1_1



CID: EN300-245061_3_1_1

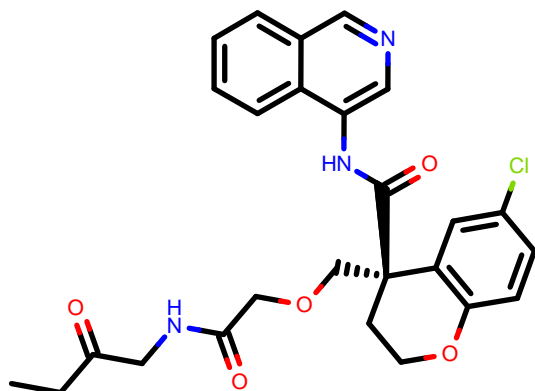
SMILES: Cc1c(en(n1)C)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN5933

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.30

EN300-132624_2_1_1



CID: EN300-132624_2_1_1

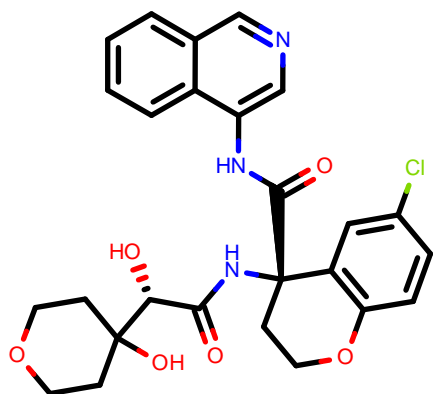
SMILES: CCC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4

RUN: RUN6301

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.35

EN300-749499_1_2_1



CID: EN300-749499_1_2_1

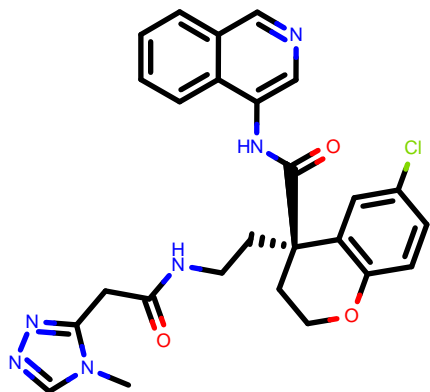
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](O)(O)C5(CCOCC5)O

RUN: RUN7759

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.31

EN300-6494474_3_1_1



CID: EN300-6494474_3_1_1

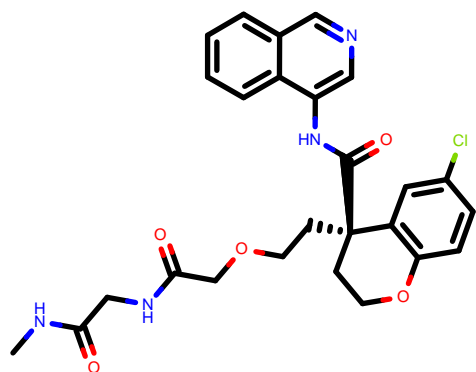
SMILES: Cn1cnc1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3094

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.24

EN300-23223_3_1_1



CID: EN300-23223_3_1_1

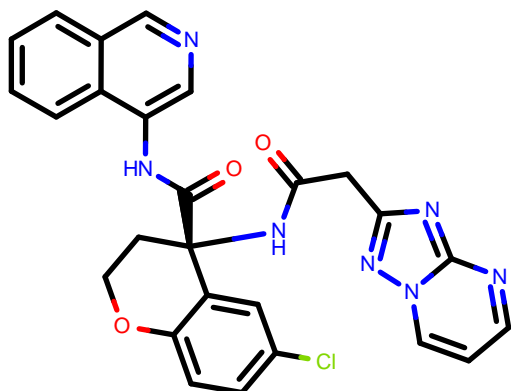
SMILES: CNC(=O)CNC(=O)COCC[C@@H](CCOC2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4819

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.27

EN300-39826_1_1_1



CID: EN300-39826_1_1_1

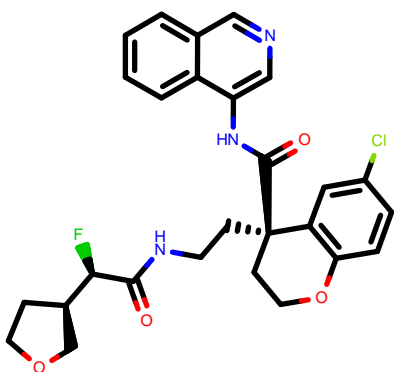
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3(CCOc4c3cc(cc4)C)NC(=O)C5nc6ncccn6n5

RUN: RUN7105

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.22

EN300-783124_3_1_1



CID: EN300-783124_3_1_1

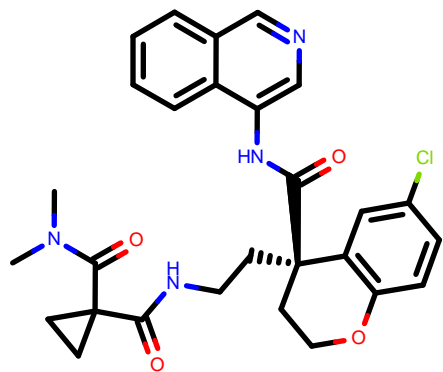
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](C@H)5c6ccoc65F

RUN: RUN3615

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.23

EN300-180875_3_1_1



CID: EN300-180875_3_1_1

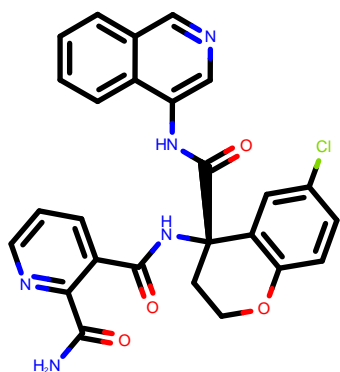
SMILES: CN(C)C(=O)C1(CC1)C(=O)NCC[C@@H](C@H)2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN7559

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.35

EN300-135530_1_1_1



CID: EN300-135530_1_1_1

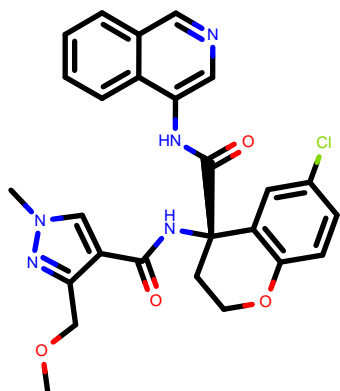
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cccnc5C(=O)N

RUN: RUN4152

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-244148_1_1_1



CID: EN300-244148_1_1_1

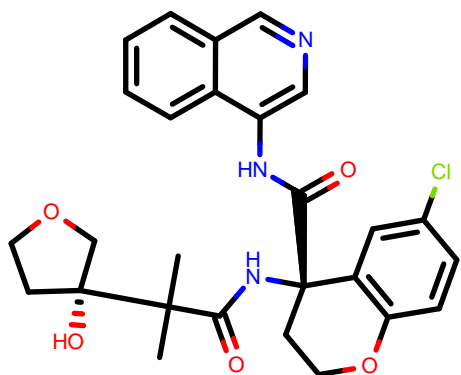
SMILES: Cn1cc(c(n1)COC)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccnc5c4ccc5

RUN: RUN2888

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-1630093_1_2_1



CID: EN300-1630093_1_2_1

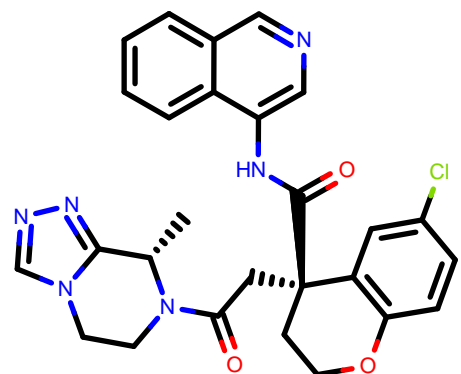
SMILES: CC(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)[C@@]5(CCOc5O

RUN: RUN6613

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-19_4



CID: EDG-MED-ba1ac7b9-19_4

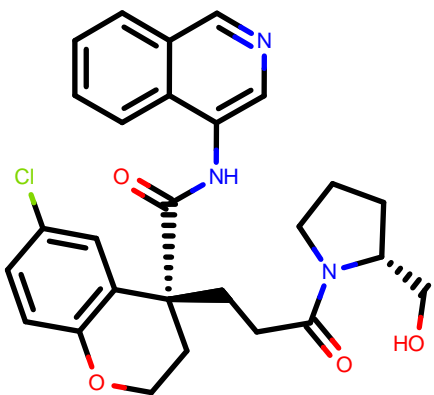
SMILES: C[C@@H]1c2nncn2CCN1C(=O)C[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cccnc6c5ccc6

RUN: RUN2499

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-55109_2_1_1



CID: EN300-55109_2_1_1

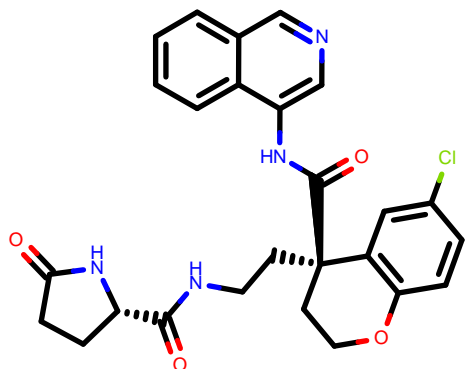
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)N5CC[C@@H]5CO

RUN: RUN5867

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-72896_3_1_1



CID: EN300-72896_3_1_1

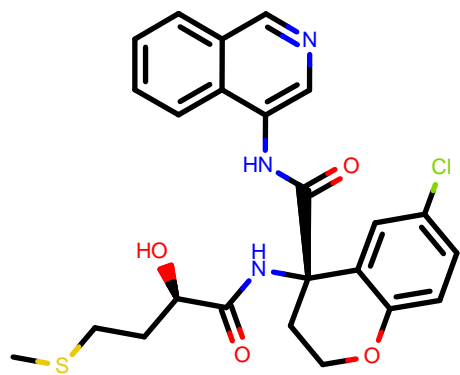
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@H]5CC(=O)N5

RUN: RUN5904

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-103144_1_2_1



CID: EN300-103144_1_2_1

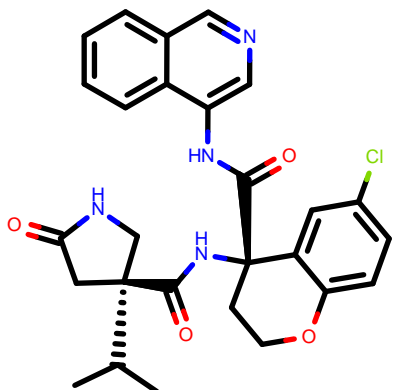
SMILES: CSCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3nccc4c3ccc4)O

RUN: RUN3943

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-211203_1_1_1



CID: EN300-211203_1_1_1

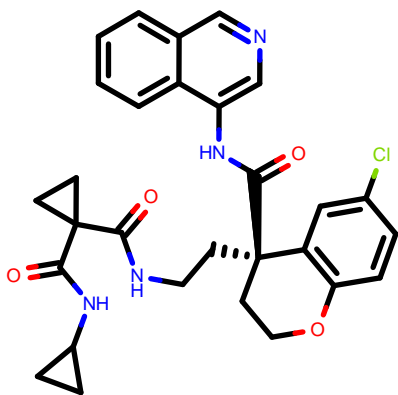
SMILES: CC(C)[C@@]1(CC(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN3018

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.25

EN300-61636_3_1_1



CID: EN300-61636_3_1_1

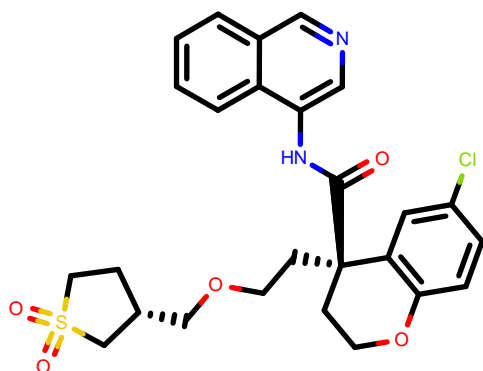
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CC5)C(=O)N6C6C6

RUN: RUN5017

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.34

EN300-1448603_3_2_1



CID: EN300-1448603_3_2_1

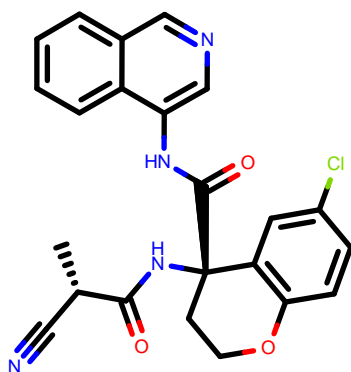
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CCS(=O)(=O)C5

RUN: RUN4926

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.30

EN300-72730_1_1_1



CID: EN300-72730_1_1_1

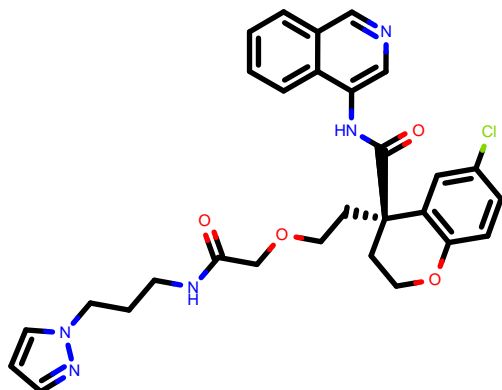
SMILES: C[C@@H](C#N)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN4991

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.21

EN300-47500_3_1_1



CID: EN300-47500_3_1_1

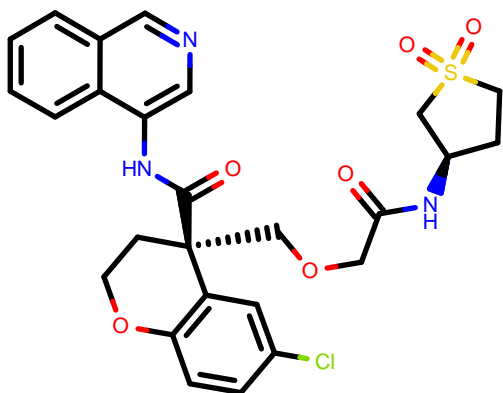
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)NCCc5ccc5

RUN: RUN4560

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.36

EN300-05512_2_1_1



CID: EN300-05512_2_1_1

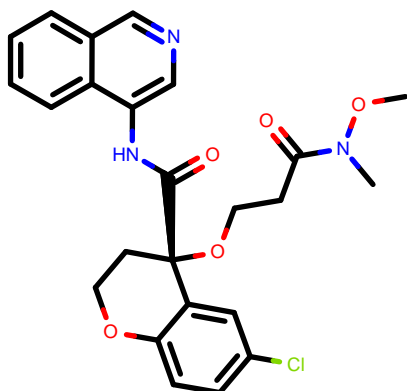
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CCS(=O)(=O)C5

RUN: RUN5201

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.33

EN300-174603_1_1_1



CID: EN300-174603_1_1_1

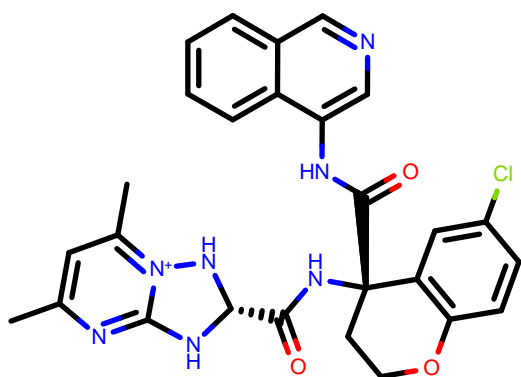
SMILES: CN(C(=O)CCO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN5076

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-00904_1_1_2



CID: EN300-00904_1_1_2

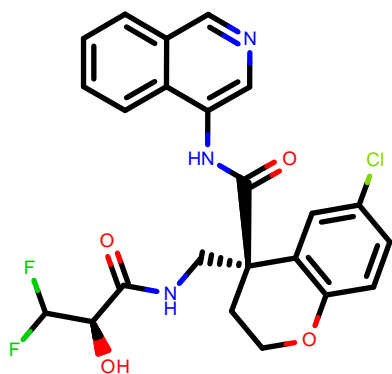
SMILES: Cc1cc([n+]2c(n1)N[C@H](N2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nccc6c5cccc6)C

RUN: RUN3381

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.35

EN300-1932780_2_2_1



CID: EN300-1932780_2_2_1

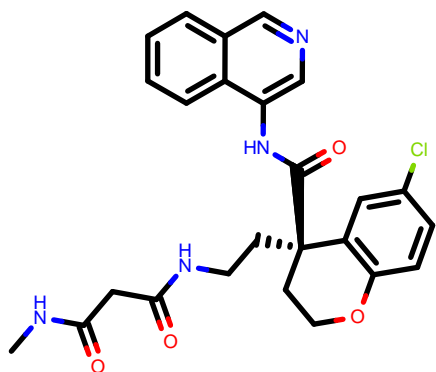
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H](C(F)F)O

RUN: RUN4954

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.21

EN300-128463_3_1_1



CID: EN300-128463_3_1_1

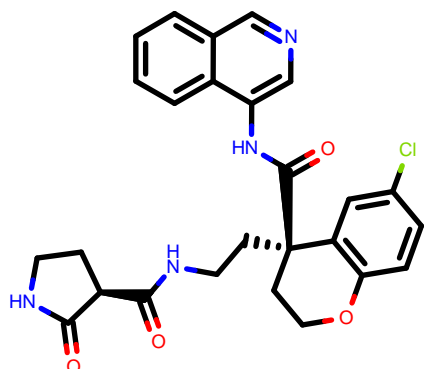
SMILES: CNC(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3858

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.31

EN300-94945_3_1_1



CID: EN300-94945_3_1_1

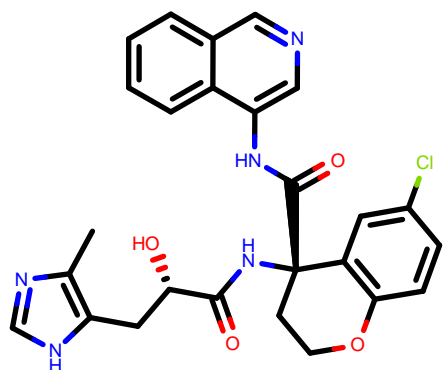
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCNC5=O

RUN: RUN6884

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.30

EN300-7494324_1_1_1



CID: EN300-7494324_1_1_1

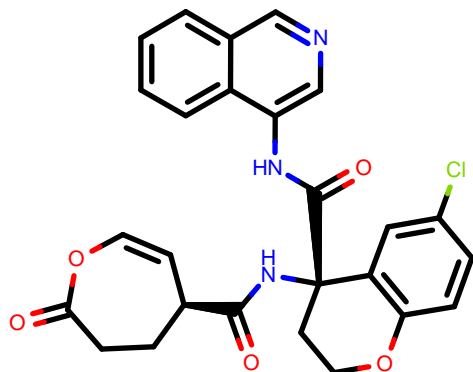
SMILES: Cc1c(nc[nH]1)C[C@@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN5034

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.26

EN300-2011083_1_2_1



CID: EN300-2011083_1_2_1

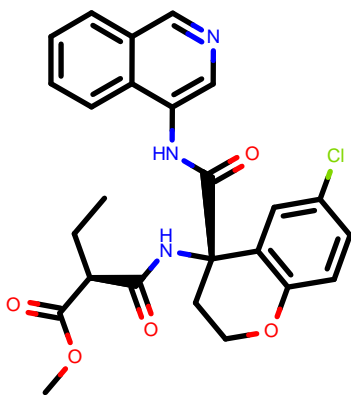
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)OCC5

RUN: RUN5708

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.27

EN300-175425_1_1_1



CID: EN300-175425_1_1_1

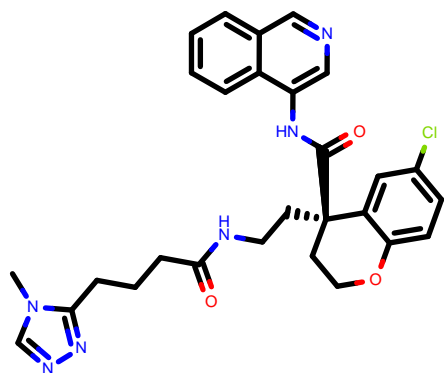
SMILES: CC[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)C(=O)OC

RUN: RUN4919

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.21

EN300-6356960_3_1_1



CID: EN300-6356960_3_1_1

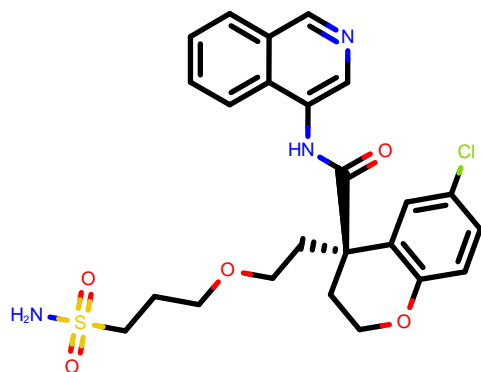
SMILES: Cn1nnc1CCCC(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN3968

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.34

EN300-79588_3_1_1



CID: EN300-79588_3_1_1

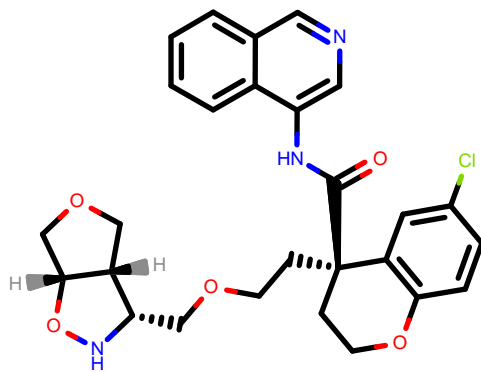
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC(CS(=O)(=O)N)=O

RUN: RUN5169

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.33

EN300-7436306_3_1_2



CID: EN300-7436306_3_1_2

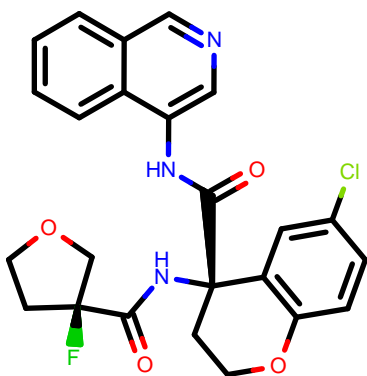
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC[C@@H]5[C@@H](COC)C@H5N

RUN: RUN3069

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.34

EN300-188356_1_1_1



CID: EN300-188356_1_1_1

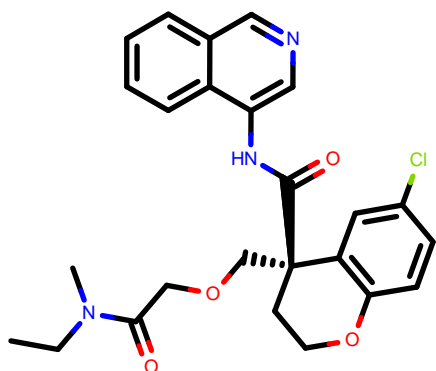
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCOc5)F

RUN: RUN5942

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.30

EN300-1253122_2_1_1



CID: EN300-1253122_2_1_1

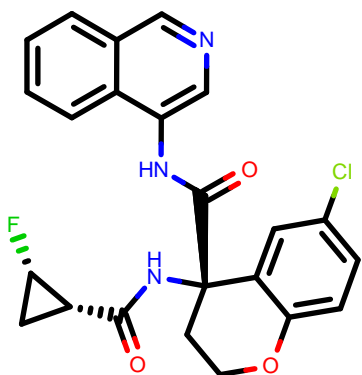
SMILES: CCN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3607

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-1654606_1_1_1



CID: EN300-1654606_1_1_1

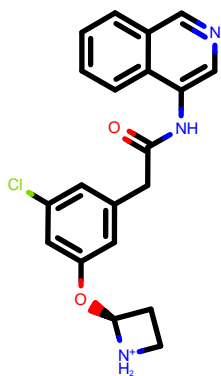
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(C)C(F)F5

RUN: RUN5095

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.17

PET-UNK-cf04cb02-1_2



CID: PET-UNK-cf04cb02-1_2

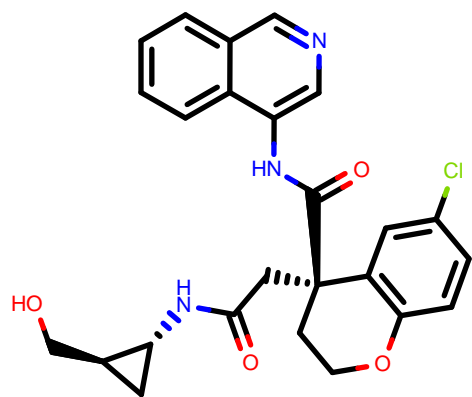
SMILES: c1ccc2c(c1)cnc2NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC[NH2+]4

RUN: RUN299

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.36

EDJ-MED-d203f206-34_1



CID: EDJ-MED-d203f206-34_1

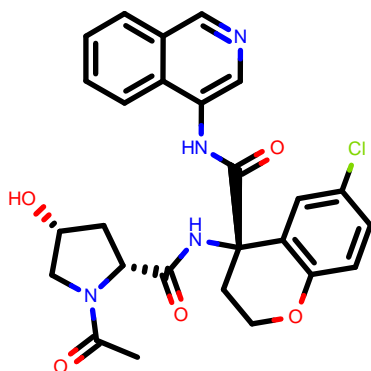
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]5CO

RUN: RUN2458

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-158260_1_1_1



CID: EN300-158260_1_1_1

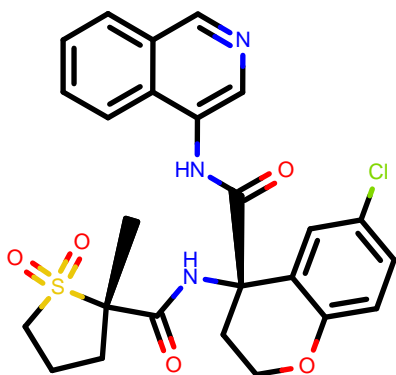
SMILES: CC(=O)N1C[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C1=O)Nc4ccc5c4ccc5O

RUN: RUN4850

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-373476_1_2_1



CID: EN300-373476_1_2_1

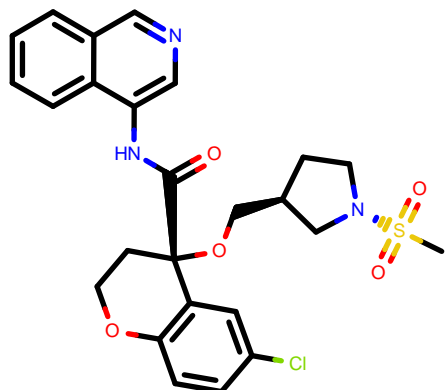
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7520

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.34

EN300-261986_1_1_1



CID: EN300-261986_1_1_1

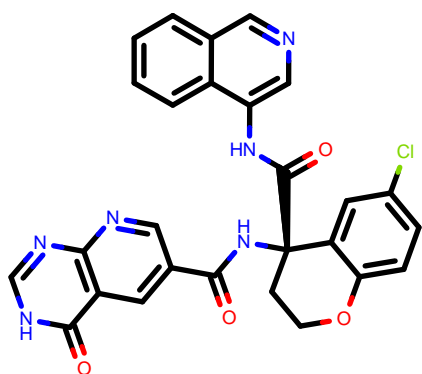
SMILES: CS(=O)(=O)N@]1CC[C@@H]1C1CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4880

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.37

EN300-7494115_1_1_1



CID: EN300-7494115_1_1_1

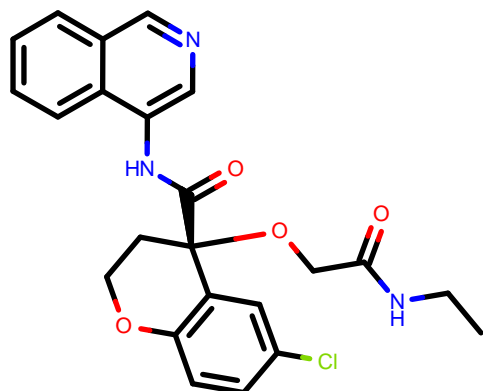
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c(=O)[nH]cnc6nc5

RUN: RUN5788

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-7003350_1_1_1



CID: EN300-7003350_1_1_1

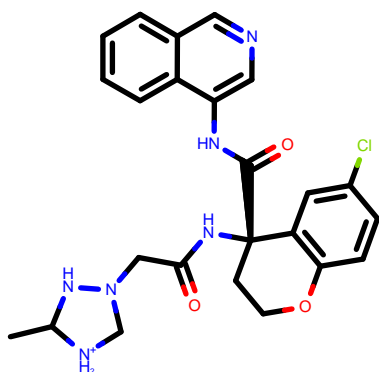
SMILES: CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4718

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.20

EN300-7473354_1_1_1



CID: EN300-7473354_1_1_1

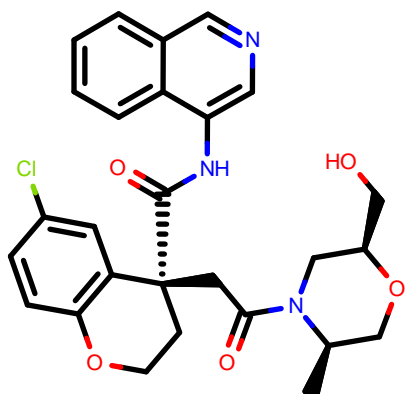
SMILES: Cc1ncn(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5780

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-109920_1_1_1



CID: EN300-109920_1_1_1

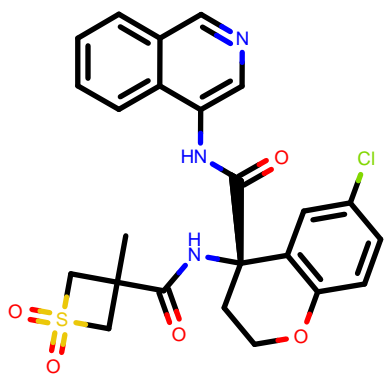
SMILES: C[C@@H]1CO[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO

RUN: RUN6103

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.49

EN300-1718364_1_1_1



CID: EN300-1718364_1_1_1

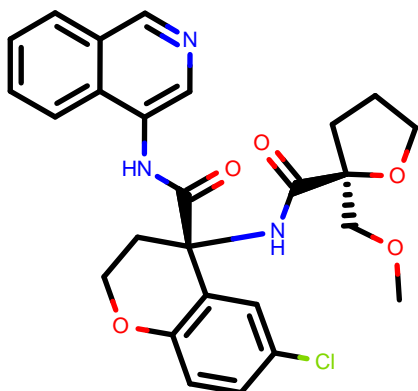
SMILES: CC1(CS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3982

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-1301381_1_1_1



CID: EN300-1301381_1_1_1

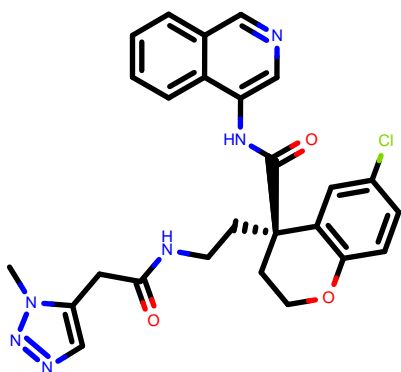
SMILES: COC[C@@]1(CCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4643

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-6486855_3_1_1



CID: EN300-6486855_3_1_1

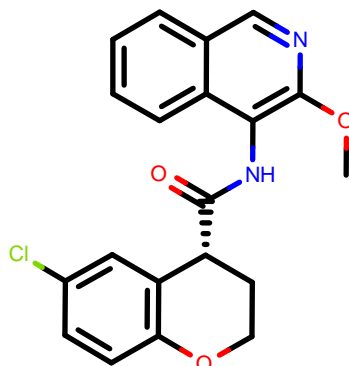
SMILES: Cn1c(cnn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN6345

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

JOH-UNI-f51e3bbc-4_1



CID: JOH-UNI-f51e3bbc-4_1

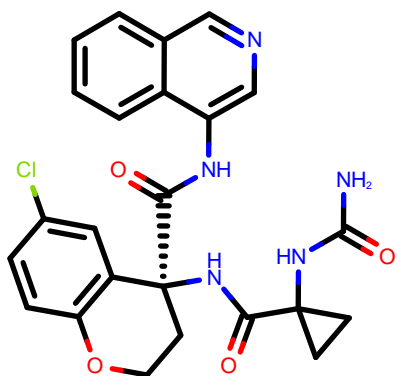
SMILES: COc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1054

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.13

EN300-123614_1_1_1



CID: EN300-123614_1_1_1

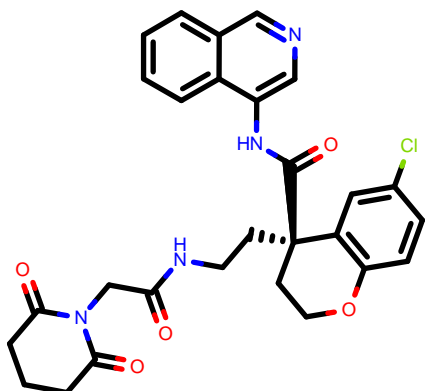
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5NC(=O)N

RUN: RUN3594

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.32

EN300-54837_3_1_1



CID: EN300-54837_3_1_1

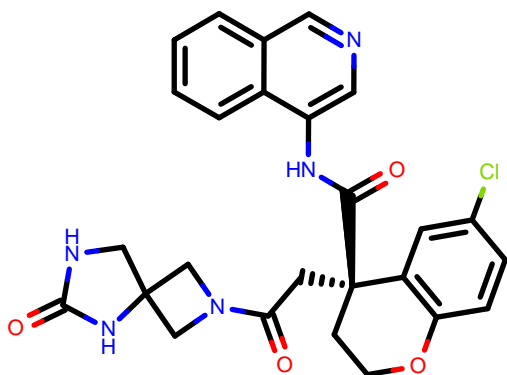
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5C(=O)CCOC5=O

RUN: RUN6495

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.33

EN300-1605226_1_1_1



CID: EN300-1605226_1_1_1

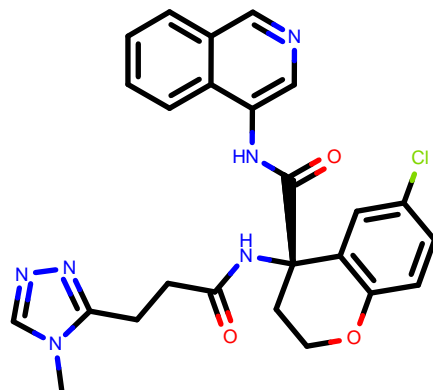
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6(C5)CNC(=O)N6

RUN: RUN7140

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.30

EN300-1138792_1_1_1



CID: EN300-1138792_1_1_1

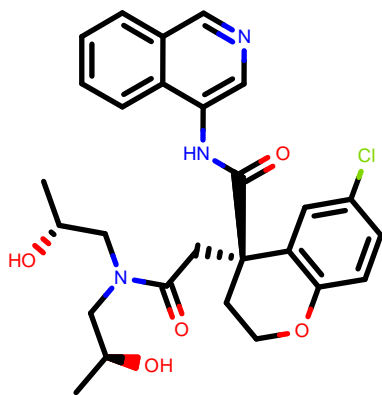
SMILES: Cn1cnnc1CCC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3216

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.23

EN300-722418_1_1_1



CID: EN300-722418_1_1_1

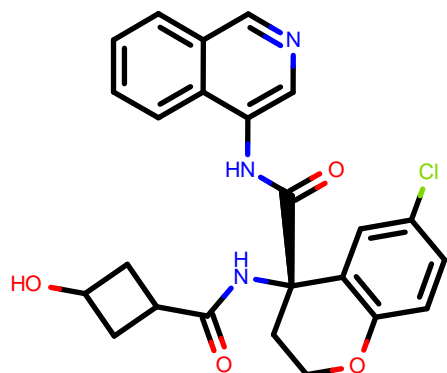
SMILES: C[C@H](CN(C[C@H](C)O)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6425

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.45

EN300-306026_1_1_1



CID: EN300-306026_1_1_1

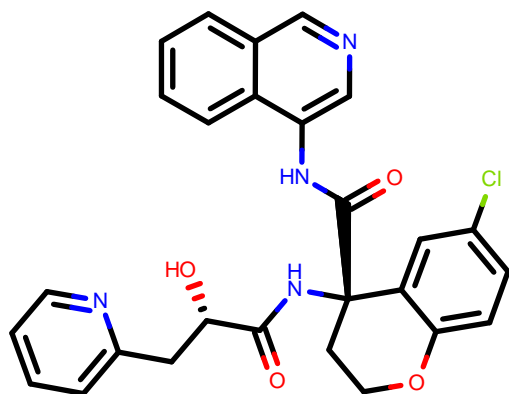
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(C)O

RUN: RUN4203

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.22

EN300-6762327_1_2_1



CID: EN300-6762327_1_2_1

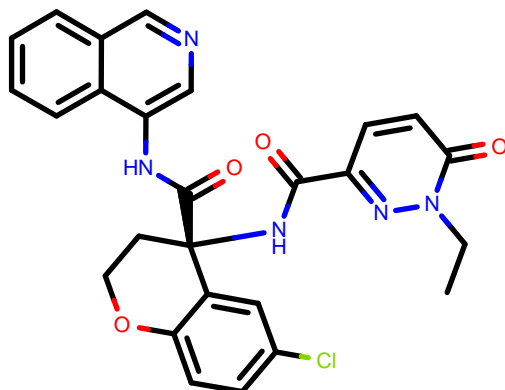
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](Cc5ccccc5)O

RUN: RUN5801

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.30

EN300-74314_1_1_1



CID: EN300-74314_1_1_1

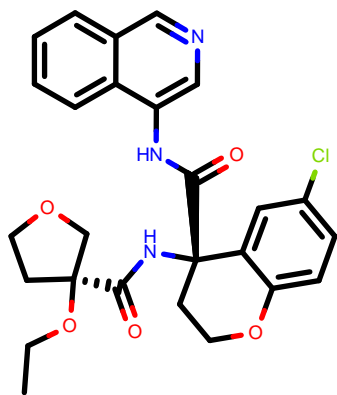
SMILES: CCn1c(O)ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3901

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.25

EN300-259694_1_2_1



CID: EN300-259694_1_2_1

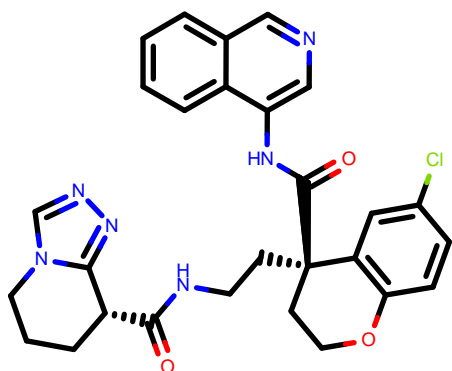
SMILES: CCOC@1(CCOC1)C(=O)N[C@@2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5248

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.35

EN300-748981_3_1_1



CID: EN300-748981_3_1_1

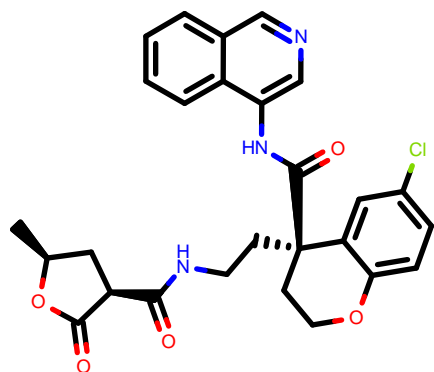
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCCN6c5nnc6

RUN: RUN3859

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.31

EN300-7444533_3_4_1



CID: EN300-7444533_3_4_1

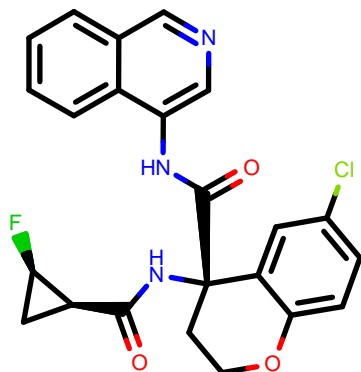
SMILES: C[C@@H]1C[C@@H](C(=O)O1)C(=O)NCC[C@@2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5650

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.36

EN300-97300_1_4_1



CID: EN300-97300_1_4_1

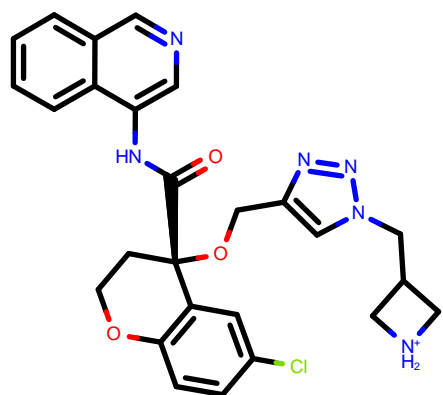
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H]5F

RUN: RUN4413

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.18

ED_-GRI-5b13fbe2-24_1



CID: ED_-GRI-5b13fbe2-24_1

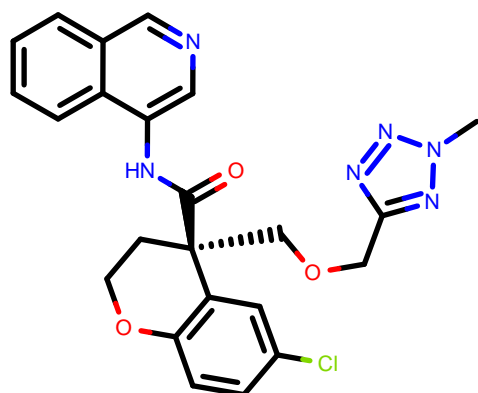
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(n5)CC6C[NH2+]C6

RUN: RUN1452

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.39

EN300-90225_2_1_1



CID: EN300-90225_2_1_1

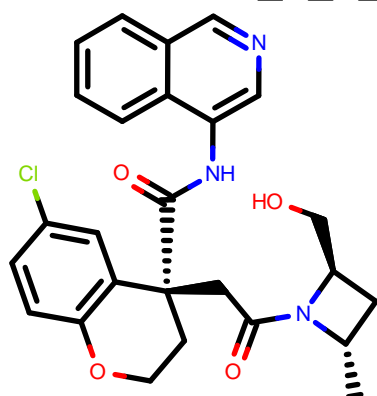
SMILES: Cn1nc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3327

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.24

EN300-1709410_1_2_1



CID: EN300-1709410_1_2_1

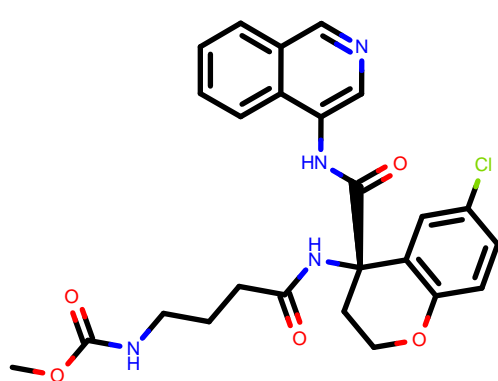
SMILES: C[C@H]1C[C@@H](N1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO

RUN: RUN4612

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.26

EN300-71560_1_1_1



CID: EN300-71560_1_1_1

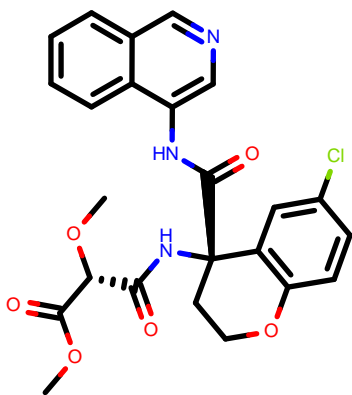
SMILES: COC(=O)NCCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6148

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.27

EN300-1718194_1_2_1



CID: EN300-1718194_1_2_1

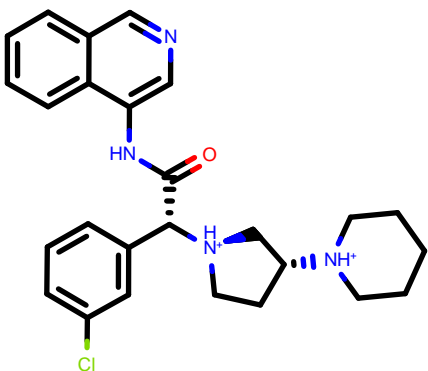
SMILES: CO[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)C(=O)OC

RUN: RUN4068

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.23

MIC-UNK-5a93dd5f-12_5



CID: MIC-UNK-5a93dd5f-12_5

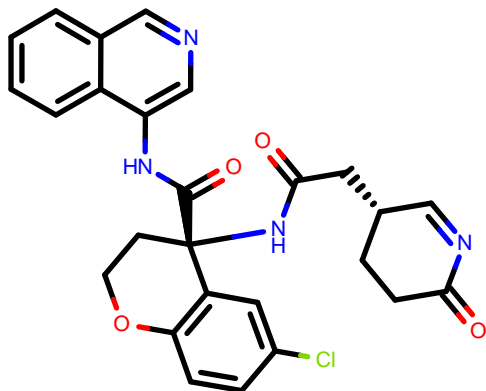
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)N@@@4CC[C@H](C4)[NH+]5CCCC5

RUN: RUN747

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.52

EN300-246992_1_2_1



CID: EN300-246992_1_2_1

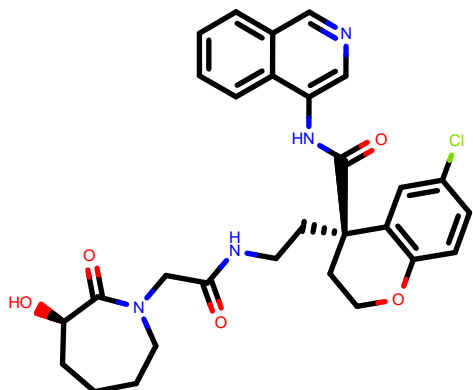
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCCC(=O)NC5

RUN: RUN4329

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.22

EN300-259849_3_2_1



CID: EN300-259849_3_2_1

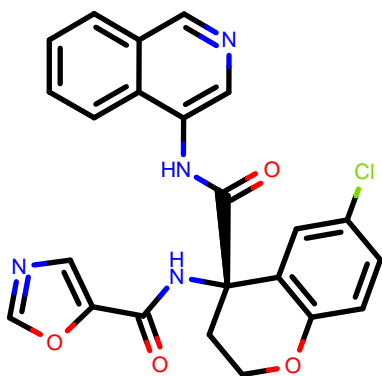
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5CCCC[C@H](C5=O)O

RUN: RUN5602

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.48

EN300-25446_1_1_1



CID: EN300-25446_1_1_1

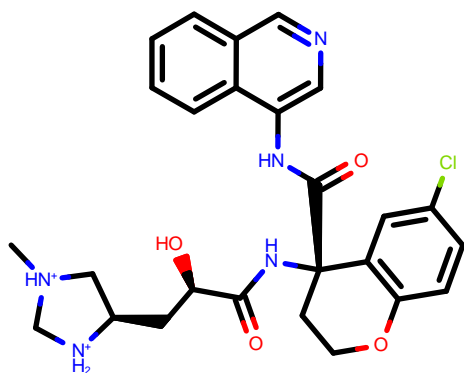
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]2(CCOc4c3cc(cc4)Cl)NC(=O)c5cnco5

RUN: RUN3051

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.17

EN300-1725538_1_2_1



CID: EN300-1725538_1_2_1

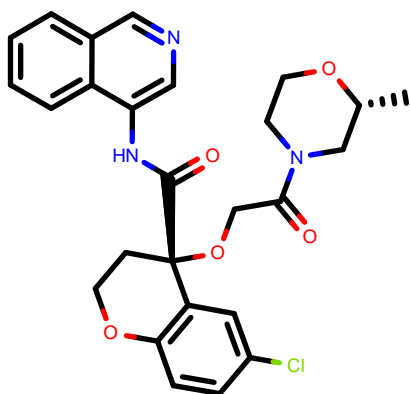
SMILES: Cn1cc(nc1)C[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN7008

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.31

EN300-25572_1_1_1



CID: EN300-25572_1_1_1

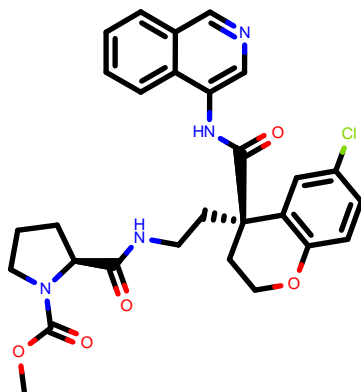
SMILES: C[C@@]1CN(CCO1)C(=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7491

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-66845_3_2_1



CID: EN300-66845_3_2_1

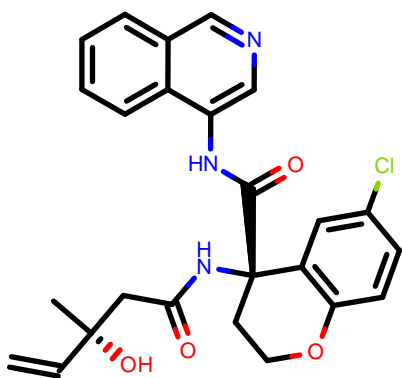
SMILES: COC(=O)N1CCC[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3261

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.34

EN300-181938_1_1_1



CID: EN300-181938_1_1_1

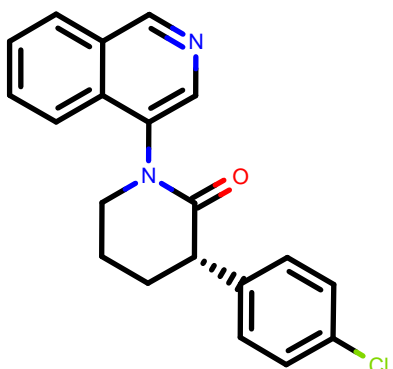
SMILES: C[C@@H](CC(=O)N[C@@H]1(CCOC2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4)(C=C)O

RUN: RUN3699

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

ALP-POS-ce760d3f-8_2



CID: ALP-POS-ce760d3f-8_2

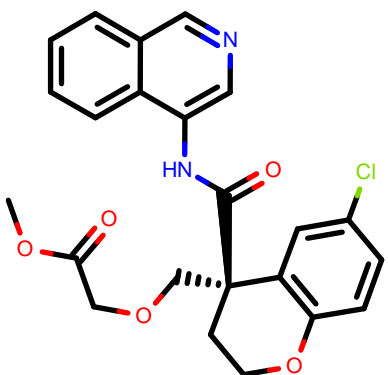
SMILES: c1ccc2c(c1)cncc2N3CCCC[C@H](C3=O)c4ccc(cc4)Cl

RUN: RUN1280

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.27

EN300-19700_2_1_1



CID: EN300-19700_2_1_1

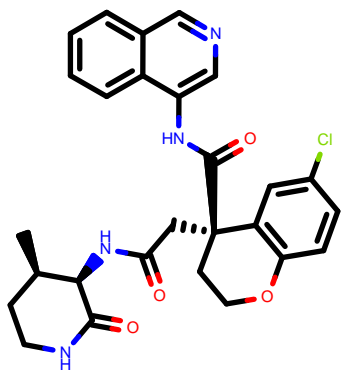
SMILES: COC(=O)COC[C@@H]1(CCOC2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4

RUN: RUN5245

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.20

EN300-91401_1_1_1



CID: EN300-91401_1_1_1

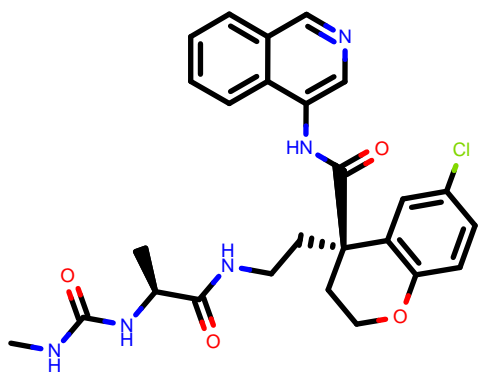
SMILES: C[C@@H]1CCNC(=O)[C@@H]1NC(=O)C[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccc5

RUN: RUN6026

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-1258964_3_1_1



CID: EN300-1258964_3_1_1

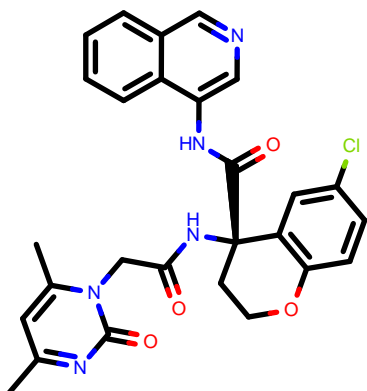
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)NC(=O)NC

RUN: RUN4414

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-137191_1_1_1



CID: EN300-137191_1_1_1

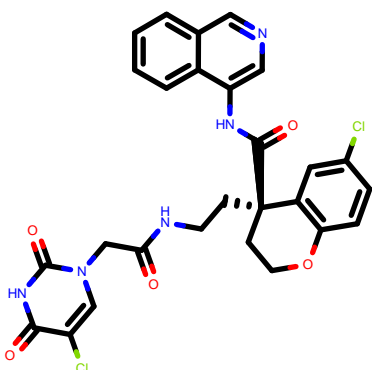
SMILES: Cc1ccn(c(=O)n1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)C

RUN: RUN3690

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-6494606_3_1_1



CID: EN300-6494606_3_1_1

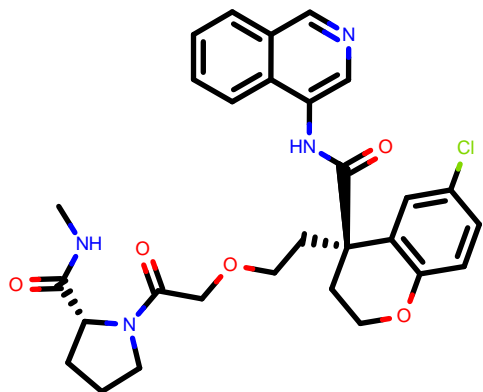
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)Cn5cc(c(=O)[nH]5=O)Cl

RUN: RUN7275

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.38

EN300-48902_3_2_1



CID: EN300-48902_3_2_1

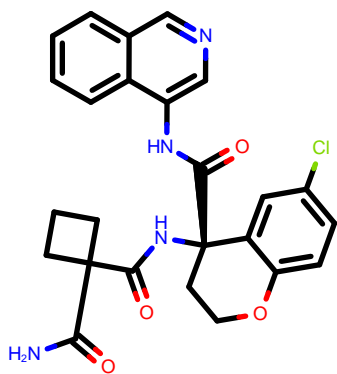
SMILES: CNC(=O)[C@@H]1CCCN1C(=O)COCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN7548

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.36

EN300-68747_1_1_1



CID: EN300-68747_1_1_1

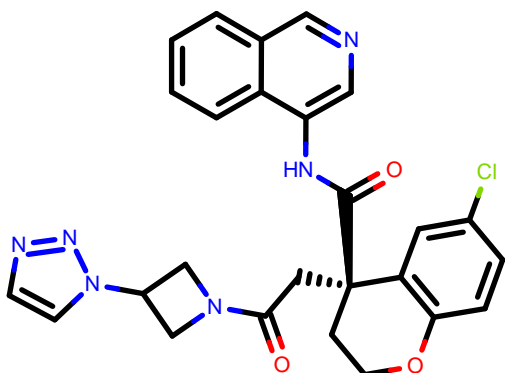
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)C(=O)N

RUN: RUN5858

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.23

EN300-367405_1_1_1



CID: EN300-367405_1_1_1

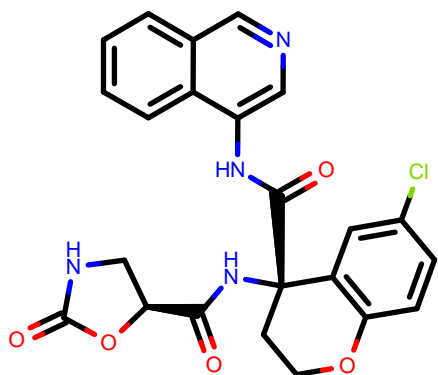
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6ccn6

RUN: RUN6862

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.31

EN300-244403_1_1_1



CID: EN300-244403_1_1_1

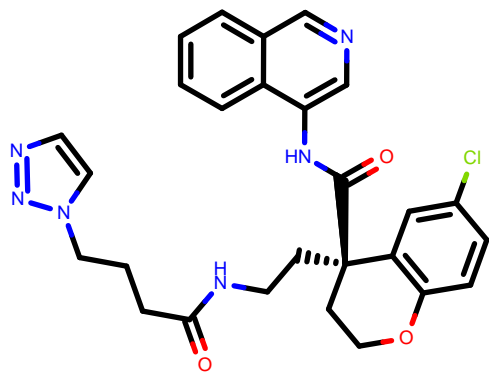
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H5CNC(=O)O5

RUN: RUN5366

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.22

EN300-124301_3_1_1



CID: EN300-124301_3_1_1

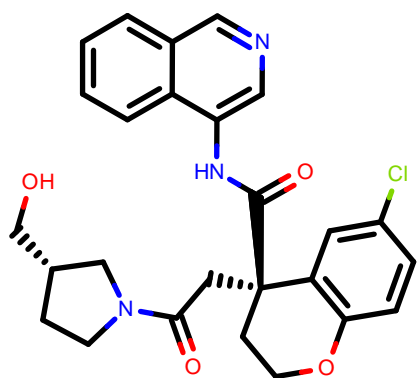
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC5C5ccn5

RUN: RUN4927

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

EN300-256053_1_1_1



CID: EN300-256053_1_1_1

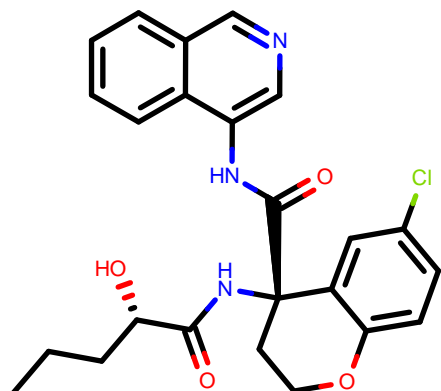
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN5492

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.27

EN300-300217_1_2_1



CID: EN300-300217_1_2_1

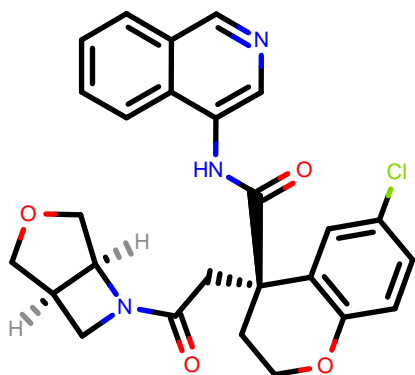
SMILES: C/C=C/[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN4697

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.29

EN300-7493296_1_1_1



CID: EN300-7493296_1_1_1

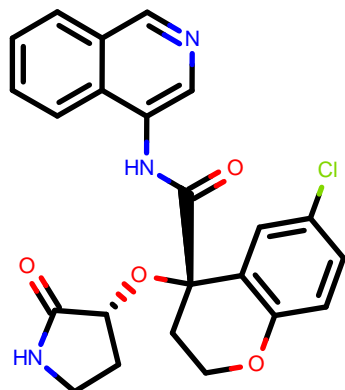
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H]5COC6

RUN: RUN6292

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.24

EN300-6736413_1_1_1



CID: EN300-6736413_1_1_1

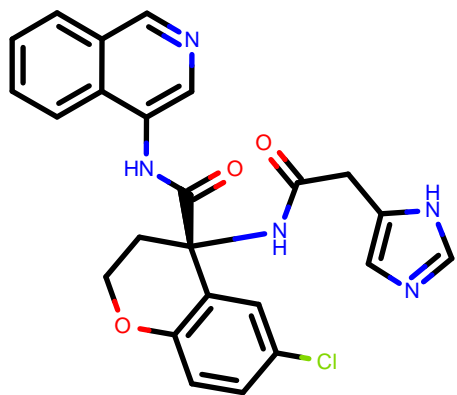
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCNC5=O

RUN: RUN7255

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.20

EN300-342226_1_1_1



CID: EN300-342226_1_1_1

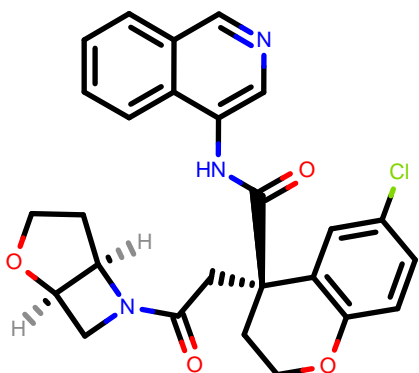
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5nc[nH]5

RUN: RUN4605

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.27

EN300-651665_1_1_1



CID: EN300-651665_1_1_1

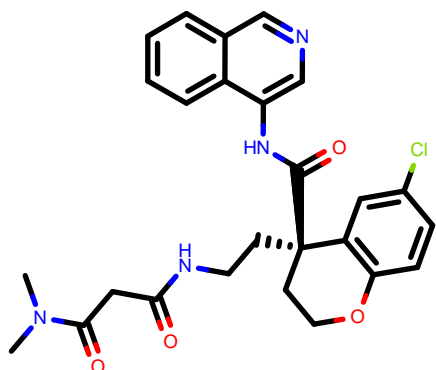
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@]H6[C@H]5CCO6

RUN: RUN3544

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-93573_3_1_1



CID: EN300-93573_3_1_1

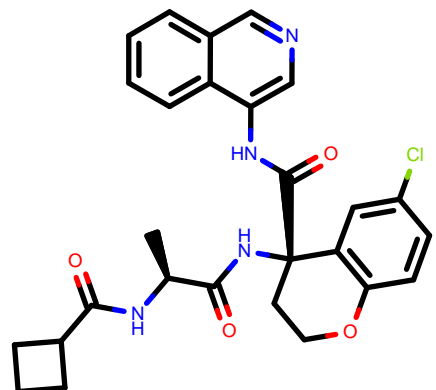
SMILES: CN(C)C(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccoc4

RUN: RUN4238

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-66082_1_1_1



CID: EN300-66082_1_1_1

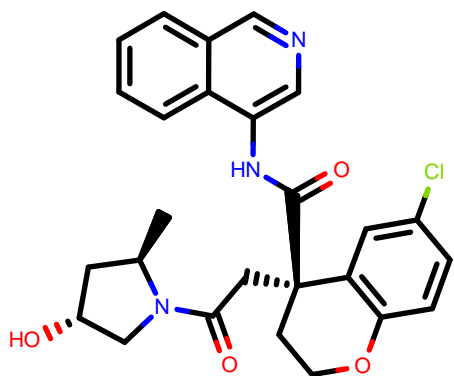
SMILES: C[C@@]H[C@]([C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccoc4)NC(=O)C5CC5

RUN: RUN6826

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-173562_1_3_1



CID: EN300-173562_1_3_1

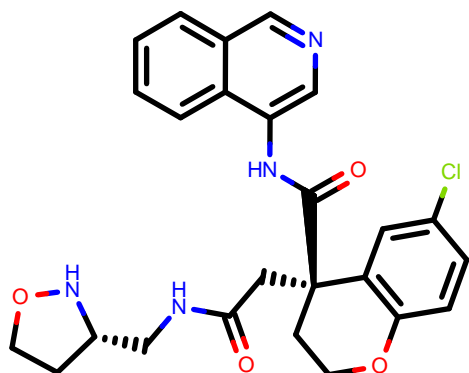
SMILES: C[C@@H]1C[C@H](CN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3091

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.27

EN300-1720418_1_1_1



CID: EN300-1720418_1_1_1

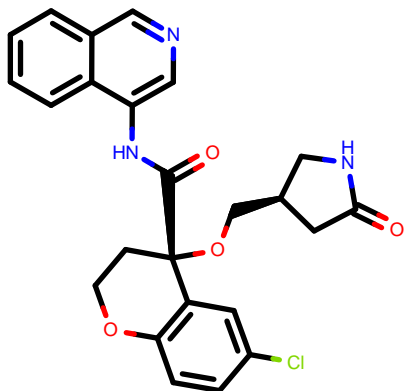
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCON5

RUN: RUN6235

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.25

EN300-246747_1_1_1



CID: EN300-246747_1_1_1

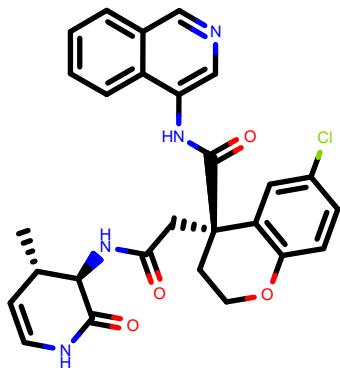
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CC(=O)NCS

RUN: RUN4887

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-91401_1_2_1



CID: EN300-91401_1_2_1

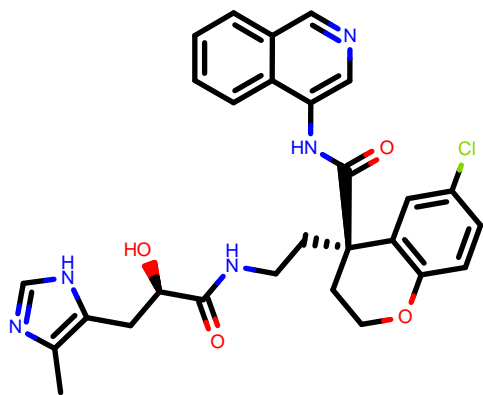
SMILES: C[C@H]1CCNC(=O)[C@@]2(CO)C[C@@]3(CCOc4c3c2cc(cc4)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4820

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.30

EN300-7494324_3_2_1



CID: EN300-7494324_3_2_1

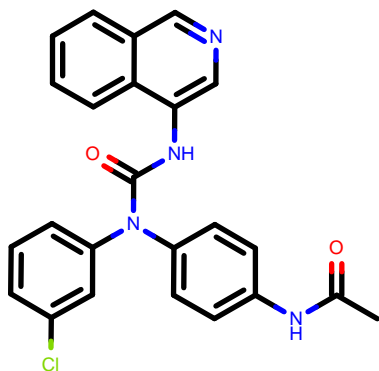
SMILES: Cc1c(nc[nH]1)C[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)O

RUN: RUN6630

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.32

MIC-UNK-d36ab305-2_1



CID: MIC-UNK-d36ab305-2_1

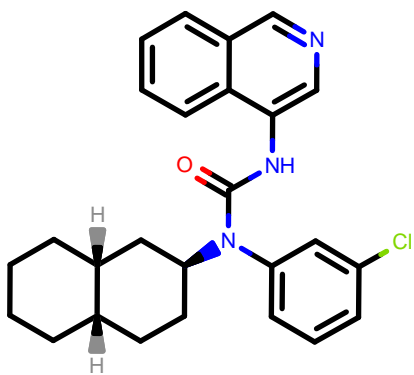
SMILES: CC(=O)Nc1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN144

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.31

MIC-UNK-cdc2493e-8_2



CID: MIC-UNK-cdc2493e-8_2

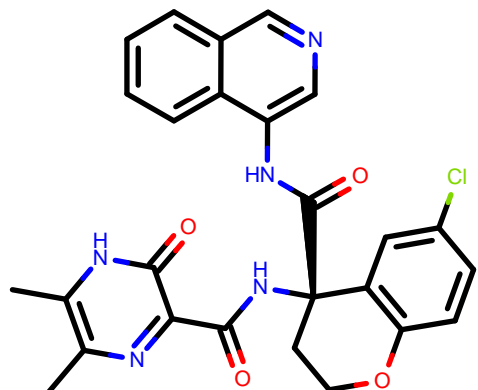
SMILES: c1ccc2c(c1)encc2NC(=O)N(c3cccc(c3)Cl)[C@H]4CC[C@@]5[H]5C[C@]6[H]5C4C6

RUN: RUN473

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.37

EN300-116885_1_1_1



CID: EN300-116885_1_1_1

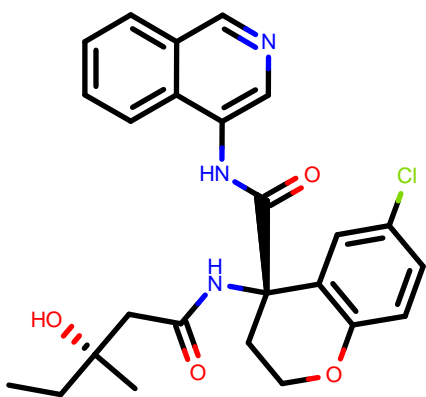
SMILES: Cc1c(nc(=O)[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)C

RUN: RUN3941

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-181938_1_2_1



CID: EN300-181938_1_2_1

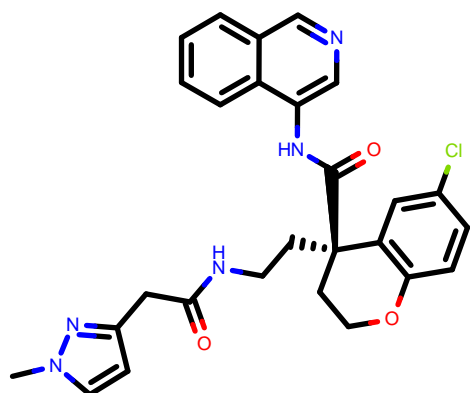
SMILES: C[C@](CC(=O)N[C@@]1(CCOC2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)(C=C)O

RUN: RUN3890

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-258702_3_1_1



CID: EN300-258702_3_1_1

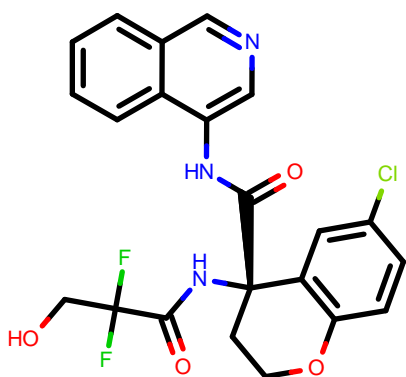
SMILES: Cn1ccc(n1)CC(=O)NCC[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4434

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-123489_1_1_1



CID: EN300-123489_1_1_1

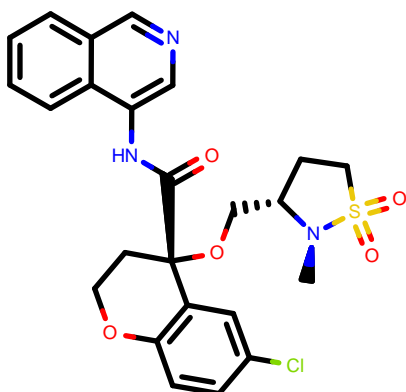
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)C(CO)(F)F

RUN: RUN5119

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.22

EN300-393148_1_1_1



CID: EN300-393148_1_1_1

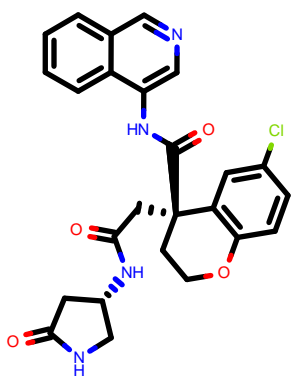
SMILES: C[N@@]1[C@@@H](CCS1(=O)=O)CO[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN6764

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-127487_1_2_1



CID: EN300-127487_1_2_1

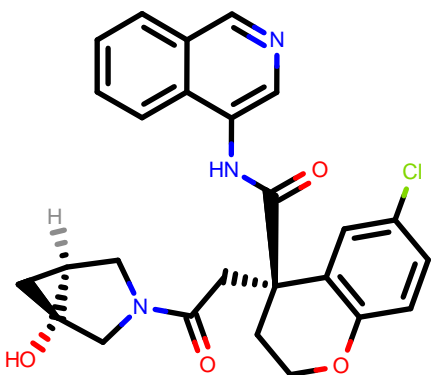
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC(=O)NCS

RUN: RUN5322

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.24

EN300-178288_1_1_1



CID: EN300-178288_1_1_1

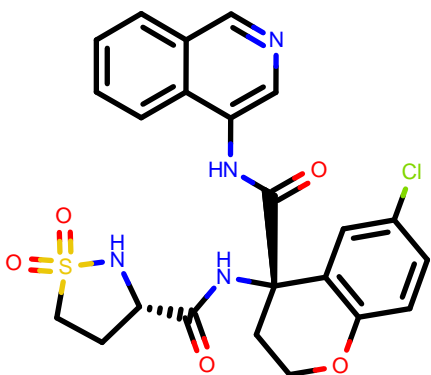
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@@]6(C5)O

RUN: RUN5697

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-45049_1_1_1



CID: EN300-45049_1_1_1

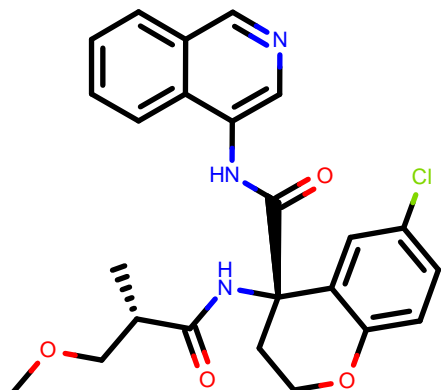
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCS(=O)(=O)N5

RUN: RUN4681

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.29

EN300-69162_1_1_1



CID: EN300-69162_1_1_1

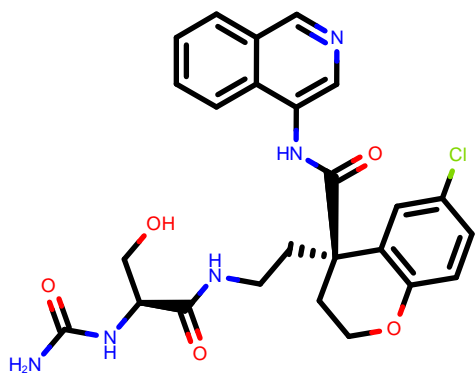
SMILES: C[C@@H](COC)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3886

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.21

EN300-10170_3_2_1



CID: EN300-10170_3_2_1

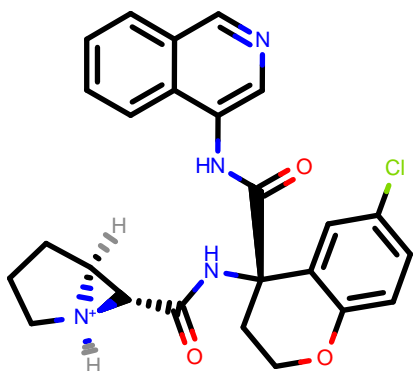
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H](CO)NC(=O)N

RUN: RUN4730

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.35

EDG-MED-90036822-73_2



CID: EDG-MED-90036822-73_2

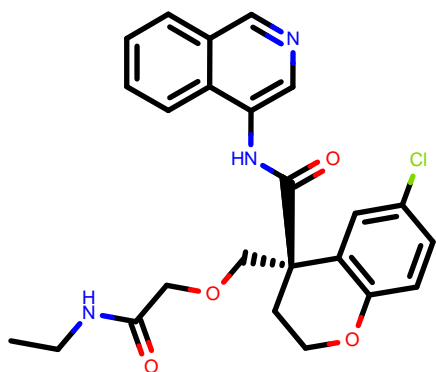
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](N)Nc4ccccc4

RUN: RUN1616

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-7003350_2_1_1



CID: EN300-7003350_2_1_1

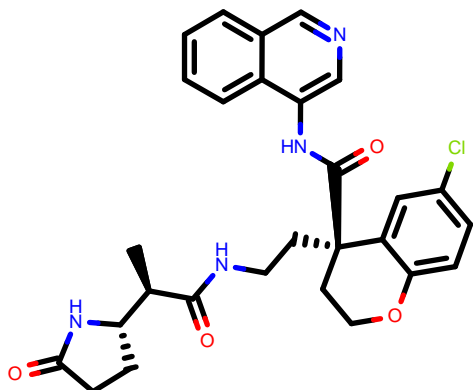
SMILES: CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN6685

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.20

EN300-249421_3_2_1



CID: EN300-249421_3_2_1

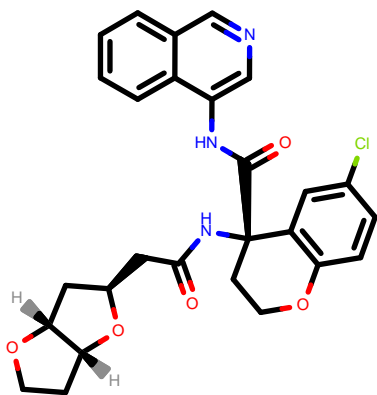
SMILES: C[C@H](C@@H)1CCC(=O)N1C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3616

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.34

EN300-735519_1_5_1



CID: EN300-735519_1_5_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C(=O)N[C@@H](O)C(=O)N[C@@H](O)C(=O)N

RUN:

RUN5585

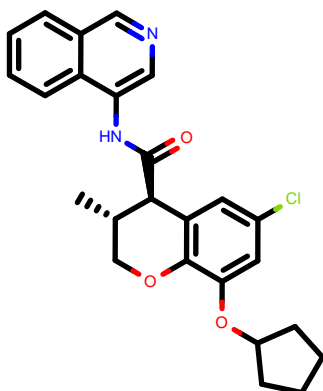
DDG (kcal/mol):

-1.09

dDDG (kcal/mol):

0.29

DAR-DIA-0d514e7d-4_1_1



CID: DAR-DIA-0d514e7d-4_1_1

SMILES:

C[C@H]1COc2c(cc2OC3CCCC3Cl)[C@@H](C(=O)Nc4cnc5c4cccc5

RUN:

RUN4177

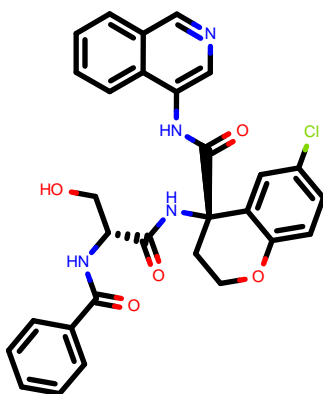
DDG (kcal/mol):

-1.09

dDDG (kcal/mol):

0.24

EN300-50228_1_2_1



CID: EN300-50228_1_2_1

SMILES:

c1ccc(cc1)C(=O)N[C@@H](CO)C(=O)N[C@@H](C(=O)Nc2cnc3c2cccc3

RUN:

RUN5104

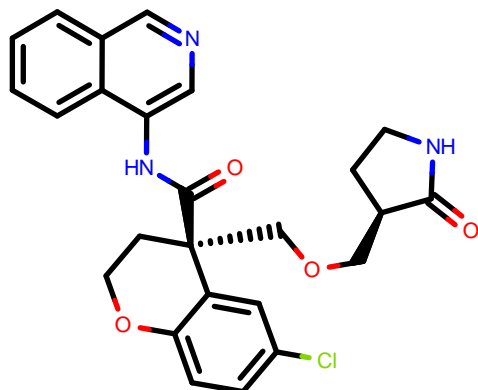
DDG (kcal/mol):

-1.09

dDDG (kcal/mol):

0.31

EDJ-MED-fcba3f31-6_1



CID: EDJ-MED-fcba3f31-6_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C(=O)N[C@@H](O)C(=O)N

RUN:

RUN2383

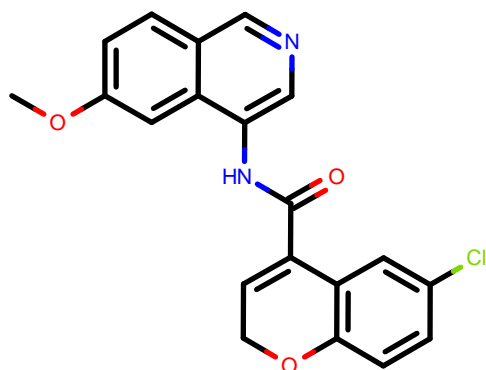
DDG (kcal/mol):

-1.09

dDDG (kcal/mol):

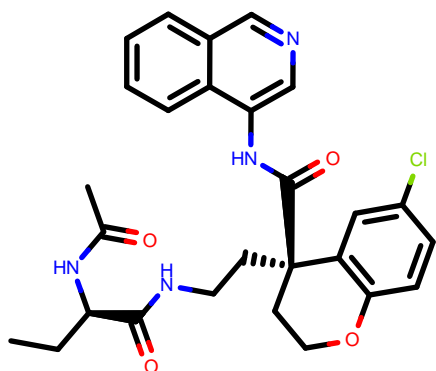
0.26

ALP-POS-ce760d3f-6_1



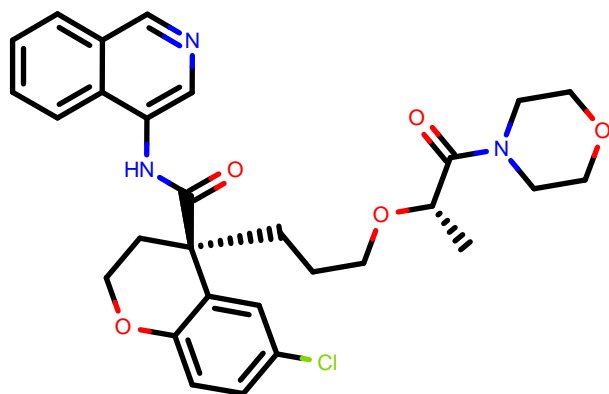
CID:	ALP-POS-ce760d3f-6_1
SMILES:	<chem>COc1ccc2cnccc(c2c1)NC(=O)C3=CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN1283
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.27

EN300-332601_3_2_1



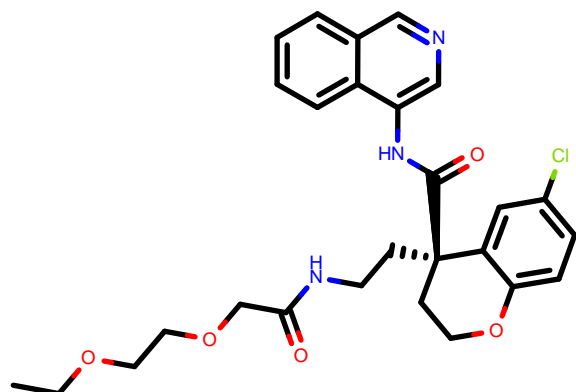
CID:	EN300-332601_3_2_1
SMILES:	<chem>CC[C@H](C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)C</chem>
RUN:	RUN3670
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.31

EN300-05754_4_1_1



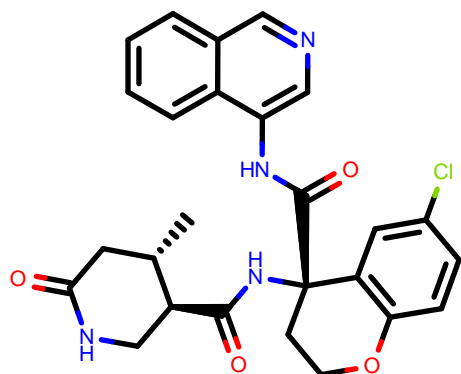
CID:	EN300-05754_4_1_1
SMILES:	<chem>C[C@]([H])(C(=O)N1CCOCC1)OCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5</chem>
RUN:	RUN7257
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.36

EN300-54304_3_1_1



CID:	EN300-54304_3_1_1
SMILES:	<chem>CCOCCOCC(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN6659
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.32

EN300-95698_1_2_1



CID: EN300-95698_1_2_1

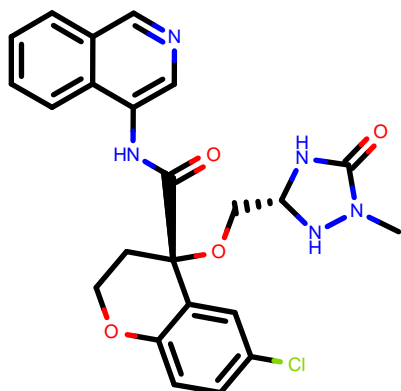
SMILES: C[C@H]1CC(=O)NC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6871

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.30

EN300-124918_1_1_2



CID: EN300-124918_1_1_2

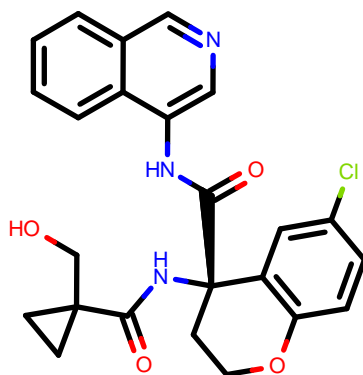
SMILES: CN1C(=O)N[C@@H]1[NH2+]1CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4058

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.33

EN300-146174_1_1_1



CID: EN300-146174_1_1_1

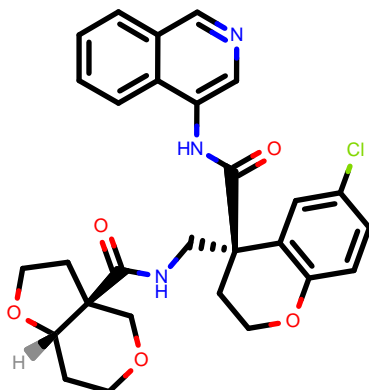
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)CO

RUN: RUN3720

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.22

EN300-341337_2_4_1



CID: EN300-341337_2_4_1

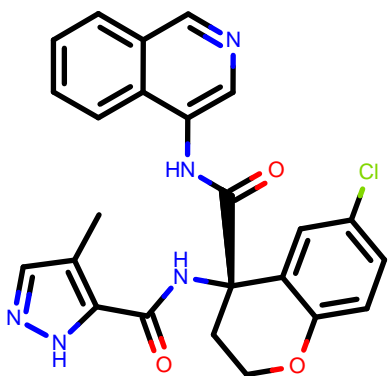
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]56CCO[C@H]5CCOC6

RUN: RUN6948

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.26

EN300-248178_1_1_1



CID: EN300-248178_1_1_1

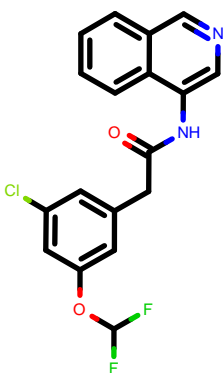
SMILES: Cc1cn[nH]c1C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5045

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.21

MIC-UNK-16ccb665-1_1



CID: MIC-UNK-16ccb665-1_1

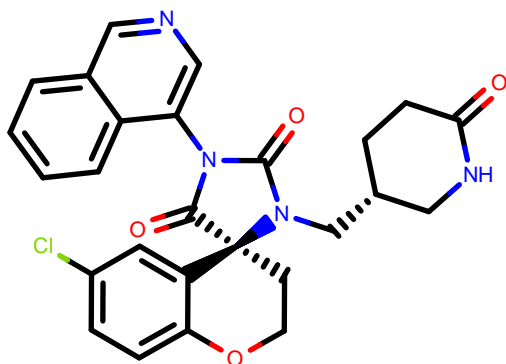
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OC(F)F

RUN: RUN2138

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.27

VLA-UNK-f702bf1c-5_1



CID: VLA-UNK-f702bf1c-5_1

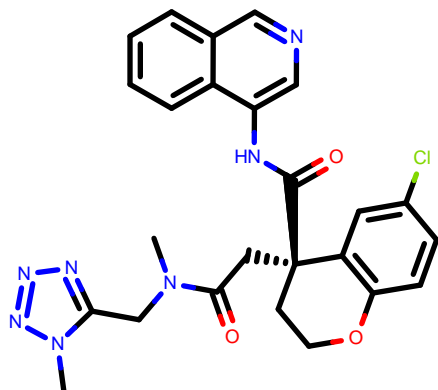
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOC5c4cc(cc5)Cl)N(C3=O)C[C@@]6CCCC(=O)NC6

RUN: RUN2117

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.30

EN300-148515_1_1_1



CID: EN300-148515_1_1_1

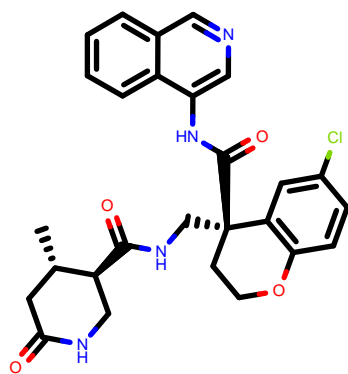
SMILES: Cn1c[nm1]CN(C)C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4481

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.29

EN300-95698_2_2_1



CID: EN300-95698_2_2_1

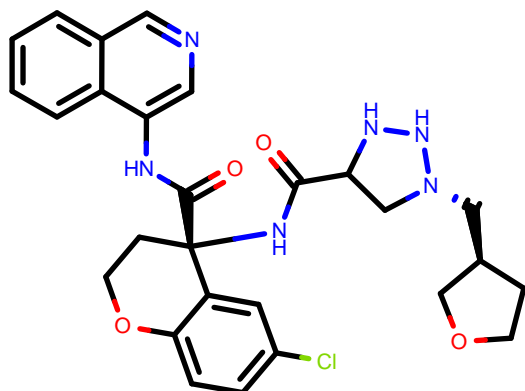
SMILES: C[C@H]1CC(=O)NC[C@@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN5008

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.35

EN300-317272_1_2_1



CID: EN300-317272_1_2_1

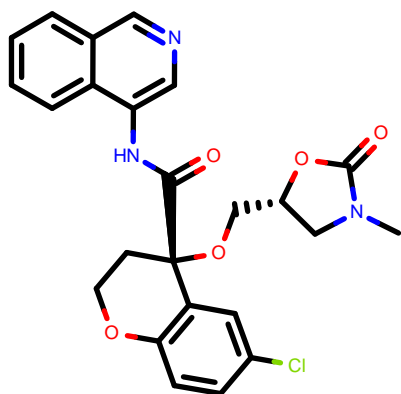
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(n5)C[C@H]6COC6

RUN: RUN4764

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.28

EN300-222969_1_1_1



CID: EN300-222969_1_1_1

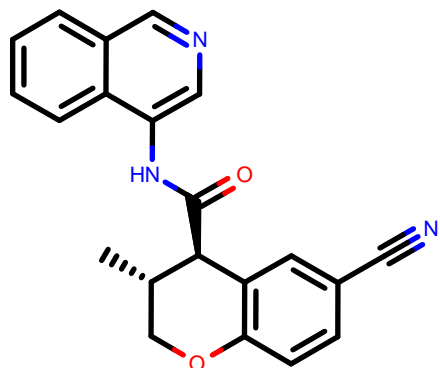
SMILES: CN1C[C@@H](OC1=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3626

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.30

DAR-DIA-0d514e7d-8_1_1



CID: DAR-DIA-0d514e7d-8_1_1

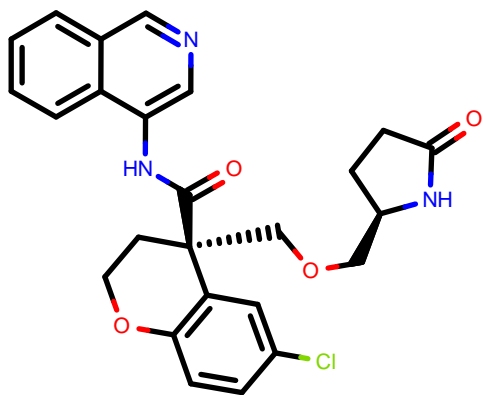
SMILES: C[C@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C#N

RUN: RUN5721

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.07

EDJ-MED-fcba3f31-9_1



CID: EDJ-MED-fcba3f31-9_1

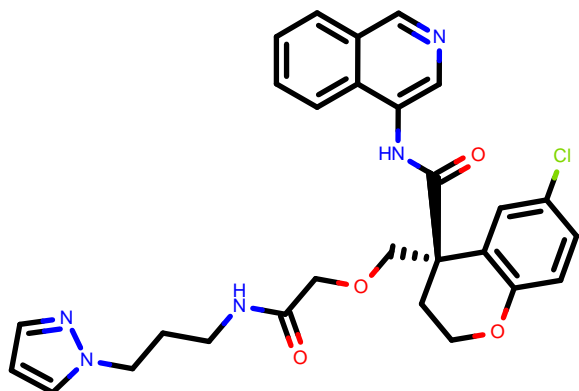
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CC(=O)N5

RUN: RUN2356

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.26

EN300-47500_2_1_1



CID: EN300-47500_2_1_1

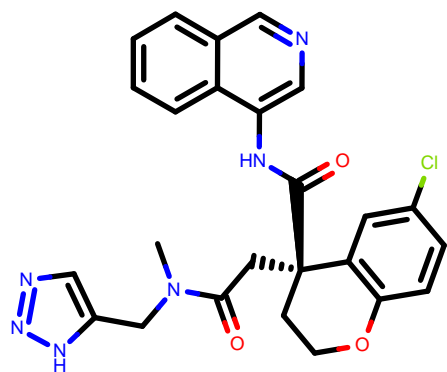
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NCCN5ccn5

RUN: RUN5748

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.36

EN300-1265071_1_1_1



CID: EN300-1265071_1_1_1

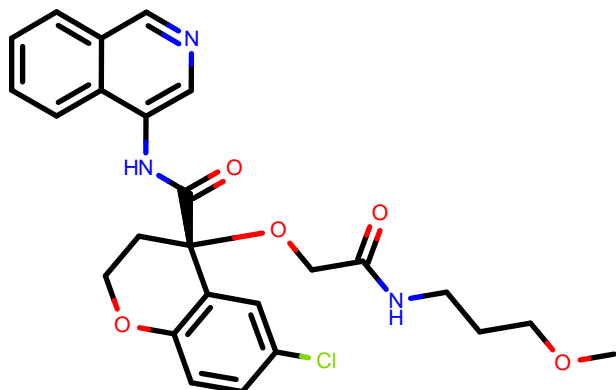
SMILES: CN(Cc1cn[nH]n1)C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN3945

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.29

EN300-04492_1_1_1



CID: EN300-04492_1_1_1

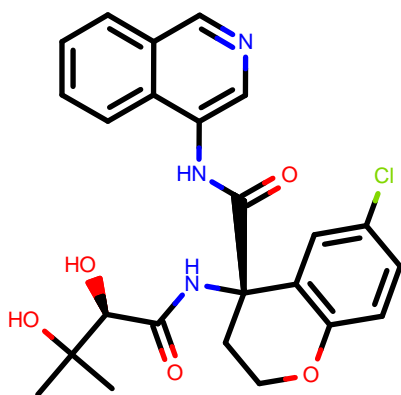
SMILES: COCCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN5646

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.24

EN300-299532_1_2_1



CID: EN300-299532_1_2_1

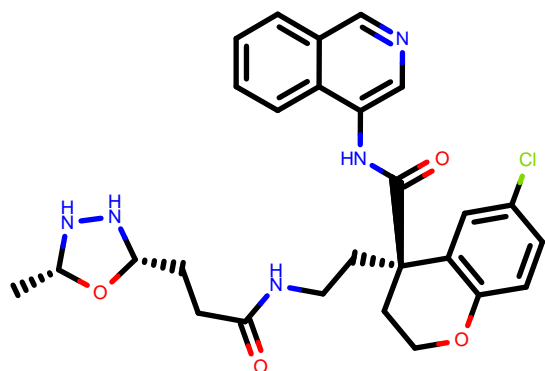
SMILES: CC(C)[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)O

RUN: RUN5912

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.23

EN300-304662_3_1_1



CID: EN300-304662_3_1_1

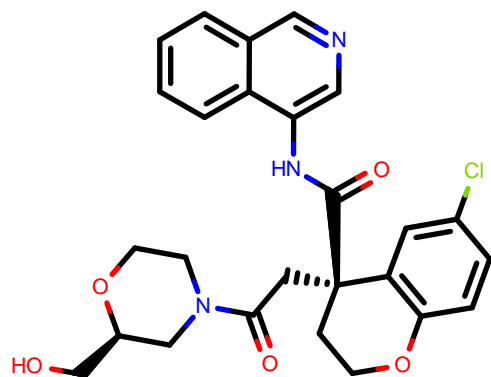
SMILES: C[C@@H]1NN[C@@H](O)CCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7015

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.31

EN300-101373_1_1_1



CID: EN300-101373_1_1_1

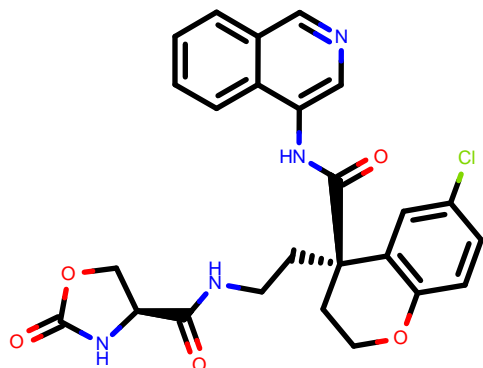
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)CO

RUN: RUN4333

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.41

EN300-126389_3_1_1



CID: EN300-126389_3_1_1

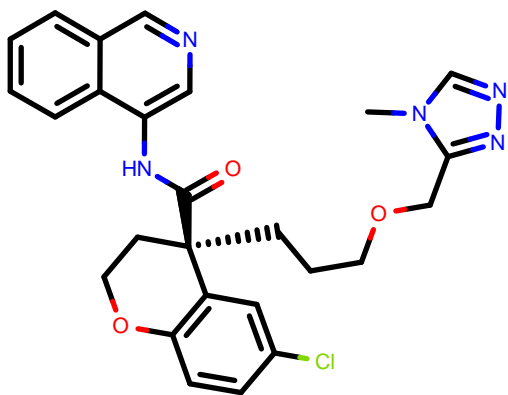
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COC(=O)N5

RUN: RUN5683

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-113112_4_1_1



CID: EN300-113112_4_1_1

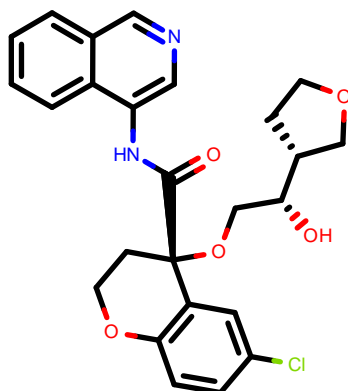
SMILES: Cn1cnnc1COCCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7357

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.38

EN300-1911992_1_2_1



CID: EN300-1911992_1_2_1

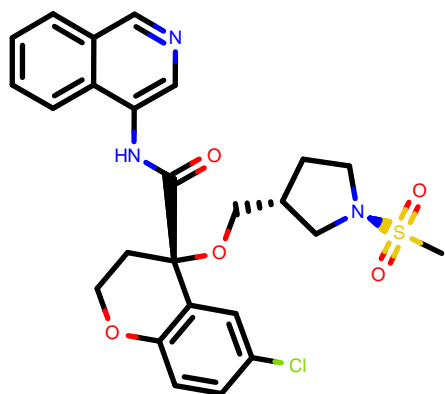
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC[C@@H](C@H)5CCOC5O

RUN: RUN7696

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.35

EN300-261986_1_2_1



CID: EN300-261986_1_2_1

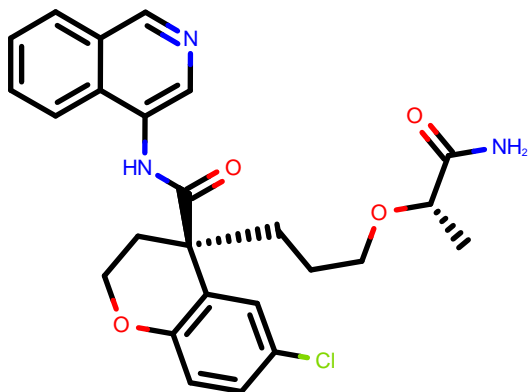
SMILES: CS(=O)(=O)[N@@]1CC[C@@H](C1)CO[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7241

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.29

EN300-17381_4_1_1



CID: EN300-17381_4_1_1

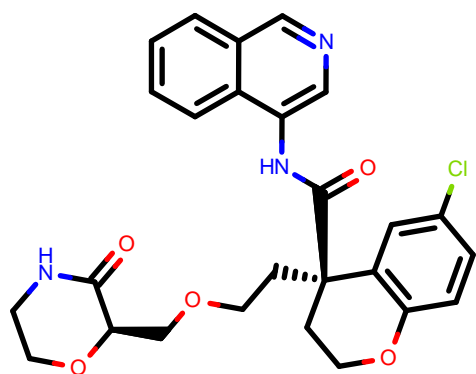
SMILES: C[C@@H](C(=O)N)OCCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6931

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-1706036_3_1_1



CID: EN300-1706036_3_1_1

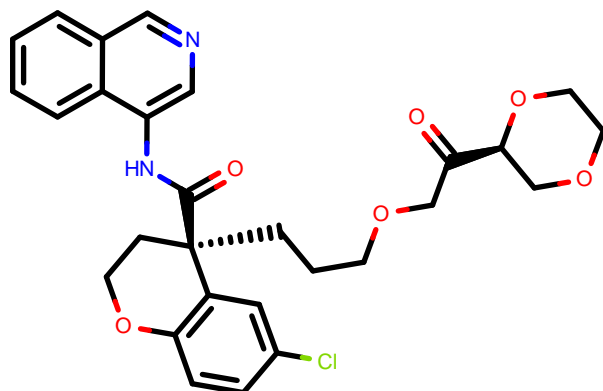
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C(=O)NCCO5

RUN: RUN5901

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.28

EN300-6238494_4_1_1



CID: EN300-6238494_4_1_1

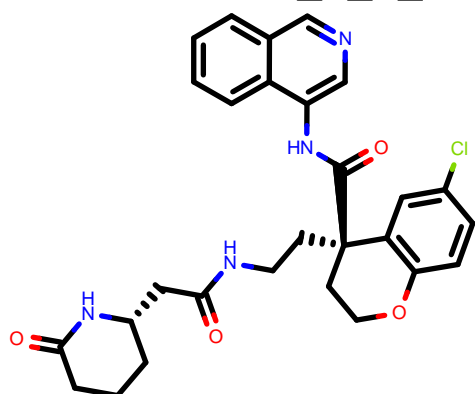
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)[C@@H]5COC(=O)O5

RUN: RUN4485

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.33

EN300-210084_3_1_1



CID: EN300-210084_3_1_1

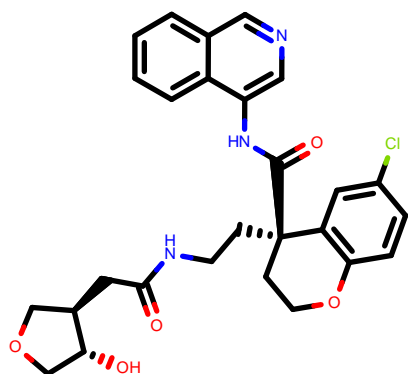
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COC(=O)N5

RUN: RUN5188

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.25

EN300-1708882_3_1_1



CID: EN300-1708882_3_1_1

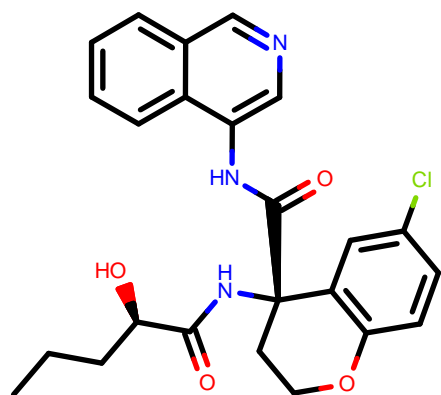
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COC[C@@H]5O

RUN: RUN5636

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.26

EN300-219531_1_2_1



CID: EN300-219531_1_2_1

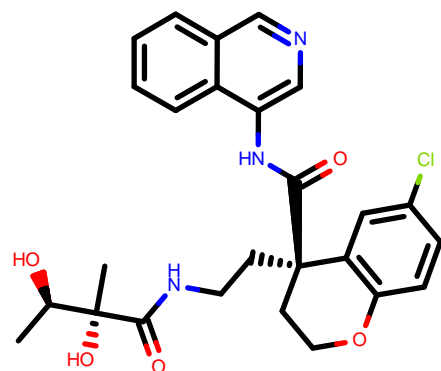
SMILES: CCC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3259

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.30

EN300-202922_3_2_1



CID: EN300-202922_3_2_1

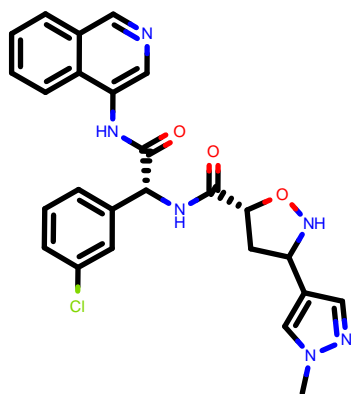
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3172

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.33

EDJ-MED-ee07cf00-6_4



CID: EDJ-MED-ee07cf00-6_4

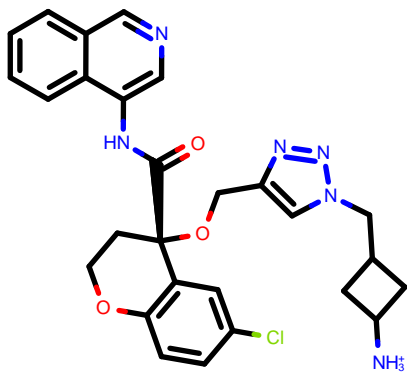
SMILES: Cn1cc(en1)C2=NO[C@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN2644

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.47

ED_-GRI-5b13fbe2-26_1



CID: ED_-GRI-5b13fbe2-26_1

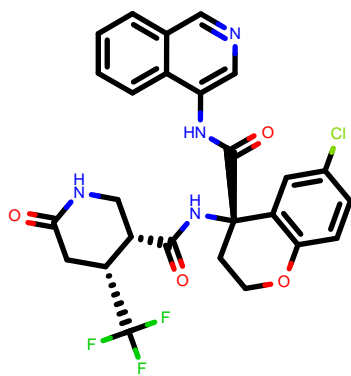
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)OCc5n(nn5)C6C6C(C6)[NH3+]

RUN: RUN1448

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-208959_1_4_1



CID: EN300-208959_1_4_1

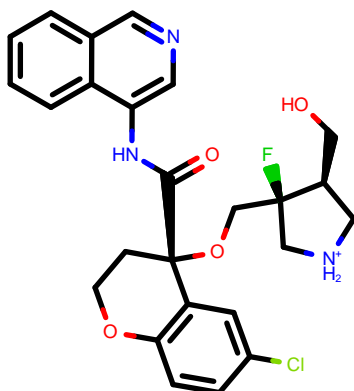
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCOC4c3ccc49C)N(C=O)[C@H]5CNC1=O[C]C@H5(C)F)F

RUN: RUN5609

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-55_2



CID: ED_-GRI-5b13fbe2-55_2

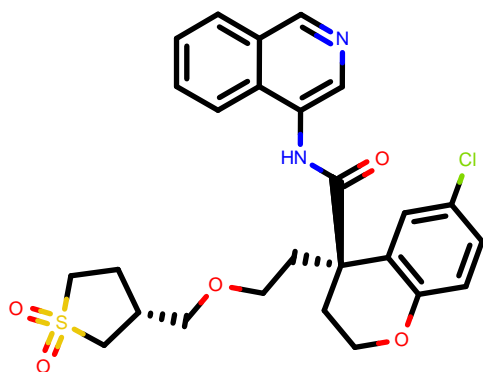
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCOC4c3ccc(cc4)C)OC[C@]5(C[NH2+])C[C@]@H5CO)F

RUN: RUN1478

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.36

EN300-1448603_3_2_1



CID: EN300-1448603_3_2_1

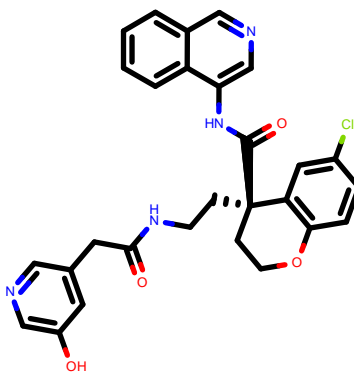
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCOC4c3ccc(cc4)C)CCOC[C@]H5CCS(=O)(=O)C5

RUN: RUN3872

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.31

EN300-222620_3_1_1



CID: EN300-222620_3_1_1

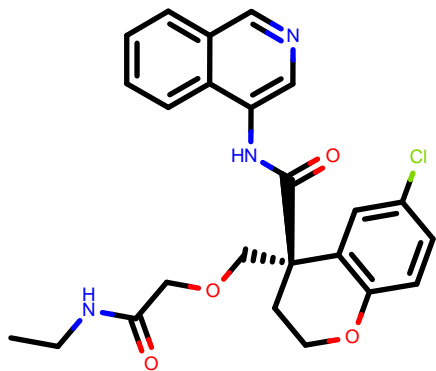
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCOC4c3ccc(cc4)C)CCNC(=O)Cc5cc(O)nc5O

RUN: RUN3428

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.43

EN300-7003350_2_1_1



CID: EN300-7003350_2_1_1

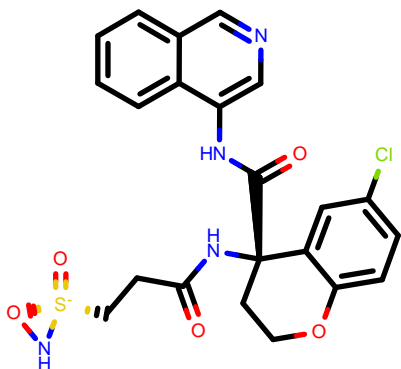
SMILES: CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN6714

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-31553_1_1_1



CID: EN300-31553_1_1_1

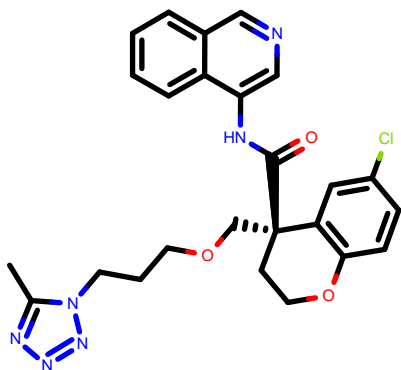
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCS(=O)(=O)N

RUN: RUN4471

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-197715_2_1_1



CID: EN300-197715_2_1_1

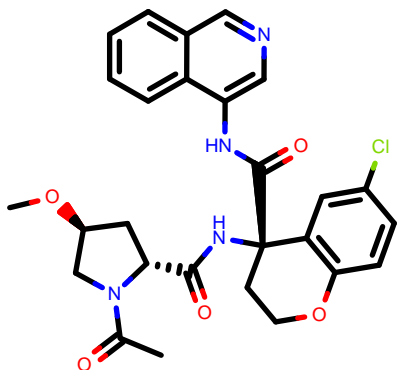
SMILES: Cc1nnnn1CCCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN2725

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.32

EN300-158272_1_1_1



CID: EN300-158272_1_1_1

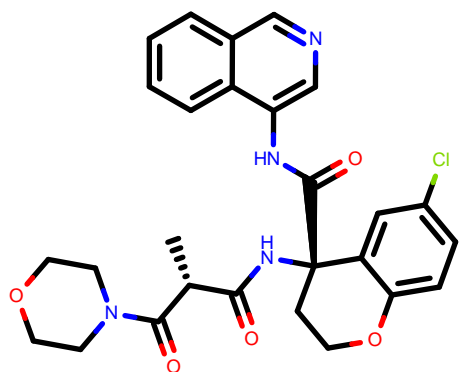
SMILES: CC(=O)N1C[C@H](C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)OC

RUN: RUN5534

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.30

EN300-2855057_1_2_1



CID: EN300-2855057_1_2_1

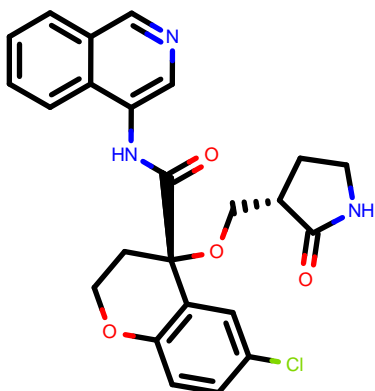
SMILES: C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)C(=O)N5CCOC5

RUN: RUN6274

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-246248_1_1_1



CID: EN300-246248_1_1_1

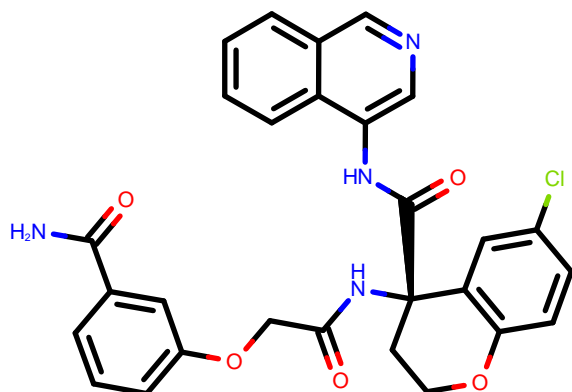
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCNC5=O

RUN: RUN5220

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-51736_1_1_1



CID: EN300-51736_1_1_1

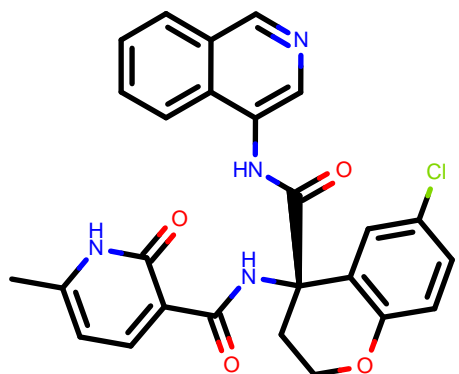
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COc5ccc(c5)C(=O)N

RUN: RUN3413

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.32

EN300-39151_1_1_1



CID: EN300-39151_1_1_1

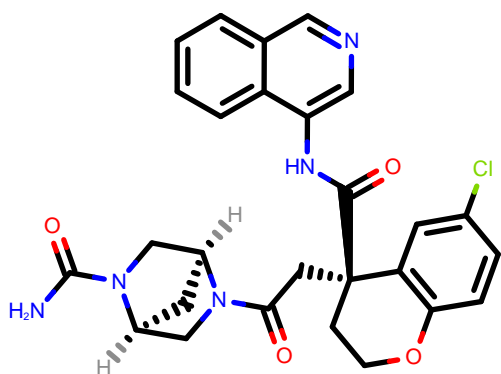
SMILES: Cc1ccc(c(=O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6097

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.33

KAD-UNI-8a629cb0-42_1



CID: KAD-UNI-8a629cb0-42_1

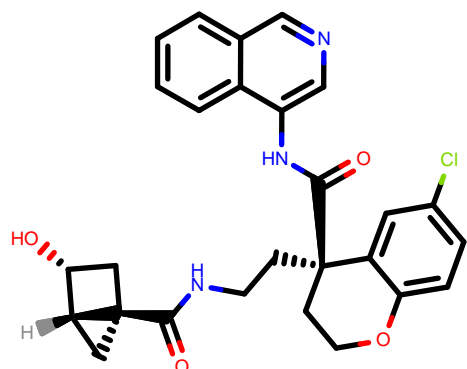
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3[C@@H](COCc4cc3cc4)CC(=O)N5C[C@@H](C)C@H5CN(C)C=O

RUN: RUN1966

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.31

EN300-7433125_3_1_1



CID: EN300-7433125_3_1_1

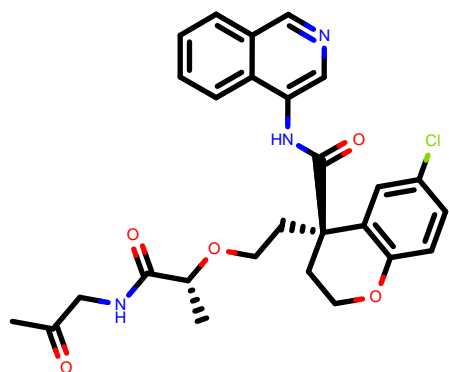
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3[C@@H](COCc4cc3cc4)CNC(=O)C@5[C@@H](C)C@H5CO

RUN: RUN6768

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.22

EN300-131093_3_2_1



CID: EN300-131093_3_2_1

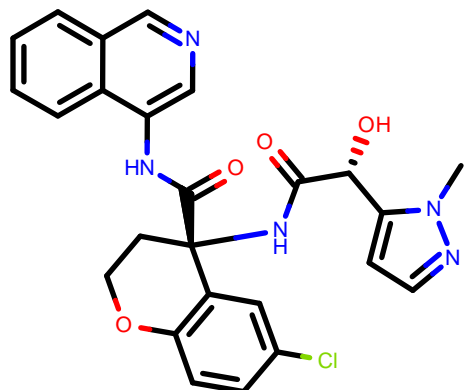
SMILES: C[C@H](C(=O)NCC(=O)C)OCC[C@1](COCc2c1cc2)C(=O)Nc3ccc4cc3ccc4

RUN: RUN3058

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-6473273_1_2_1



CID: EN300-6473273_1_2_1

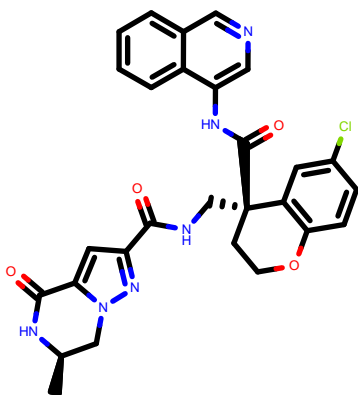
SMILES: Cn1c(ccn1)[C@H](C(=O)N[C@2](COCc3cc2cc3)C)C(=O)Nc4ccc5cc4ccc5O

RUN: RUN5285

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-265285_2_1_1



CID: EN300-265285_2_1_1

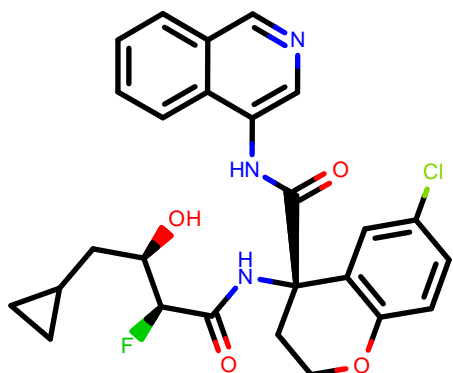
SMILES: C[C@@H]1Cn2c(ccn2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)C(=O)N1

RUN: RUN5147

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.36

EDG-MED-90036822-108_2



CID: EDG-MED-90036822-108_2

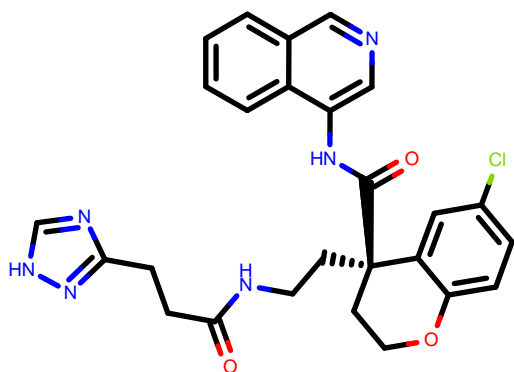
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)O(F)

RUN: RUN1715

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-101197_3_1_1



CID: EN300-101197_3_1_1

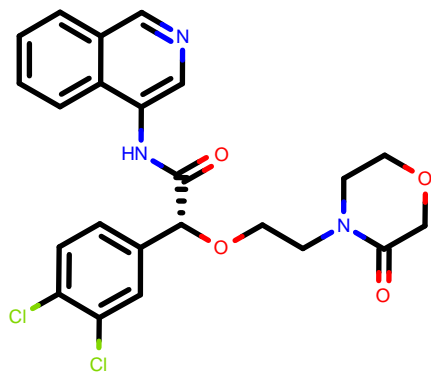
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5[nH]nnc5

RUN: RUN4884

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.30

MAT-POS-de59a476-3_1



CID: MAT-POS-de59a476-3_1

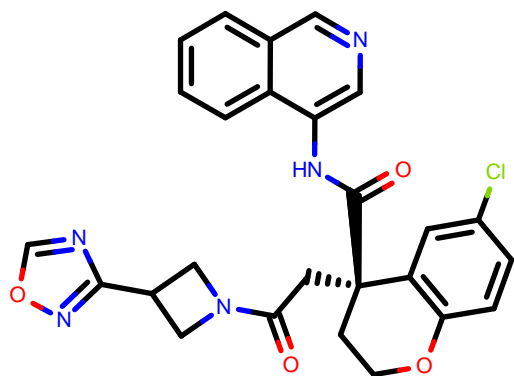
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c(c3)Cl)Cl)OCCN4CCOCC4=O

RUN: RUN2071

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.45

EN300-1700143_1_1_1



CID: EN300-1700143_1_1_1

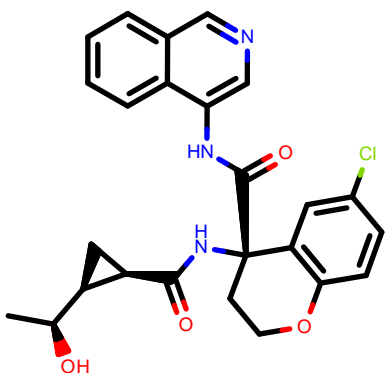
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)c6ncn6

RUN: RUN6350

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-6729572_1_7_1



CID: EN300-6729572_1_7_1

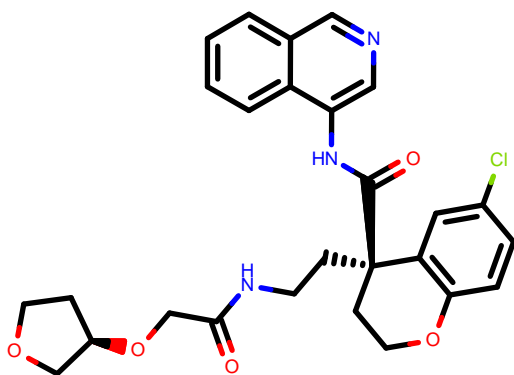
SMILES: C[C@@H]([C@H]1C[C@H]1C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5O

RUN: RUN5484

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.26

EN300-99391_3_1_1



CID: EN300-99391_3_1_1

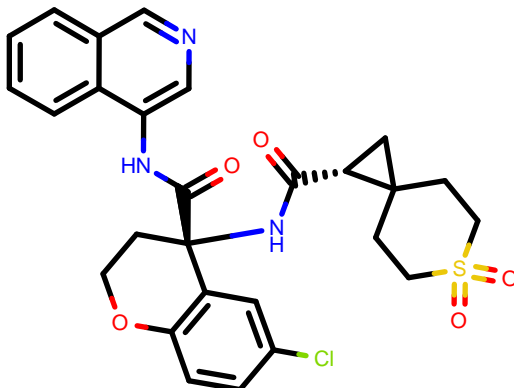
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@]5COC5

RUN: RUN4035

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.34

EN300-141809_1_1_1



CID: EN300-141809_1_1_1

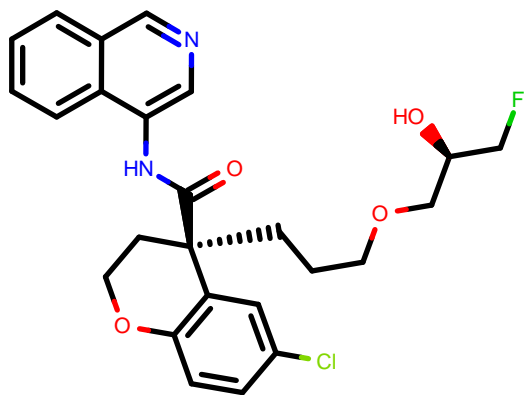
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C5S(=O)(=O)C5=O

RUN: RUN5790

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.31

EN300-1968342_4_2_1



CID: EN300-1968342_4_2_1

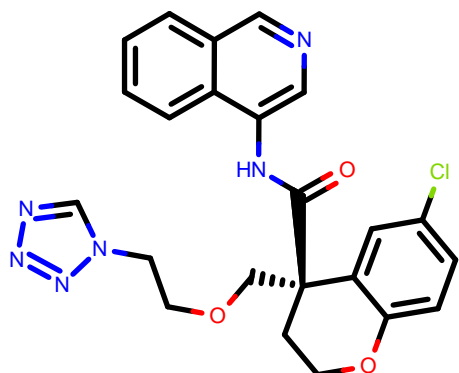
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN5061

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.43

EN300-364679_2_1_1



CID: EN300-364679_2_1_1

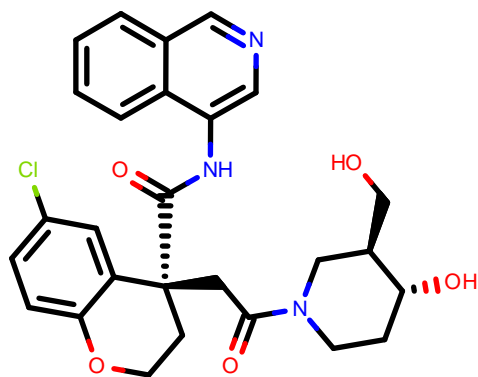
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCN5nnn5

RUN: RUN3246

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-233678_1_2_1



CID: EN300-233678_1_2_1

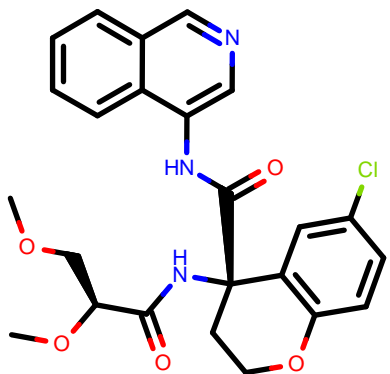
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C)[C@H](C5)CO

RUN: RUN3773

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.29

EN300-305282_1_1_1



CID: EN300-305282_1_1_1

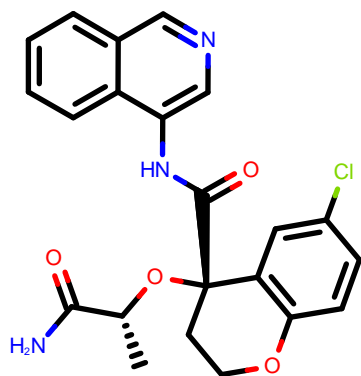
SMILES: COC[C@]3(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)OC

RUN: RUN5979

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.42

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

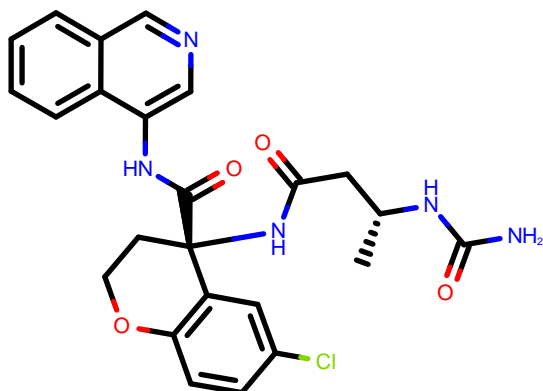
SMILES: C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cccc4c3ccc4

RUN: RUN5906

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.18

EN300-268198_1_2_1



CID: EN300-268198_1_2_1

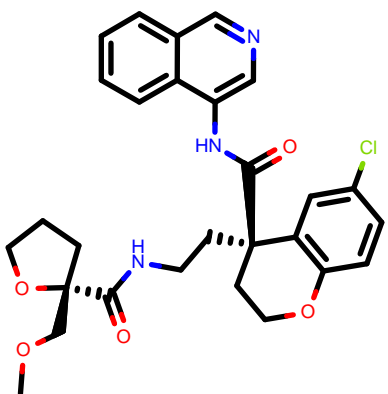
SMILES: C[C@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cccc4c3ccc4)NC(=O)N

RUN: RUN4534

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.29

EN300-1301381_3_1_1



CID: EN300-1301381_3_1_1

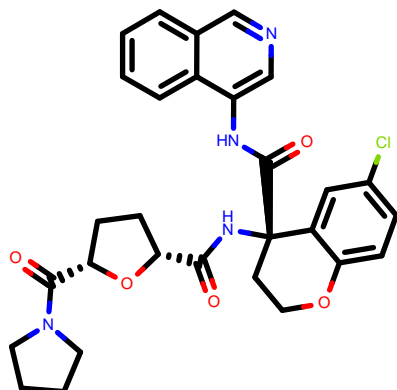
SMILES: CO[C@]1(CCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccc5c4ccc5

RUN: RUN3166

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.38

ALP-UNI-dbbfd3db-6_4



CID: ALP-UNI-dbbfd3db-6_4

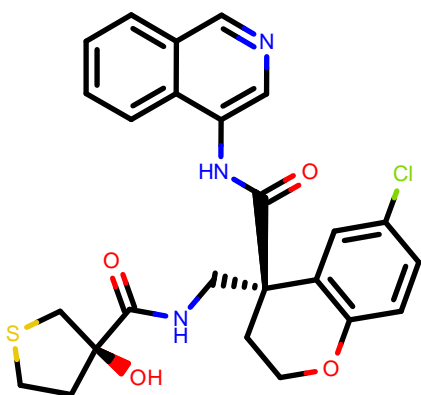
SMILES: c1ccc2c(1)nc2NC(=O)[C@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[C@H](O5)C(=O)N6CCCC6

RUN: RUN2612

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.39

EDJ-MED-4c7486ba-9_1



CID: EDJ-MED-4c7486ba-9_1

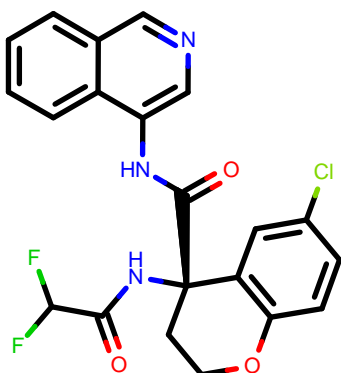
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCSC5)O

RUN: RUN1822

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.37

EN300-19507_1_1_1



CID: EN300-19507_1_1_1

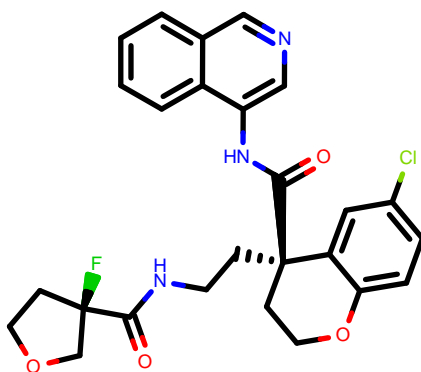
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(F)F

RUN: RUN6558

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.15

EN300-188356_3_2_1



CID: EN300-188356_3_2_1

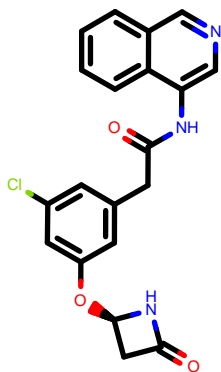
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCOC5)F

RUN: RUN5713

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.28

EDJ-MED-7320d5d2-1_1



CID: EDJ-MED-7320d5d2-1_1

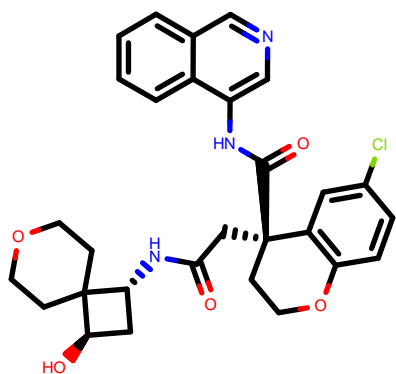
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@]4CC(=O)N4

RUN: RUN88

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.44

EN300-640503_1_1_1



CID: EN300-640503_1_1_1

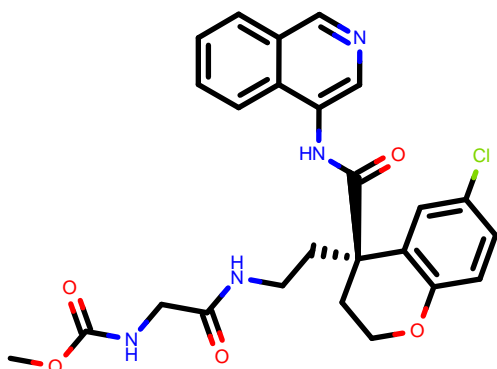
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@H3(CCOc4ccc(cc4)C)C(=O)N[C@@H]5C[C@@H](C56CCCC6)O

RUN: RUN5632

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.39

EN300-50009_3_1_1



CID: EN300-50009_3_1_1

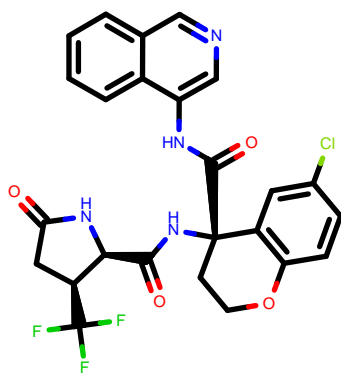
SMILES: COC(=O)NCC(=O)NCC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN3676

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.31

EN300-169955_1_4_1



CID: EN300-169955_1_4_1

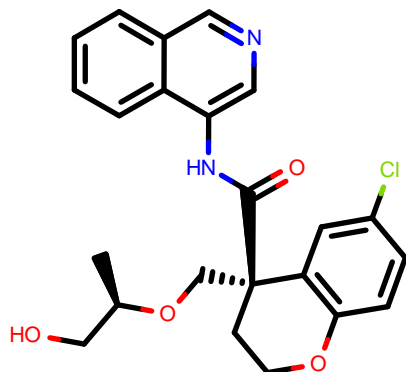
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@H3(CCOc4ccc(cc4)C)NC(=O)C@H5C[C@@H](C5)C(F)F(F)F

RUN: RUN5738

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.25

EN300-175186_2_2_1



CID: EN300-175186_2_2_1

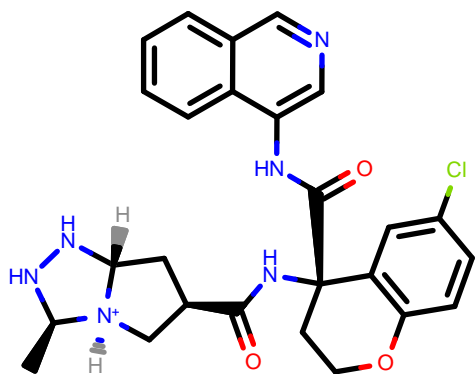
SMILES: C[C@@H](CO)OC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN7616

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.25

EN300-6729747_1_1_4



CID: EN300-6729747_1_1_4

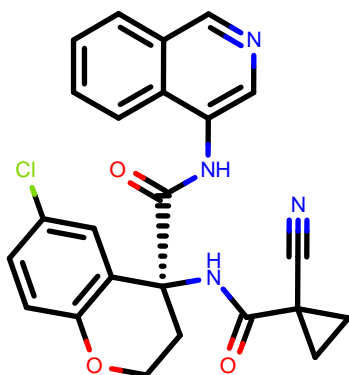
SMILES: C[C@H]1NNC@H2[NH+]1C[C@@H]2C(=O)NC@3(CCOc4c3cc(cc4Cl)Cl=O)N5cnc6c5ccc6

RUN: RUN3148

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.43

EN300-114082_1_1_1



CID: EN300-114082_1_1_1

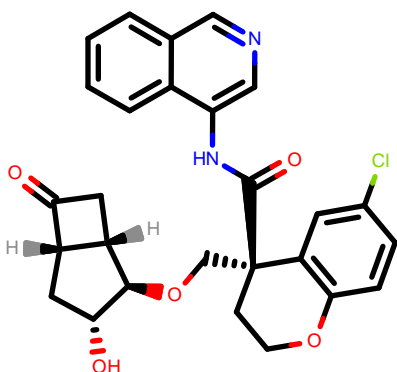
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)C5(C)C5#N

RUN: RUN3561

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.21

EN300-6481287_2_1_1



CID: EN300-6481287_2_1_1

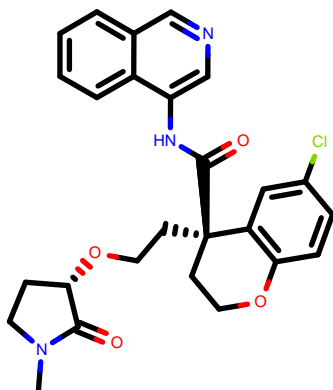
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)C[C@H]5[C@@H]1C[C@@H]2[C@]3(C)C5=O

RUN: RUN5303

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.27

EN300-98648_3_1_1



CID: EN300-98648_3_1_1

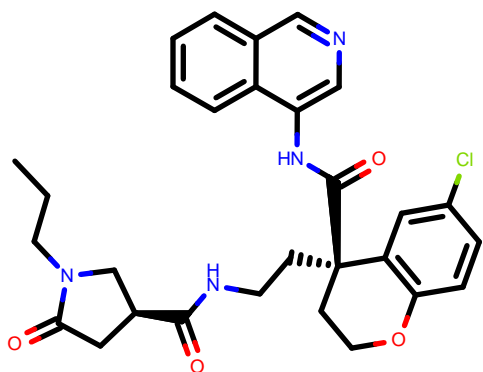
SMILES: CN1CC[C@@H](C1=O)OCC[C@@]2(CCOc3c2cc(cc3Cl)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4013

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.24

EN300-253443_3_2_1



CID: EN300-253443_3_2_1

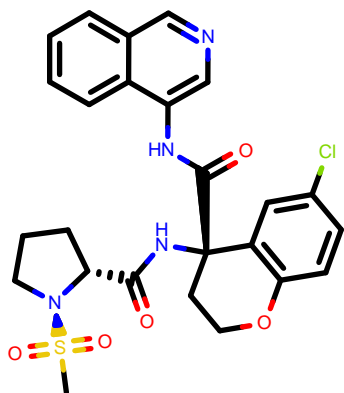
SMILES: CCCN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5961

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.33

EN300-10402_1_1_1



CID: EN300-10402_1_1_1

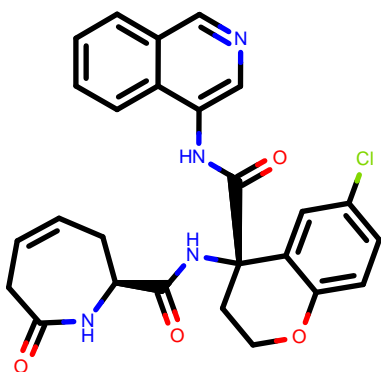
SMILES: CS(=O)(=O)N@1CCCC[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3297

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.39

EN300-80083_1_1_1



CID: EN300-80083_1_1_1

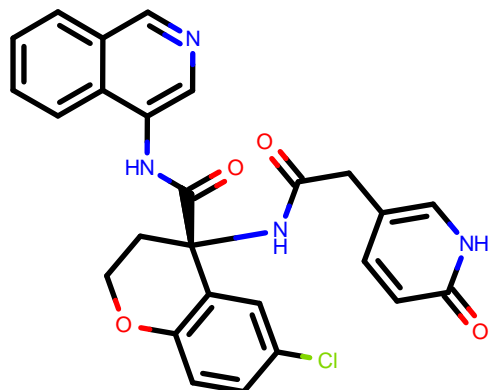
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCCC(=O)N5

RUN: RUN4497

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.30

EN300-189672_1_1_1



CID: EN300-189672_1_1_1

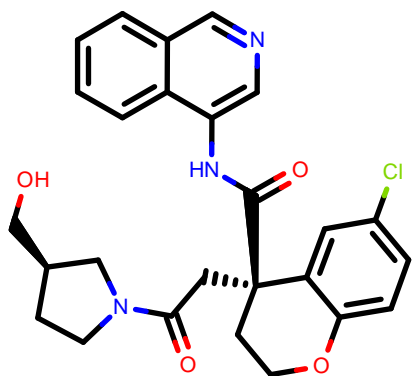
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(=O)[nH]5

RUN: RUN3906

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-144970_1_1_1



CID: EN300-144970_1_1_1

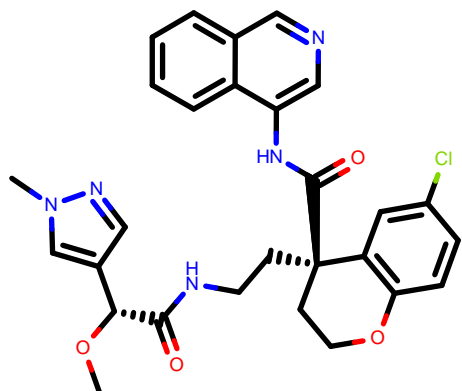
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)CO

RUN: RUN4597

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

EN300-198240_3_2_1



CID: EN300-198240_3_2_1

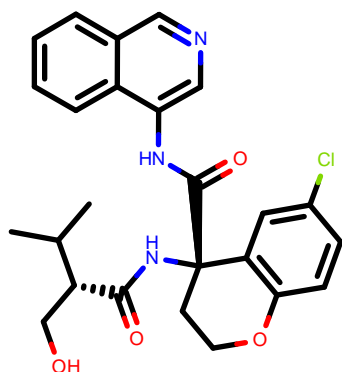
SMILES: Cn1cc(en1)[C@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5)OC

RUN: RUN6390

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

EN300-153257_1_1_1



CID: EN300-153257_1_1_1

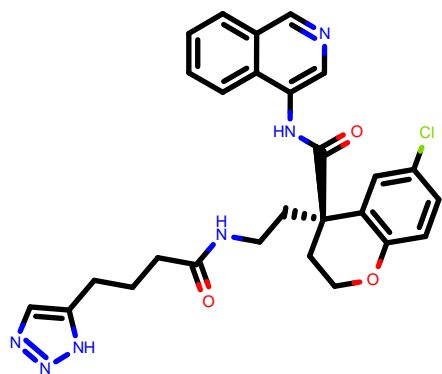
SMILES: CC(C)[C@@H](CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccc4

RUN: RUN3577

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.26

EN300-156995_3_1_1



CID: EN300-156995_3_1_1

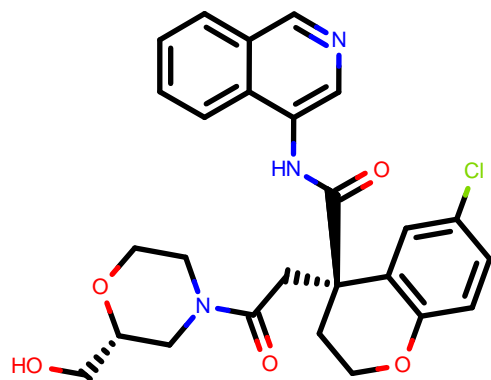
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCCc5cn[nH]5

RUN: RUN3900

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.29

EN300-175485_1_1_1



CID: EN300-175485_1_1_1

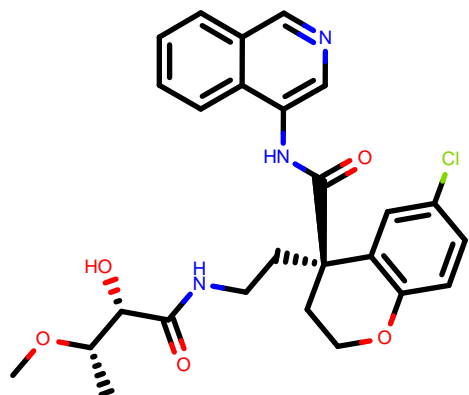
SMILES: c1ccc2c(c1)nc(=O)nc2N[C@@H](C(=O)N3CCOC3)C(=O)N5CCO[C@H](C5)CO

RUN: RUN4813

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.38

EN300-220194_3_1_1



CID: EN300-220194_3_1_1

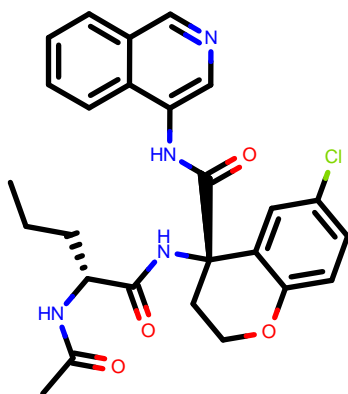
SMILES: C[C@@H](C(=O)N[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4)O)OC

RUN: RUN4175

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.34

EN300-43047_1_2_1



CID: EN300-43047_1_2_1

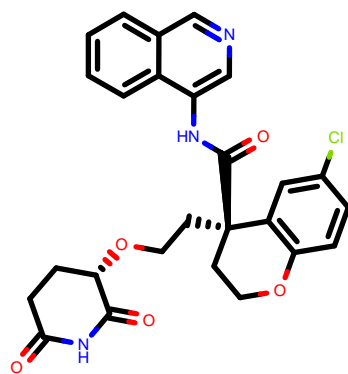
SMILES: CC(=O)N[C@@H](C(=O)N[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4)C)CC

RUN: RUN7283

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

EN300-120920_3_2_1



CID: EN300-120920_3_2_1

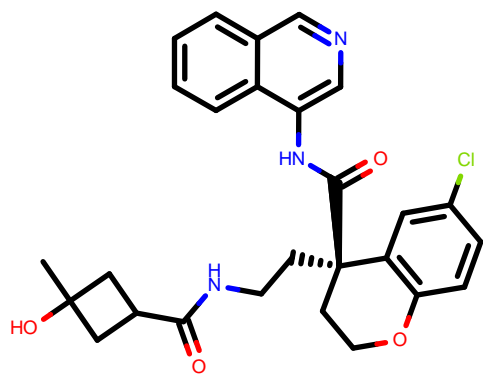
SMILES: c1ccc2c(c1)nc(=O)nc2N[C@@H](C(=O)N3CCOC3)C(=O)N5CCCC(=O)NCS=O

RUN: RUN3634

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-247343_3_1_1



CID: EN300-247343_3_1_1

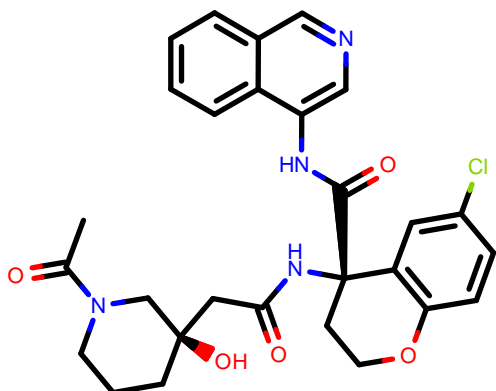
SMILES: CC1(CC(C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN7043

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.29

EN300-259063_1_2_1



CID: EN300-259063_1_2_1

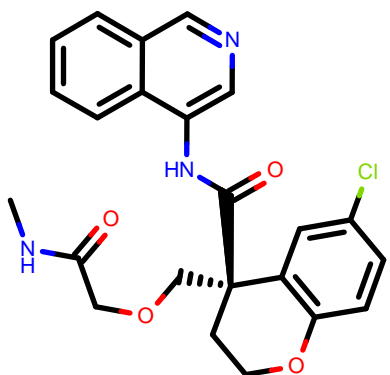
SMILES: CC(=O)N1CCC[C@](C1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN7506

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.35

EN300-2977549_2_1_1



CID: EN300-2977549_2_1_1

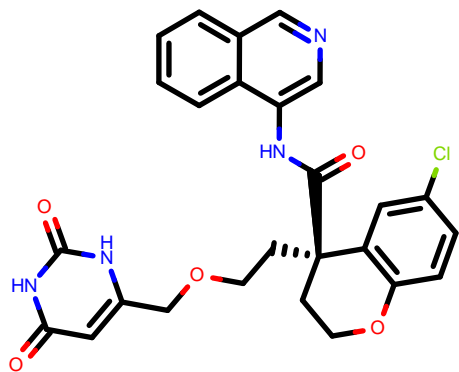
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4642

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.20

EN300-11300_3_1_1



CID: EN300-11300_3_1_1

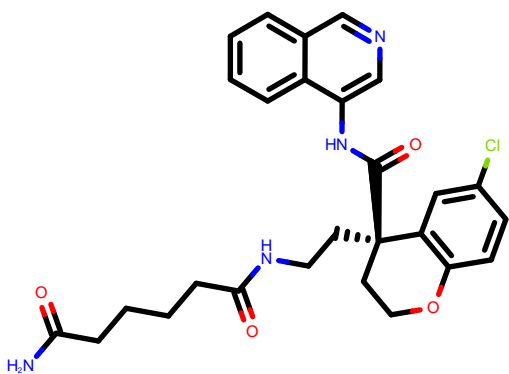
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN4522

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

EN300-142412_3_1_1



CID: EN300-142412_3_1_1

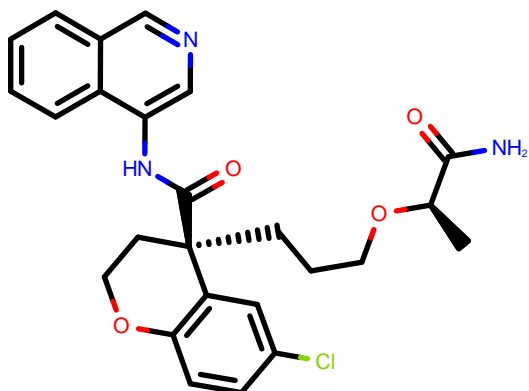
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CCCC(=O)N

RUN: RUN4334

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.33

EN300-17381_4_2_1



CID: EN300-17381_4_2_1

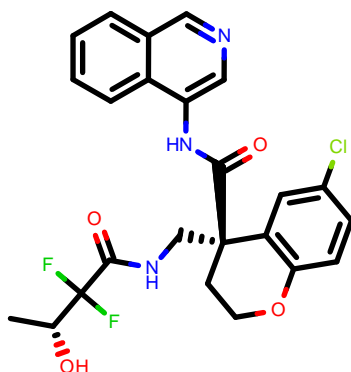
SMILES: C[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3076

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-185398_2_2_1



CID: EN300-185398_2_2_1

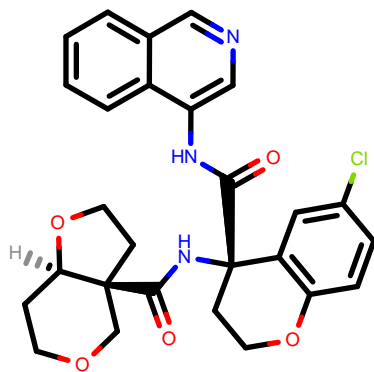
SMILES: C[C@H](C(=O)N)C[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cnc4c3cccc4(F)F)O

RUN: RUN5479

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.22

EN300-341337_1_2_1



CID: EN300-341337_1_2_1

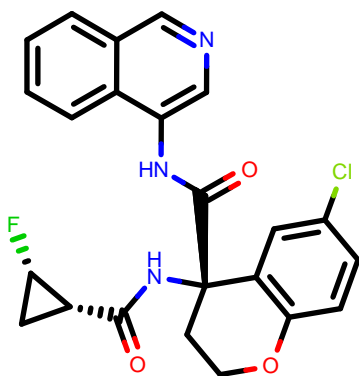
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@]56CCO[C@@]@H)5CCOC6

RUN: RUN2847

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-1654606_1_1_1



CID: EN300-1654606_1_1_1

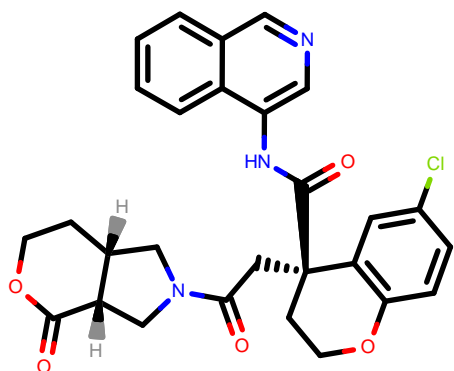
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H]5F

RUN: RUN5148

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.17

EN300-7426520_1_1_1



CID: EN300-7426520_1_1_1

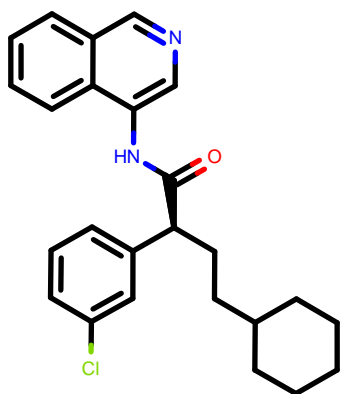
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6CCOC(=O)[C@@H]6C5

RUN: RUN7240

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.25

MIC-UNK-c66144cb-3_1



CID: MIC-UNK-c66144cb-3_1

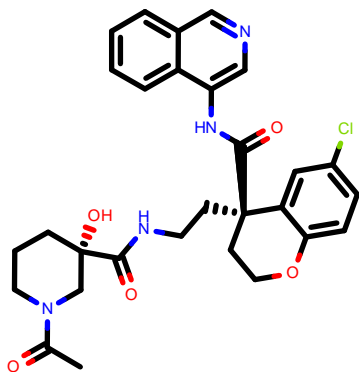
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)[C@@H](CCC3CCCCC3)c4ccc(cc4)Cl

RUN: RUN94

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.32

EN300-210552_3_2_1



CID: EN300-210552_3_2_1

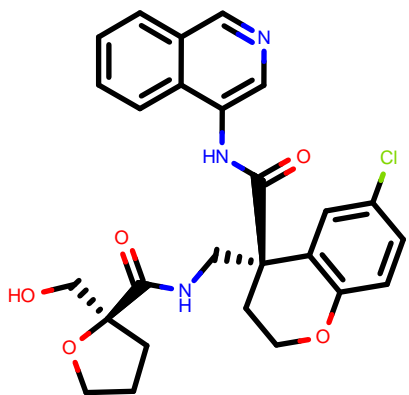
SMILES: CC(=O)N1CCC[C@](C1)(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3191

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.52

EN300-1425677_2_2_1



CID: EN300-1425677_2_2_1

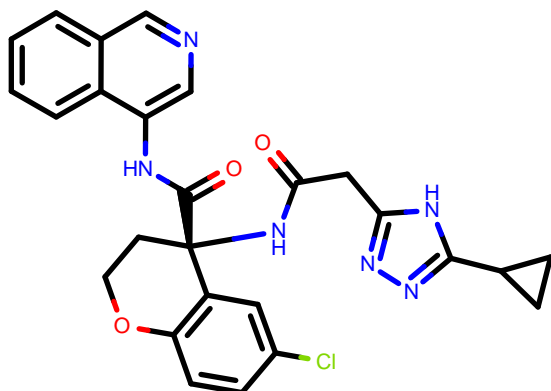
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCCO5)CO

RUN: RUN6283

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-657211_1_1_1



CID: EN300-657211_1_1_1

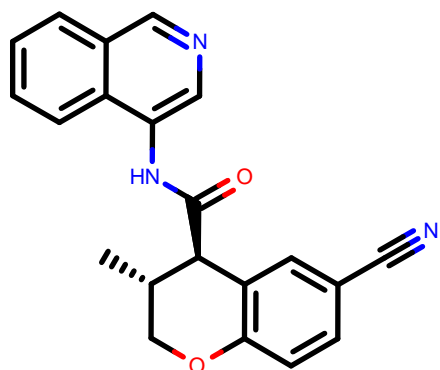
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]ne(n5)C6CC6

RUN: RUN4236

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.27

DAR-DIA-0d514e7d-8_1



CID: DAR-DIA-0d514e7d-8_1

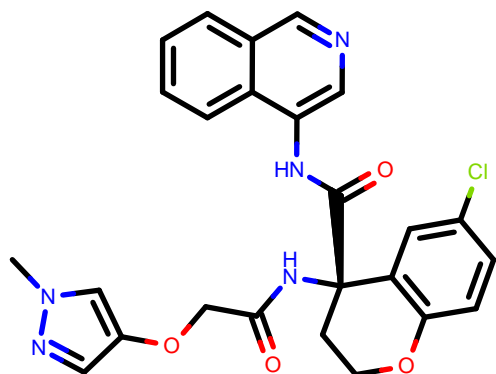
SMILES: C[C@H]1COc2ccc(cc2[C@@]3(C)C(=O)Nc3ncc4c3ccc4)C#N

RUN: RUN745

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.07

EN300-201553_1_1_1



CID: EN300-201553_1_1_1

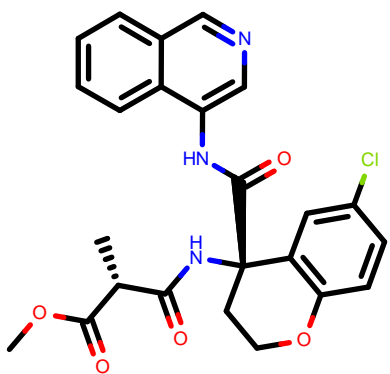
SMILES: C[n+][1]cc(c[nH]1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN5330

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.30

EN300-1239522_1_2_1



CID: EN300-1239522_1_2_1

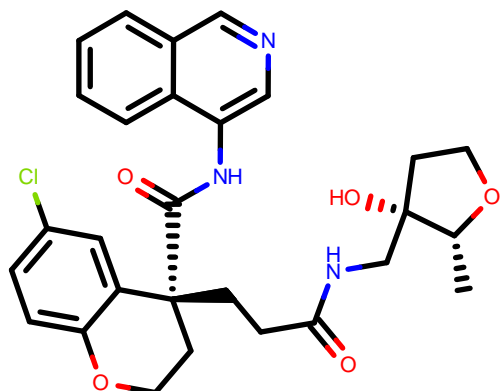
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)C(=O)OC

RUN: RUN4023

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.25

EN300-188324_2_3_1



CID: EN300-188324_2_3_1

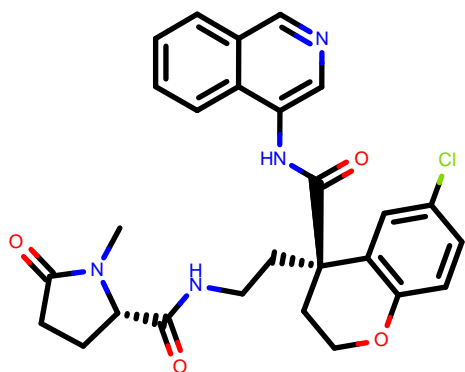
SMILES: C[C@@H]1[C@](CO1)(CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5)O

RUN: RUN7431

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

EN300-132963_3_1_1



CID: EN300-132963_3_1_1

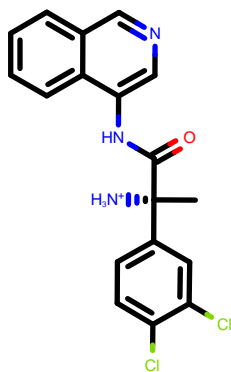
SMILES: CN1[C@@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN5126

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.29

MAT-POS-fce787c2-7_1



CID: MAT-POS-fce787c2-7_1

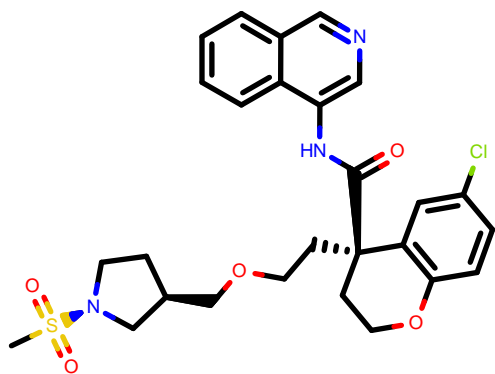
SMILES: C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)[NH3+]

RUN: RUN1945

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.35

EN300-261986_3_2_1



CID: EN300-261986_3_2_1

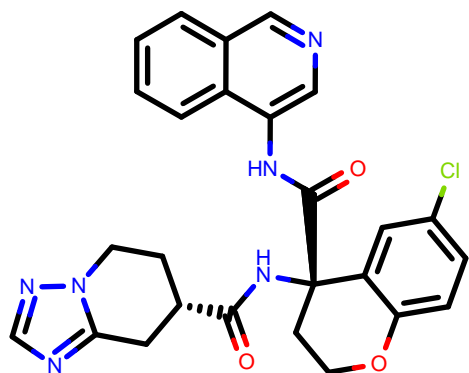
SMILES: CS(=O)(=O)N@@[1]CC[C@H](C1)COCC[C@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4539

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.37

EN300-1448674_1_2_1



CID: EN300-1448674_1_2_1

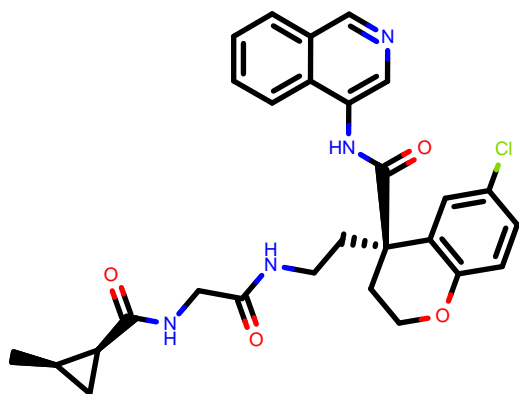
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5Cn6c(ncn6)C5

RUN: RUN3068

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

EN300-30768_3_1_1



CID: EN300-30768_3_1_1

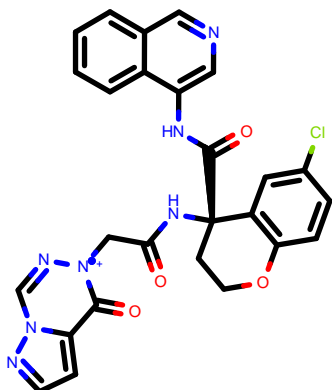
SMILES: C[C@@H]1C[C@@H]1C1=O)NC1=O)NCC[C@2](CCOc3c2cc(cc3)Cl)C1=O)Nc4cncc5c4cccc5

RUN: RUN6012

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.26

ALP-UNI-dbbfd3db-9_1



CID: ALP-UNI-dbbfd3db-9_1

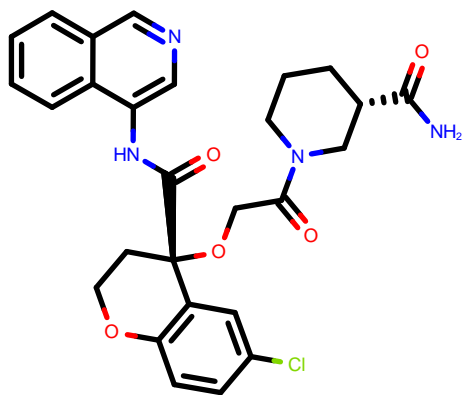
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(c=O)c6ccnn6c5

RUN: RUN2614

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.33

EN300-22880_1_1_1



CID: EN300-22880_1_1_1

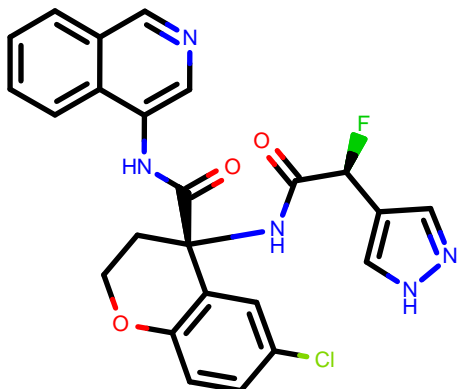
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@@H](C5)C(=O)N

RUN: RUN7079

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.32

EDG-MED-90036822-8_2



CID: EDG-MED-90036822-8_2

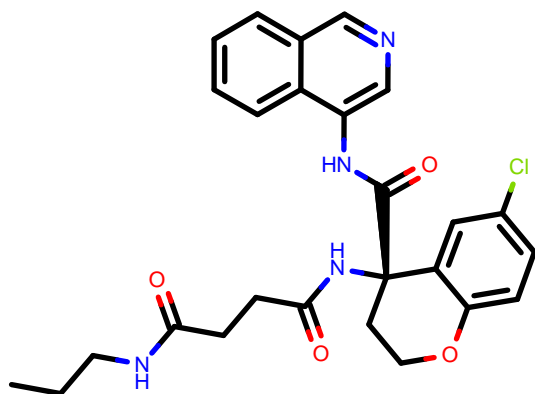
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5c[nH]nc5)F

RUN: RUN1549

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.30

EN300-68740_1_1_1



CID: EN300-68740_1_1_1

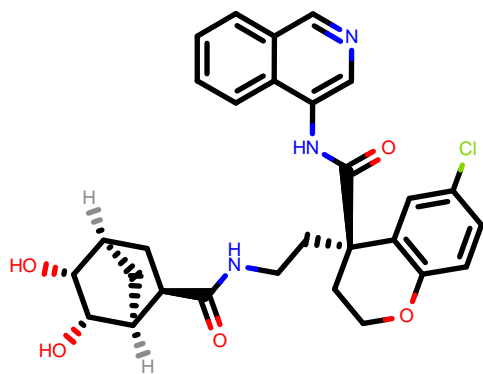
SMILES: CCCC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7659

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.30

EN300-6744028_3_1_1



CID: EN300-6744028_3_1_1

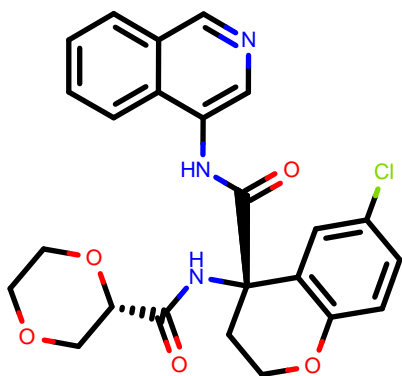
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C=C[C@@H](C)C)C(=O)N

RUN: RUN6241

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.34

EN300-36158_1_1_1



CID: EN300-36158_1_1_1

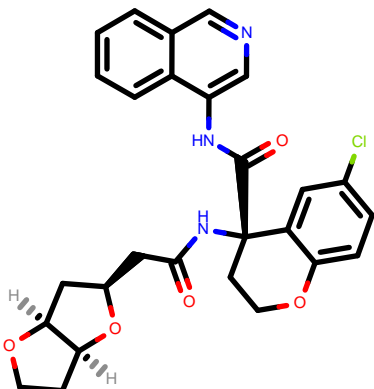
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COCOC5

RUN: RUN2848

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.20

EN300-735519_1_3_1



CID: EN300-735519_1_3_1

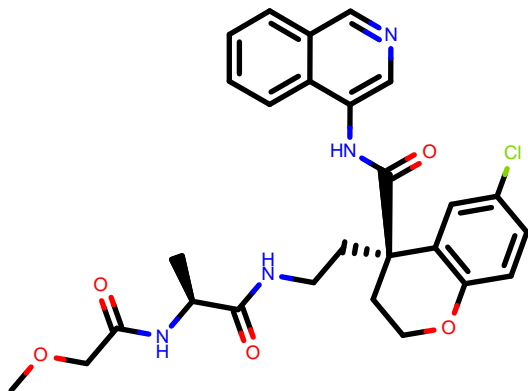
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H]6C[C@H](O)COC6

RUN: RUN4545

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.30

EN300-31183_3_1_1



CID: EN300-31183_3_1_1

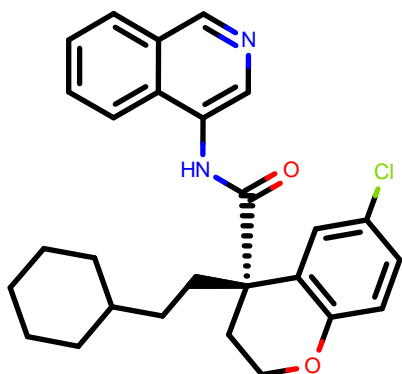
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)NC(=O)COC

RUN: RUN5525

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.35

DAR-DIA-6a508060-9_2



CID: DAR-DIA-6a508060-9_2

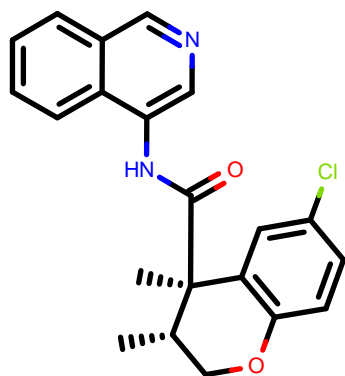
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCC5

RUN: RUN318

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.39

DAR-DIA-0d514e7d-28_1_1



CID: DAR-DIA-0d514e7d-28_1_1

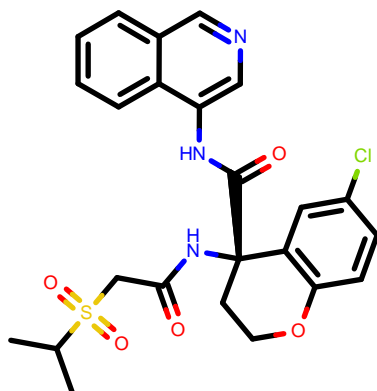
SMILES: C[C@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN4579

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.10

EN300-51028_1_1_1



CID: EN300-51028_1_1_1

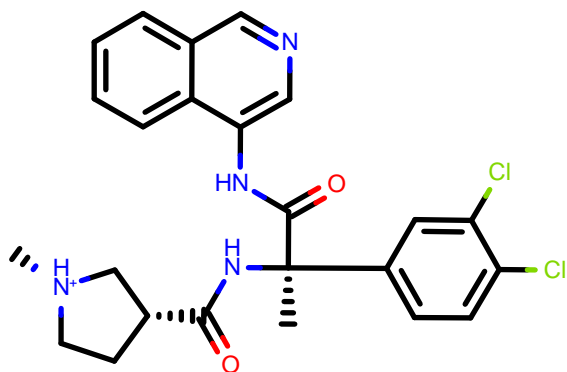
SMILES: CC(C)S(=O)(=O)CC(=O)N[C@]1(C)COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4845

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

MAT-POS-e9e99895-13_1



CID: MAT-POS-e9e99895-13_1

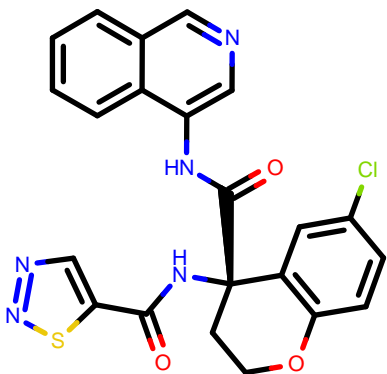
SMILES: C[C@@]1(c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CCN1@H4)C4C

RUN: RUN2110

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.32

EN300-42269_1_1_1



CID: EN300-42269_1_1_1

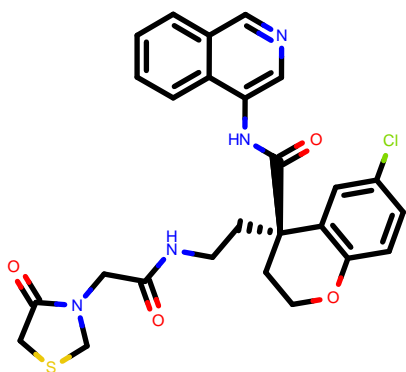
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnns5

RUN: RUN3649

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.19

EN300-10747_3_1_1



CID: EN300-10747_3_1_1

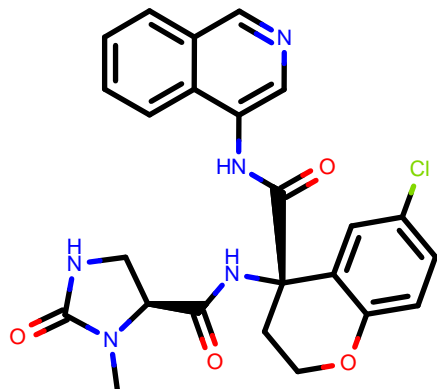
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CSCC5=O

RUN: RUN3643

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

EN300-307008_1_1_1



CID: EN300-307008_1_1_1

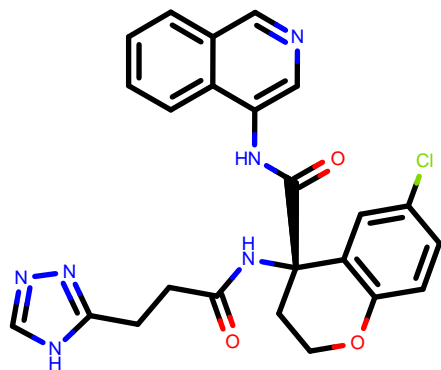
SMILES: CN1[C@@H](CNC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN5132

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.22

EN300-101197_1_1_1



CID: EN300-101197_1_1_1

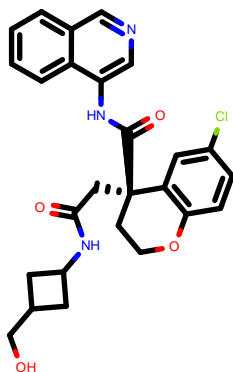
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5[nH]nnc5

RUN: RUN3389

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.23

EN300-331593_1_1_1



CID: EN300-331593_1_1_1

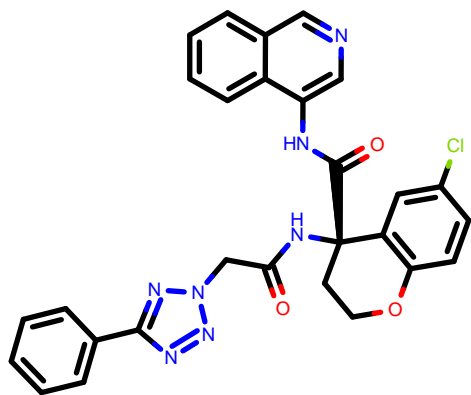
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)CO

RUN: RUN6352

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.29

ALP-UNI-dbbfd3db-8_1



CID: ALP-UNI-dbbfd3db-8_1

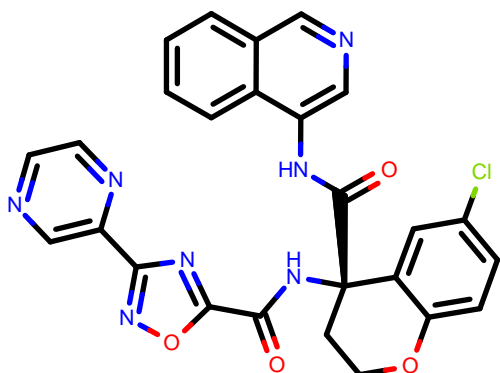
SMILES: c1ccc(cc1)c2nnn(n2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN2622

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.32

EN300-239219_1_1_1



CID: EN300-239219_1_1_1

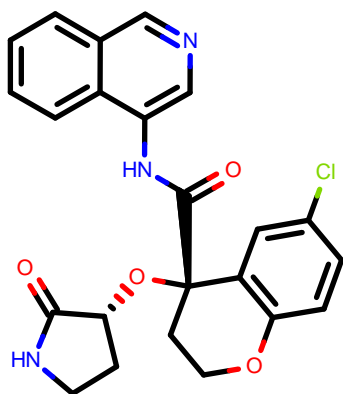
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc(nc5)c6cnc6

RUN: RUN6300

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.20

EN300-6736413_1_1_1



CID: EN300-6736413_1_1_1

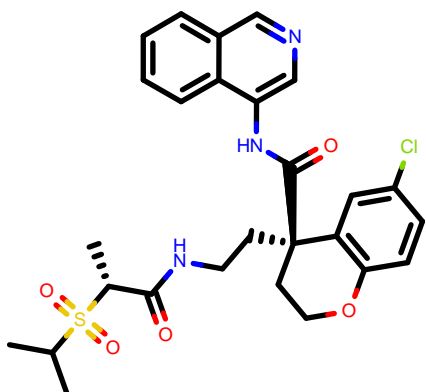
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCNC5=O

RUN: RUN5861

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.19

EN300-40947_3_2_1



CID: EN300-40947_3_2_1

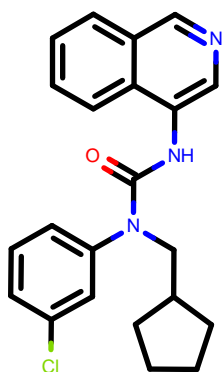
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)S(=O)(=O)C(C)C

RUN: RUN6893

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.65

MIC-UNK-bcd487e9-3_1



CID: MIC-UNK-bcd487e9-3_1

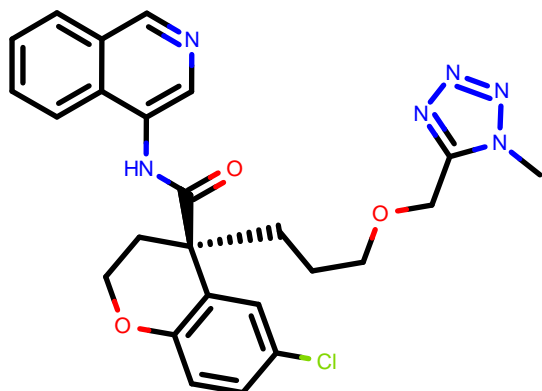
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CC3CCCC3)c4cccc(c4)Cl

RUN: RUN540

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.36

EN300-62574_4_1_1



CID: EN300-62574_4_1_1

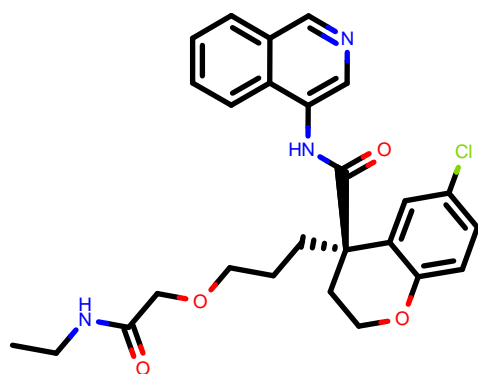
SMILES: Cn1c(nnn1)COCCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5612

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.35

EN300-7003350_4_1_1



CID: EN300-7003350_4_1_1

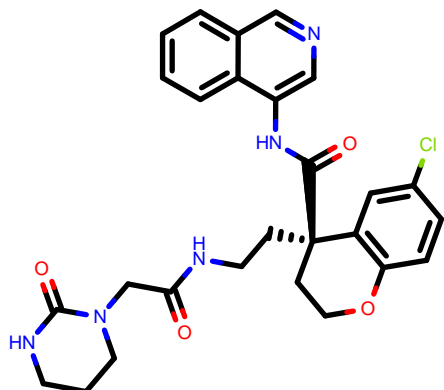
SMILES: CCNC(=O)COCCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4624

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.28

EN300-36096_3_1_1



CID: EN300-36096_3_1_1

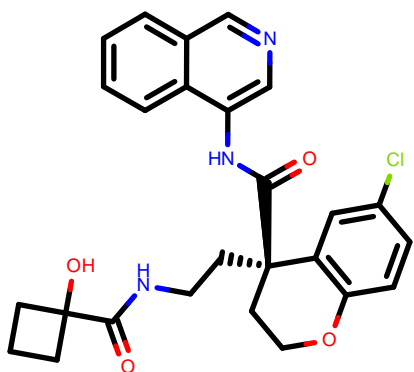
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCC5=O

RUN: RUN4407

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.39

EN300-52009_3_1_1



CID: EN300-52009_3_1_1

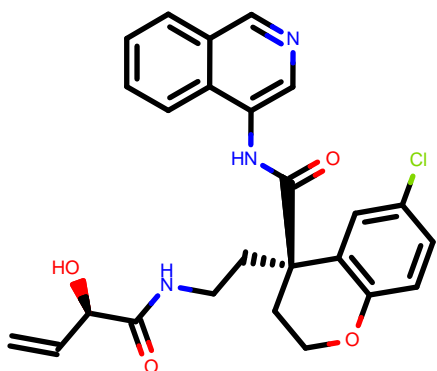
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)O

RUN: RUN4751

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-181492_3_2_1



CID: EN300-181492_3_2_1

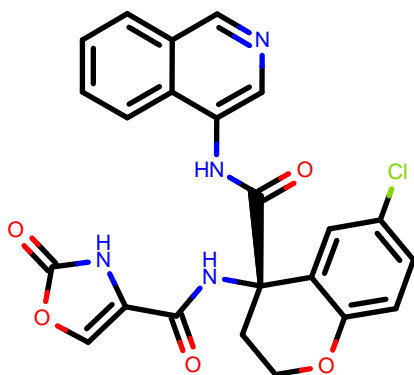
SMILES: C=C[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN4439

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.30

EN300-246486_1_1_1



CID: EN300-246486_1_1_1

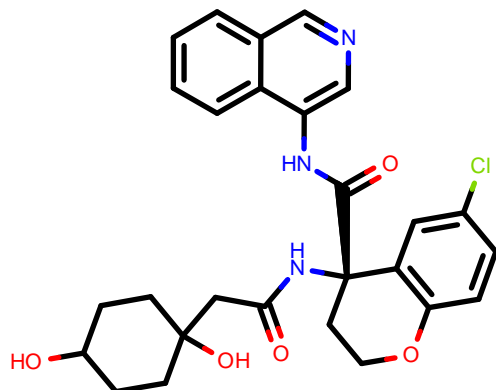
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5occc(=O)[nH]5

RUN: RUN7155

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.20

EN300-181558_1_1_1



CID: EN300-181558_1_1_1

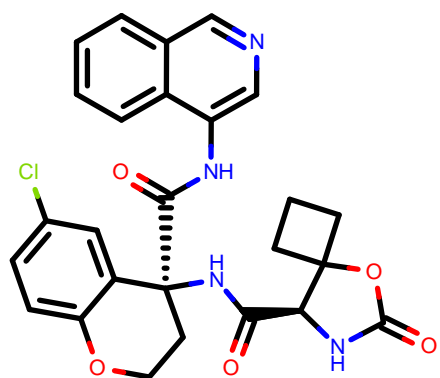
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCC(C)C5)O

RUN: RUN7565

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-7432415_1_2_1



CID: EN300-7432415_1_2_1

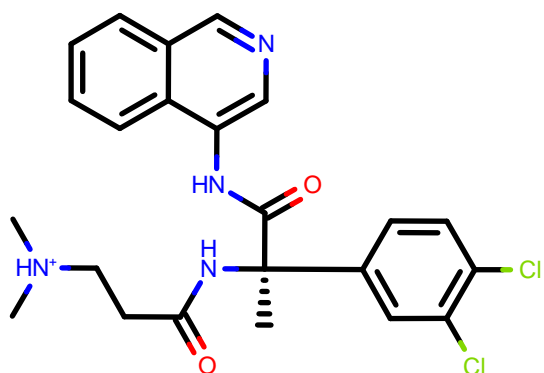
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C6(CCC6)OC(=O)N5

RUN: RUN2921

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.22

MAT-POS-e9e99895-12_1



CID: MAT-POS-e9e99895-12_1

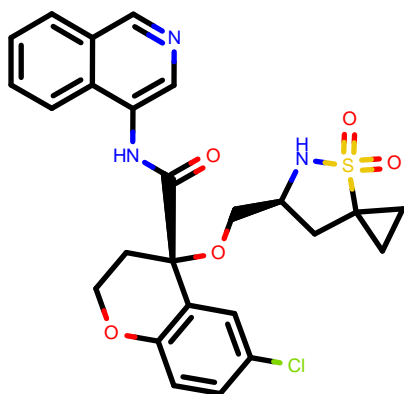
SMILES: C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2ncnc3c2ccc3)NC(=O)CC[NH+](C)C

RUN: RUN2158

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.47

EN300-6504697_1_1_1



CID: EN300-6504697_1_1_1

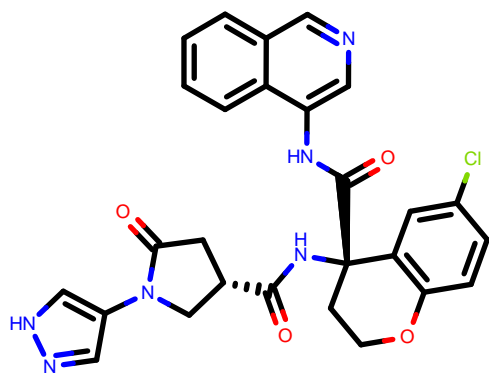
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5CC6(CC6)S(=O)(=O)N5

RUN: RUN4150

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.29

EN300-99064_1_2_1



CID: EN300-99064_1_2_1

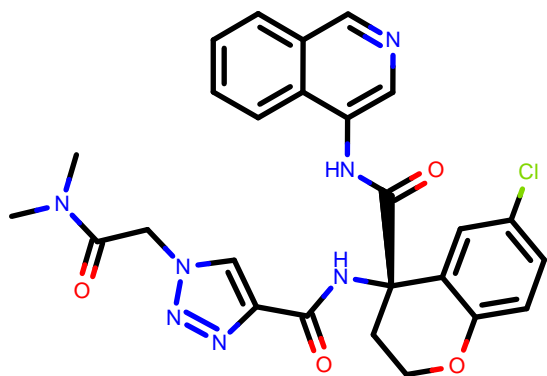
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC(=O)N(C5)c6c[nH]n6

RUN: RUN7419

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.35

EN300-52382_1_1_1



CID: EN300-52382_1_1_1

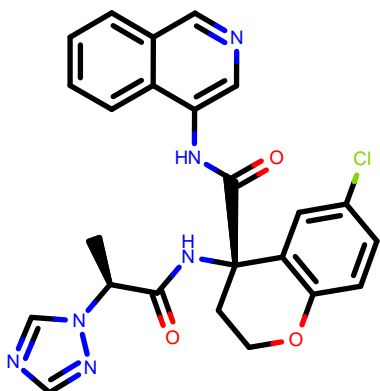
SMILES: CN(C)C(=O)Cn1cc(nn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5

RUN: RUN3547

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.29

EN300-30397_1_1_1



CID: EN300-30397_1_1_1

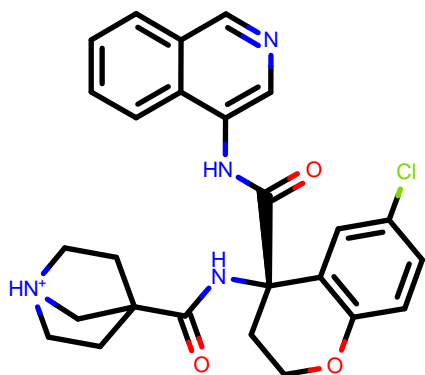
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)n5cnm5

RUN: RUN3815

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-313366_1_1_1



CID: EN300-313366_1_1_1

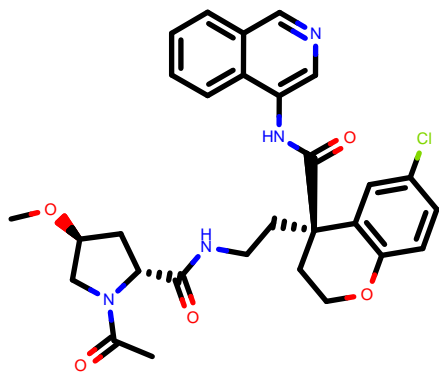
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC[NH+]([C5])C6

RUN: RUN4762

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.32

EN300-158272_3_1_1



CID: EN300-158272_3_1_1

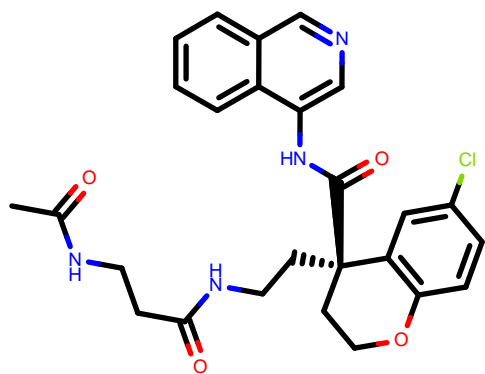
SMILES: CC(=O)N1C[C@@H](C[C@@H]1C(=O)NC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccc5)OC

RUN: RUN6157

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.32

EN300-04073_3_1_1



CID: EN300-04073_3_1_1

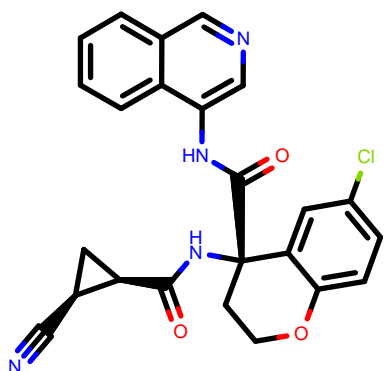
SMILES: CC(=O)NCCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7581

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-1588617_1_1_1



CID: EN300-1588617_1_1_1

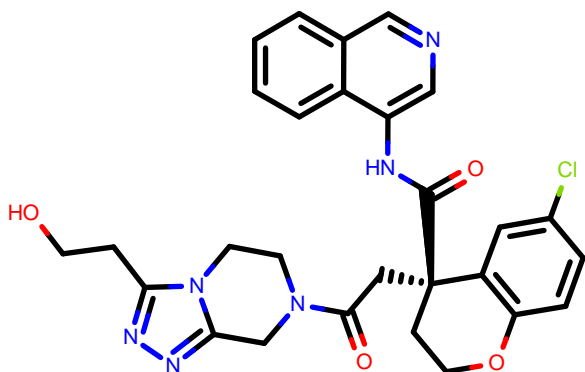
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5C[C@@]HJ5C#N

RUN: RUN4601

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.18

EN300-6472558_1_1_1



CID: EN300-6472558_1_1_1

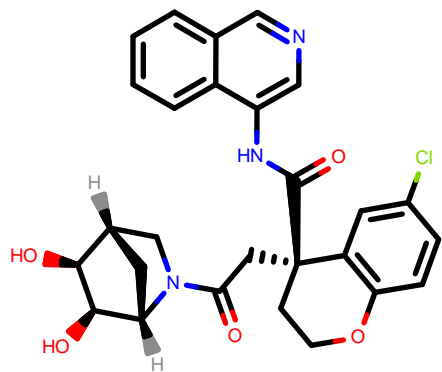
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cn6c(nnc6CCO)C5

RUN: RUN6559

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.32

EN300-1722072_1_1_1



CID: EN300-1722072_1_1_1

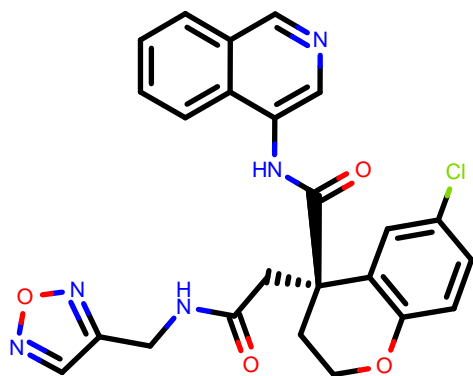
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]H6C[C@@]H5[C@@]H[C@@]H6O

RUN: RUN4190

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.30

EN300-1068239_1_1_1



CID: EN300-1068239_1_1_1

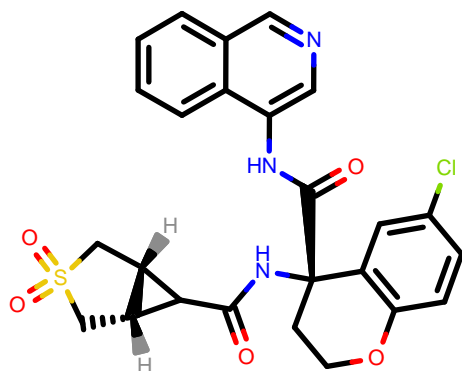
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)NCc5cnon5

RUN: RUN5891

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.23

EN300-6779469_1_2_1



CID: EN300-6779469_1_2_1

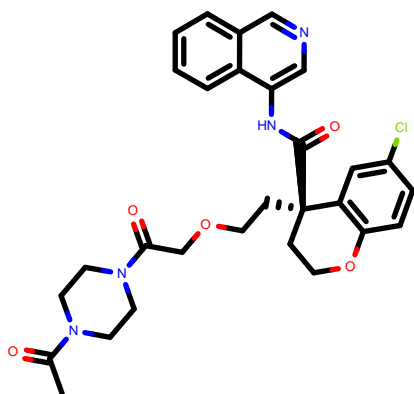
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)CS(=O)N

RUN: RUN5870

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.27

EN300-1724771_3_1_1



CID: EN300-1724771_3_1_1

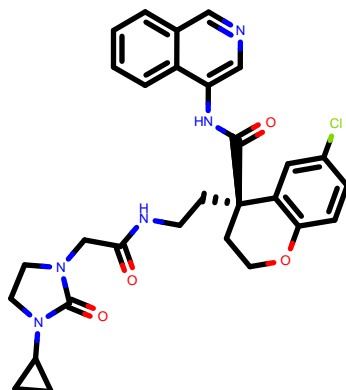
SMILES: CC(=O)N1CCN(CC1)C(=O)COCC[C@@]2(C)CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5o4ccoc5

RUN: RUN5976

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.29

EN300-304771_3_1_1



CID: EN300-304771_3_1_1

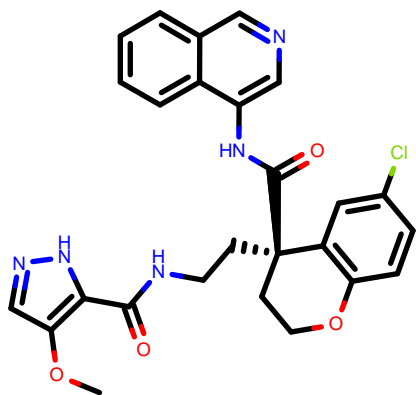
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)CN5CCN(C5=O)C6C6

RUN: RUN4828

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.40

EN300-7439284_3_1_1



CID: EN300-7439284_3_1_1

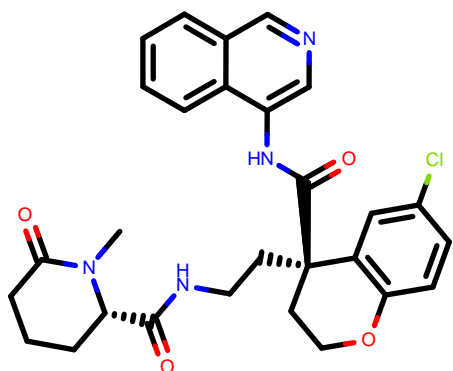
SMILES: COc1cn[nH]c1C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN5583

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.29

EN300-325738_3_1_1



CID: EN300-325738_3_1_1

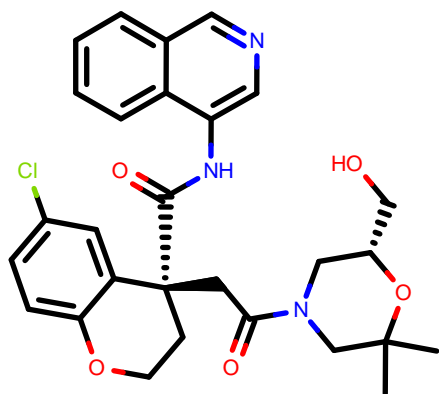
SMILES: CN1[C@@H](CCCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN4626

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.27

EN300-158082_1_1_1



CID: EN300-158082_1_1_1

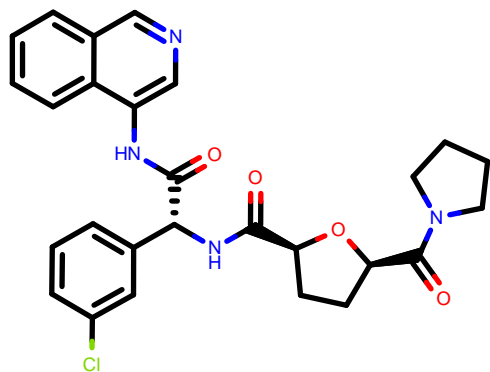
SMILES: CC1(CN(C)C[C@@H](O1)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN4860

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.42

EDJ-MED-ee07cf00-11_1



CID: EDJ-MED-ee07cf00-11_1

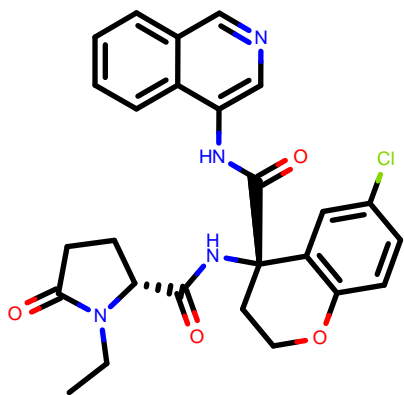
SMILES: c1ccc2c(c1)nc2NC(=O)C[C@@H](c3ccc(c3)NC(=O)C[C@@H](O)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN2668

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.65

EN300-718785_1_2_1



CID: EN300-718785_1_2_1

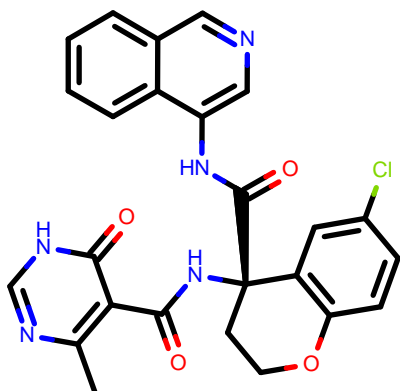
SMILES: CCN1C@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN6255

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.25

EN300-256762_1_1_1



CID: EN300-256762_1_1_1

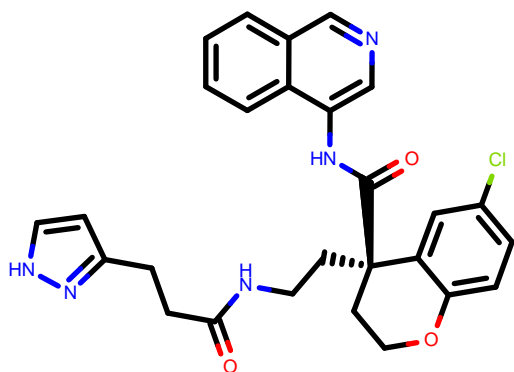
SMILES: Cc1c(c(=O)[nH]cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN3254

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.27

EN300-1664603_3_1_1



CID: EN300-1664603_3_1_1

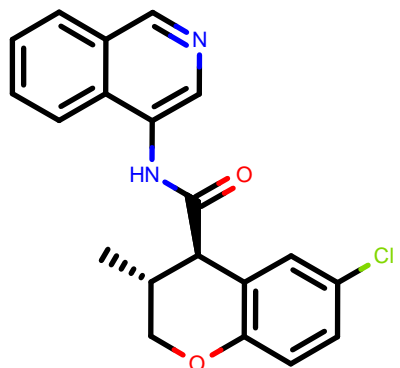
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCc5ccn[nH]5

RUN: RUN4167

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.24

MAT-POS-8a69d52e-4_2



CID: MAT-POS-8a69d52e-4_2

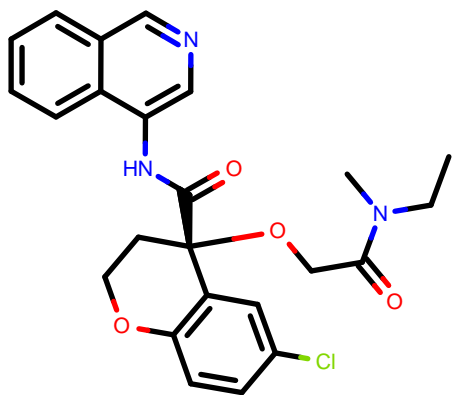
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cnccc4c3cccc4)Cl

RUN: RUN288

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.05

EN300-1253122_1_1_1



CID: EN300-1253122_1_1_1

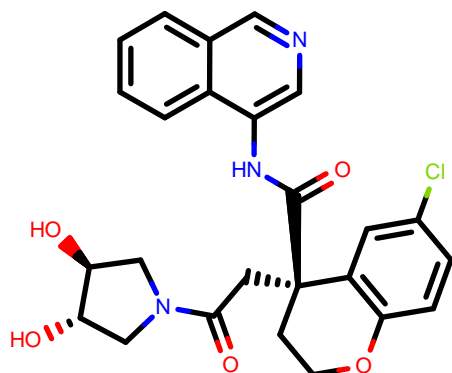
SMILES: CCN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN5172

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.23

EN300-96037_1_1_1



CID: EN300-96037_1_1_1

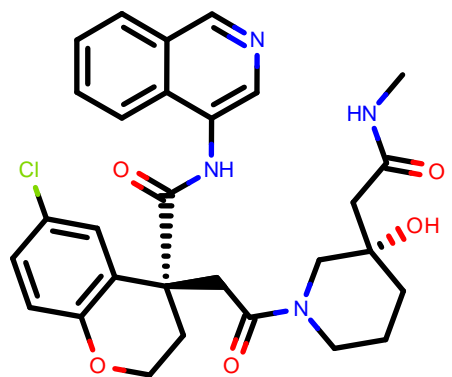
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@H](C5)O)O

RUN: RUN5696

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.26

EN300-259062_1_2_1



CID: EN300-259062_1_2_1

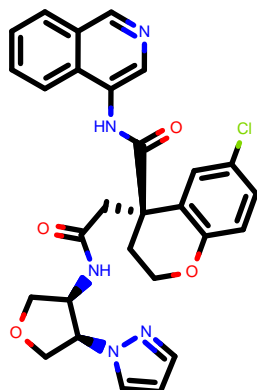
SMILES: CNC(=O)C[C@]1(CCCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)O

RUN: RUN3631

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.34

EN300-1086925_1_1_1



CID: EN300-1086925_1_1_1

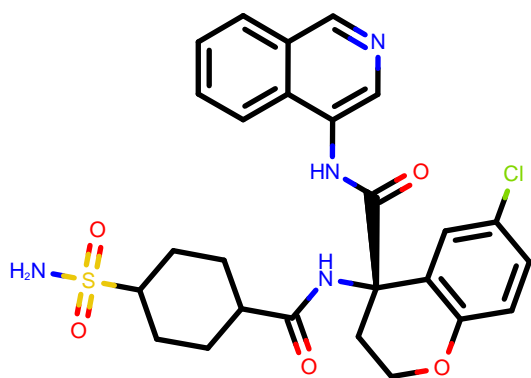
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CO)C[C@H]5Nc6cnc6

RUN: RUN5822

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.35

EN300-83864_1_1_1



CID: EN300-83864_1_1_1

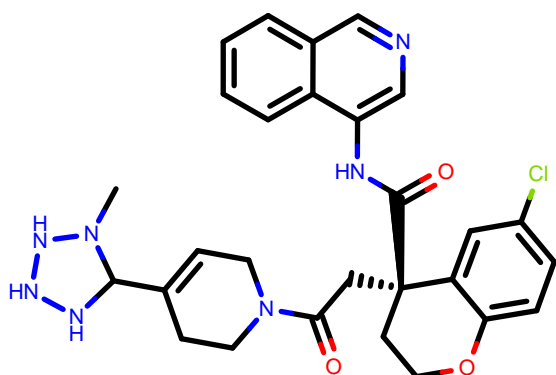
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCCC(C5)S(=O)(=O)N

RUN: RUN3212

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.38

ALP-POS-5bb456a5-3_2



CID: ALP-POS-5bb456a5-3_2

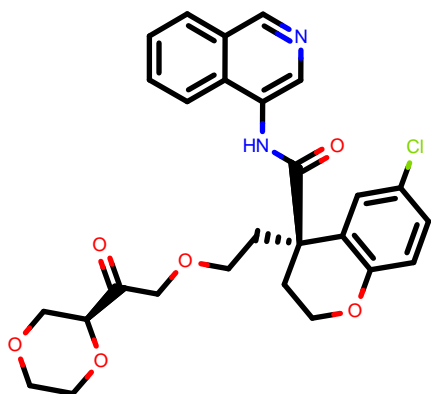
SMILES: Cn1c(nnn1)C2=CCN(CC2)C(=O)[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cccc6c5cccc6

RUN: RUN2269

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.28

EN300-6238494_3_1_1



CID: EN300-6238494_3_1_1

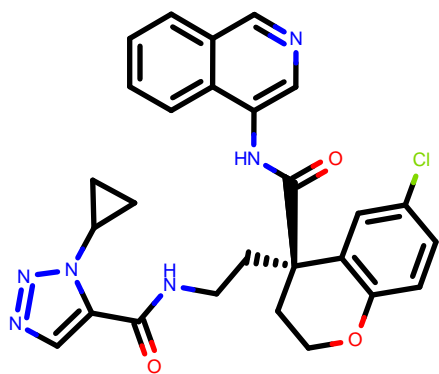
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)O[C@@]5OCOC5

RUN: RUN5381

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.25

EN300-1718675_3_1_1



CID: EN300-1718675_3_1_1

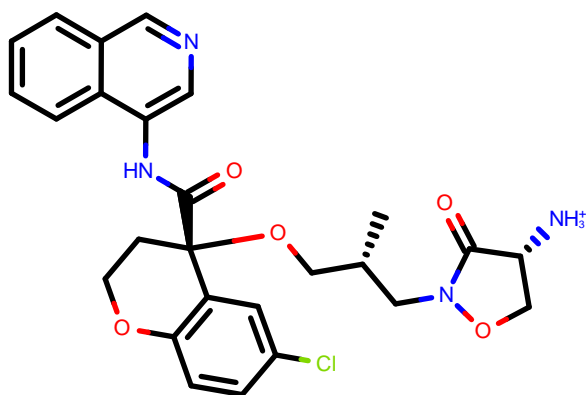
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5nnnn5C6C6

RUN: RUN5476

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.35

EDG-MED-4c68219f-1_2



CID: EDG-MED-4c68219f-1_2

SMILES:

C[C@@H](CN1C(=O)C[C@@H](CO1)N)C(=O)C[C@@H](CO)C(=O)Nc4ccc5c4ccc5

RUN:

RUN1513

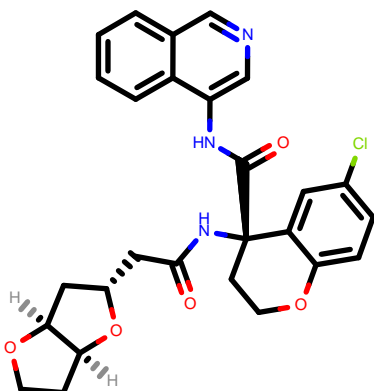
DDG (kcal/mol):

-1.01

dDDG (kcal/mol):

0.40

EN300-7355519_1_4_1



CID: EN300-7355519_1_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C[C@@H](CO)C(=O)Nc4ccc5c4ccc5

RUN:

RUN4720

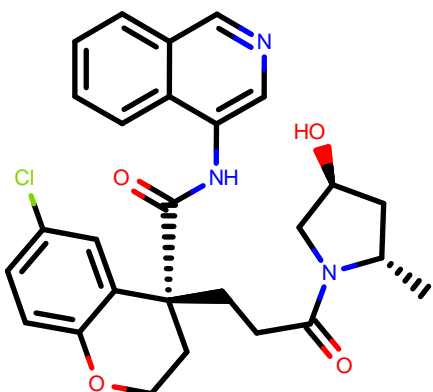
DDG (kcal/mol):

-1.01

dDDG (kcal/mol):

0.28

EN300-173562_2_2_1



CID: EN300-173562_2_2_1

SMILES:

C[C@@H]1C[C@@H](CN1C(=O)CC)C(=O)C[C@@H](CO)C(=O)Nc4ccc5c4ccc5

RUN:

RUN5840

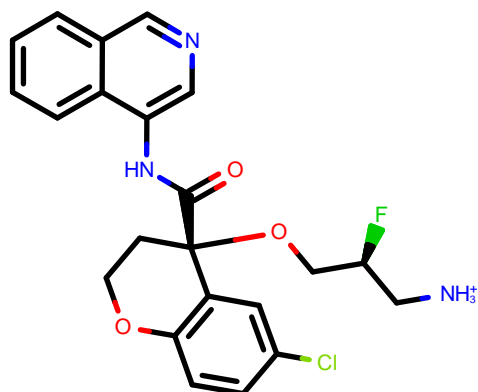
DDG (kcal/mol):

-1.01

dDDG (kcal/mol):

0.23

ED_-GRI-5b13fbe2-40_1



CID: ED_-GRI-5b13fbe2-40_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C[C@@H](CO)C(=O)Nc4ccc5c4ccc5

RUN:

RUN1419

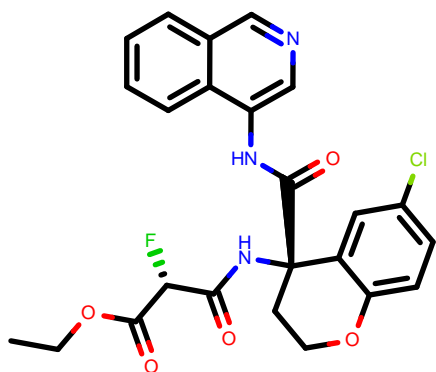
DDG (kcal/mol):

-1.01

dDDG (kcal/mol):

0.45

EN300-123398_1_1_1



CID: EN300-123398_1_1_1

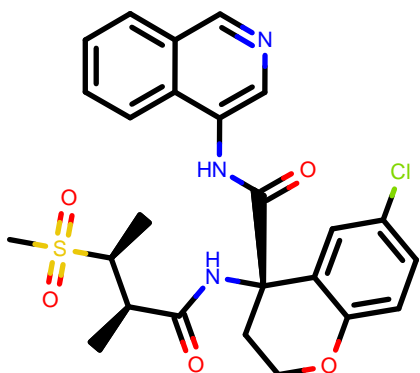
SMILES: CCOC(=O)[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)F

RUN: RUN6619

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.22

EN300-182725_1_3_1



CID: EN300-182725_1_3_1

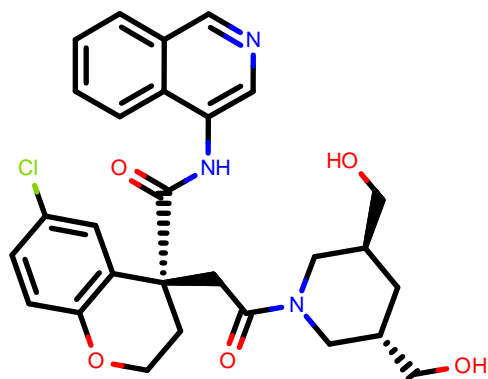
SMILES: C[C@@H](C[C@@H](C)S(=O)(=O)C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)C

RUN: RUN5352

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.29

EN300-2007627_1_2_1



CID: EN300-2007627_1_2_1

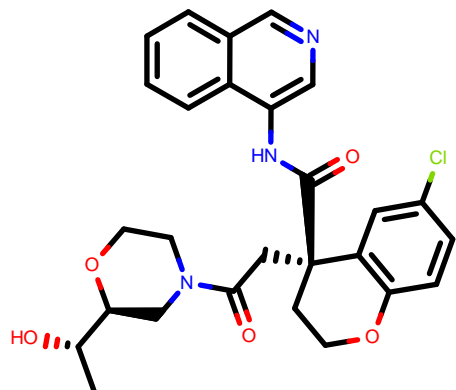
SMILES: C1CCc2c1ncc2NC(=O)[C@@H](C)C(=O)N[C@@H]1(CCOc3c1cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5O

RUN: RUN4144

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.38

EN300-1708848_1_1_1



CID: EN300-1708848_1_1_1

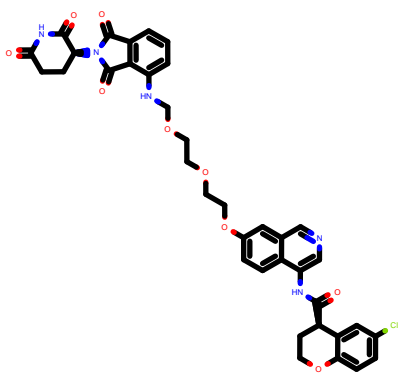
SMILES: C[C@@H](C[C@@H](C)CN(CCO1)C(=O)C[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN4080

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.37

DAR-DIA-9e4459de-11_7



CID: DAR-DIA-9e4459de-11_7

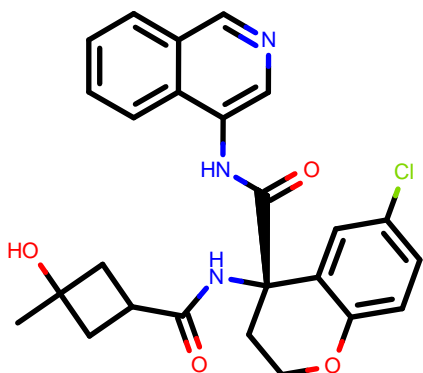
SMILES: c1cc2c(c1)NC(=O)CCOCc3ccc4c(c3)ncnc4NC(=O)[C@@H]5COCc6cc(c(c6)Cl)C(=O)Nc7cc1(O)NC7=O

RUN: RUN1326

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.36

EN300-7183657_1_1_1



CID: EN300-7183657_1_1_1

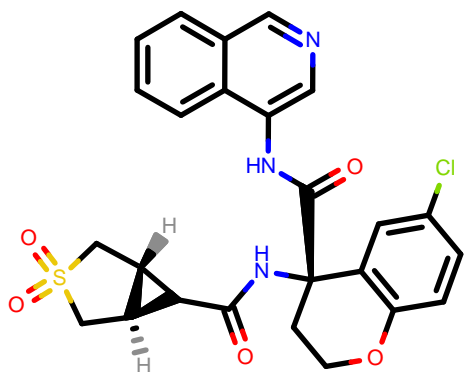
SMILES: CC1(CC(C1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5)O

RUN: RUN4092

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.22

EN300-6779469_1_1_1



CID: EN300-6779469_1_1_1

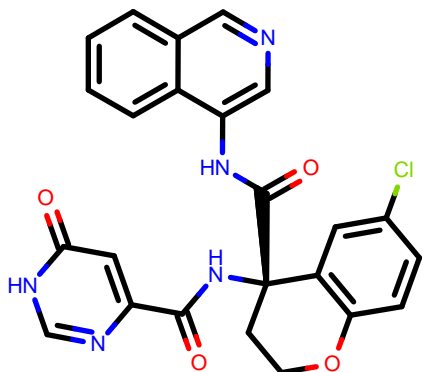
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)N[C@@]5(C)C(=O)Nc6cccc7c6cccc7

RUN: RUN5975

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.22

EN300-817811_1_1_1



CID: EN300-817811_1_1_1

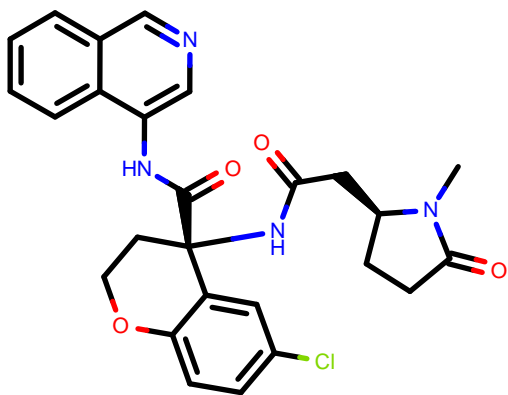
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5(C)C(=O)Nc6cccc7c6cccc7

RUN: RUN5538

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.21

EN300-207765_1_1_1



CID: EN300-207765_1_1_1

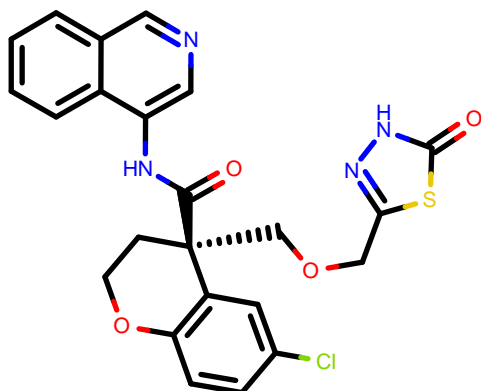
SMILES: CN1[C@@H](CCC1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5

RUN: RUN5439

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.27

EDJ-MED-fcba3f31-12_1



CID: EDJ-MED-fcba3f31-12_1

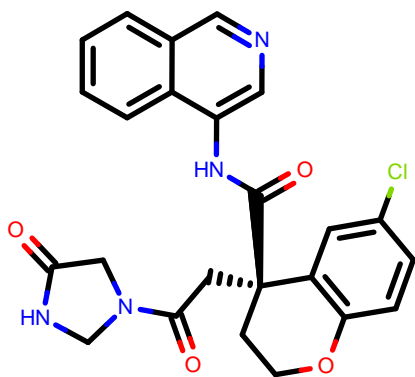
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCc5n[nH]c(=O)s5

RUN: RUN2387

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-154156_1_1_1



CID: EN300-154156_1_1_1

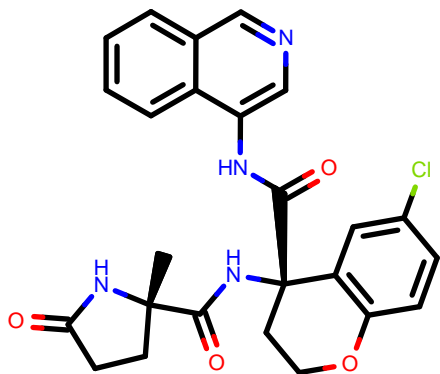
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(=O)N5

RUN: RUN4088

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.22

EN300-177118_1_2_1



CID: EN300-177118_1_2_1

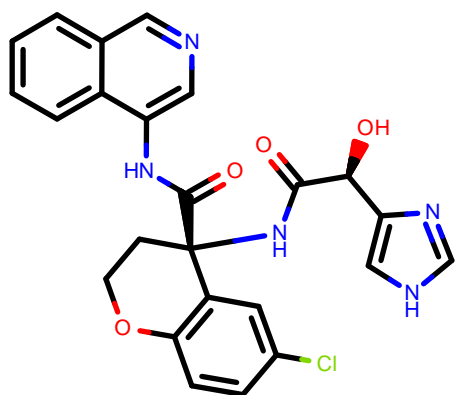
SMILES: C[C@@]1(CCC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5

RUN: RUN4899

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-254121_1_2_1



CID: EN300-254121_1_2_1

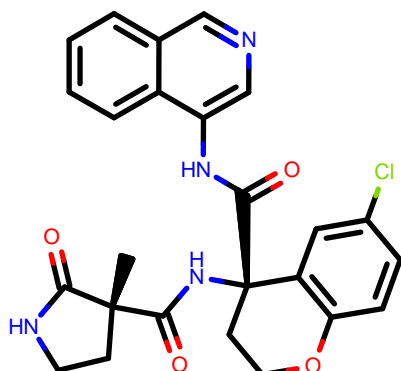
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](c5cnc[nH]5)O

RUN: RUN5909

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.35

EN300-207959_1_2_1



CID: EN300-207959_1_2_1

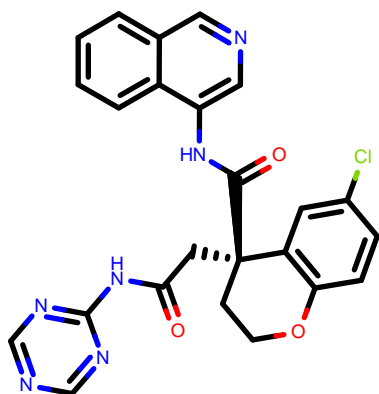
SMILES: C[C@@]1(CCN1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5

RUN: RUN3749

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.35

EDJ-MED-d203f206-20_1



CID: EDJ-MED-d203f206-20_1

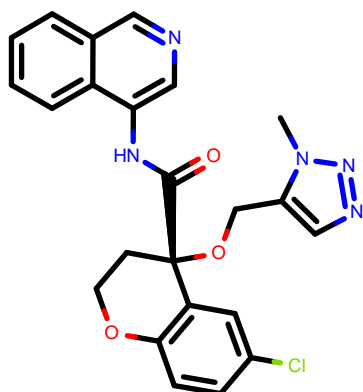
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5ncnc5

RUN: RUN2385

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.26

EN300-216673_1_1_1



CID: EN300-216673_1_1_1

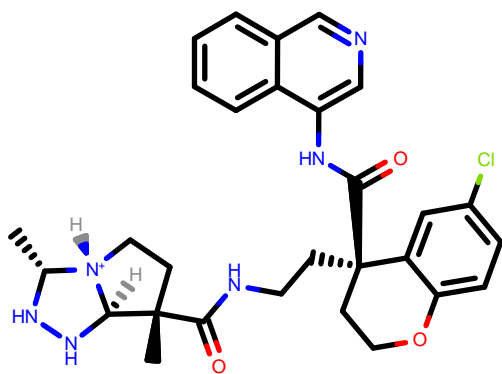
SMILES: Cn1c(cnn1)CO[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncnc4cccc5

RUN: RUN5326

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-7431629_3_2_4



CID: EN300-7431629_3_2_4

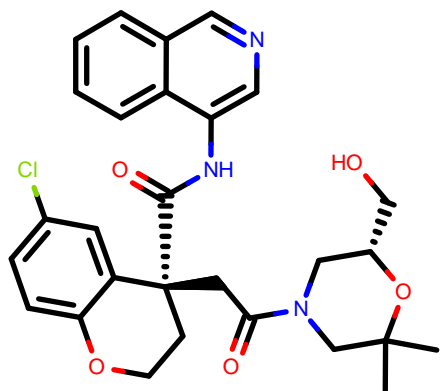
SMILES: C[C@@H]1NN[C@@H]2[NB]H1CC[C@]2(C)C(=O)NCC[C@@]3(C)CCOC4C3C(=O)C1C(=O)N5C6OC65CCCC6

RUN: RUN3194

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.87

EN300-7412943_1_1_1



CID: EN300-7412943_1_1_1

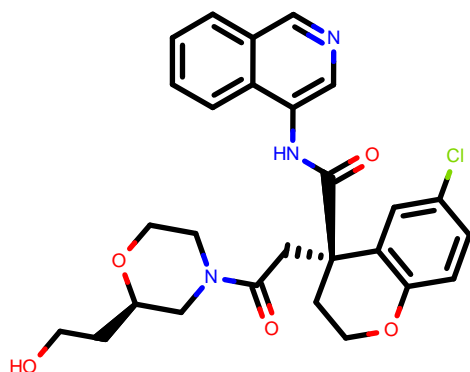
SMILES: CC1(CN(C)C[C@@H](O)CO)C(=O)C[C@]2(C)CCOC3C2C(=O)C1C(=O)N4C5OC54CCCC5

RUN: RUN2962

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.39

EN300-102007_1_1_1



CID: EN300-102007_1_1_1

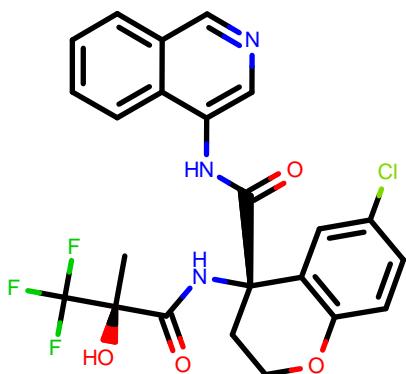
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@]3(C)CCOC4C3C(=O)N5CCOC[C@@H](C5)CCO

RUN: RUN4996

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.34

EN300-159633_1_2_1



CID: EN300-159633_1_2_1

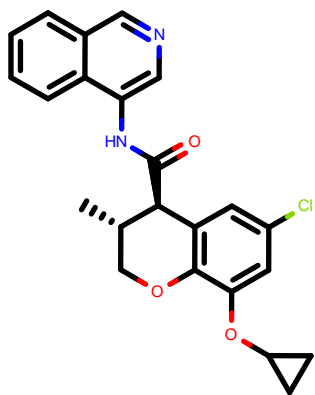
SMILES: C[C@](C(=O)N[C@@]1(C)CCOC2C1CC(=O)C1C(=O)N3C4OC4C3CCCC4)(C(F)(F)F)O

RUN: RUN4377

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.25

DAR-DIA-0d514e7d-6_1_1



CID: DAR-DIA-0d514e7d-6_1_1

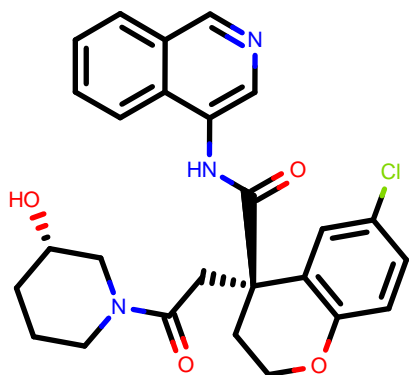
SMILES: C[C@H]1COc2c(cc2OC3CC3)Cl[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN4430

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.17

EDJ-MED-d203f206-43_1



CID: EDJ-MED-d203f206-43_1

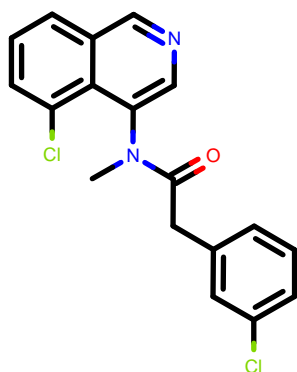
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN2460

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.27

MIC-UNK-67d4a29a-1_1



CID: MIC-UNK-67d4a29a-1_1

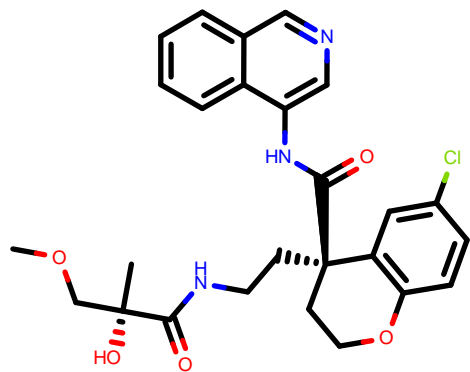
SMILES: CN(c1cncc2c1c(ccc2)Cl)C(=O)Cc3cccc(c3)Cl

RUN: RUN976

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-76841_3_2_1



CID: EN300-76841_3_2_1

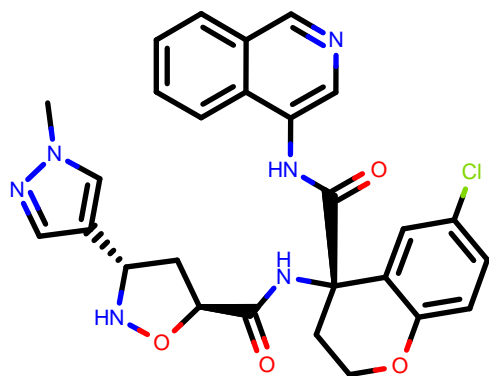
SMILES: C[C@](COC)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN6008

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.41

EN300-92605_1_1_1



CID: EN300-92605_1_1_1

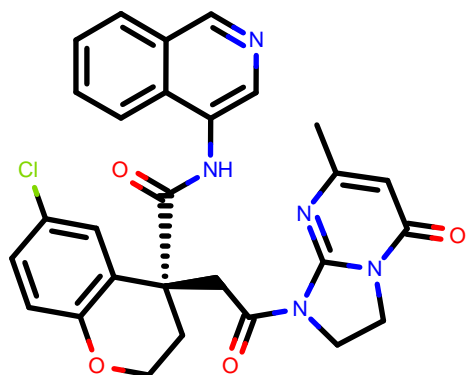
SMILES: Cn1cc(m1)[C@@H]2[C@@H](ON2)C(=O)NC@3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccc6

RUN: RUN4196

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.40

EN300-124973_1_1_1



CID: EN300-124973_1_1_1

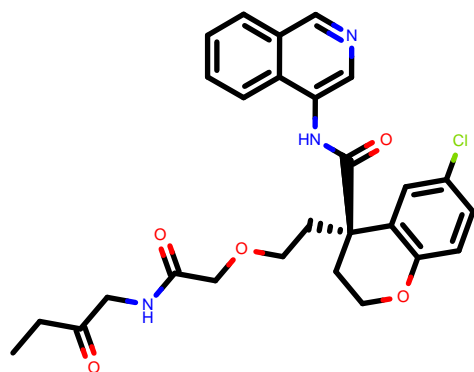
SMILES: Cc1cc(=O)n2c(n1)N(CC2)C(=O)C[C@@3](CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccc6

RUN: RUN5350

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.24

EN300-132624_3_1_1



CID: EN300-132624_3_1_1

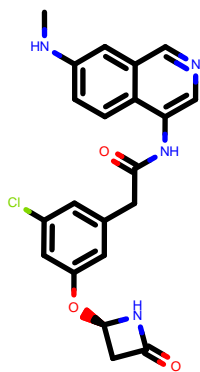
SMILES: CCC(=O)CNC(=O)COCC[C@@1](CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN4556

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.33

ALF-EVA-0b412456-6_1



CID: ALF-EVA-0b412456-6_1

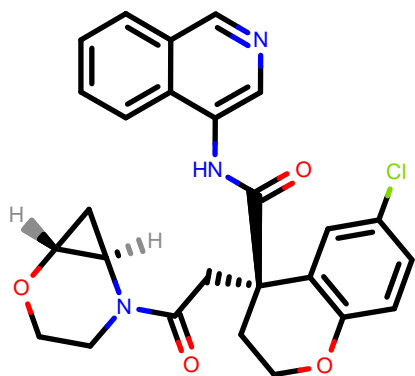
SMILES: CNc1ccc2c(c1)ncnc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN2574

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.36

EN300-91609_1_4_1



CID: EN300-91609_1_4_1

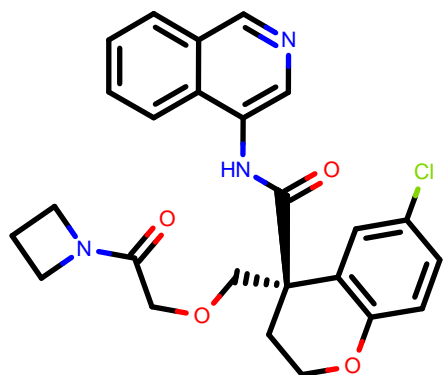
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]6[C@H]5C6

RUN: RUN4470

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EN300-11195_2_1_1



CID: EN300-11195_2_1_1

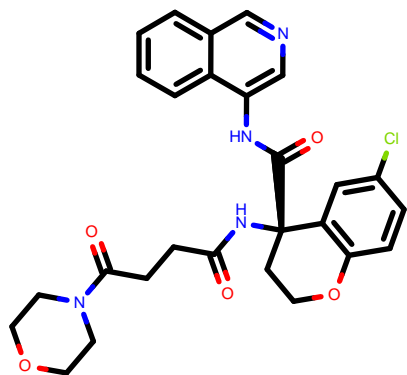
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCCC5

RUN: RUN4896

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.21

EN300-05277_1_1_1



CID: EN300-05277_1_1_1

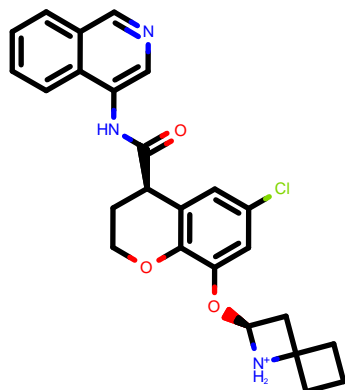
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCC(=O)N5CCOCC5

RUN: RUN3958

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.27

DAR-DIA-23e5a6a0-2_2



CID: DAR-DIA-23e5a6a0-2_2

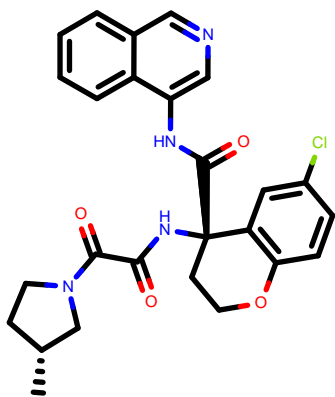
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[C@H]5CC6([NH2+][5]C)CC6]Cl

RUN: RUN412

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EN300-138170_1_1_1



CID: EN300-138170_1_1_1

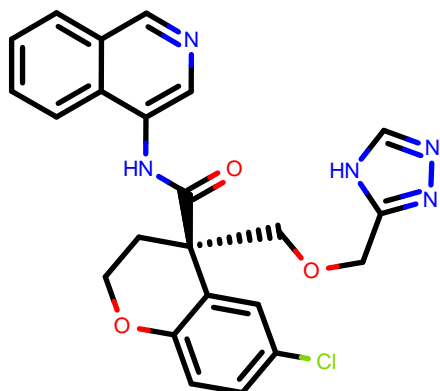
SMILES: C[C@@H]1CCN(C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN7678

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-306316_2_1_1



CID: EN300-306316_2_1_1

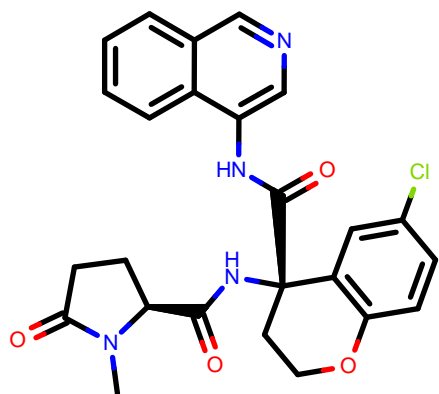
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCc5[nH]ncn5

RUN: RUN4586

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.20

EN300-132963_1_1_1



CID: EN300-132963_1_1_1

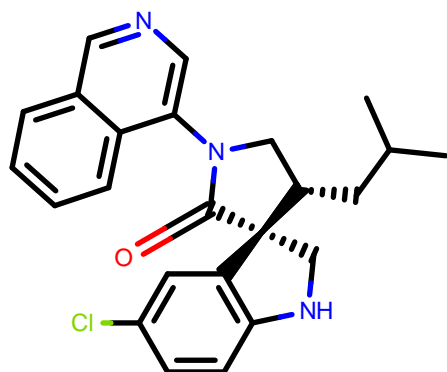
SMILES: CN1[C@@H](CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN7580

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

DAR-DIA-6be260fc-2_1



CID: DAR-DIA-6be260fc-2_1

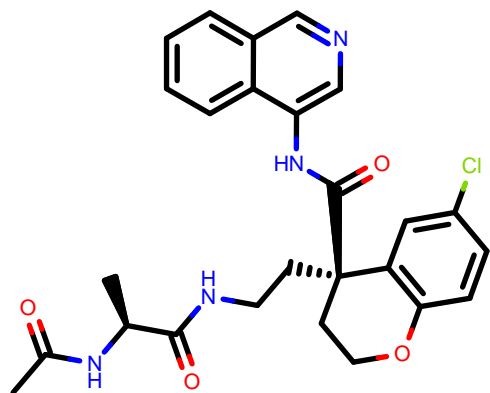
SMILES: CC(C)C[C@H]1CN(C(=O)[C@@]2(CCOc3c2cc(cc3)C)c4ncoc5c4cccc5

RUN: RUN1935

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.32

EN300-862647_3_1_1



CID: EN300-862647_3_1_1

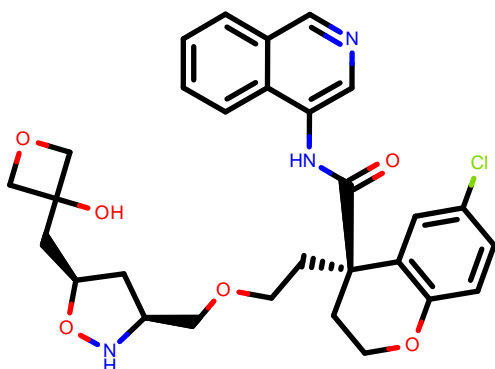
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)C

RUN: RUN4783

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

EN300-7457160_3_2_1



CID: EN300-7457160_3_2_1

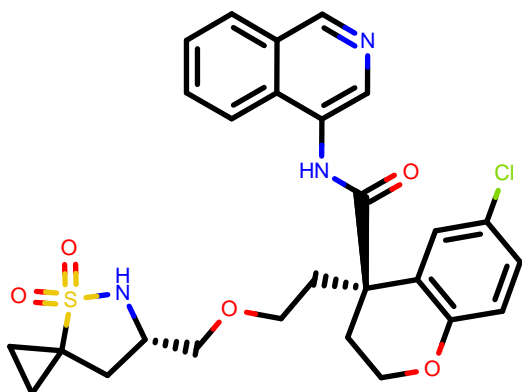
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CCOC[C@@H]5C[C@@H](O)N5C6COC6

RUN: RUN6859

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.36

KAD-UNI-8a629cb0-29_1



CID: KAD-UNI-8a629cb0-29_1

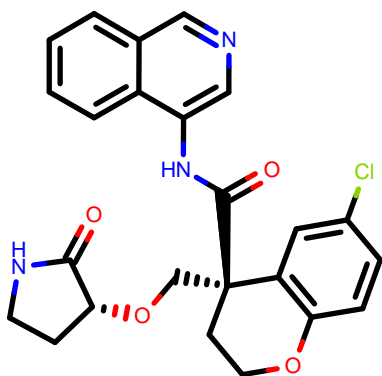
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CCOC[C@@H]5C6C(C6)S(=O)(=O)N5

RUN: RUN2030

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-6736413_2_1_1



CID: EN300-6736413_2_1_1

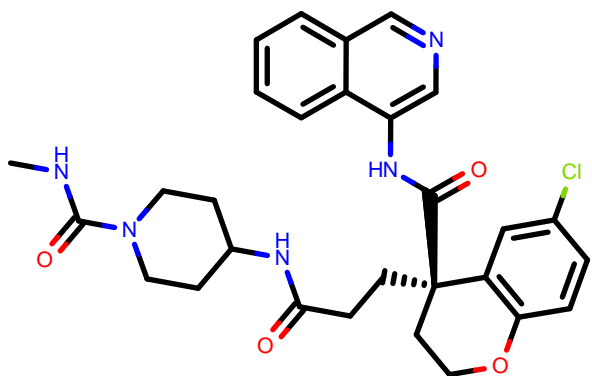
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CO[C@@H]5CCNC5=O

RUN: RUN4277

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.22

EN300-6764450_2_1_1



CID: EN300-6764450_2_1_1

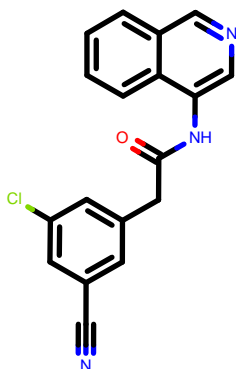
SMILES: CNC(=O)N1CCC(CC1)NC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN6456

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.32

RAL-THA-2d450e86-17_1



CID: RAL-THA-2d450e86-17_1

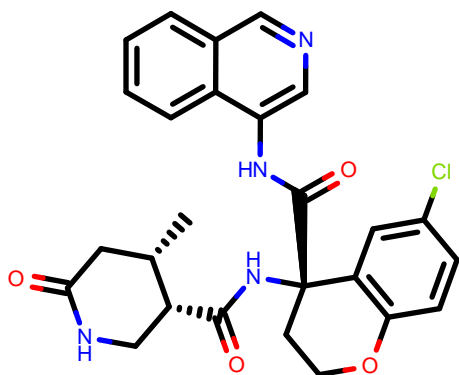
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C#N

RUN: RUN1796

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-95698_1_4_1



CID: EN300-95698_1_4_1

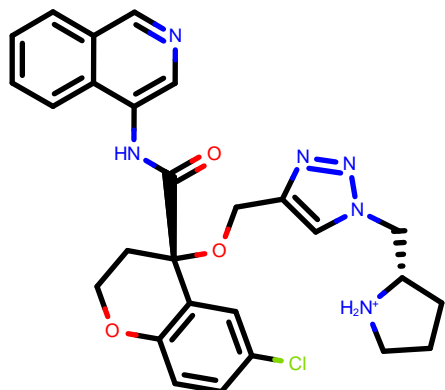
SMILES: C[C@H]1CC(=O)N[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN4016

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-37_1



CID: ED_-GRI-5b13fbe2-37_1

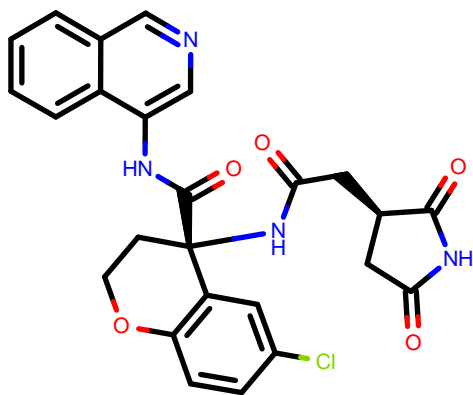
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(nn5)C[C@@H]6CCCC[NH2+][6]

RUN: RUN1466

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.32

EN300-227055_1_1_1



CID: EN300-227055_1_1_1

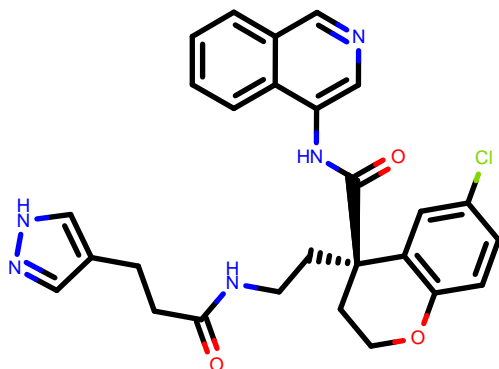
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]5H5CC(=O)NC5=O

RUN: RUN5196

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-250836_3_1_1



CID: EN300-250836_3_1_1

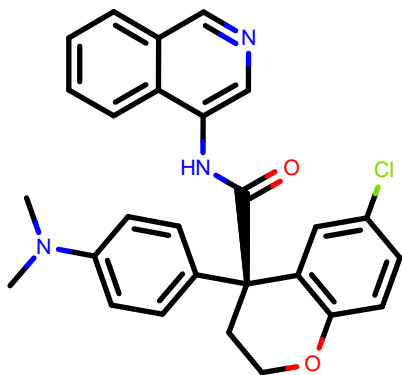
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCc5c[nH]jnc5

RUN: RUN4416

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.31

FRA-DIA-13af2da5-2_1_1



CID: FRA-DIA-13af2da5-2_1_1

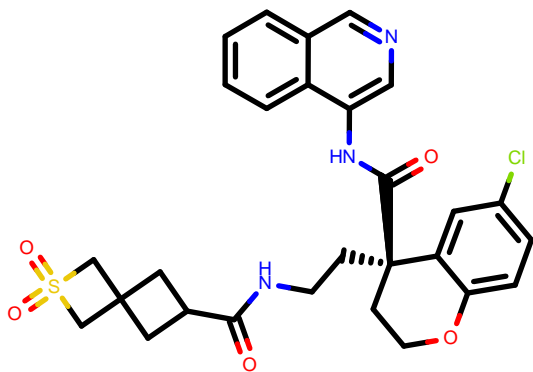
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2882

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.21

KAD-UNI-8a629cb0-24_1



CID: KAD-UNI-8a629cb0-24_1

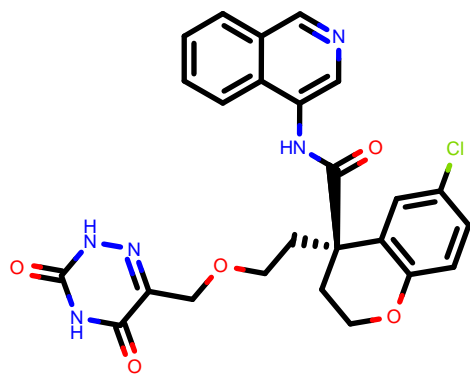
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5CC6(C5)CS(=O)(=O)C6

RUN: RUN1975

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-761746_3_1_1



CID: EN300-761746_3_1_1

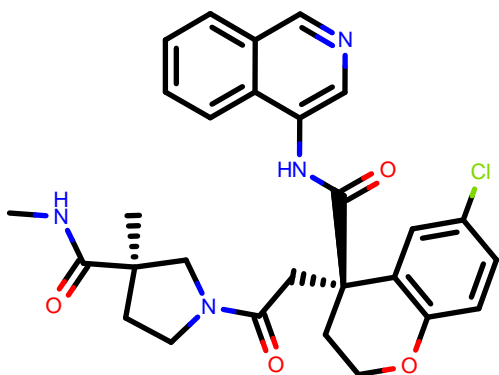
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5c(=O)[nH]c(=O)[nH]n5

RUN: RUN3473

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.31

EN300-196140_1_2_1



CID: EN300-196140_1_2_1

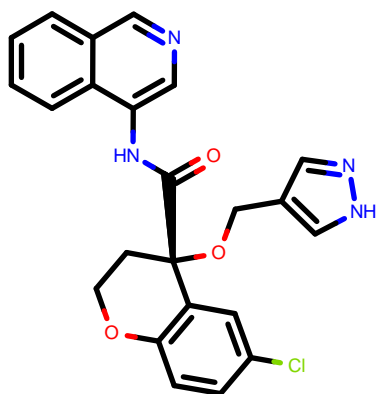
SMILES: C[C@@]1(CCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C(=O)Nc4

RUN: RUN4596

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.42

EDJ-MED-28ec730d-4_1



CID: EDJ-MED-28ec730d-4_1

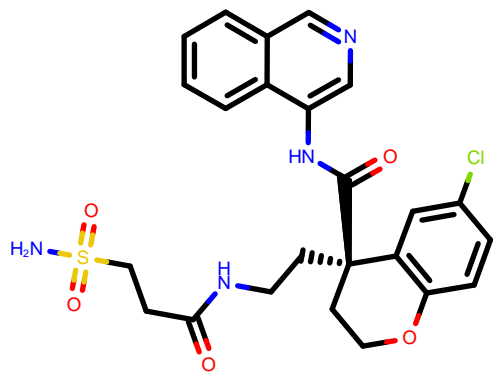
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5

RUN: RUN571

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-31553_3_1_1



CID: EN300-31553_3_1_1

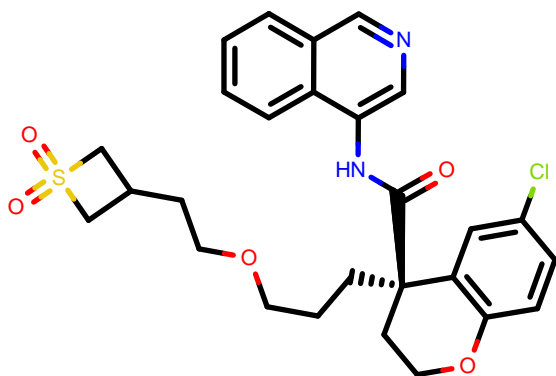
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCS(=O)(=O)N

RUN: RUN5365

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.35

EN300-189563_4_1_1



CID: EN300-189563_4_1_1

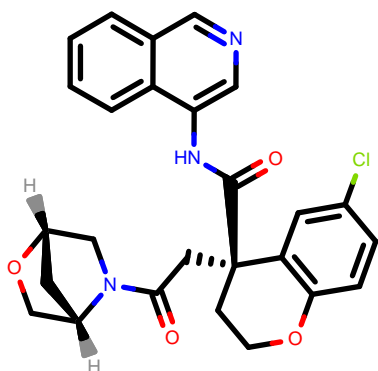
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCCCSCS(=O)(=O)C5

RUN: RUN7304

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.33

EN300-321790_1_1_1



CID: EN300-321790_1_1_1

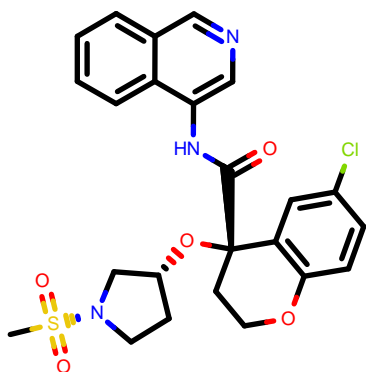
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@]H6[C@]H5O6

RUN: RUN4861

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.25

EN300-301690_1_2_1



CID: EN300-301690_1_2_1

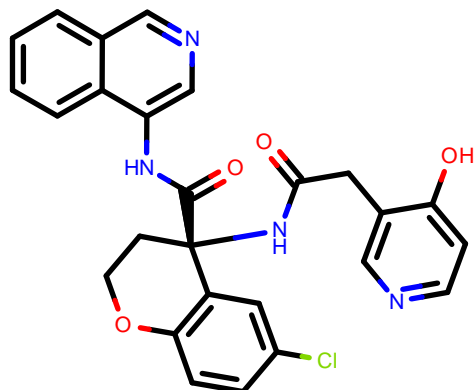
SMILES: CS(=O)(=O)[N@]1CC[C@H]1O[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN7564

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.31

EN300-205486_1_1_1



CID: EN300-205486_1_1_1

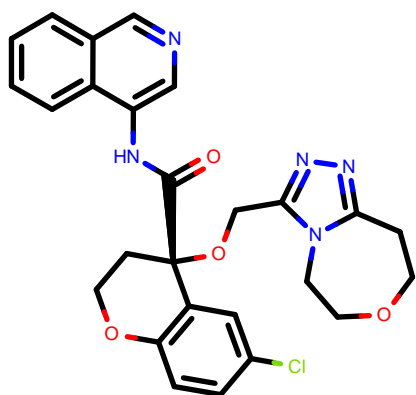
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5c[nH]ccc5=O

RUN: RUN6855

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-310888_1_1_1



CID: EN300-310888_1_1_1

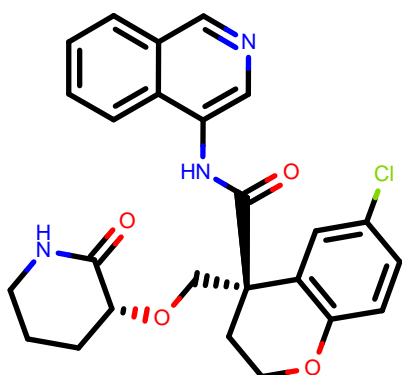
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nnc6n5CCOC6

RUN: RUN5478

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.26

EDJ-MED-fcba3f31-1_1



CID: EDJ-MED-fcba3f31-1_1

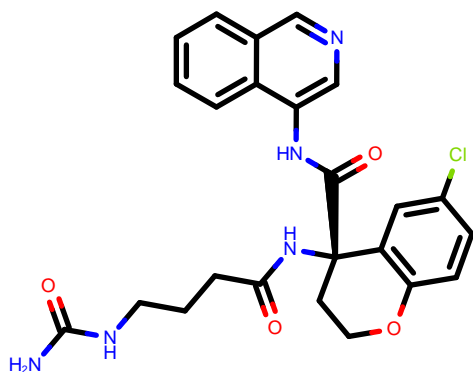
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@]5H5CCNC5=O

RUN: RUN2353

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-05620_1_1_1



CID: EN300-05620_1_1_1

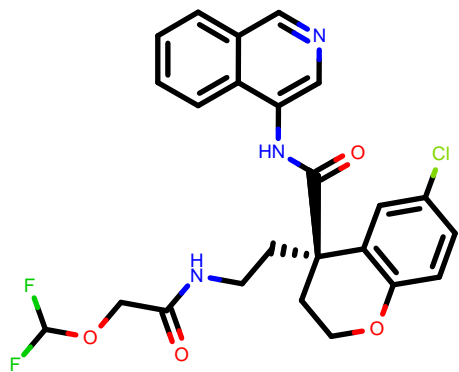
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)N

RUN: RUN6087

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.30

EN300-179091_3_1_1



CID: EN300-179091_3_1_1

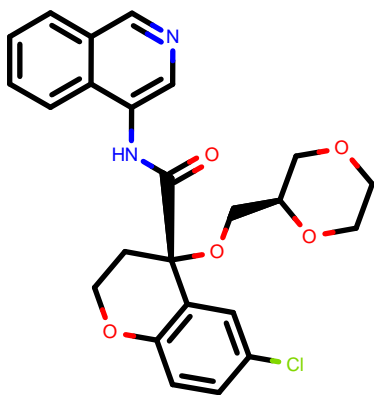
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC(F)F

RUN: RUN3933

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

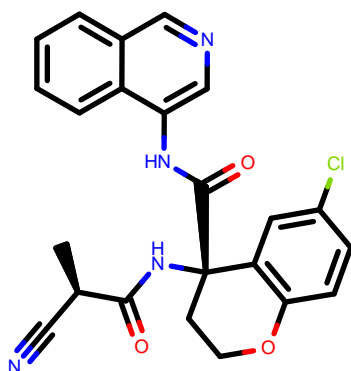
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCCO5

RUN: RUN3817

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EDG-MED-90036822-80_2



CID: EDG-MED-90036822-80_2

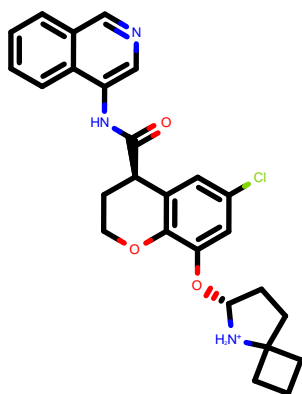
SMILES: C[C@H](C#N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN1636

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.17

DAR-DIA-23e5a6a0-1_1



CID: DAR-DIA-23e5a6a0-1_1

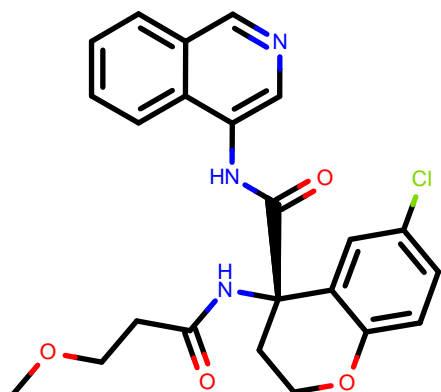
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6([NH2+][5])CCO6Cl

RUN: RUN417

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.34

EN300-64536_1_1_1



CID: EN300-64536_1_1_1

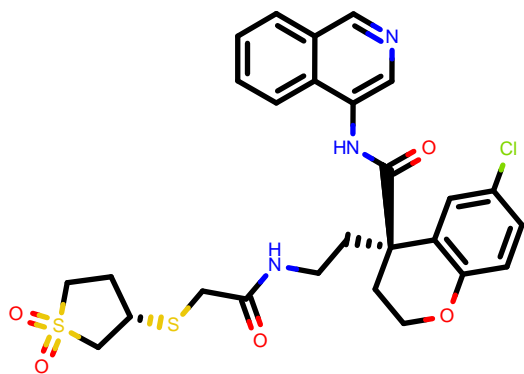
SMILES: COCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4565

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-13890_3_2_1



CID: EN300-13890_3_2_1

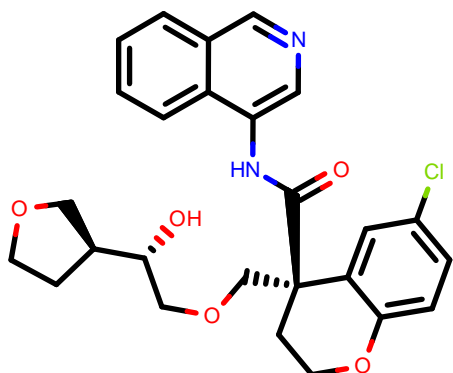
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@H]5CCS(=O)(=O)C5

RUN: RUN4760

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.34

EN300-1911992_2_4_1



CID: EN300-1911992_2_4_1

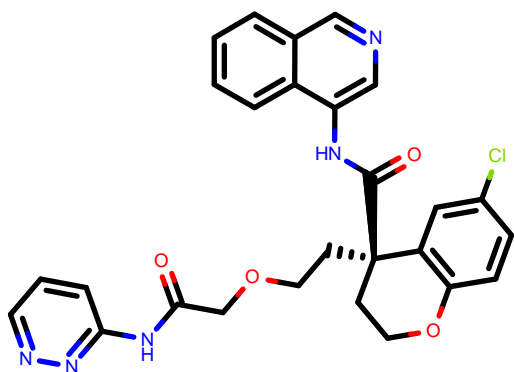
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5COCCO5

RUN: RUN4531

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.33

EN300-761618_3_1_1



CID: EN300-761618_3_1_1

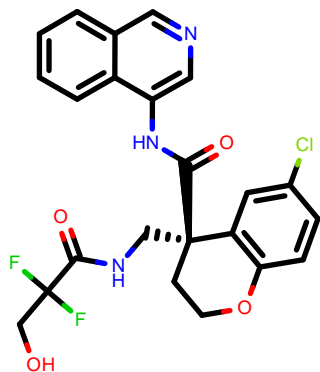
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5ccnnc5

RUN: RUN3931

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.27

EN300-123489_2_1_1



CID: EN300-123489_2_1_1

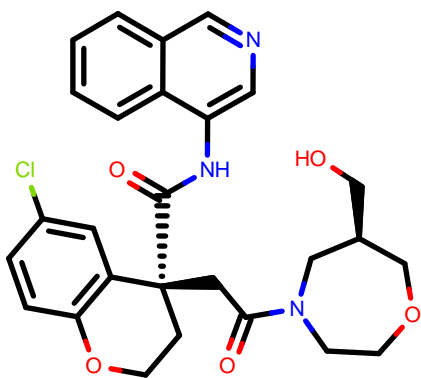
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(CO)(F)F

RUN: RUN3873

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.21

EN300-6478054_1_1_1



CID: EN300-6478054_1_1_1

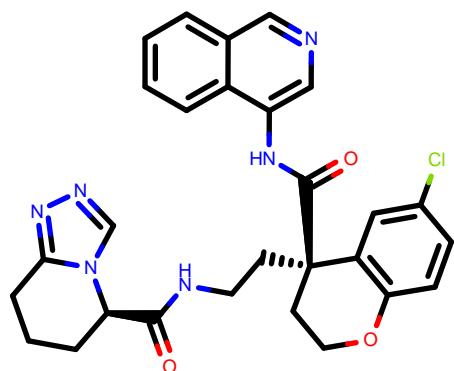
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)CO

RUN: RUN6401

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.37

EN300-6478631_3_2_1



CID: EN300-6478631_3_2_1

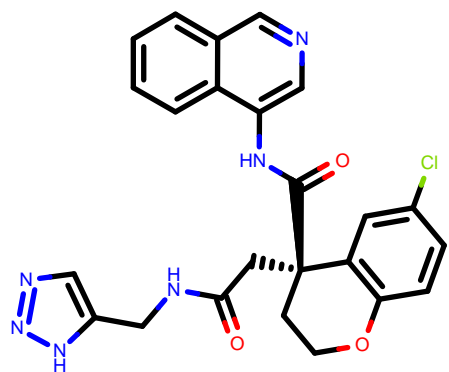
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCc6n5n6

RUN: RUN6328

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.29

EN300-98429_1_1_1



CID: EN300-98429_1_1_1

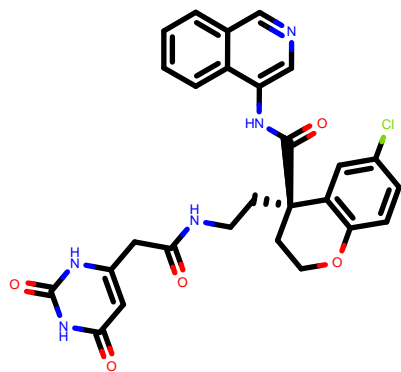
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5cn[nH]5

RUN: RUN5190

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.29

EN300-11441_3_1_1



CID: EN300-11441_3_1_1

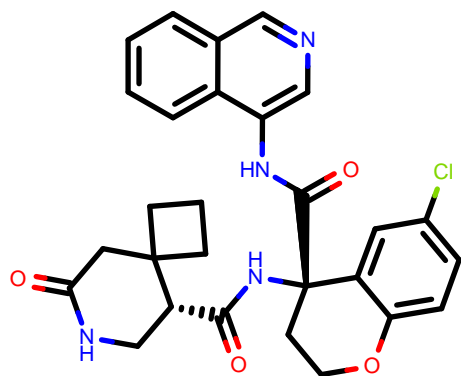
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN4538

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.31

EN300-1704404_1_1_1



CID: EN300-1704404_1_1_1

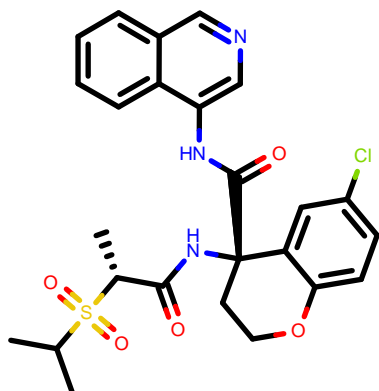
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNC(=O)CC56CC6

RUN: RUN3834

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.23

EN300-40947_1_2_1



CID: EN300-40947_1_2_1

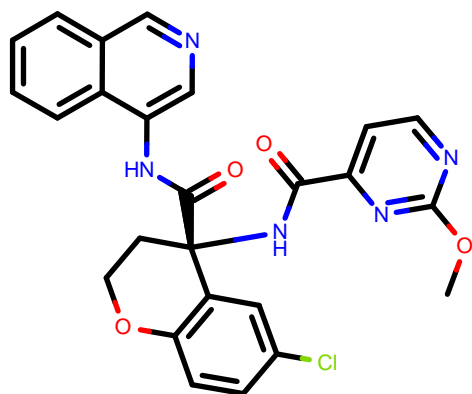
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)S(=O)(=O)C(C)C

RUN: RUN6240

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-154912_1_1_1



CID: EN300-154912_1_1_1

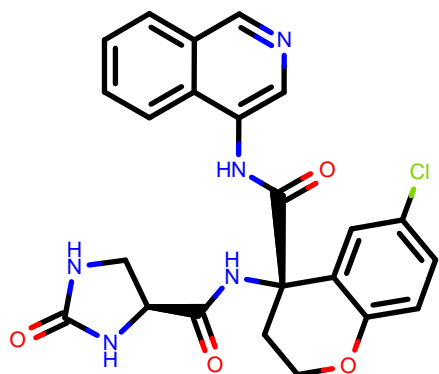
SMILES: COc1nccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5464

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.26

EN300-66461_1_1_1



CID: EN300-66461_1_1_1

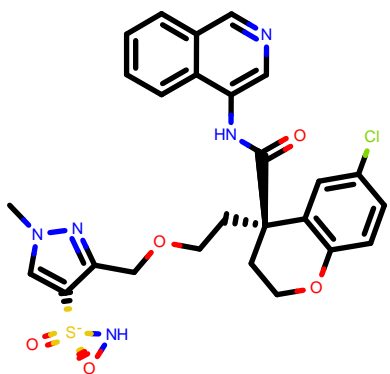
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNC(=O)N5

RUN: RUN5829

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.20

EN300-7355737_3_1_1



CID: EN300-7355737_3_1_1

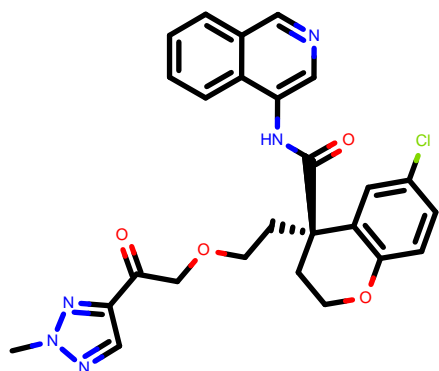
SMILES: Cn1cc(c(n1)COC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5)S(=O)(=O)N

RUN: RUN6414

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.42

EN300-204935_3_1_1



CID: EN300-204935_3_1_1

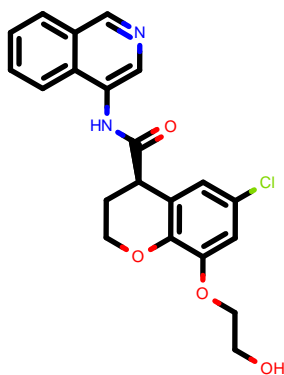
SMILES: Cn1ncc(n1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN3031

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.31

LAU-MED-88a3970a-1_1



CID: LAU-MED-88a3970a-1_1

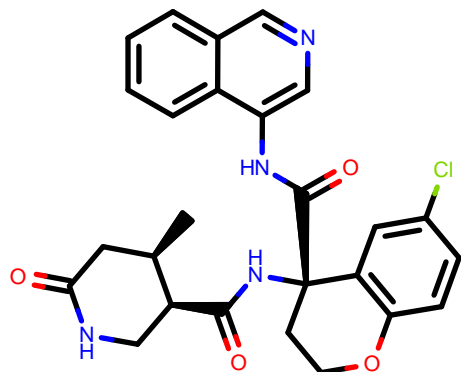
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4OCCO)Cl

RUN: RUN1314

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-95698_1_1_1



CID: EN300-95698_1_1_1

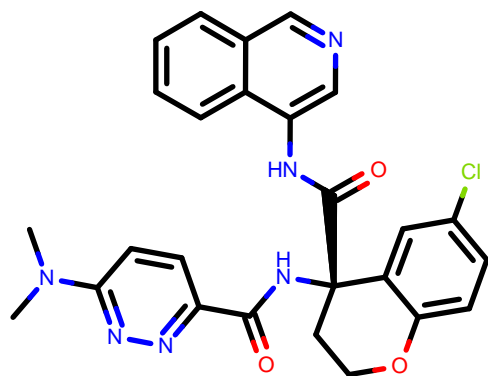
SMILES: C[C@@H]1CC(=O)NC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN5931

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.25

EN300-7535922_1_1_1



CID: EN300-7535922_1_1_1

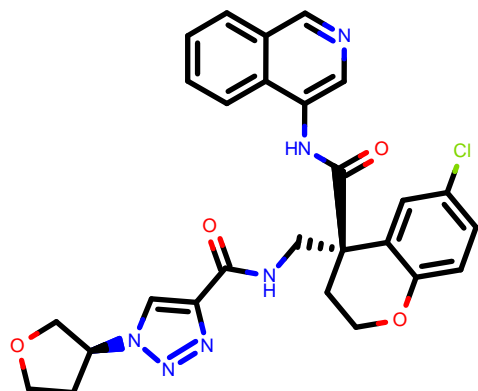
SMILES: CN(C)c1ccc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4206

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.25

EN300-151461_2_2_1



CID: EN300-151461_2_2_1

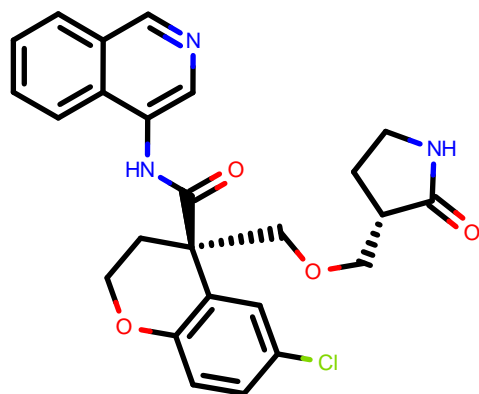
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nc5)[C@H]6CCOC6

RUN: RUN6605

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.37

EN300-246248_2_1_1



CID: EN300-246248_2_1_1

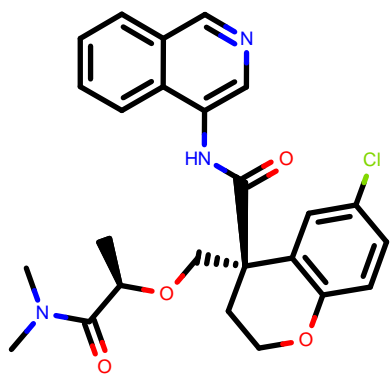
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNC5=O

RUN: RUN4589

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.24

EN300-14458_2_2_1



CID: EN300-14458_2_2_1

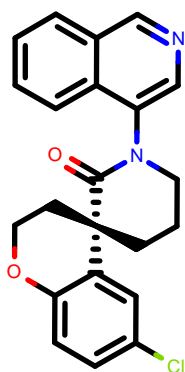
SMILES: C[C@H](C(=O)N(C)C)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4703

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.25

ALP-POS-477dc5b7-5_1



CID: ALP-POS-477dc5b7-5_1

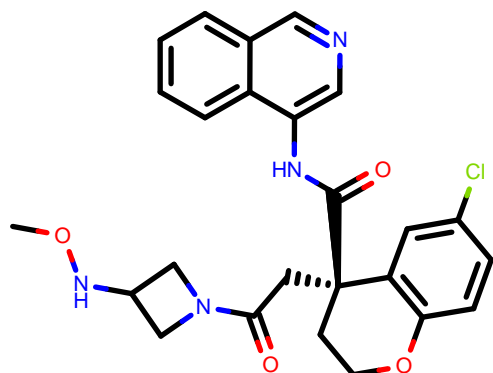
SMILES: c1ccc2c(c1)cncc2N3CCCC[C@]4(C3=O)CCOc5c4cc(cc5)Cl

RUN: RUN209

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.33

EN300-6745214_1_1_1



CID: EN300-6745214_1_1_1

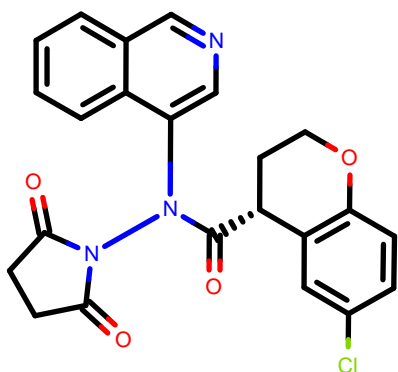
SMILES: CONC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6603

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.24

JOH-UNI-ea72002d-1_1



CID: JOH-UNI-ea72002d-1_1

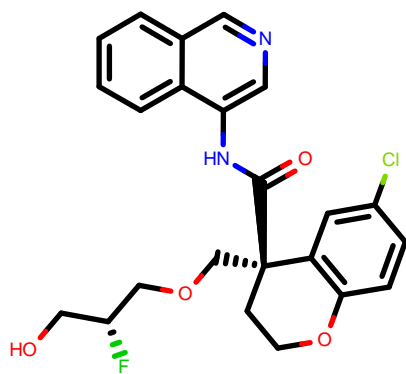
SMILES: c1ccc2c(c1)cncc2N(C(=O)C[C@@H]3CCOC4c3cc(cc4)Cl)N5C(=O)C=CC5=O

RUN: RUN2302

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.21

EN300-1600517_2_1_1



CID: EN300-1600517_2_1_1

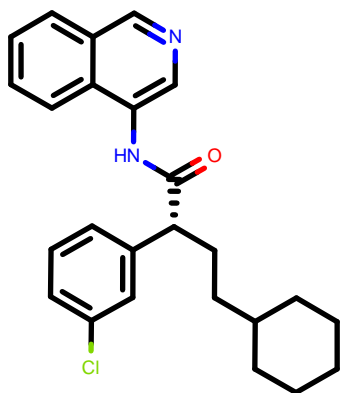
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CO)F

RUN: RUN4654

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.31

MIC-UNK-c66144cb-3_2



CID: MIC-UNK-c66144cb-3_2

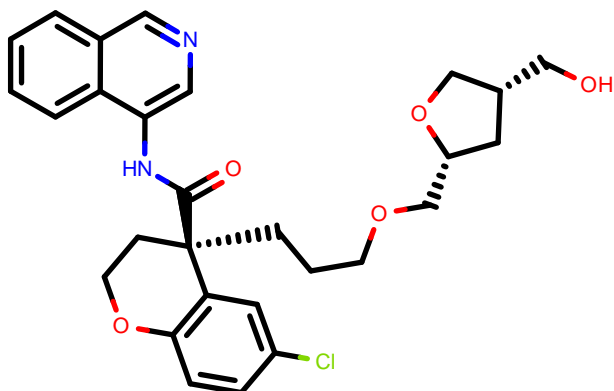
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](CCCCCCCC3)c4cccc(c4)Cl

RUN: RUN130

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.33

EN300-6494158_4_4_1



CID: EN300-6494158_4_4_1

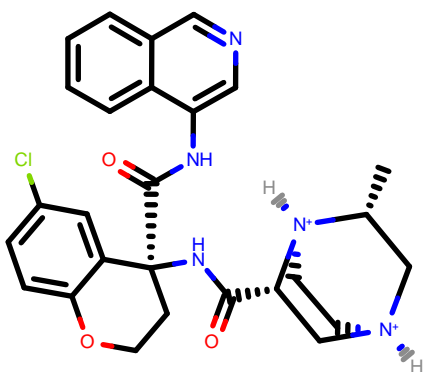
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCOC[C@H]5C[C@H](CO)5CO

RUN: RUN7713

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.33

EN300-120562_1_3_1



CID: EN300-120562_1_3_1

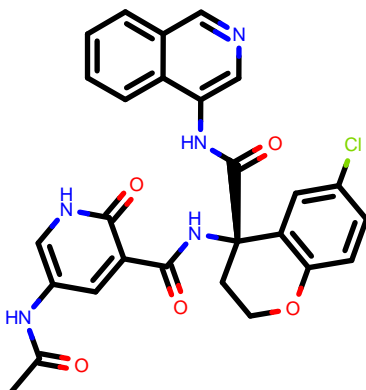
SMILES: C[C@]H1CN[C@@]2CCN[C@H]1[C@H](C2)C(=O)N[C@@]3(CCOc4c3cc(c4)Cl)C(=O)N5CCCC5

RUN: RUN7494

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.34

EN300-307053_1_1_1



CID: EN300-307053_1_1_1

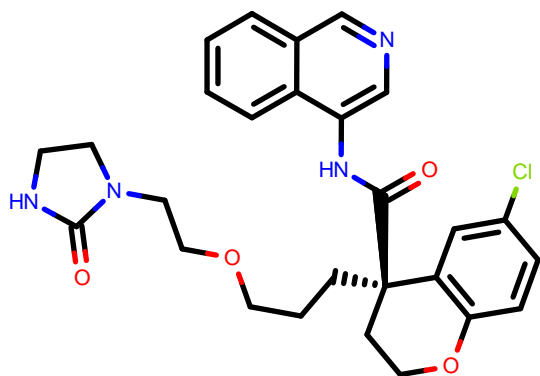
SMILES: CC(=O)Nc1cc(c(=O)[nH]c1)C(=O)N[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5055

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.31

EN300-214800_4_1_1



CID: EN300-214800_4_1_1

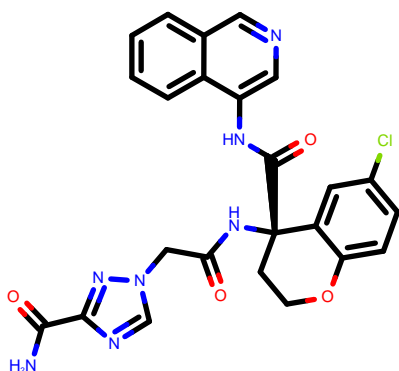
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c24)Cl)CCCCOCCN5CNC5=O

RUN: RUN4340

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.32

EN300-262604_1_1_1



CID: EN300-262604_1_1_1

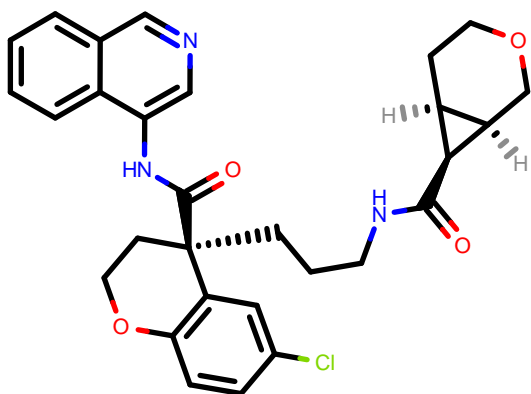
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c24)Cl)NC(=O)Cn5ncnc5C(=O)N

RUN: RUN3640

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.42

EN300-1644723_4_6_1



CID: EN300-1644723_4_6_1

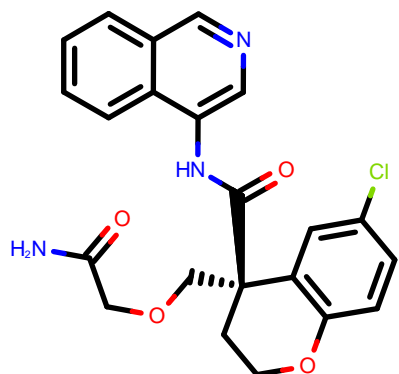
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c24)Cl)CCNC(=O)[C@@]5[C@@]6(C)H9[C@@]6H[C@@]5COCC6

RUN: RUN4155

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.39

EN300-18249_2_1_1



CID: EN300-18249_2_1_1

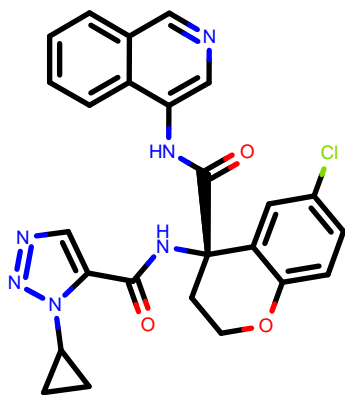
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(c24)Cl)COCC(=O)N

RUN: RUN5286

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.19

EN300-1718675_1_1_1



CID: EN300-1718675_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)c5cnnn5C6C6

RUN:

RUN5686

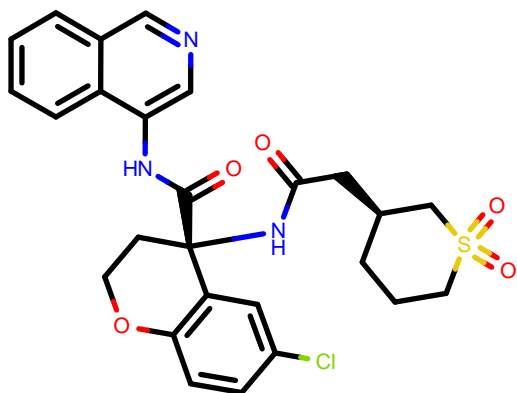
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.26

EN300-220676_1_1_1



CID: EN300-220676_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCS(=O)(=O)C5

RUN:

RUN3080

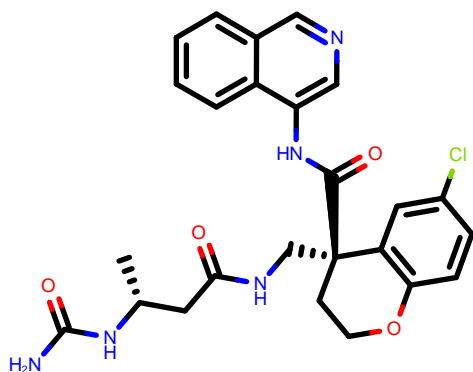
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.24

EN300-268198_2_2_1



CID: EN300-268198_2_2_1

SMILES:

C[C@@H](CC(=O)N)C@1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4NC(=O)N

RUN:

RUN7348

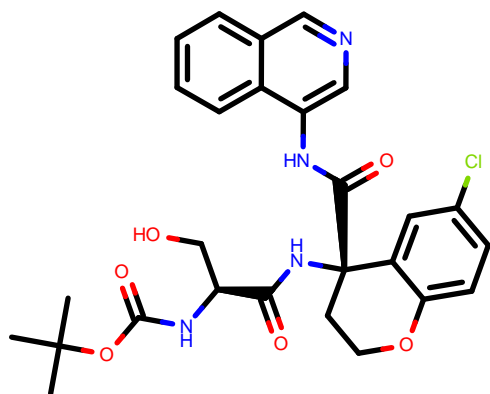
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.18

EN300-72109_1_1_1



CID: EN300-72109_1_1_1

SMILES:

CC(C)(C)OC(=O)N[C@@H](CO)C(=O)N[C@1](CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN:

RUN5228

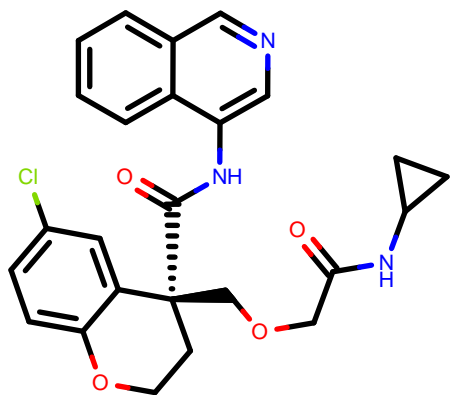
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.29

EN300-1253178_2_1_1



CID: EN300-1253178_2_1_1

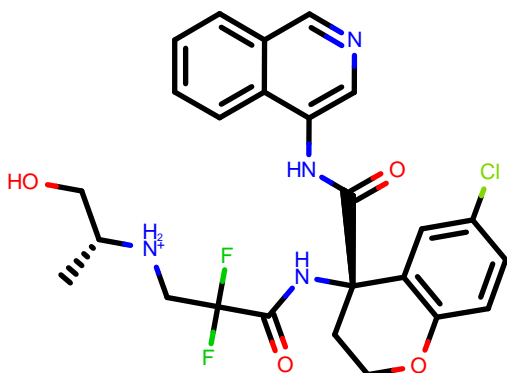
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CC5

RUN: RUN4656

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EDG-MED-90036822-39_2



CID: EDG-MED-90036822-39_2

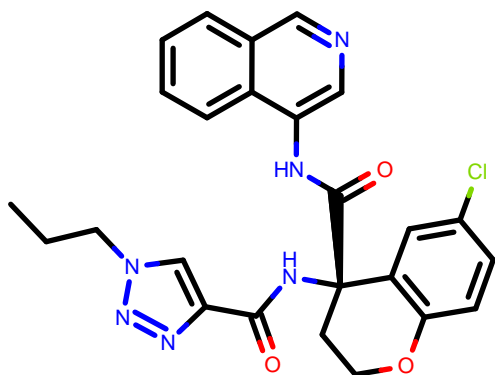
SMILES: C[C@H](CO)NCC(C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)F

RUN: RUN1678

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.36

EN300-261596_1_1_1



CID: EN300-261596_1_1_1

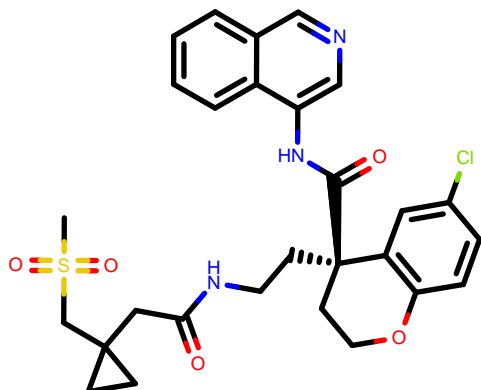
SMILES: C=CCn1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN2820

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.22

EN300-97904_3_1_1



CID: EN300-97904_3_1_1

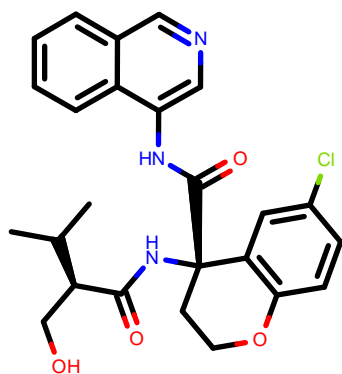
SMILES: CS(=O)(=O)CC1(CC1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5425

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.34

EN300-153257_1_2_1



CID: EN300-153257_1_2_1

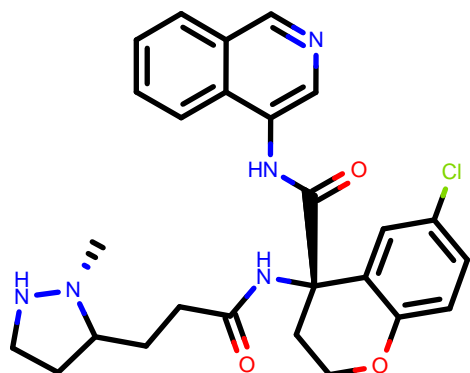
SMILES: CC(C)[C@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5945

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.24

EN300-92662_1_1_1



CID: EN300-92662_1_1_1

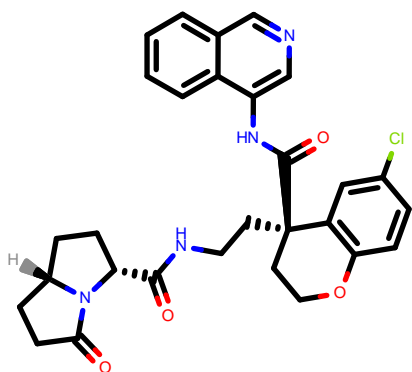
SMILES: Cn1c(ccn1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN5006

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.25

EN300-6479181_3_2_1



CID: EN300-6479181_3_2_1

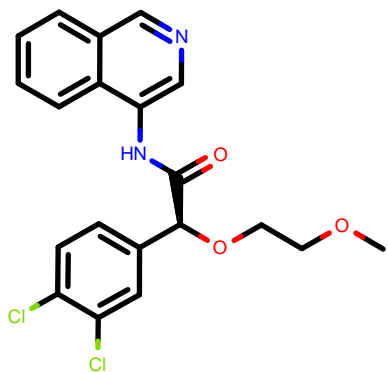
SMILES: c1ccc2c(c1)ncnc2N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN6752

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.28

MAT-POS-de59a476-4_1



CID: MAT-POS-de59a476-4_1

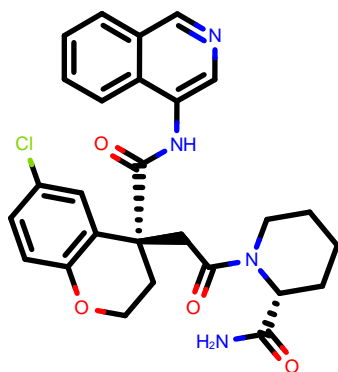
SMILES: COCCOC[C@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cnc3c2cccc3

RUN: RUN2068

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.28

EDJ-MED-d203f206-30_1



CID: EDJ-MED-d203f206-30_1

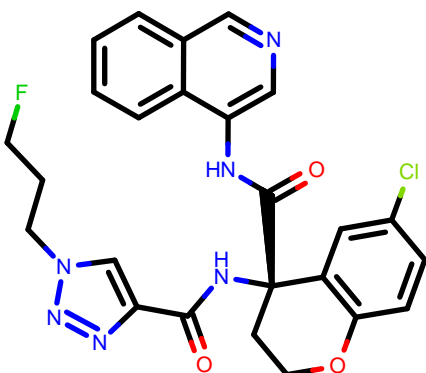
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN2428

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

EN300-1704723_1_1_1



CID: EN300-1704723_1_1_1

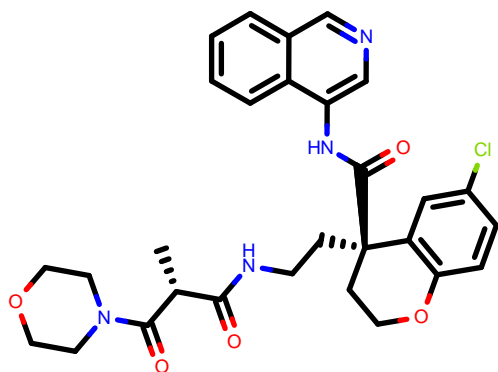
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(mn5)CCF

RUN: RUN5193

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-2855057_3_2_1



CID: EN300-2855057_3_2_1

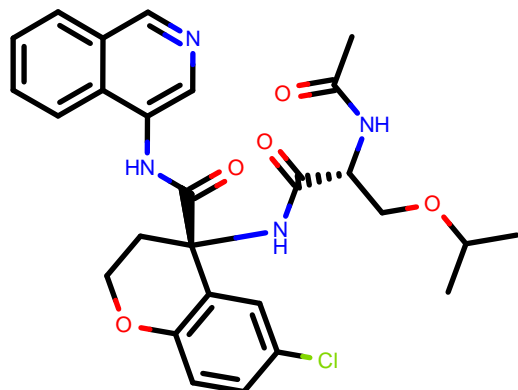
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)N5CCOCC5

RUN: RUN5659

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.42

EN300-1299691_1_2_1



CID: EN300-1299691_1_2_1

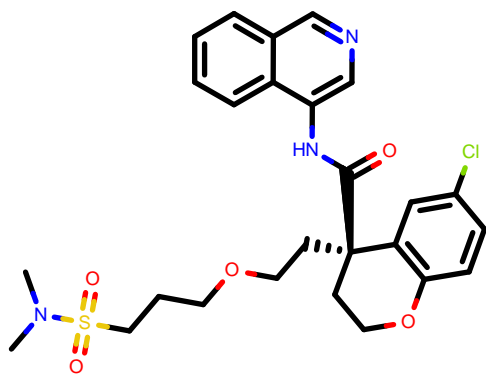
SMILES: CC(C)OC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C

RUN: RUN6402

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-66432_3_1_1



CID: EN300-66432_3_1_1

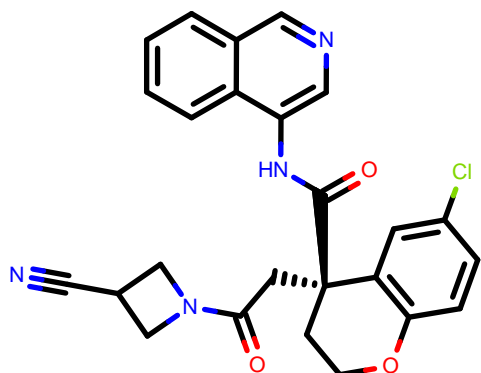
SMILES: CN(C)S(=O)(=O)CCCCOC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6263

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.34

EN300-206282_1_1_1



CID: EN300-206282_1_1_1

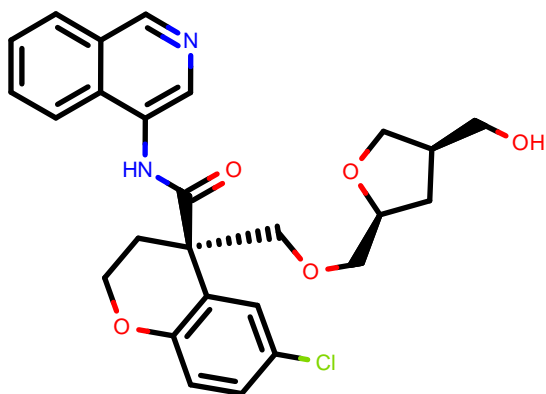
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C#N

RUN: RUN5434

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.24

EN300-6494158_2_1_1



CID: EN300-6494158_2_1_1

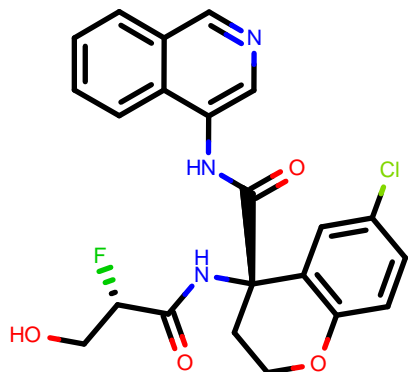
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5C[C@@H](CO)O5

RUN: RUN6059

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.30

EDG-MED-90036822-15_2



CID: EDG-MED-90036822-15_2

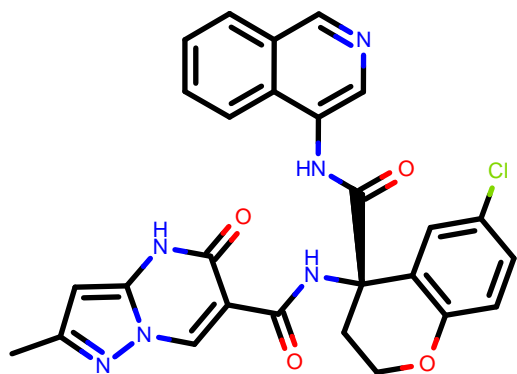
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CO)F

RUN: RUN1541

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.23

EN300-61860_1_1_1



CID: EN300-61860_1_1_1

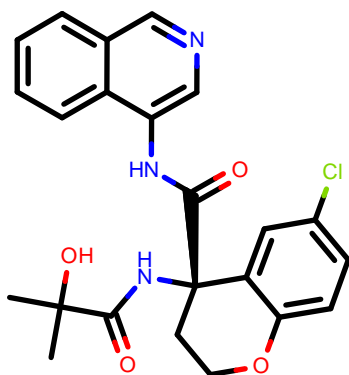
SMILES: Cc1cc2[nH]c(=O)c(en2n1)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4269

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-59285_1_1_1



CID: EN300-59285_1_1_1

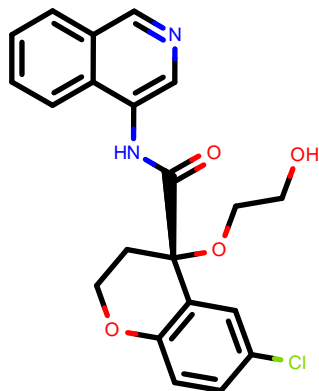
SMILES: CC(C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4O

RUN: RUN5844

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-21258_1_1_1



CID: EN300-21258_1_1_1

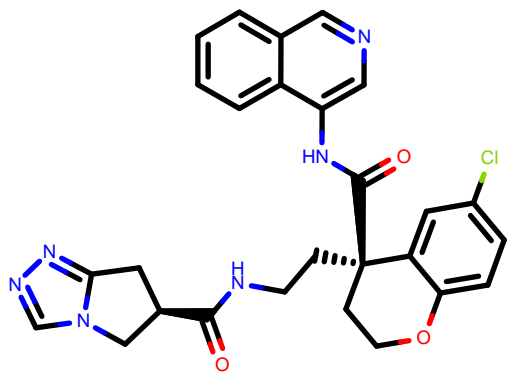
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO

RUN: RUN7590

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.18

EN300-6745453_3_1_1



CID: EN300-6745453_3_1_1

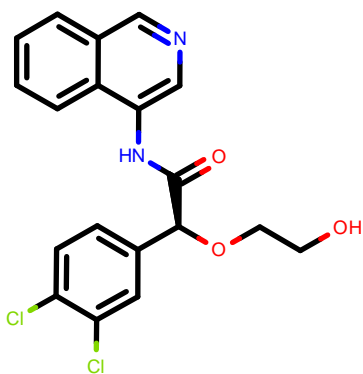
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5C@H5C6nncn6C5

RUN: RUN5539

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.30

MAT-POS-de59a476-5_2



CID: MAT-POS-de59a476-5_2

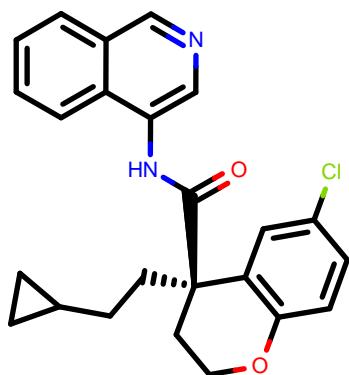
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)OCCO

RUN: RUN2041

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.31

ALP-POS-477dc5b7-3_1



CID: ALP-POS-477dc5b7-3_1

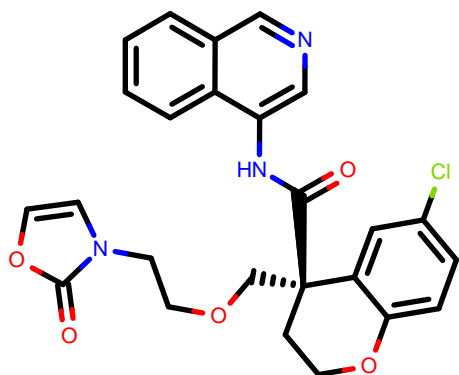
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CC5

RUN: RUN249

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.20

EN300-370967_2_1_1



CID: EN300-370967_2_1_1

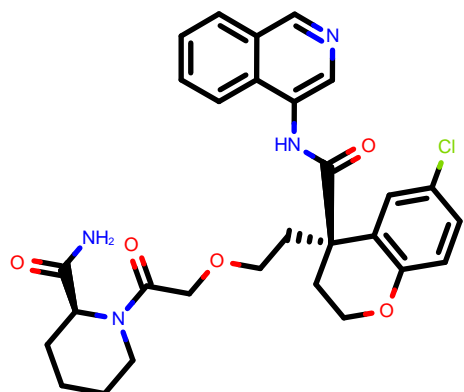
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5COC(=O)C5=O

RUN: RUN4632

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-22879_3_2_1



CID: EN300-22879_3_2_1

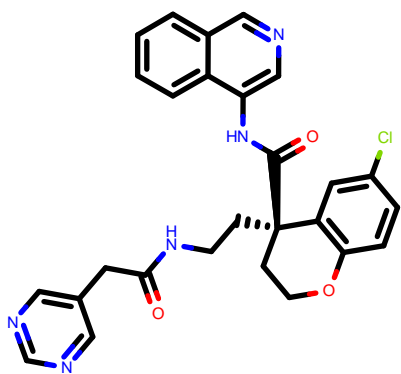
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N5C(=O)C[C@H]5C(=O)N

RUN: RUN4025

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.37

EN300-185751_3_1_1



CID: EN300-185751_3_1_1

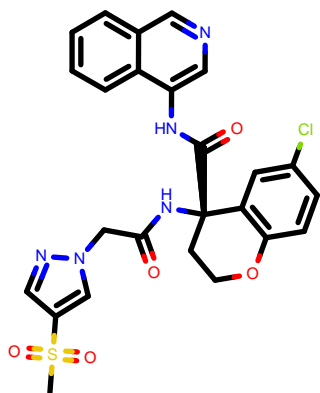
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cncc5

RUN: RUN3969

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.27

EN300-78121_1_1_1



CID: EN300-78121_1_1_1

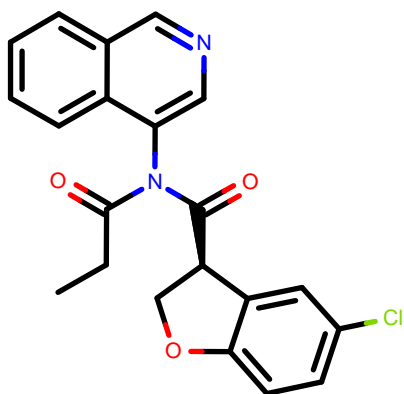
SMILES: CS(=O)(=O)c1nnc(c1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN5142

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.34

MAT-POS-e69ad64a-2_1



CID: MAT-POS-e69ad64a-2_1

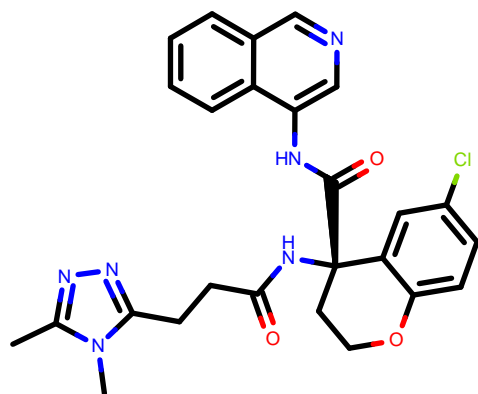
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@](C)(H)3COc4c3cc(cc4)Cl

RUN: RUN2153

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.27

EN300-1721328_1_1_1



CID: EN300-1721328_1_1_1

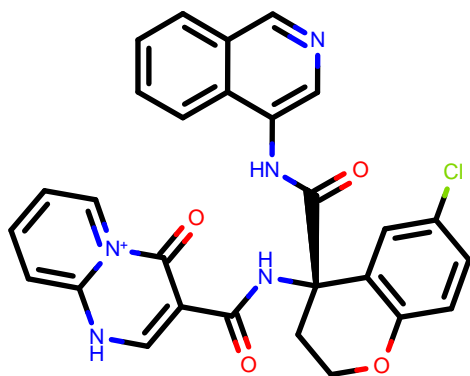
SMILES: Cc1nnc(n1C)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN3971

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-35781_1_1_1



CID: EN300-35781_1_1_1

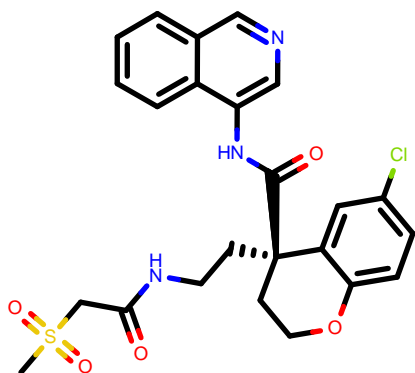
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6ccccc6c5=O

RUN: RUN3796

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.31

EN300-53677_3_1_1



CID: EN300-53677_3_1_1

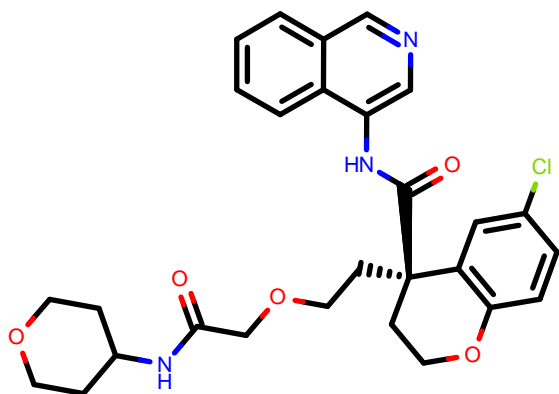
SMILES: CS(=O)(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN: RUN6221

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

EN300-67573_3_1_1



CID: EN300-67573_3_1_1

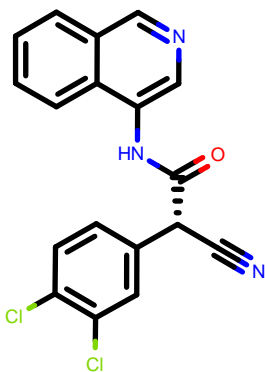
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC5CCOCC5

RUN: RUN5744

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.34

MAT-POS-fce787c2-8_2



CID: MAT-POS-fce787c2-8_2

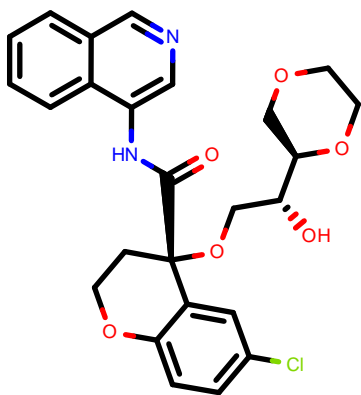
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](C#N)c3ccc(c(c3)Cl)Cl

RUN: RUN1959

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.27

EN300-6238494_1_2_2



CID: EN300-6238494_1_2_2

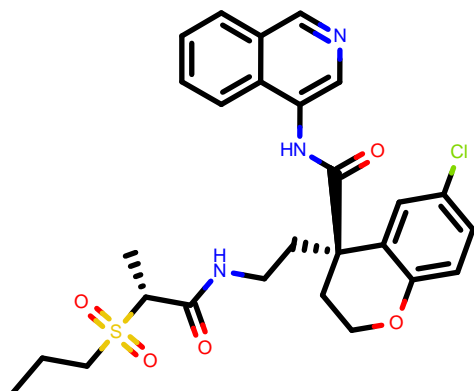
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC@H5COCOCOS5O

RUN: RUN5103

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.46

EN300-52768_3_2_1



CID: EN300-52768_3_2_1

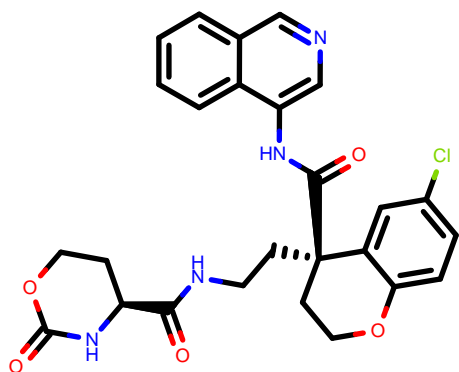
SMILES: CCCS(=O)(=O)[C@H](C)C=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN6032

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.47

EN300-249804_3_1_1



CID: EN300-249804_3_1_1

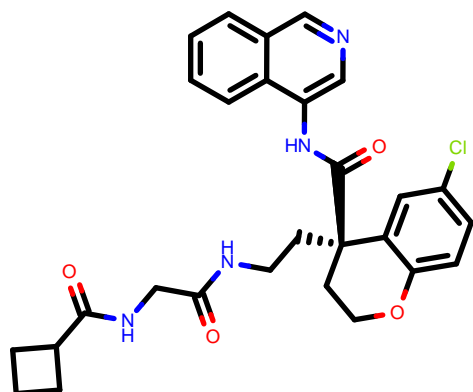
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5COCOC(=O)N5

RUN: RUN4047

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.26

EN300-62448_3_1_1



CID: EN300-62448_3_1_1

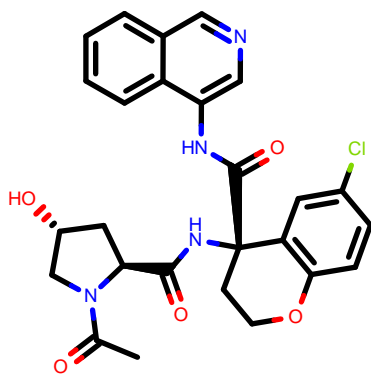
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CC5

RUN: RUN4652

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.34

EN300-1703718_1_1_1



CID: EN300-1703718_1_1_1

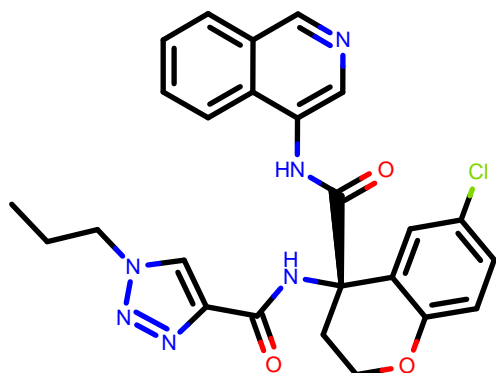
SMILES: CC(=O)N1C[C@@H](C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN5409

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.37

EN300-123416_1_1_1



CID: EN300-123416_1_1_1

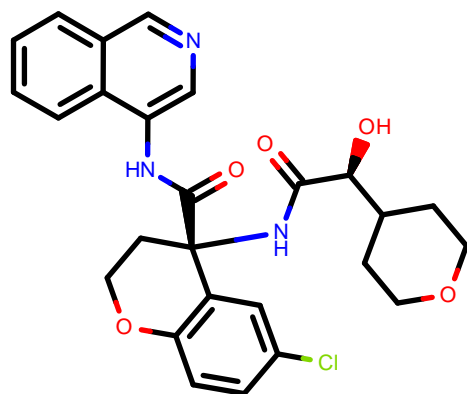
SMILES: CCCN1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3215

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.25

EN300-6792206_1_1_1



CID: EN300-6792206_1_1_1

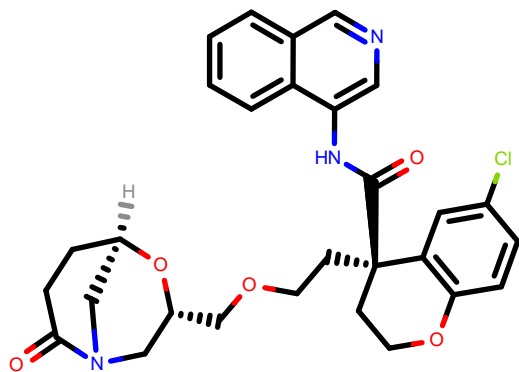
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]3(O)C5COC5)O

RUN: RUN6291

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.32

EN300-2008102_3_1_1



CID: EN300-2008102_3_1_1

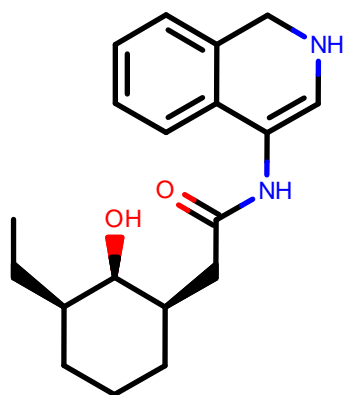
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)COC3C@H]5N6C[C@H]5O)CC6=O

RUN: RUN6537

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.31

MAK-UNK-c749d764-2_1



CID: MAK-UNK-c749d764-2_1

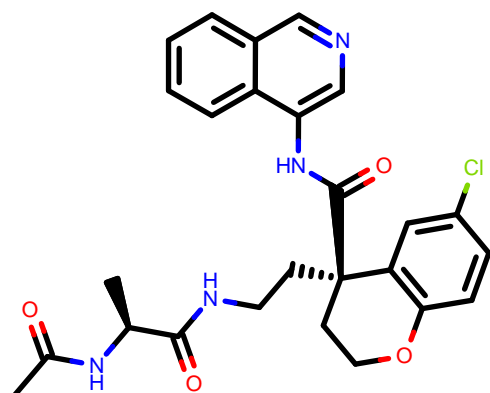
SMILES: CC[C@@H]1CCC[C@@H]([C@@H]1O)CC(=O)Nc2cncc3c2ccc3

RUN: RUN818

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.47

EN300-18569_3_1_1



CID: EN300-18569_3_1_1

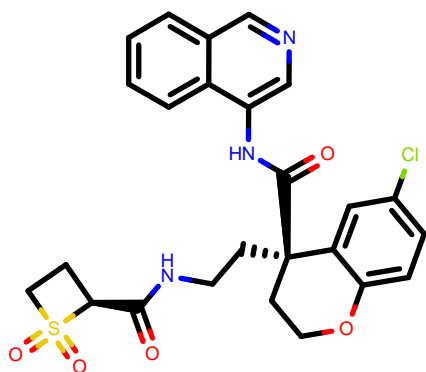
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)NC(=O)C

RUN: RUN5687

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.29

EN300-1387104_3_1_1



CID: EN300-1387104_3_1_1

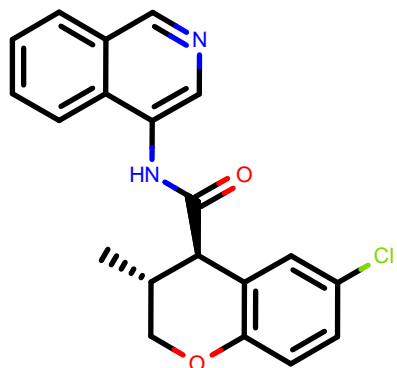
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCSS5(=O)=O

RUN: RUN3786

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.24

MAT-POS-8a69d52e-4_2_1



CID: MAT-POS-8a69d52e-4_2_1

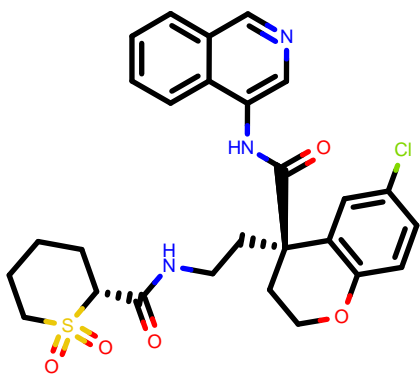
SMILES: C[C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3ccc4)Cl

RUN: RUN5655

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.05

EN300-107435_3_2_1



CID: EN300-107435_3_2_1

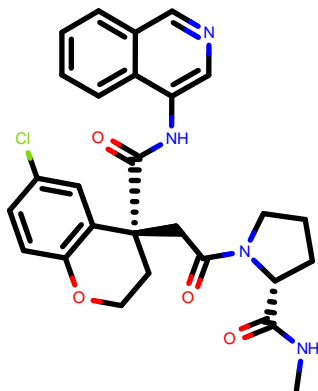
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCCS(=O)=O

RUN: RUN4758

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-6492197_1_1_1



CID: EN300-6492197_1_1_1

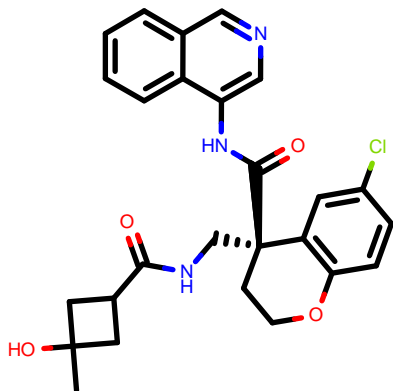
SMILES: CNC(=O)[C@H]1CCCN1C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN6461

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.32

EN300-247343_2_1_1



CID: EN300-247343_2_1_1

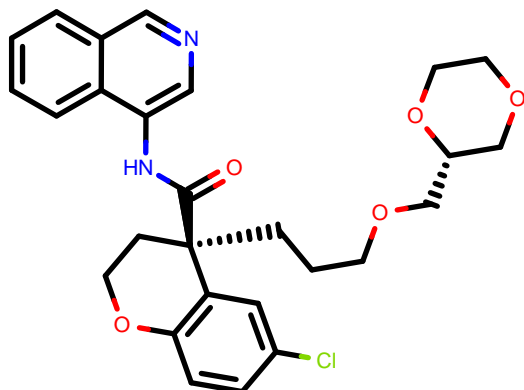
SMILES: CC1(CC(C1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5)O

RUN: RUN5371

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.21

EN300-139167_4_2_1



CID: EN300-139167_4_2_1

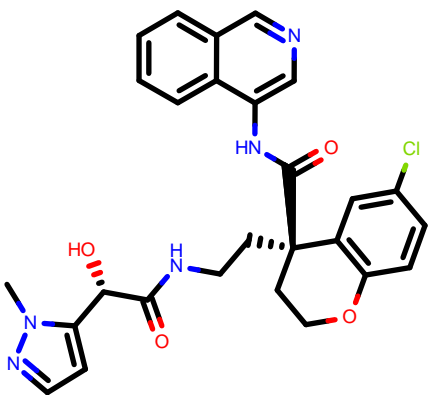
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5CCOCC5

RUN: RUN7141

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.36

EN300-6473273_3_1_1



CID: EN300-6473273_3_1_1

SMILES:

Cn1c(ccn1)[C@@H](C(=O)NCC[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O

RUN:

RUN4399

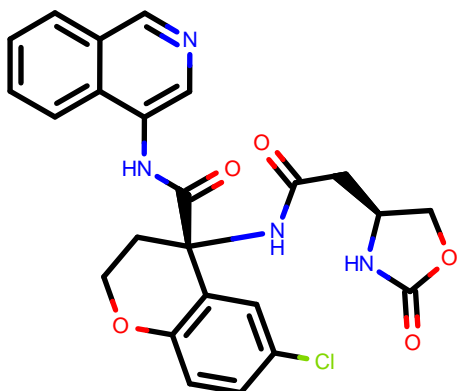
DDG (kcal/mol):

-0.94

dDDG (kcal/mol):

0.33

EN300-1703852_1_1_1



CID: EN300-1703852_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5COC(=O)N5

RUN:

RUN4722

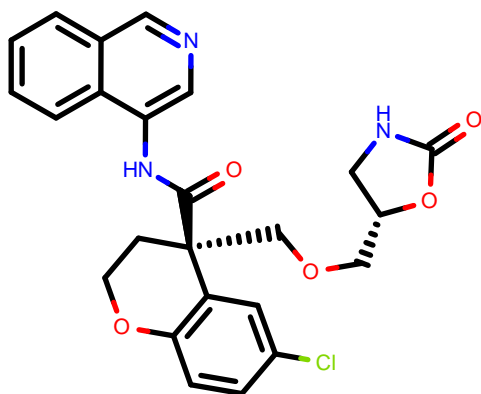
DDG (kcal/mol):

-0.94

dDDG (kcal/mol):

0.29

EN300-203293_2_1_1



CID: EN300-203293_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CNC(=O)O5

RUN:

RUN4179

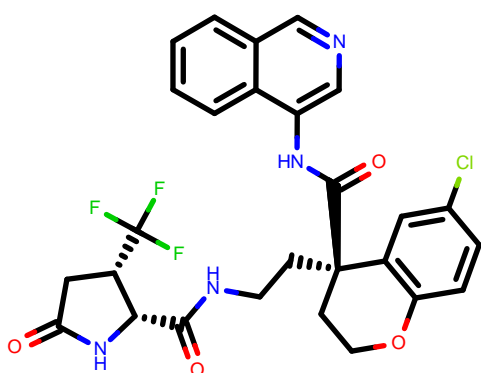
DDG (kcal/mol):

-0.94

dDDG (kcal/mol):

0.27

EN300-169955_3_4_1



CID: EN300-169955_3_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@@H](O)N5C(F)F(F)F

RUN:

RUN7820

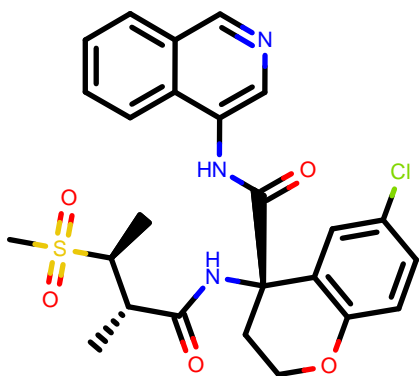
DDG (kcal/mol):

-0.94

dDDG (kcal/mol):

0.40

EN300-182725_1_4_1



CID: EN300-182725_1_4_1

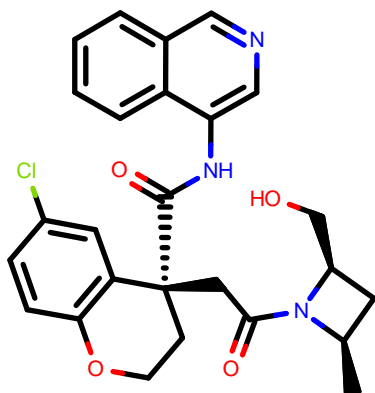
SMILES: C[C@H]([C@H](C)S(=O)(=O)C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN6672

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.30

EN300-1709410_1_1_1



CID: EN300-1709410_1_1_1

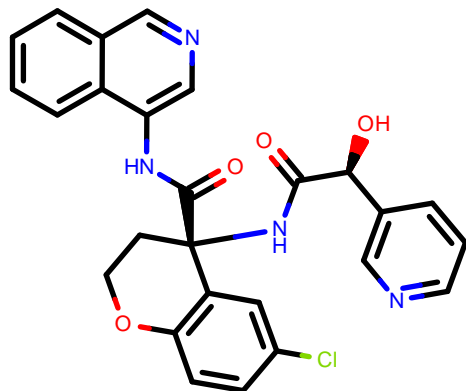
SMILES: C[C@@]([C@H]1[C@@]([C@H](N1C(=O)C)C)2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)CO

RUN: RUN4265

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.31

EN300-134855_1_2_1



CID: EN300-134855_1_2_1

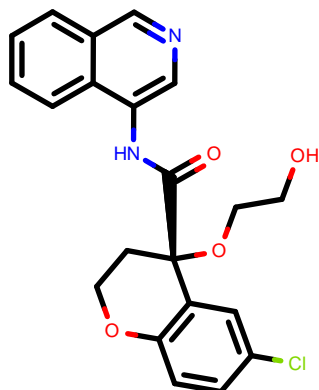
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](c5cccnc5)O

RUN: RUN5793

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-72_1



CID: ED_-GRI-5b13fbe2-72_1

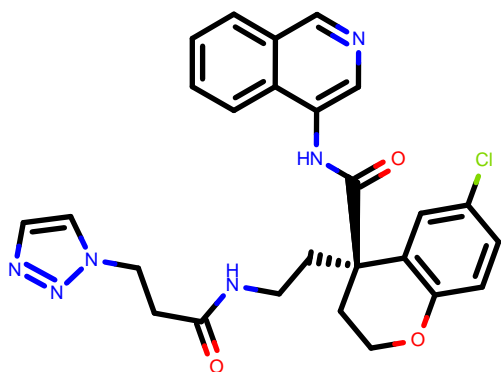
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO

RUN: RUN1451

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.19

EN300-28871_3_1_1



CID: EN300-28871_3_1_1

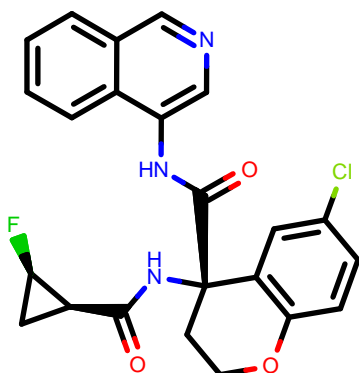
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5ccnn5

RUN: RUN3020

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.30

EN300-6953121_1_1_1



CID: EN300-6953121_1_1_1

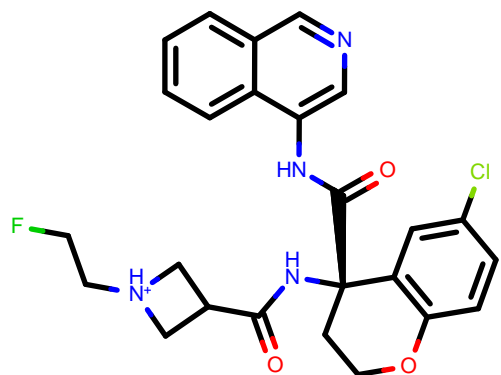
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[C@H]5F

RUN: RUN5647

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.20

EDG-MED-90036822-65_1



CID: EDG-MED-90036822-65_1

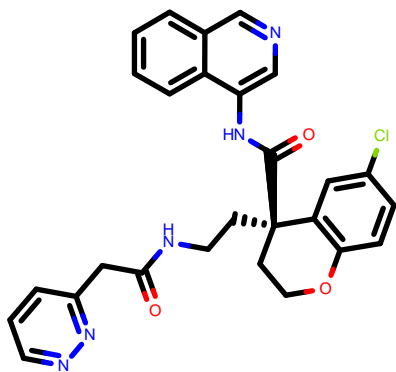
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C5]C[NH+]5CCF

RUN: RUN1647

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.34

EN300-7456948_3_1_1



CID: EN300-7456948_3_1_1

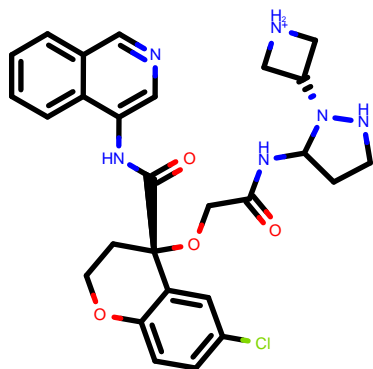
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5ccnn5

RUN: RUN3410

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EDG-MED-4c68219f-9_1



CID: EDG-MED-4c68219f-9_1

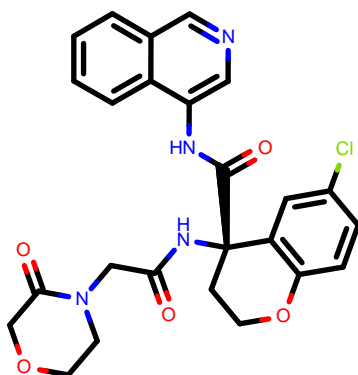
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5ccnn5C6C[NH2+]C6

RUN: RUN1569

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.36

EN300-186943_1_1_1



CID: EN300-186943_1_1_1

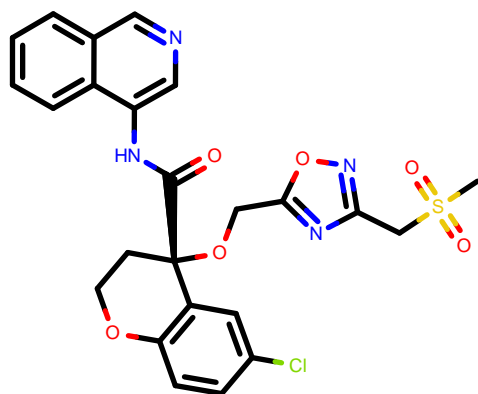
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCOCC5=O

RUN: RUN2944

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.27

EN300-94900_1_1_1



CID: EN300-94900_1_1_1

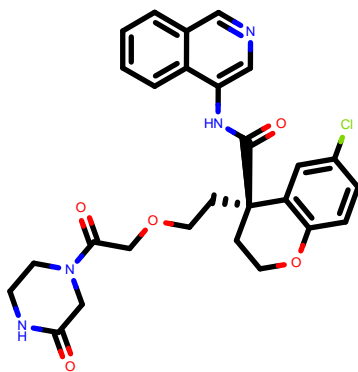
SMILES: CS(=O)(=O)Cc1nc(on1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nnc5c4ccccc5

RUN: RUN6464

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.35

EN300-22884_3_1_1



CID: EN300-22884_3_1_1

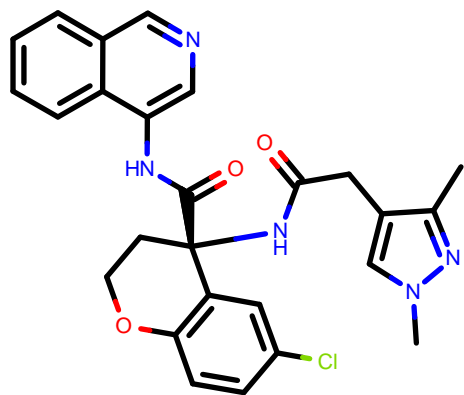
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CCNC(=O)C5

RUN: RUN4771

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-245061_1_1_1



CID: EN300-245061_1_1_1

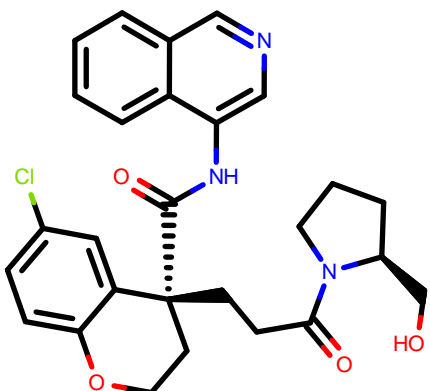
SMILES: Cc1c(cn(n1)C)CC(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN6483

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.24

EN300-55109_2_2_1



CID: EN300-55109_2_2_1

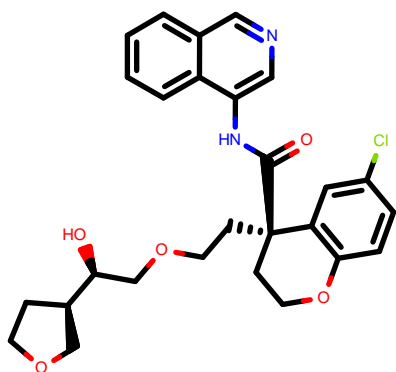
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CCC(=O)N5CCCC[C@H]5CO

RUN: RUN7807

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.27

EN300-1911992_3_1_1



CID: EN300-1911992_3_1_1

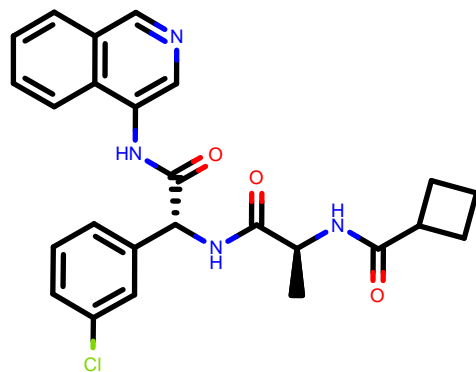
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CCOC[C@@H]([C@@H]5COCOC5)O

RUN: RUN5682

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.30

EDJ-MED-ee07cf00-4_3



CID: EDJ-MED-ee07cf00-4_3

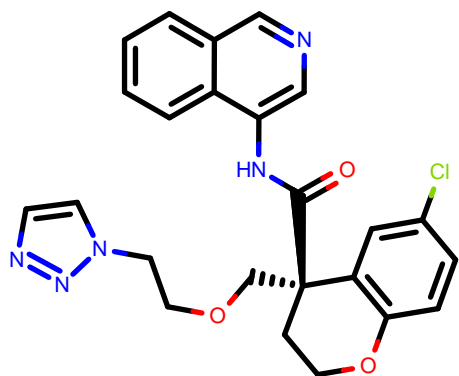
SMILES: C[C@@H](C(=O)N[C@@H](c1cccc(c1)C)C(=O)Nc2cncc3c2cccc3)NC(=O)C4CCCC4

RUN: RUN2645

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.45

EN300-1715993_2_1_1



CID: EN300-1715993_2_1_1

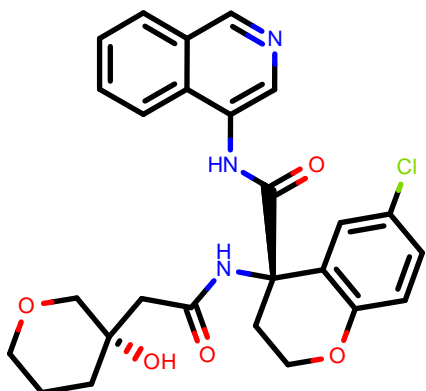
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cenn5

RUN: RUN5131

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.25

EN300-1071940_1_2_1



CID: EN300-1071940_1_2_1

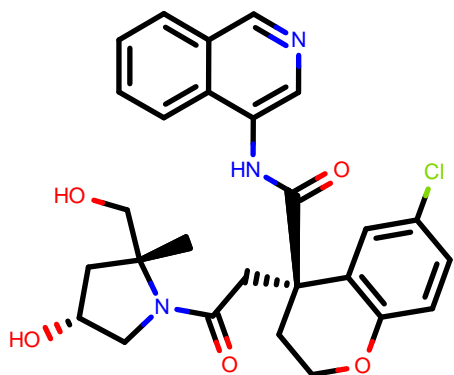
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCCOC5)O

RUN: RUN4495

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-307336_1_3_1



CID: EN300-307336_1_3_1

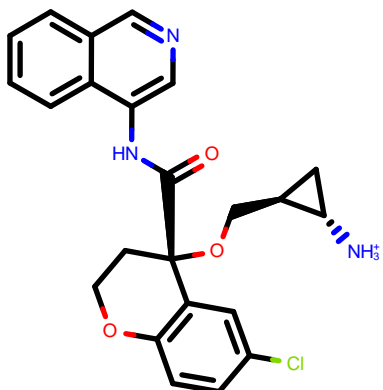
SMILES: C[C@@]1(C[C@H](CN1C(=O)C)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O)CO

RUN: RUN7099

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.29

ED_-GRI-5b13fbe2-69_2



CID: ED_-GRI-5b13fbe2-69_2

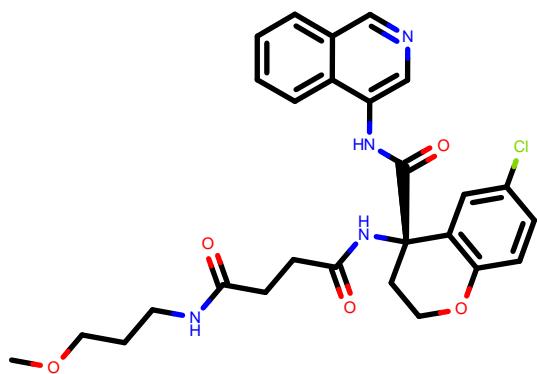
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[C@@H]5[NH3+]

RUN: RUN1477

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.21

EN300-175251_1_1_1



CID: EN300-175251_1_1_1

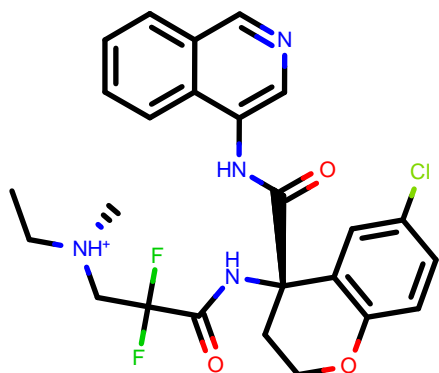
SMILES: COC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4

RUN: RUN7453

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.35

EDG-MED-90036822-110_2



CID: EDG-MED-90036822-110_2

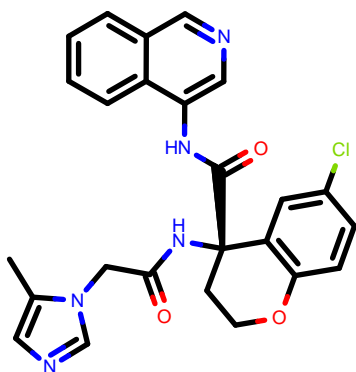
SMILES: CC[N+](C)CC(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4)F(F)F

RUN: RUN1801

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-315453_1_1_1



CID: EN300-315453_1_1_1

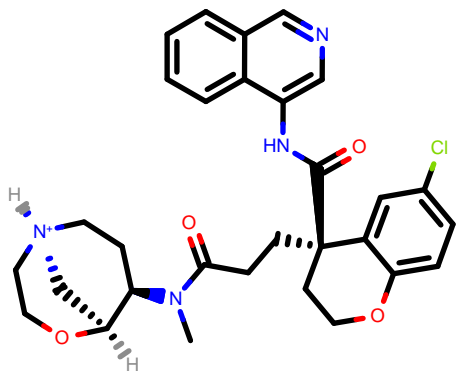
SMILES: Cc1cn[n1]CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccoc5

RUN: RUN4508

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.23

EN300-159953_2_1_1



CID: EN300-159953_2_1_1

SMILES: CN[C@@H]1CC[N@@H+]2CCO[C@@H]1C2[C@@]3(C)CCO[C@@H]3C(=O)Nc4ccc5c4ccoc5

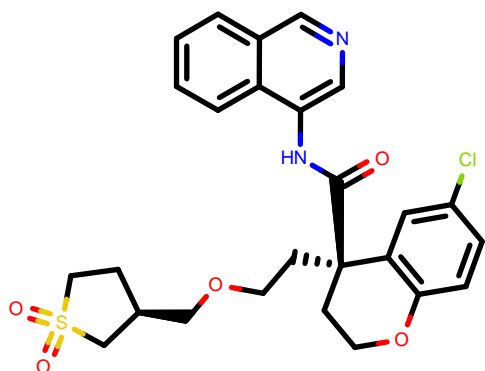
RUN: RUN6970

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.35

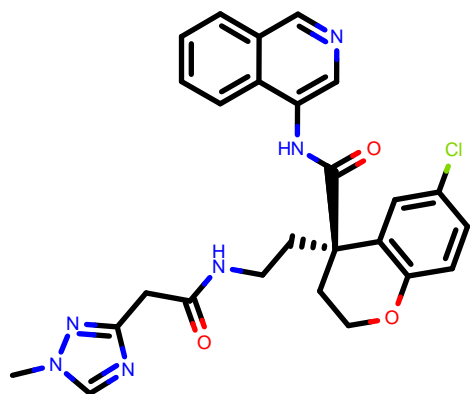
CID:	EN300-198515_3_1_1
SMILES:	<chem>C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)n5nc(nc5)C#N</chem>
RUN:	RUN2891
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.30

EN300-1448603_3_1_1



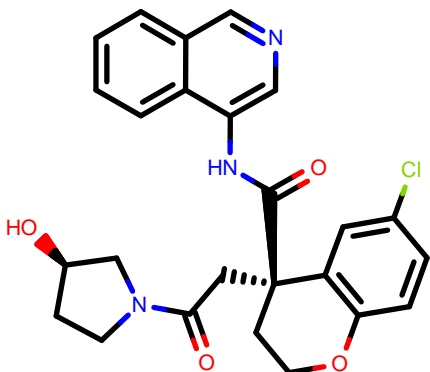
CID:	EN300-1448603_3_1_1
SMILES:	<chem>c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)C5</chem>
RUN:	RUN7025
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.29

EN300-7493922_3_1_1



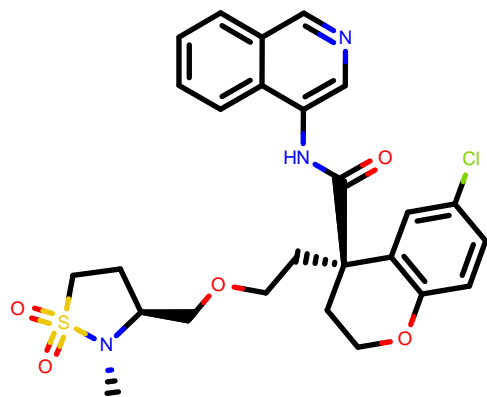
CID:	EN300-7493922_3_1_1
SMILES:	<chem>Cn1nc(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5</chem>
RUN:	RUN4341
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.30

EN300-69313_1_1_1



CID:	EN300-69313_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O</chem>
RUN:	RUN5547
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.25

EN300-393148_3_1_1



CID: EN300-393148_3_1_1

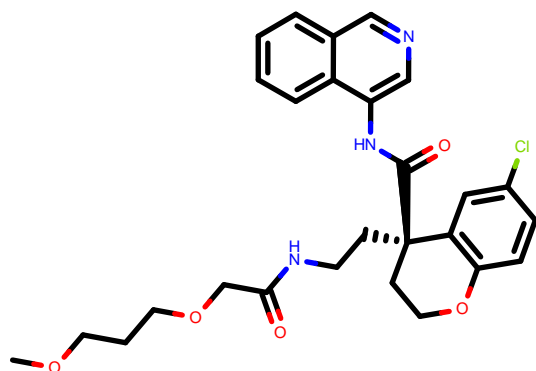
SMILES: C[N@@]1[C@@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN4517

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

EN300-125769_3_1_1



CID: EN300-125769_3_1_1

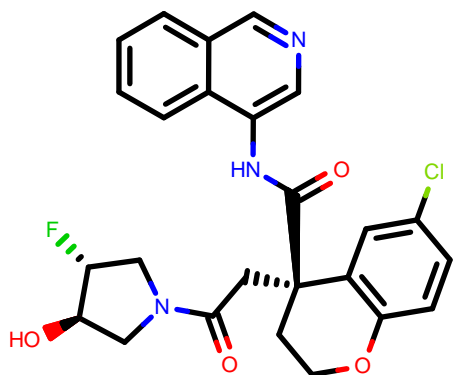
SMILES: COCCCOCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN4603

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.28

EN300-317085_1_1_1



CID: EN300-317085_1_1_1

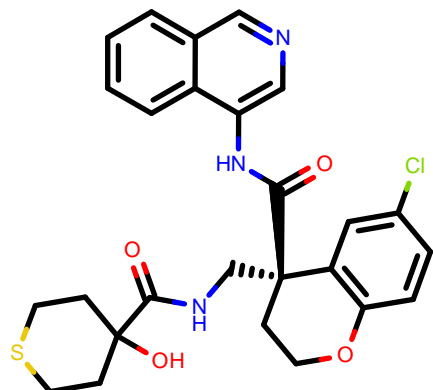
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]([C@@H](C5)F)O

RUN: RUN6121

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-122340_2_1_1



CID: EN300-122340_2_1_1

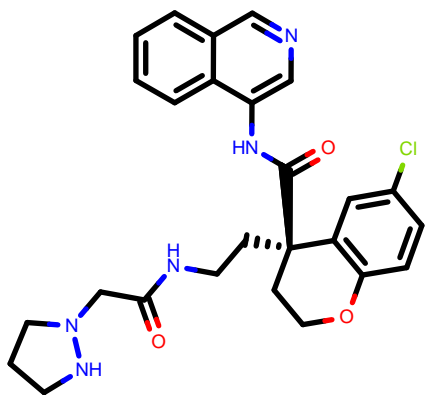
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCS5)O

RUN: RUN5499

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.32

EN300-23942_3_1_1



CID: EN300-23942_3_1_1

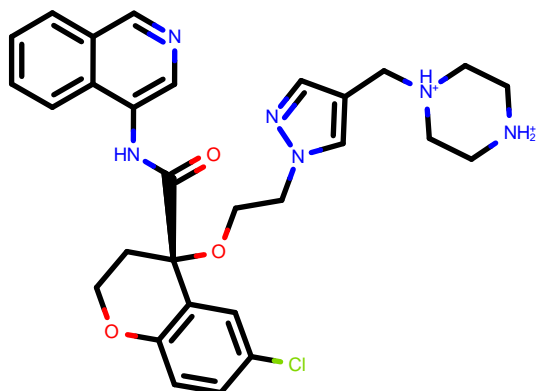
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ccn5

RUN: RUN4046

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-27_1



CID: ED_-GRI-5b13fbe2-27_1

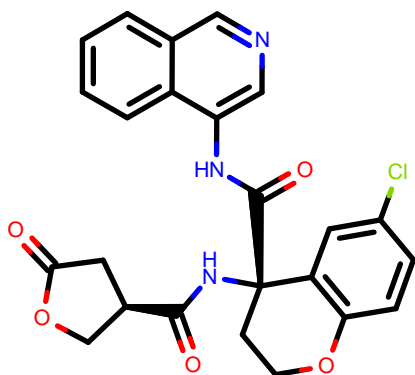
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCn5cc(cn5)CN6CC[NH2+]CC6

RUN: RUN1473

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.36

EN300-113234_1_1_1



CID: EN300-113234_1_1_1

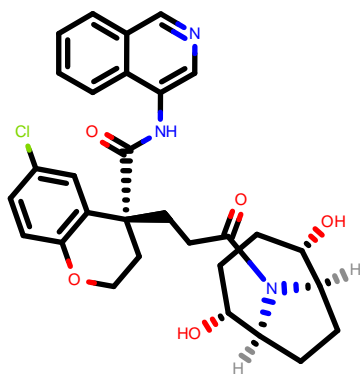
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H5CC(=O)OC5

RUN: RUN3574

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-6738887_2_1_1



CID: EN300-6738887_2_1_1

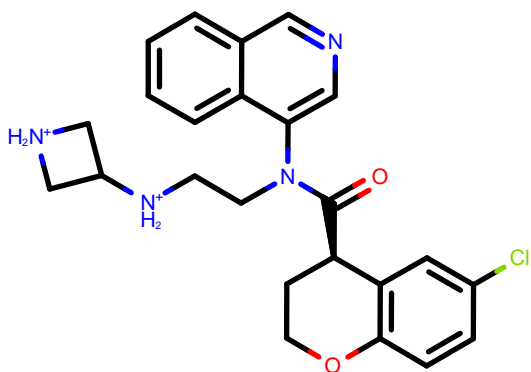
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5[C@@]H6CC[C@@]H5[C@@]H7[C@@]H8O

RUN: RUN7100

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

MAK-UNK-83e0a0b4-3_1



CID: MAK-UNK-83e0a0b4-3_1

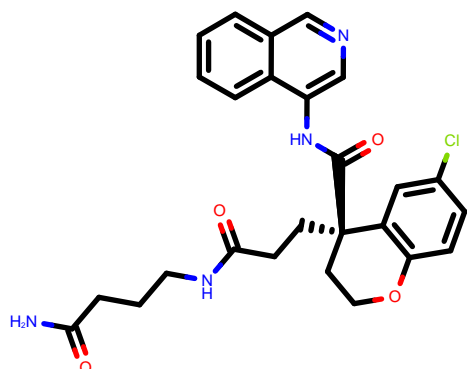
SMILES: c1ccc2c(c1)cncc2N(CCN(C)C)C(=O)C[C@@H](C)COCc5ccccc5Cl

RUN: RUN755

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.31

EN300-39439_2_1_1



CID: EN300-39439_2_1_1

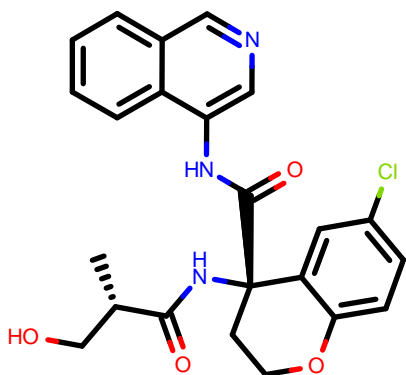
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@H](C)COCc5ccccc5Cl

RUN: RUN2756

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-55072_1_1_1



CID: EN300-55072_1_1_1

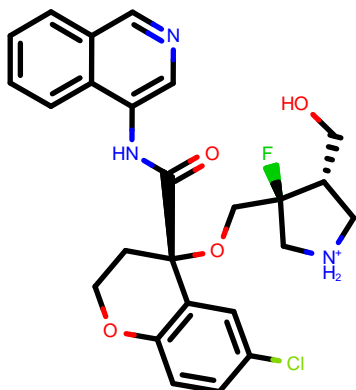
SMILES: C[C@@H](CO)C(=O)N[C@@H](C)COCc5ccccc5Cl

RUN: RUN4343

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-55_4



CID: ED_-GRI-5b13fbe2-55_4

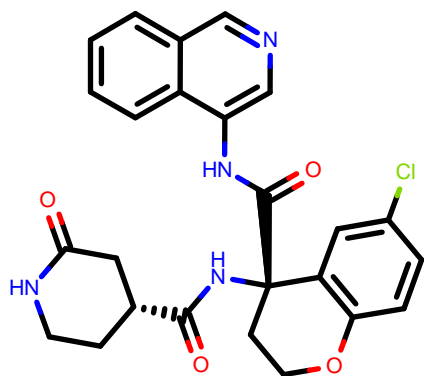
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@H](C)COCc5ccccc5Cl

RUN: RUN1487

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.35

EN300-107493_1_1_1



CID: EN300-107493_1_1_1

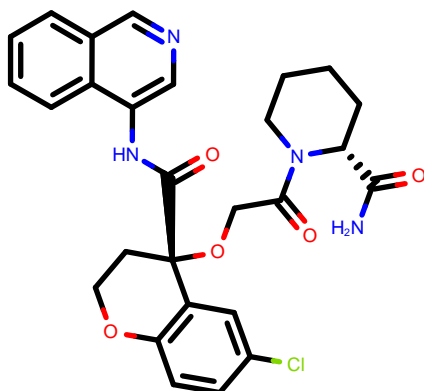
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCNC(=O)C5

RUN: RUN6117

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.26

EN300-22879_1_1_1



CID: EN300-22879_1_1_1

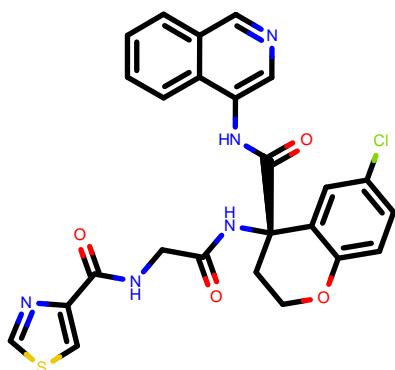
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN5027

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.24

EN300-182084_1_1_1



CID: EN300-182084_1_1_1

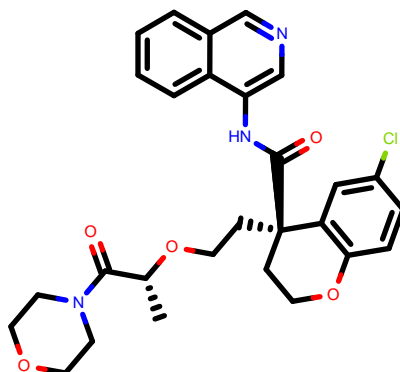
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)c5ccsn5

RUN: RUN7760

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-05754_3_2_1



CID: EN300-05754_3_2_1

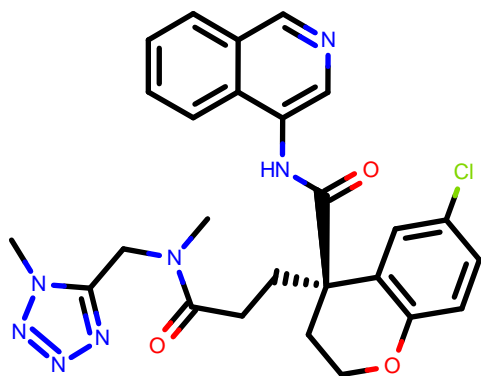
SMILES: C[C@H](C(=O)N1CCOCC1)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN4072

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.34

EN300-148515_2_1_1



CID: EN300-148515_2_1_1

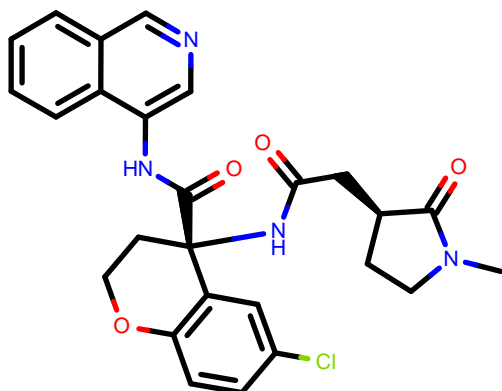
SMILES: Cn1c(nnn1)CN(C)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6900

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-378722_1_2_1



CID: EN300-378722_1_2_1

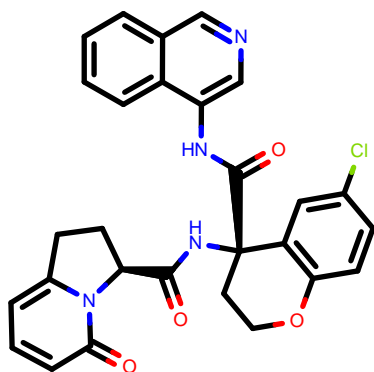
SMILES: CN1CC[C@@H](C1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6926

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.25

EN300-332002_1_1_1



CID: EN300-332002_1_1_1

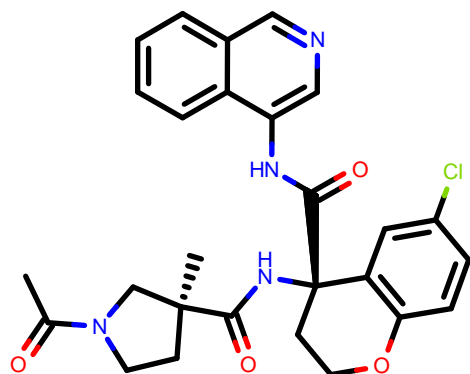
SMILES: c1ccc2c(c1)ncc2N[C@@]([C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]([C@@]5C5CC6n5c(=O)ccc6

RUN: RUN3460

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.31

EN300-98018_1_2_1



CID: EN300-98018_1_2_1

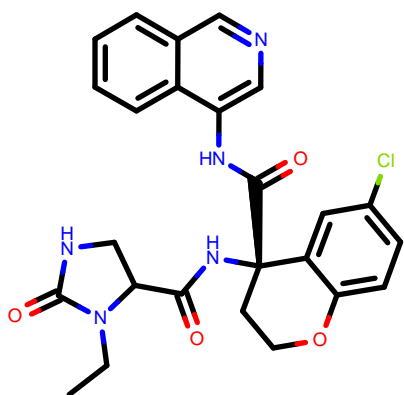
SMILES: CC(=O)N1CC[C@@](C1)(C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4282

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.27

EN300-264184_1_1_1



CID: EN300-264184_1_1_1

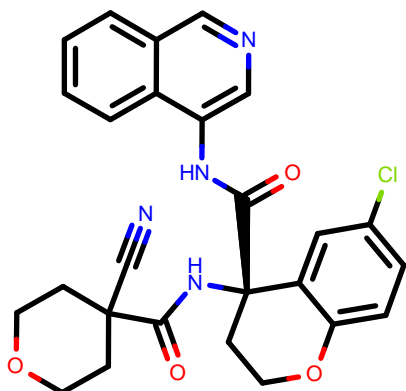
SMILES: CCn1c(c[nH]c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccoc5

RUN: RUN5392

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.22

EN300-74089_1_1_1



CID: EN300-74089_1_1_1

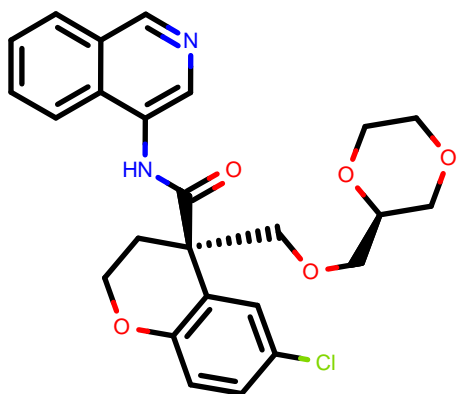
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCOCC5)C#N

RUN: RUN2771

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-139167_2_1_1



CID: EN300-139167_2_1_1

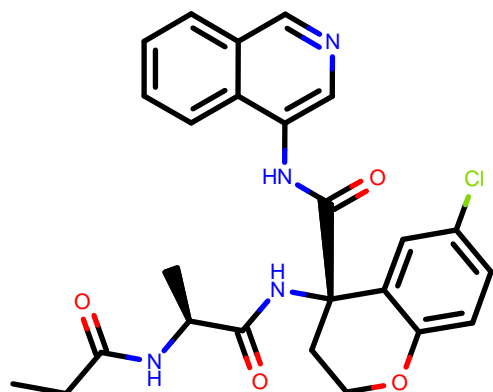
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@H]5COCOC5

RUN: RUN6614

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.24

EN300-31148_1_1_1



CID: EN300-31148_1_1_1

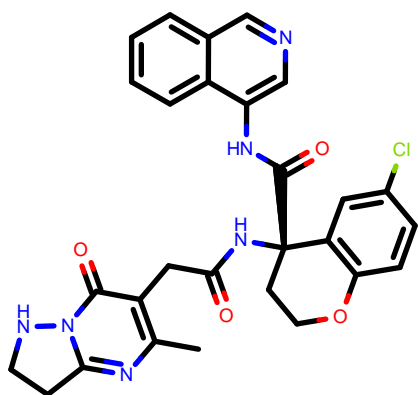
SMILES: CCC(=O)N[C@@H](C)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccoc4

RUN: RUN7150

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.27

ALP-UNI-dbbfd3db-17_1



CID: ALP-UNI-dbbfd3db-17_1

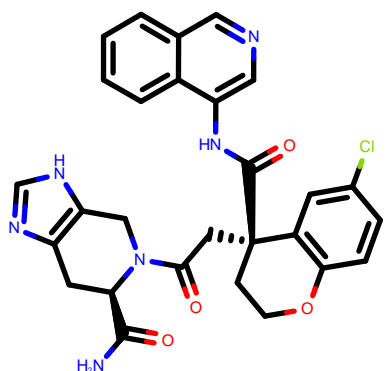
SMILES: Cc1c(c(O)n2c(n1)cd[nH]2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN2643

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.33

EDG-MED-ba1ac7b9-22_1



CID: EDG-MED-ba1ac7b9-22_1

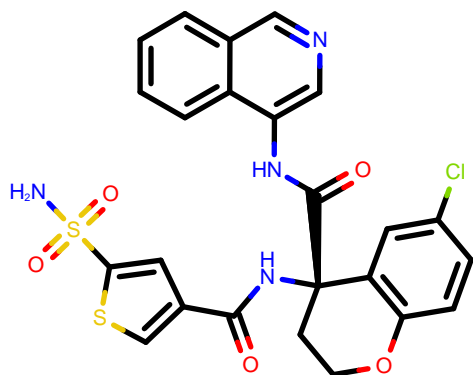
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6cnc[nH]6[C@@]3(C)N

RUN: RUN2547

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.36

EN300-23792_1_1_1



CID: EN300-23792_1_1_1

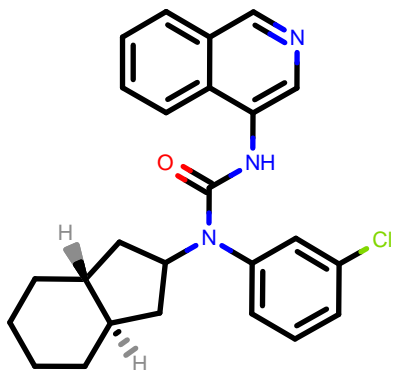
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5csc(s5)S(=O)(=O)N

RUN: RUN6259

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.23

MIC-UNK-cdc2493e-5_2



CID: MIC-UNK-cdc2493e-5_2

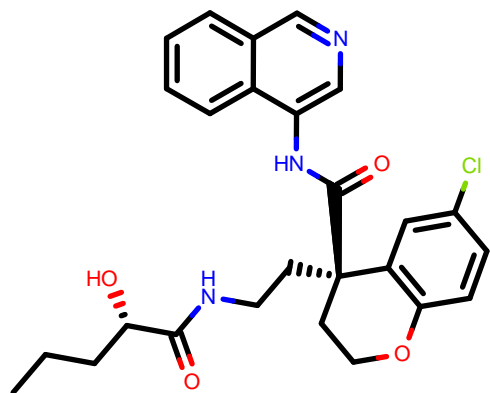
SMILES: c1ccc2c(c1)ncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCCC[C@]4(C)N5

RUN: RUN478

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.41

EN300-316679_3_1_1



CID: EN300-316679_3_1_1

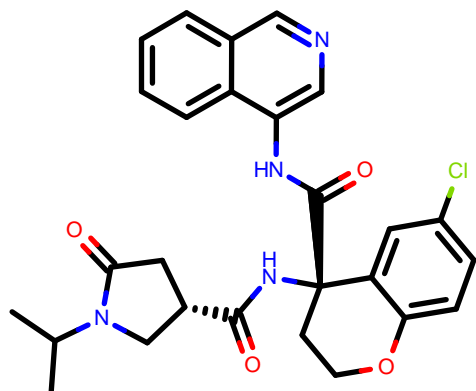
SMILES: CCC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)O

RUN: RUN6961

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.37

EN300-33398_1_2_1



CID: EN300-33398_1_2_1

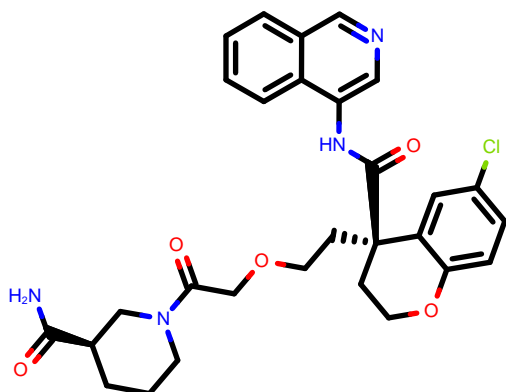
SMILES: CC(C)N1C[C@@H](CC1=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nnc5c4ccc5

RUN: RUN5562

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.28

EN300-22880_3_2_1



CID: EN300-22880_3_2_1

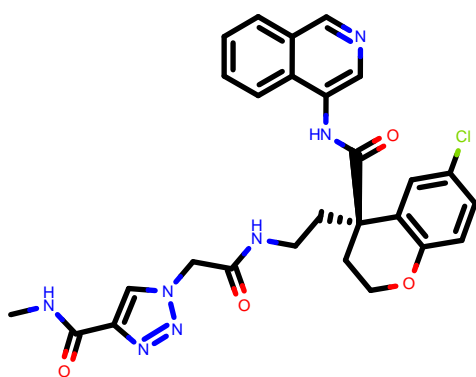
SMILES: c1ccc2c(c1)nnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCC[C@@H](C5)C(=O)N

RUN: RUN6237

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.31

EN300-2617222_3_1_1



CID: EN300-2617222_3_1_1

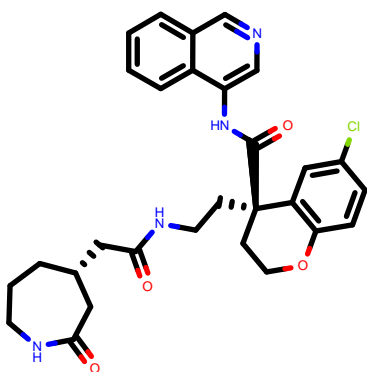
SMILES: CNC(=O)c1cn(nn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nnc5c4ccc5

RUN: RUN4807

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

EN300-195590_3_2_1



CID: EN300-195590_3_2_1

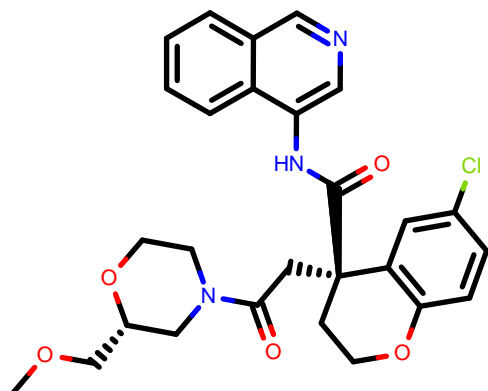
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCCNC(=O)C5

RUN: RUN5735

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.32

EN300-85707_1_2_1



CID: EN300-85707_1_2_1

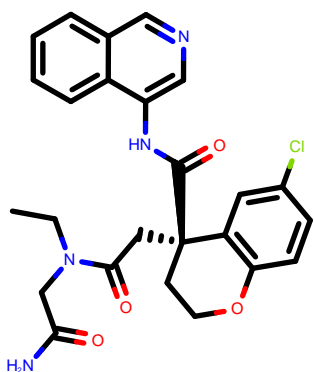
SMILES: CO[C@@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4561

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.32

EN300-174763_1_1_1



CID: EN300-174763_1_1_1

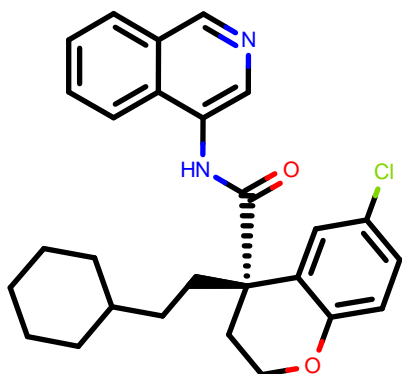
SMILES: CCN(CC(=O)N)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3275

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

VLA-UCB-05e51b3f-13_1



CID: VLA-UCB-05e51b3f-13_1

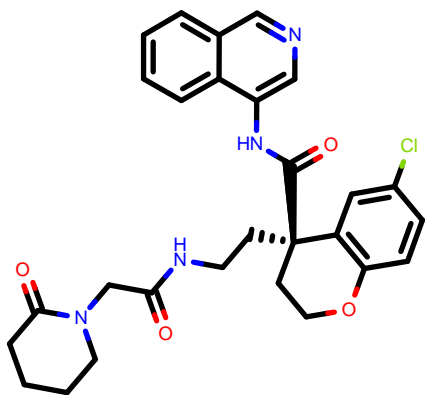
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCCCCC5

RUN: RUN267

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.38

EN300-36111_3_1_1



CID: EN300-36111_3_1_1

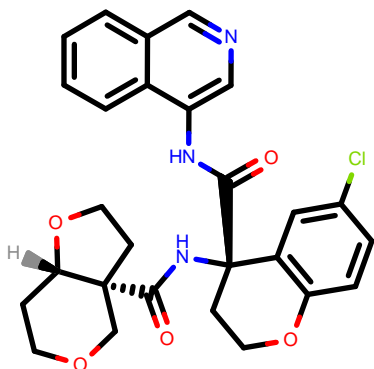
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCCC5=O

RUN: RUN5940

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

EN300-341337_1_3_1



CID: EN300-341337_1_3_1

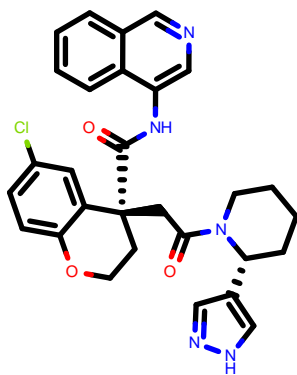
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCO[C@H]5CCOC6

RUN: RUN4600

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-11_1



CID: EDG-MED-ba1ac7b9-11_1

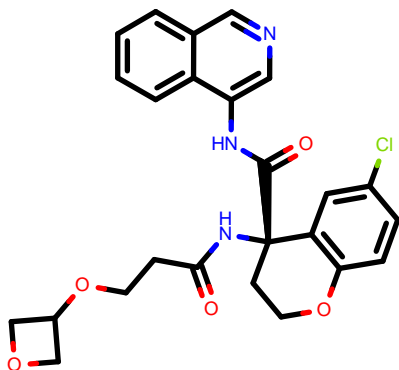
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5c6c[nH]nc6

RUN: RUN2493

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.31

EN300-321703_1_1_1



CID: EN300-321703_1_1_1

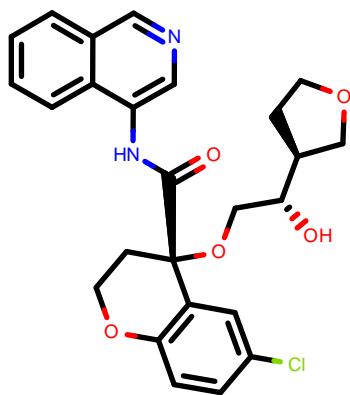
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCOC5COCS

RUN: RUN4201

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.25

EN300-1911992_1_4_1



CID: EN300-1911992_1_4_1

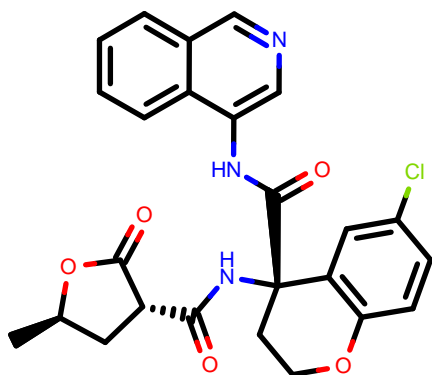
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C@H)5CCOC5O

RUN: RUN4272

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.30

EN300-7444533_1_3_1



CID: EN300-7444533_1_3_1

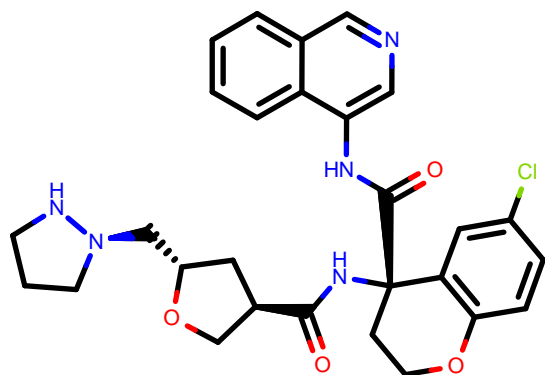
SMILES: C[C@@H]1C[C@@H](C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN6183

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.25

EN300-6494859_1_3_1



CID: EN300-6494859_1_3_1

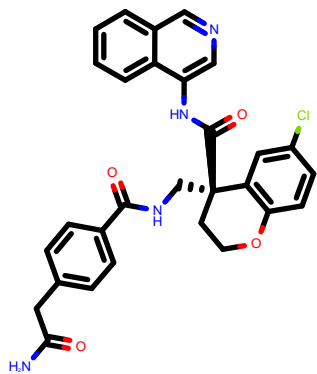
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H](O)C5

RUN: RUN3850

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.31

EN300-2924757_2_1_1



CID: EN300-2924757_2_1_1

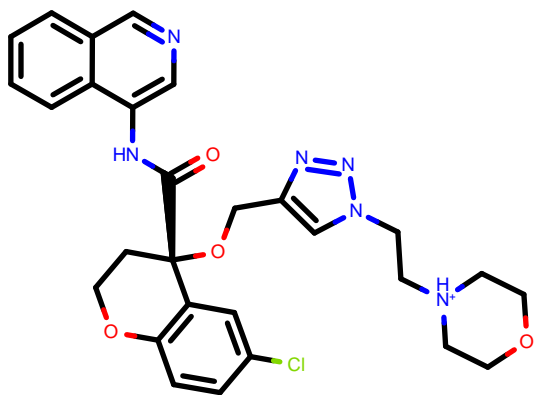
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cc5)CC(=O)N

RUN: RUN6671

DDG (kcal/mol): -0.89

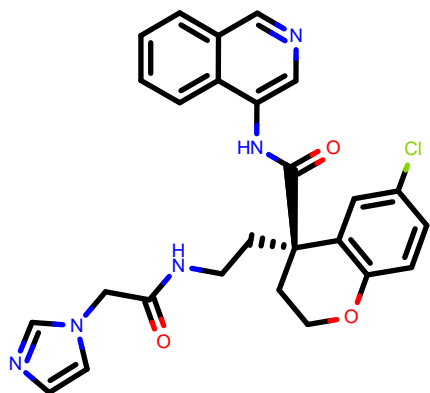
dDDG (kcal/mol): 0.28

EDG-MED-4c68219f-4_1



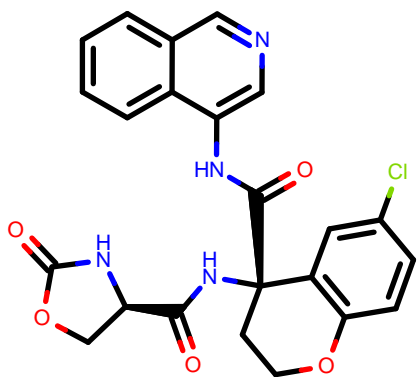
CID:	EDG-MED-4c68219f-4_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(n5)CC[NH+]6COCOC6</chem>
RUN:	RUN1573
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.38

EN300-38979_3_1_1



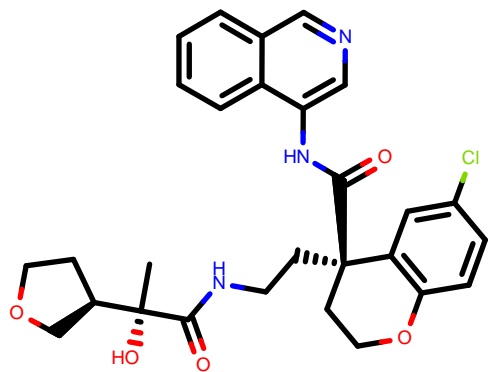
CID:	EN300-38979_3_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc5</chem>
RUN:	RUN3754
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.27

EN300-201346_1_2_1



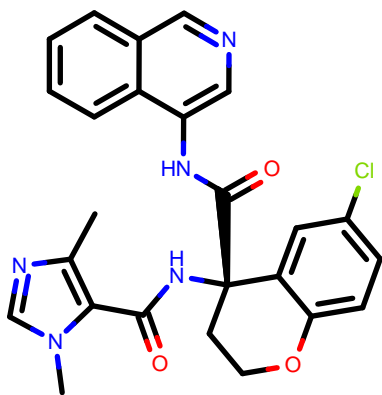
CID:	EN300-201346_1_2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COC(=O)N5</chem>
RUN:	RUN4091
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.19

EN300-217494_3_2_1



CID:	EN300-217494_3_2_1
SMILES:	<chem>C[C@@]([C@@H]1CCOC1)(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5)O</chem>
RUN:	RUN4182
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.33

EN300-6498351_1_1_1



CID: EN300-6498351_1_1_1

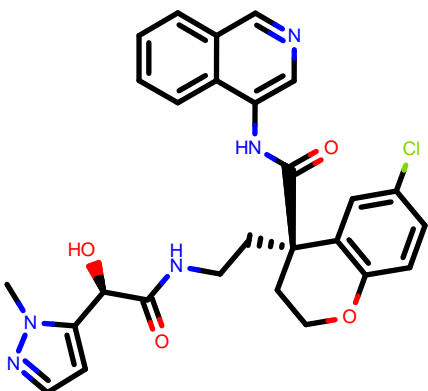
SMILES: Cc1c(n(en1)C)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5572

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-6473273_3_2_1



CID: EN300-6473273_3_2_1

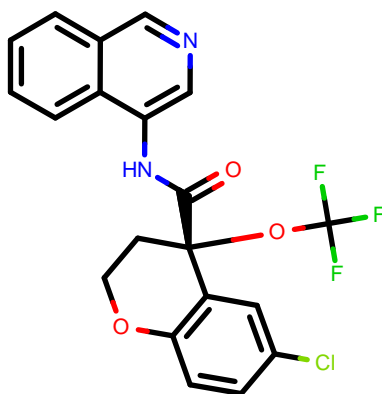
SMILES: Cn1c(en1)[C@H](C(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN6591

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.33

DAR-DIA-e7614d05-2_1



CID: DAR-DIA-e7614d05-2_1

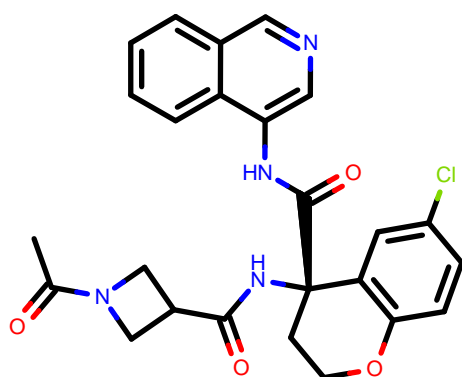
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC(F)(F)F

RUN: RUN2293

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.17

EN300-74876_1_1_1



CID: EN300-74876_1_1_1

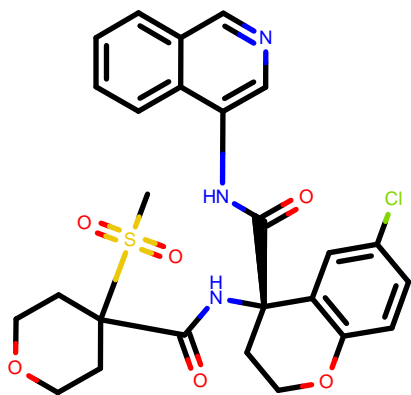
SMILES: CC(=O)N1CC(C1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5022

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-220536_1_1_1



CID: EN300-220536_1_1_1

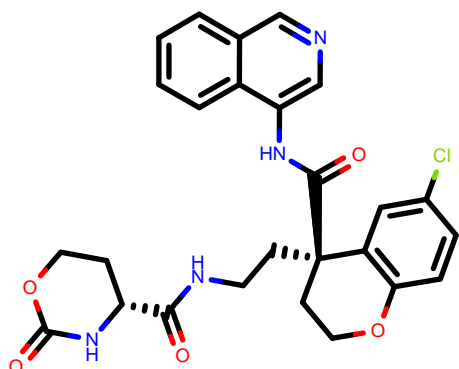
SMILES: CS(=O)(=O)C1(CCOCC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4cccc5c4ccccc5

RUN: RUN4513

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.32

EN300-249804_3_2_1



CID: EN300-249804_3_2_1

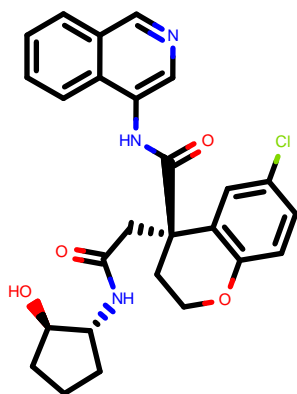
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC(=O)N5

RUN: RUN5805

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-60314_1_1_1



CID: EN300-60314_1_1_1

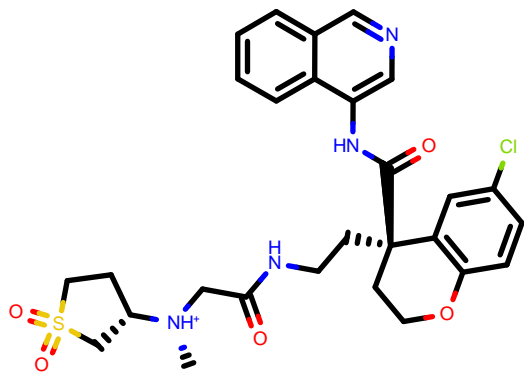
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4H5CC[C@]4H5O

RUN: RUN6419

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.23

EN300-14628_3_2_1



CID: EN300-14628_3_2_1

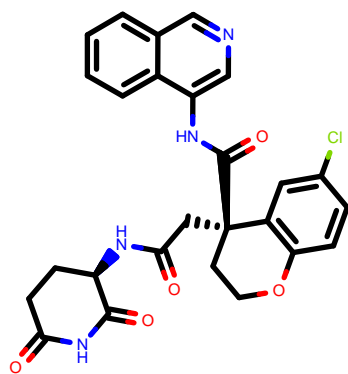
SMILES: C[N+]([O-])CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4[C@H]5CCS(=O)(=O)N5

RUN: RUN6896

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.46

EN300-113633_1_1_1



CID: EN300-113633_1_1_1

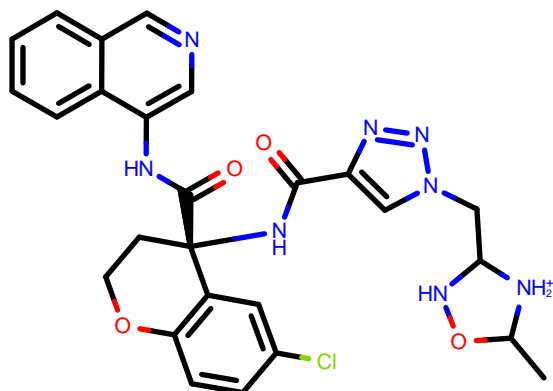
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCC(=O)NC5=O

RUN: RUN6711

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.23

EN300-182758_1_1_1



CID: EN300-182758_1_1_1

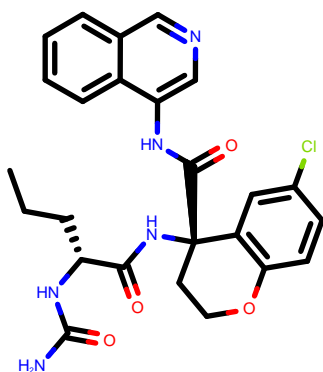
SMILES: Cc1nc(nc1)Cn2cc(nc2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN3740

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.26

EN300-102901_1_1_1



CID: EN300-102901_1_1_1

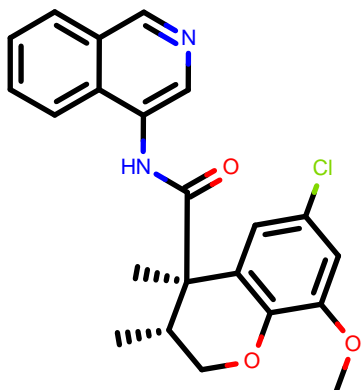
SMILES: CCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)N

RUN: RUN2876

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.24

DAR-DIA-0d514e7d-25_1_1



CID: DAR-DIA-0d514e7d-25_1_1

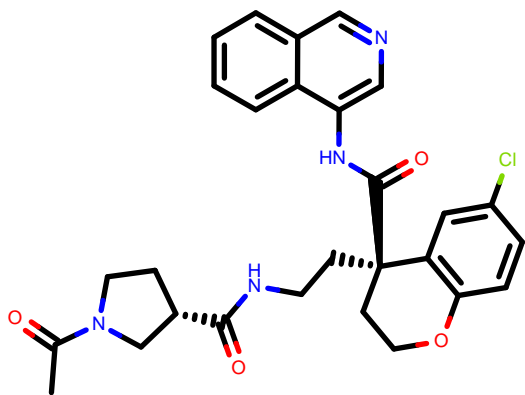
SMILES: C[C@@H]1COc2c(cc(cc2OC)Cl)[C@@]1(C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5838

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.13

EN300-100180_3_1_1



CID: EN300-100180_3_1_1

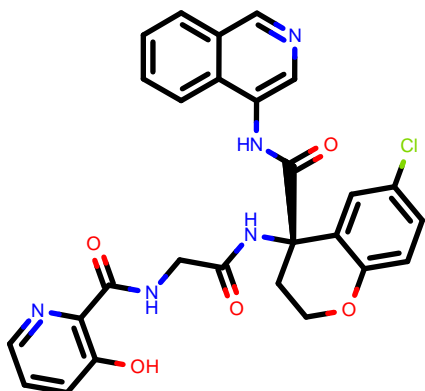
SMILES: CC(=O)N1CC[C@@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6330

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.45

EN300-115421_1_1_1



CID: EN300-115421_1_1_1

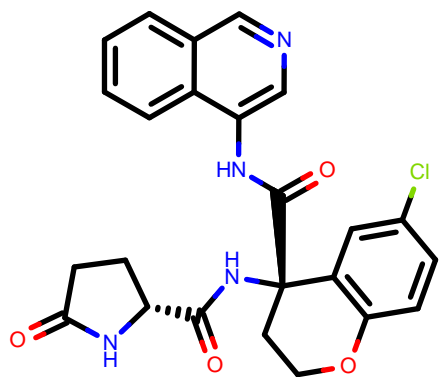
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5c(cccn5)O

RUN: RUN6459

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.28

EN300-19515_1_2_1



CID: EN300-19515_1_2_1

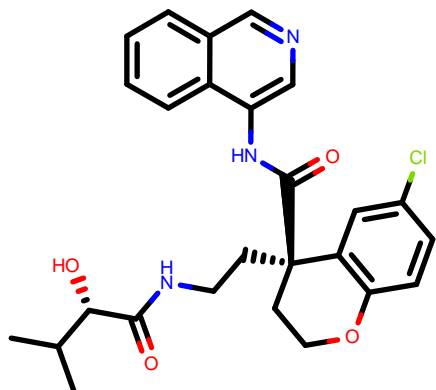
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCC(=O)N5

RUN: RUN3930

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.19

EN300-199359_3_1_1



CID: EN300-199359_3_1_1

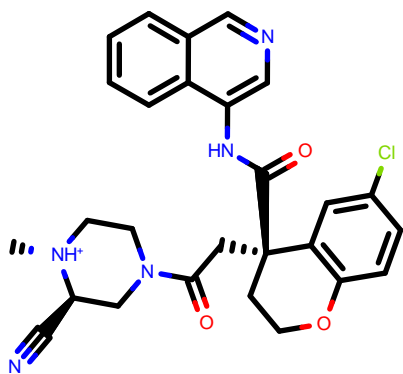
SMILES: CC(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN7702

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.30

EDG-MED-ba1ac7b9-14_7



CID: EDG-MED-ba1ac7b9-14_7

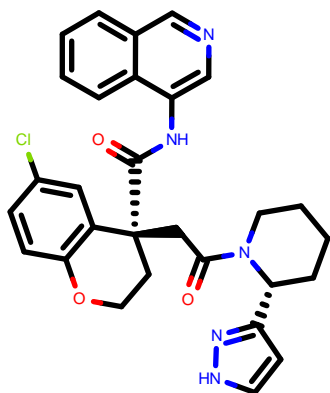
SMILES: C#N[C@@H]1CCN(C[C@H]1C#N)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5

RUN: RUN2478

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.28

EDG-MED-ba1ac7b9-10_1



CID: EDG-MED-ba1ac7b9-10_1

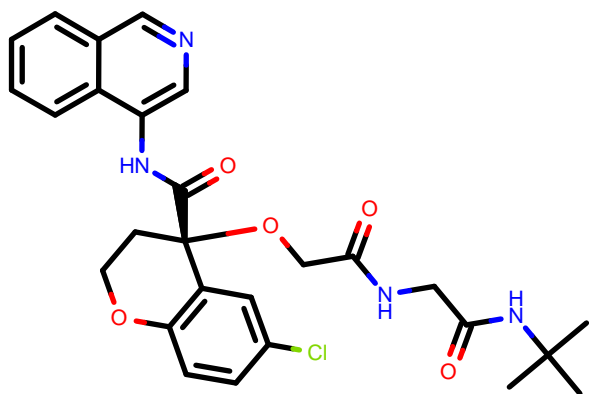
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5c6cn[nH]6

RUN: RUN2485

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.41

EN300-48760_1_1_1



CID: EN300-48760_1_1_1

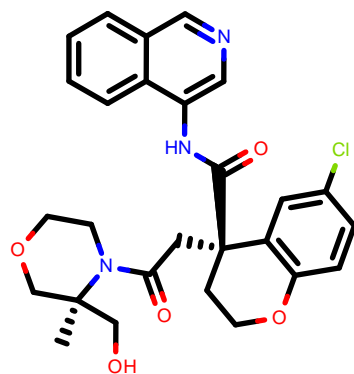
SMILES: CC(C)(C)NC(=O)CNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccc4

RUN: RUN6841

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.36

EN300-127629_1_1_1



CID: EN300-127629_1_1_1

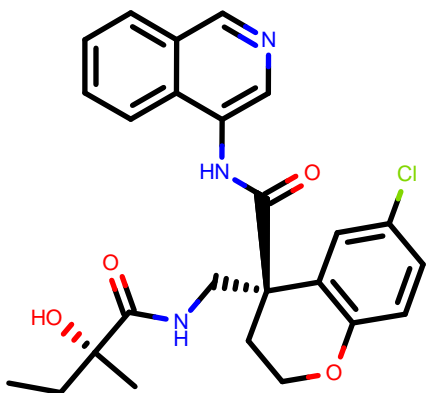
SMILES: C[C@@]1(COCCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5)CO

RUN: RUN4883

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.31

EN300-104746_2_2_1



CID: EN300-104746_2_2_1

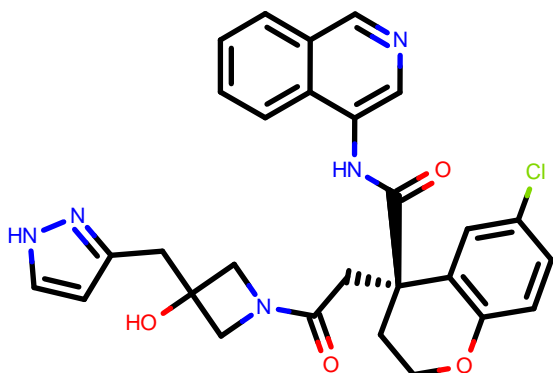
SMILES: CC[C@](C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN5893

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.28

EN300-6489696_1_1_1



CID: EN300-6489696_1_1_1

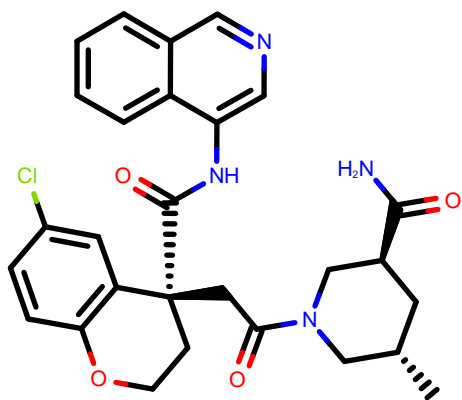
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)(Cc6cn[nH]6)O

RUN: RUN5284

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-1724086_1_2_1



CID: EN300-1724086_1_2_1

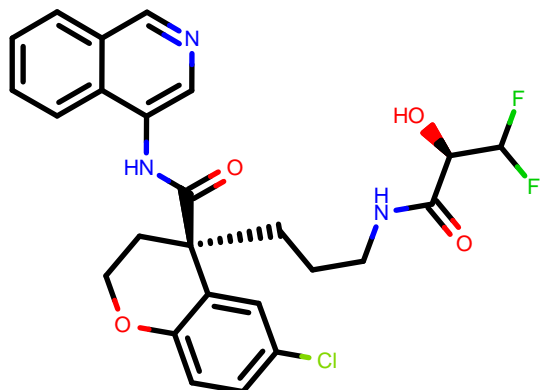
SMILES: C[C@@H]1C[C@@]2(C)C[C@@]3(CCOc4c3cc(cc4)C)C[C@@]4(C)N4cnc5c4cccc5)C1=O

RUN: RUN5430

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-1932780_4_2_1



CID: EN300-1932780_4_2_1

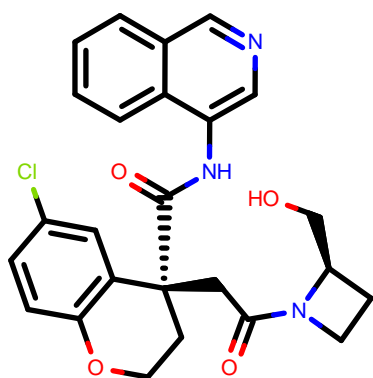
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C(F)F)O

RUN: RUN6734

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.20

EN300-154332_1_1_1



CID: EN300-154332_1_1_1

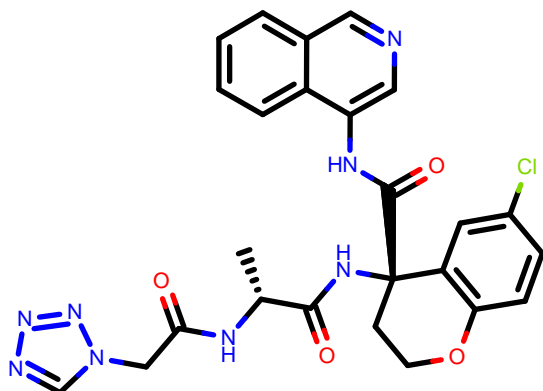
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO

RUN: RUN5797

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-649743_1_1_1



CID: EN300-649743_1_1_1

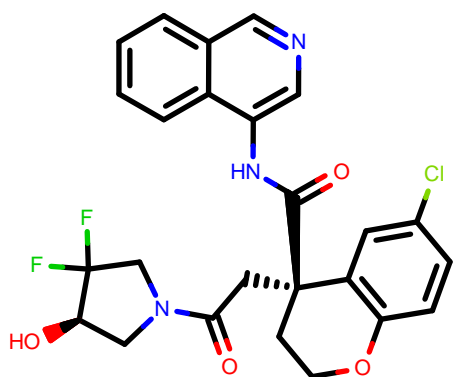
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4)NC(=O)Cn5nncn5

RUN: RUN3929

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.37

EN300-1710153_1_2_1



CID: EN300-1710153_1_2_1

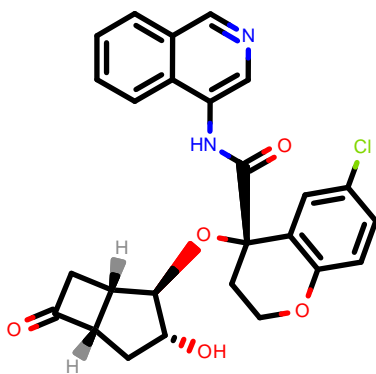
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C5)(F)F

RUN: RUN7384

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.23

EN300-6481287_1_1_1



CID: EN300-6481287_1_1_1

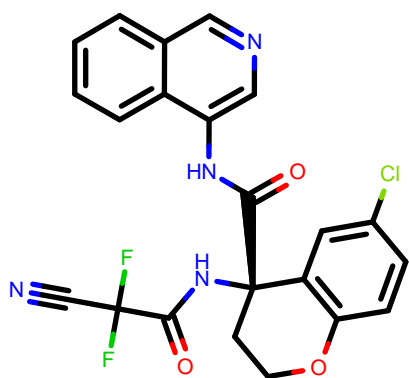
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5[C@H](C5)C[C@H]6[C@@H]5C(=O)O

RUN: RUN7482

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.29

EDG-MED-90036822-84_1



CID: EDG-MED-90036822-84_1

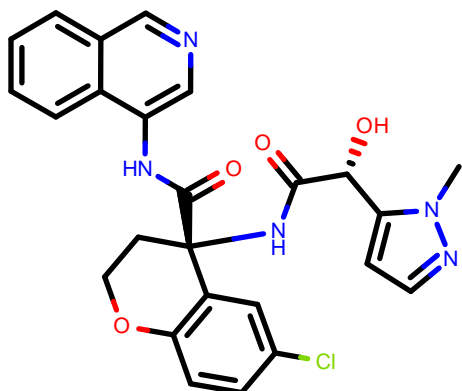
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(C#N)(F)F

RUN: RUN1622

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.22

EN300-6473273_1_2_1



CID: EN300-6473273_1_2_1

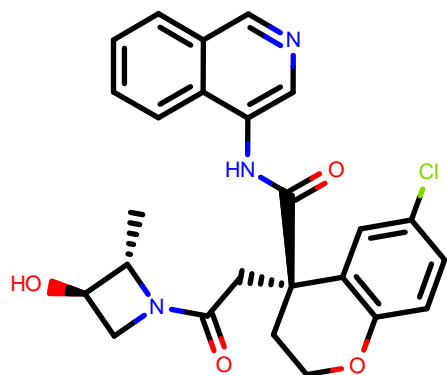
SMILES: Cn1c(cn1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN5161

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.23

EN300-7471076_1_2_1



CID: EN300-7471076_1_2_1

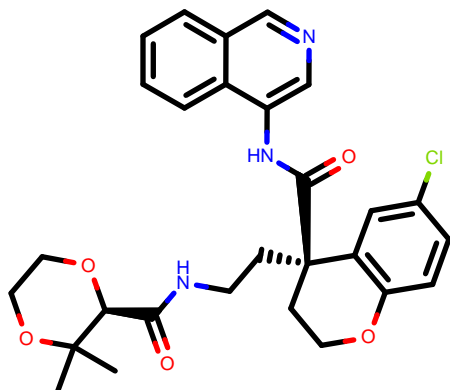
SMILES: C[C@H]1[C@@H](CN1C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN5423

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-1601684_3_1_1



CID: EN300-1601684_3_1_1

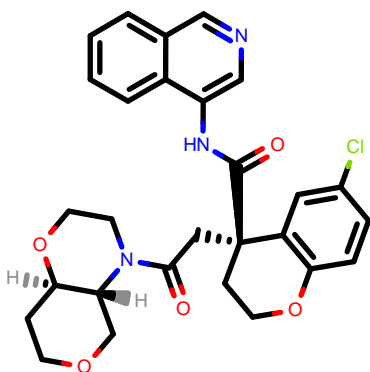
SMILES: CC1([C@@H](OCCO1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN5184

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.40

EN300-1387243_1_1_1



CID: EN300-1387243_1_1_1

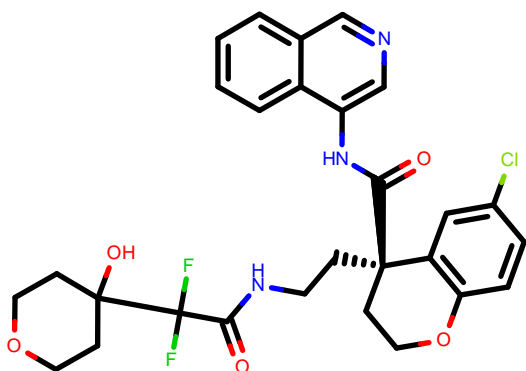
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@H]6[C@H]5COCC6

RUN: RUN5513

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.31

EN300-706065_3_1_1



CID: EN300-706065_3_1_1

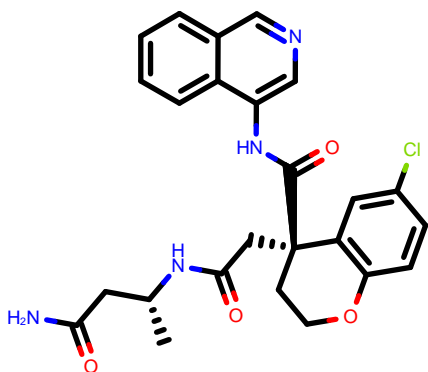
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCOCC5)O(F)F

RUN: RUN7708

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.35

EN300-84785_1_2_1



CID: EN300-84785_1_2_1

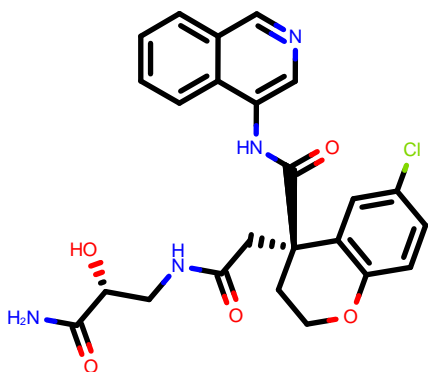
SMILES: C[C@H](C(=O)N)NC(=O)[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN3301

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-184355_1_2_1



CID: EN300-184355_1_2_1

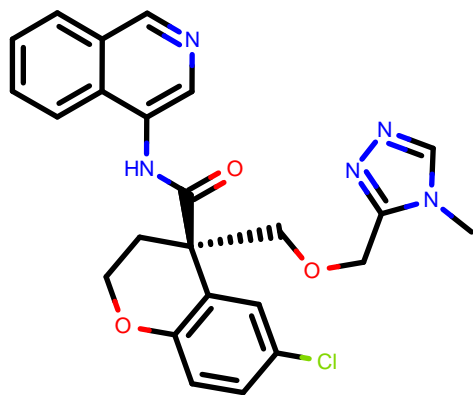
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@H](C(=O)N)O

RUN: RUN5535

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.39

EN300-113112_2_1_1



CID: EN300-113112_2_1_1

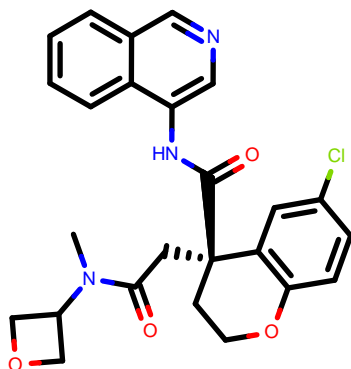
SMILES: Cn1cnnc1COC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3170

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.22

EN300-1091444_1_1_1



CID: EN300-1091444_1_1_1

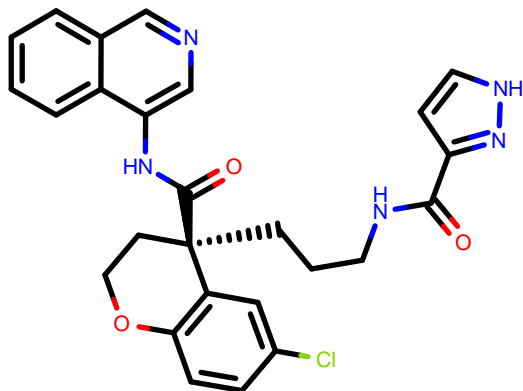
SMILES: CN(C1COC1)C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3832

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.28

EN300-37077_4_1_1



CID: EN300-37077_4_1_1

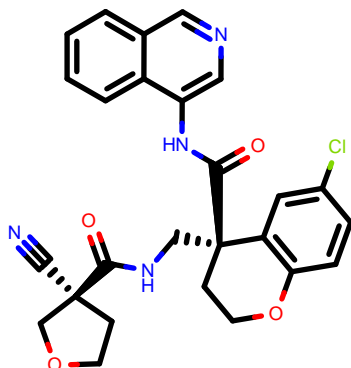
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cn[nH]5

RUN: RUN6378

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.32

EDJ-MED-40433386-8_1



CID: EDJ-MED-40433386-8_1

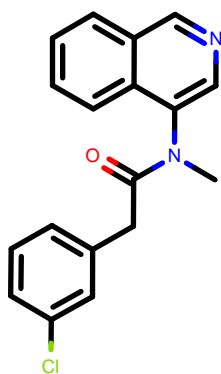
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOc5)C#N

RUN: RUN2386

DDG (kcal/mol): -0.87

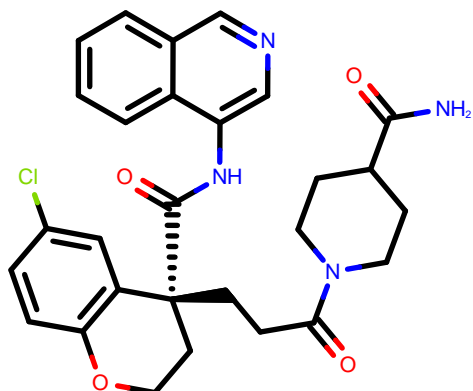
dDDG (kcal/mol): 0.29

MAT-POS-bb423b95-7_1



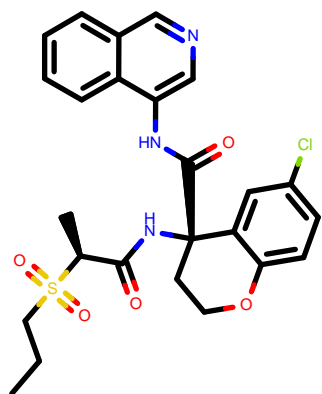
CID:	MAT-POS-bb423b95-7_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN146
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.24

EN300-1265946_2_1_1



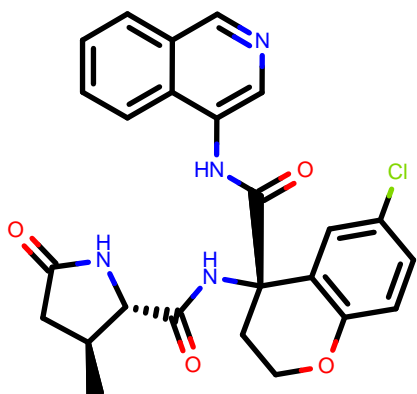
CID:	EN300-1265946_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCCC(C5)C(=O)N</chem>
RUN:	RUN7720
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.29

EN300-52768_1_1_1



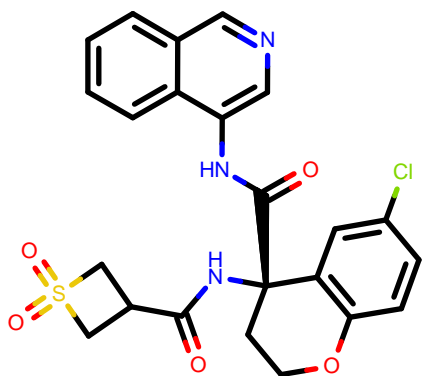
CID:	EN300-52768_1_1_1
SMILES:	<chem>CCCS(=O)(=O)[C@@H](C)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN4977
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.39

EN300-155362_1_2_1



CID:	EN300-155362_1_2_1
SMILES:	<chem>C[C@H]1CC(=O)N[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5</chem>
RUN:	RUN6709
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.21

EN300-261365_1_1_1



CID: EN300-261365_1_1_1

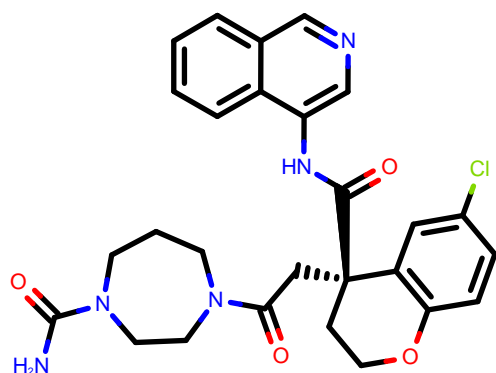
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CS(=O)C5=O

RUN: RUN4142

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.21

EN300-65063_1_1_1



CID: EN300-65063_1_1_1

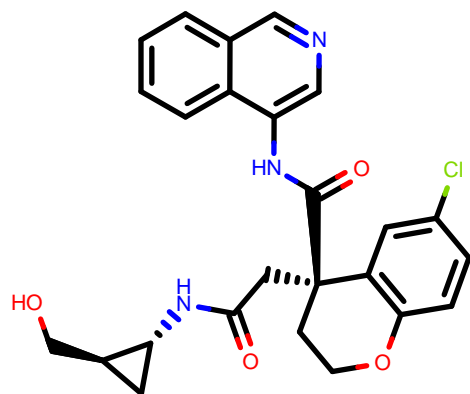
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN(C5)C(=O)N

RUN: RUN5396

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.26

EN300-196962_1_1_1



CID: EN300-196962_1_1_1

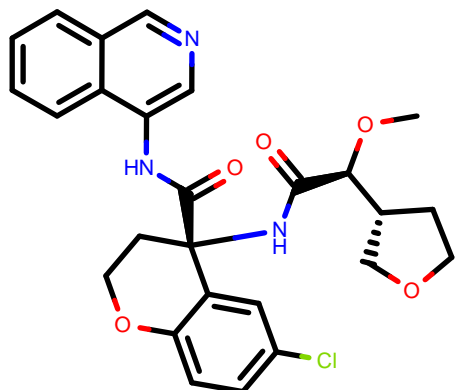
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5C[C@H]5CO

RUN: RUN5723

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.23

EN300-298552_1_1_1



CID: EN300-298552_1_1_1

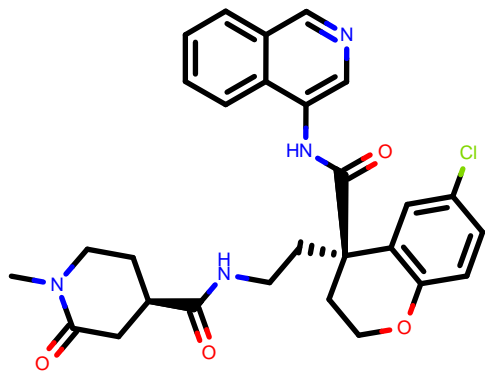
SMILES: CO[C@@H]([C@@H]1CCOC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c5c4ccc5

RUN: RUN2989

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.20

EN300-30458_3_2_1



CID: EN300-30458_3_2_1

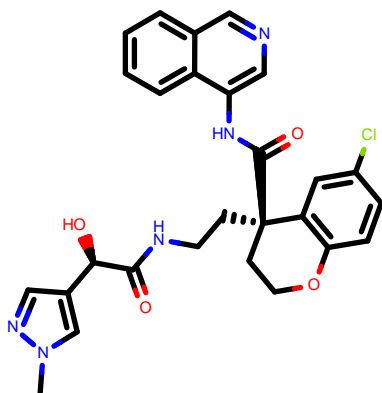
SMILES: CN1CC[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN7262

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.33

EN300-198540_3_2_1



CID: EN300-198540_3_2_1

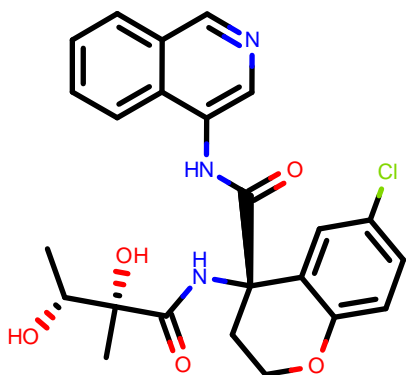
SMILES: C[n+1]1cc(c[nH]1)[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5)O

RUN: RUN4636

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.46

EN300-202922_1_4_1



CID: EN300-202922_1_4_1

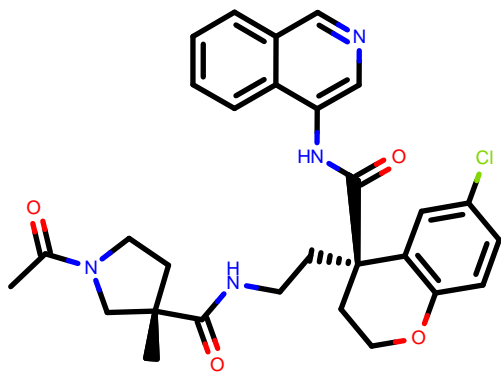
SMILES: C[C@H](C[C@](C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccccc4)O)O

RUN: RUN5720

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.27

EN300-98018_3_2_1



CID: EN300-98018_3_2_1

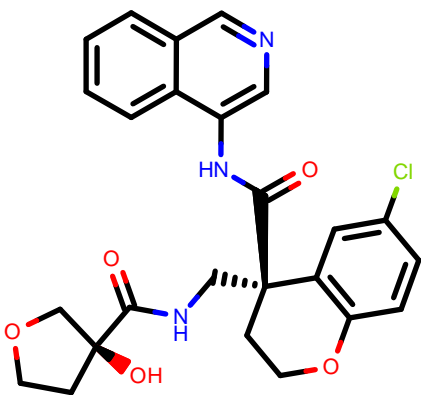
SMILES: CC(=O)N1CC[C@](C1)(C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN3672

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.35

EN300-148421_2_1_1



CID: EN300-148421_2_1_1

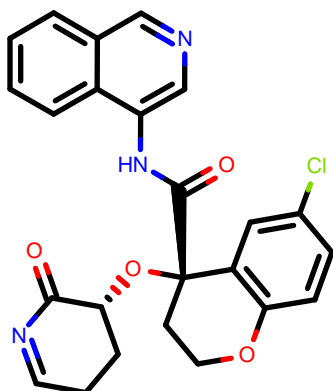
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOC5)O

RUN: RUN4864

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.32

EN300-107267_1_1_1



CID: EN300-107267_1_1_1

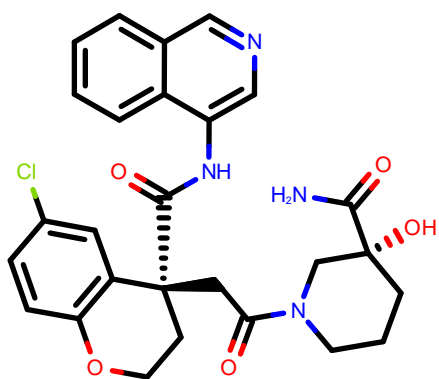
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@]5H5CCNC5=O

RUN: RUN6765

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.26

EN300-210553_1_1_1



CID: EN300-210553_1_1_1

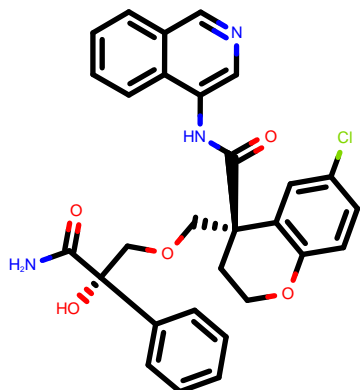
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]5(C)N)O

RUN: RUN7680

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.45

EN300-248526_2_2_1



CID: EN300-248526_2_2_1

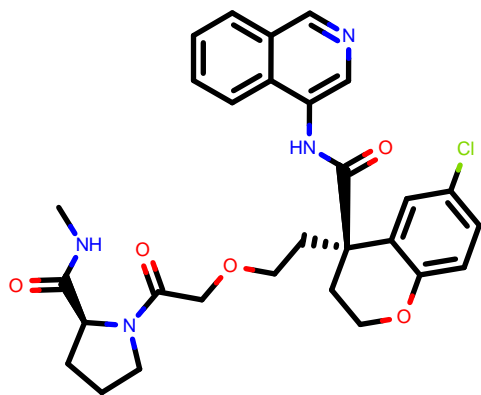
SMILES: c1ccc(cc1)[C@@]1COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5(C)C(=O)N)O

RUN: RUN4042

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.33

EN300-48902_3_1_1



CID: EN300-48902_3_1_1

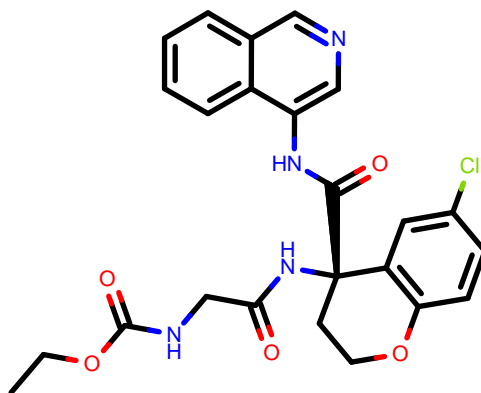
SMILES: CNC(=O)[C@@H](CCCN1C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN6513

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.40

EN300-36390_1_1_1



CID: EN300-36390_1_1_1

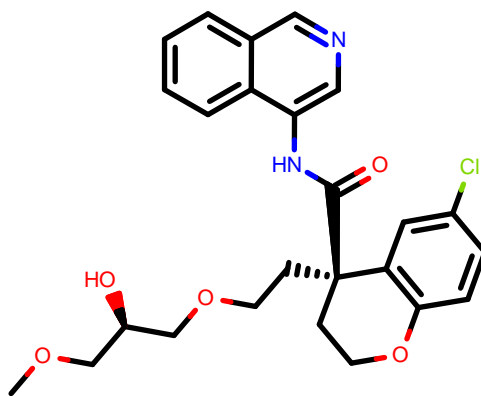
SMILES: CCOC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN6254

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.23

EN300-1915260_3_2_1



CID: EN300-1915260_3_2_1

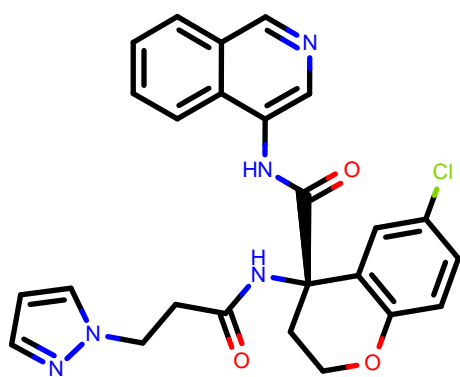
SMILES: COC[C@H](COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)O

RUN: RUN6133

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.32

EN300-25986_1_1_1



CID: EN300-25986_1_1_1

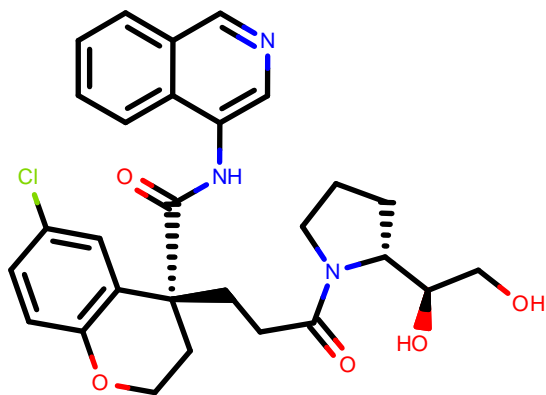
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cccn5

RUN: RUN4143

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.21

EN300-7459540_2_1_1



CID: EN300-7459540_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4=CC=CC=C4)C(C)C(=O)N5CC[C@H]3C5

RUN:

RUN6119

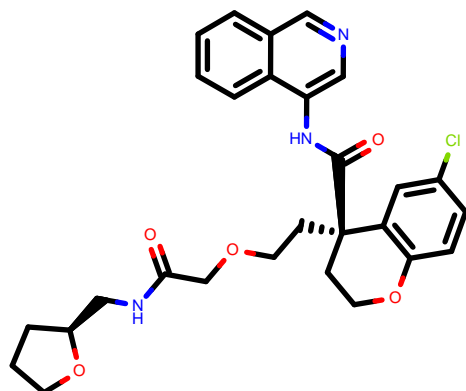
DDG (kcal/mol):

-0.85

dDDG (kcal/mol):

0.39

EN300-01527_3_1_1



CID: EN300-01527_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4=CC=CC=C4)C(C)C(=O)N5CC[C@H]3C5

RUN:

RUN4818

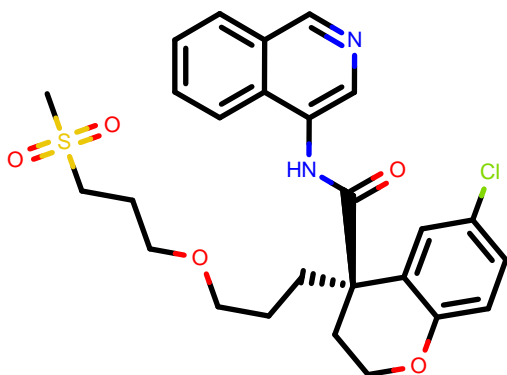
DDG (kcal/mol):

-0.85

dDDG (kcal/mol):

0.36

EN300-68794_4_1_1



CID: EN300-68794_4_1_1

SMILES:

CS(=O)(=O)CCOC[C@]1(C)C(C)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN7328

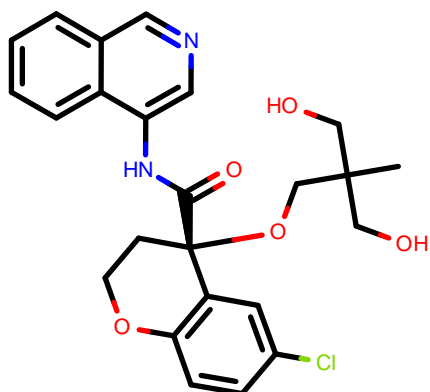
DDG (kcal/mol):

-0.85

dDDG (kcal/mol):

0.36

EN300-218116_1_1_1



CID: EN300-218116_1_1_1

SMILES:

CC(CO)(CO)CO[C@]1(C)C(C)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN5872

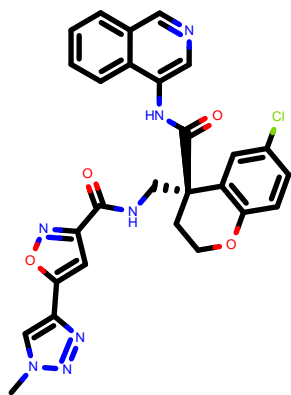
DDG (kcal/mol):

-0.85

dDDG (kcal/mol):

0.38

ALP-UNI-0676e700-23_1



CID: ALP-UNI-0676e700-23_1

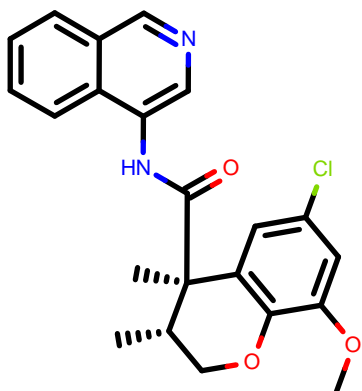
SMILES: Cn1cc(nn1)c2cc(n2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN2331

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-25_1



CID: DAR-DIA-0d514e7d-25_1

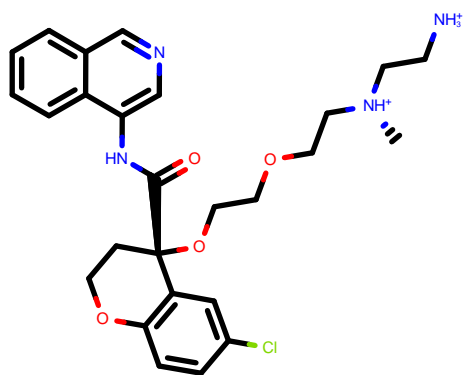
SMILES: C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3ccc4c3ccc4

RUN: RUN763

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.12

ED_-GRI-5b13fbe2-15_1



CID: ED_-GRI-5b13fbe2-15_1

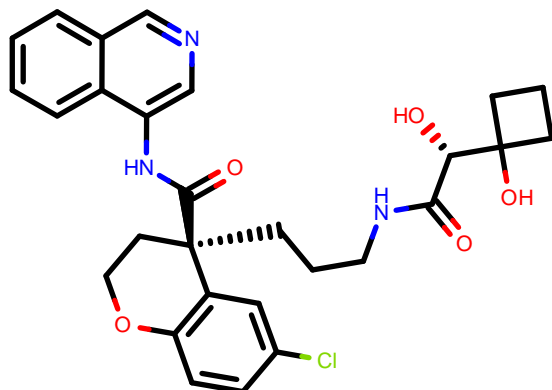
SMILES: C[N@]([CC[NH3+])CCOCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN1414

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.50

EN300-1073320_4_1_1



CID: EN300-1073320_4_1_1

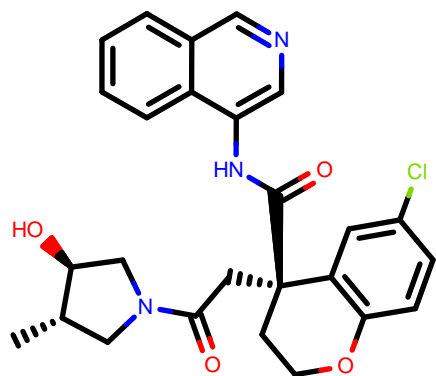
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN7256

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.40

EN300-124052_1_2_1



CID: EN300-124052_1_2_1

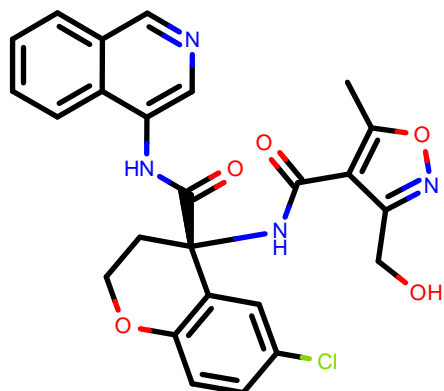
SMILES: C[C@H]1CN(C[C@@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4288

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.25

EN300-215799_1_1_1



CID: EN300-215799_1_1_1

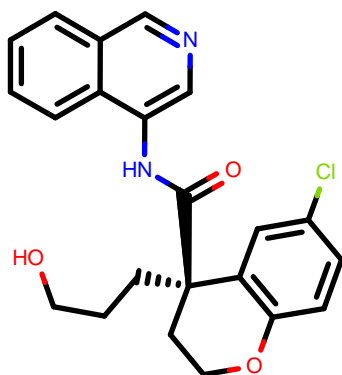
SMILES: Cc1c(c(no1)CO)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4846

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.25

EDG-MED-971238d3-8_1



CID: EDG-MED-971238d3-8_1

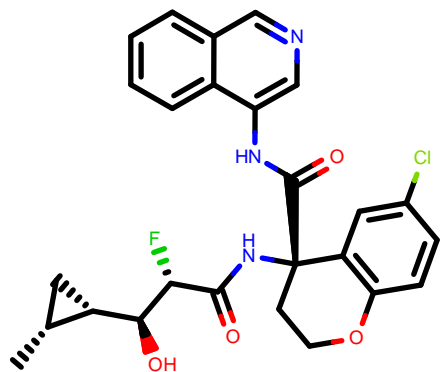
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO

RUN: RUN1306

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.20

EDG-MED-90036822-94_1



CID: EDG-MED-90036822-94_1

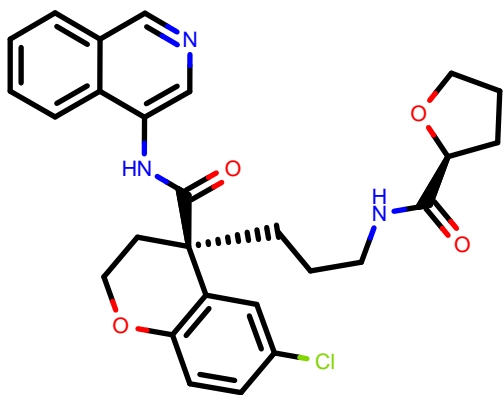
SMILES: C[C@@H]1C[C@@H]1[C@@H](C(F)O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5F

RUN: RUN1679

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.34

EN300-21009_4_1_1



CID: EN300-21009_4_1_1

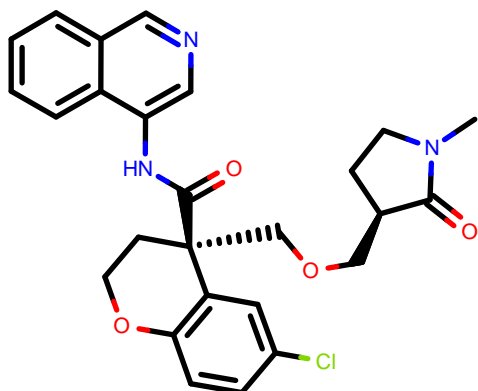
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCCCO5

RUN: RUN6038

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.33

EN300-260816_2_1_1



CID: EN300-260816_2_1_1

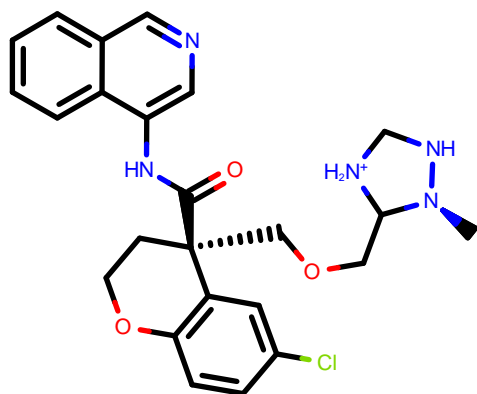
SMILES: CN1CC[C@@H](C1=O)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN4178

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.24

EN300-87334_2_1_1



CID: EN300-87334_2_1_1

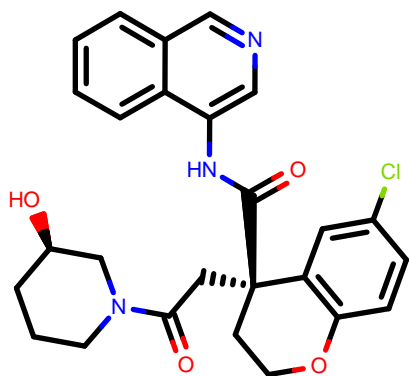
SMILES: Cn1c(ncn1)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN6606

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.28

EN300-266117_1_1_1



CID: EN300-266117_1_1_1

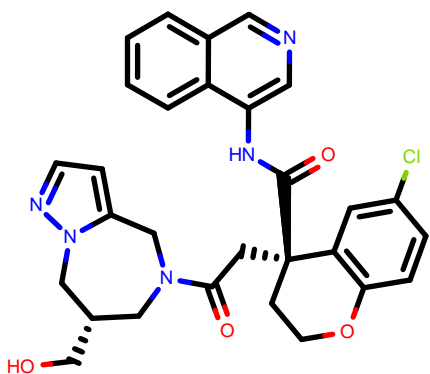
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN4829

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.31

EN300-6739414_1_2_1



CID: EN300-6739414_1_2_1

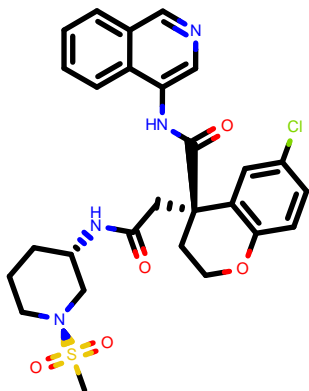
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C6ccnn6[C@H](C5)CO

RUN: RUN7553

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.28

EN300-54922_1_1_1



CID: EN300-54922_1_1_1

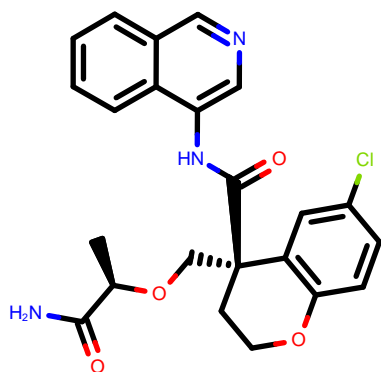
SMILES: CS(=O)(=O)N1[C@H](C)C[C@@H](C1)NC(=O)[C@]2(COCc3c2cc(cc3)C)C(=O)N4ccc5c4ccccc5

RUN: RUN6099

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.24

EN300-17381_2_2_1



CID: EN300-17381_2_2_1

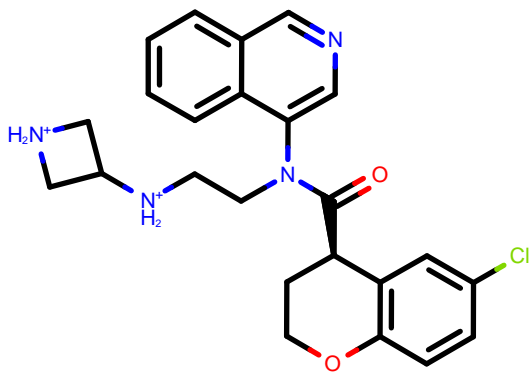
SMILES: C[C@H](C(=O)N)OC[C@]1(C)COCc2c1cc(cc2)C(=O)Nc3ccc4c3ccccc4

RUN: RUN4799

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.23

MAK-UNK-83e0a0b4-3_1_1



CID: MAK-UNK-83e0a0b4-3_1_1

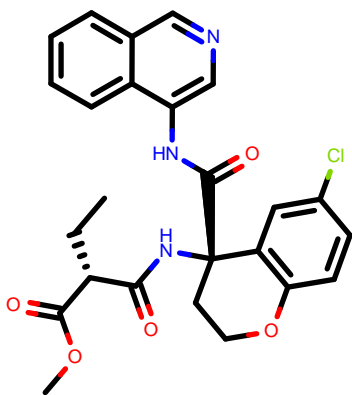
SMILES: c1ccc2c(c1)ncoc2N(CN(C)N)C(=O)[C@]3(C)C(=O)[C@@H](C4CCOC5c4cc(cc5)Cl

RUN: RUN7605

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.46

EN300-175425_1_2_1



CID: EN300-175425_1_2_1

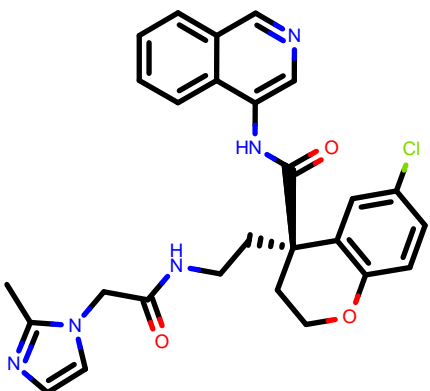
SMILES: CC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)C(=O)OC

RUN: RUN3153

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.22

EN300-41507_3_1_1



CID: EN300-41507_3_1_1

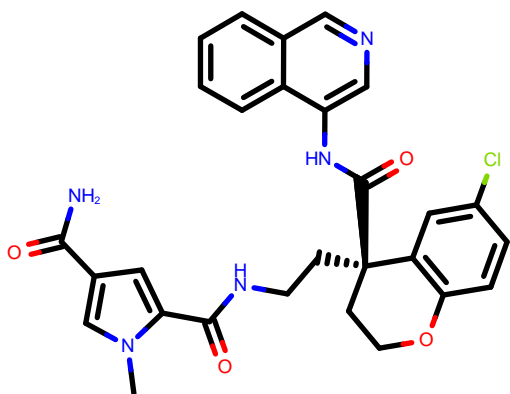
SMILES: Cc1nccn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN5753

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.31

KAD-UNI-8a629cb0-4_1



CID: KAD-UNI-8a629cb0-4_1

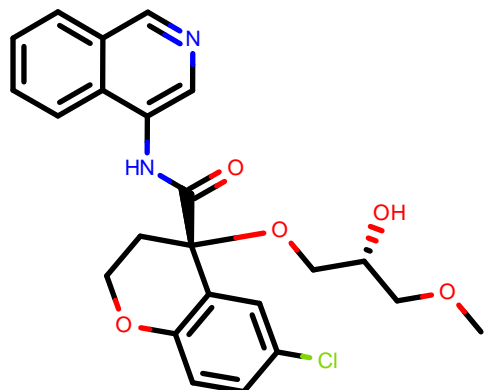
SMILES: Cn1cc(cc1C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5)C(=O)N

RUN: RUN1946

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-1915260_1_2_1



CID: EN300-1915260_1_2_1

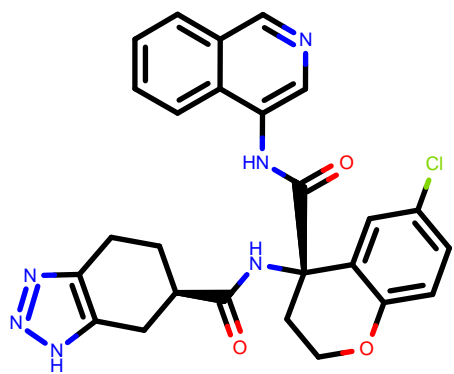
SMILES: COC[C@H](CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccc4)O

RUN: RUN5252

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.32

EN300-185729_1_1_1



CID: EN300-185729_1_1_1

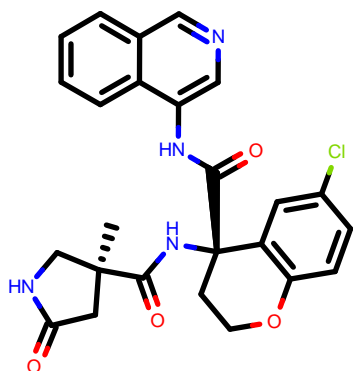
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4C)NC(=O)C@H)5CC6c6c(nH)n6)C5

RUN: RUN3045

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.23

EN300-132157_1_1_1



CID: EN300-132157_1_1_1

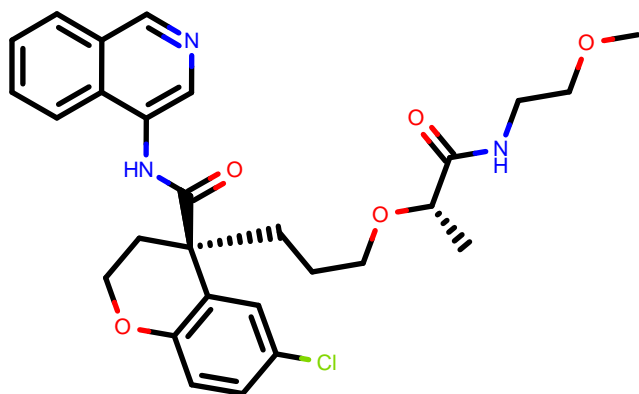
SMILES: C[C@@H]1(CC(=O)NC1)C(=O)N[C@@2](CCOc3c2cc(cc3C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN4966

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-23317_4_1_1



CID: EN300-23317_4_1_1

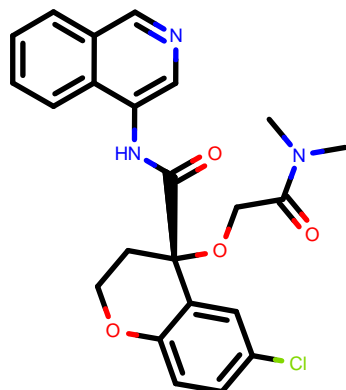
SMILES: C[C@@H](C(=O)NCCOC)OCC[C@@H]1(CCOc2c1cc(cc2C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN6585

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.38

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

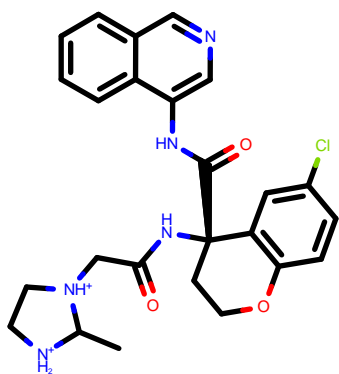
SMILES: CN(C)C(=O)CO[C@@H]1(CCOc2c1cc(cc2C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN6561

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.20

EN300-41507_1_1_1



CID: EN300-41507_1_1_1

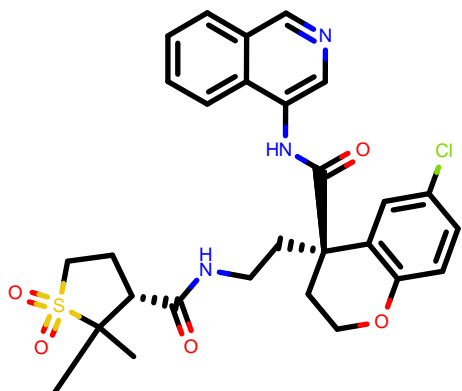
SMILES: Cc1nccn1CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5643

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.25

EN300-2007564_3_2_1



CID: EN300-2007564_3_2_1

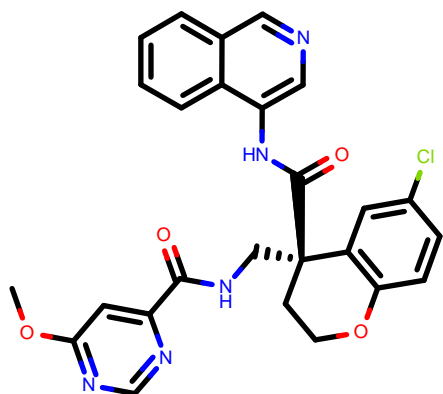
SMILES: CC1([C@H](CCS1(=O)=O)C(=O)N)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3866

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.35

EN300-131943_2_1_1



CID: EN300-131943_2_1_1

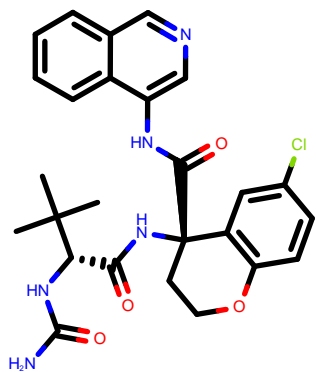
SMILES: COc1cc(ncn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7768

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.34

EN300-201164_1_2_1



CID: EN300-201164_1_2_1

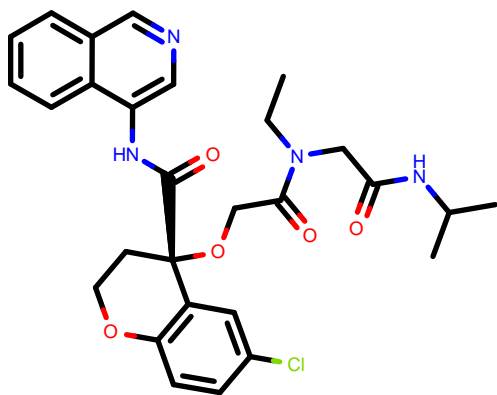
SMILES: CC(C)C[C@H](C(=O)N)C@1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4NC(=O)N

RUN: RUN3887

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.25

EN300-07936_1_1_1



CID: EN300-07936_1_1_1

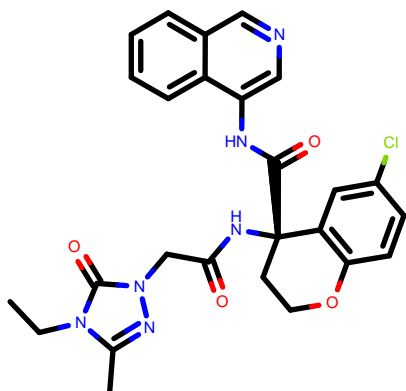
SMILES: CCN(CC(=O)NC(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5136

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.36

EN300-6478433_1_1_1



CID: EN300-6478433_1_1_1

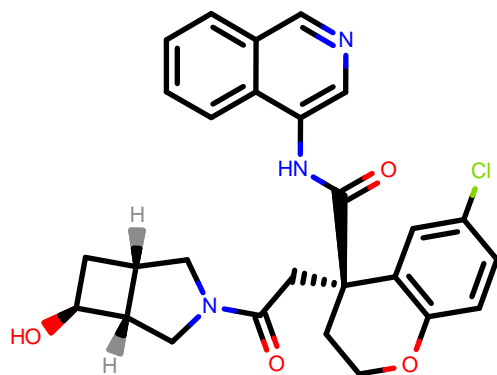
SMILES: CCn1c(nn(c1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN5716

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.35

EN300-305294_1_6_1



CID: EN300-305294_1_6_1

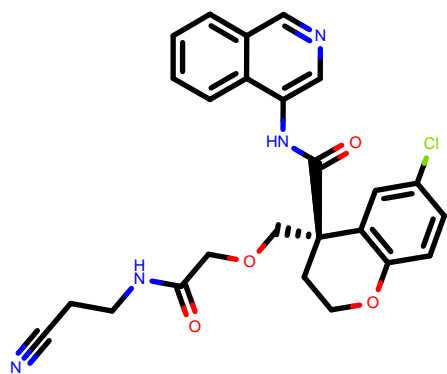
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@@H]7[C@@H]8C5O

RUN: RUN4981

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-10895_2_1_1



CID: EN300-10895_2_1_1

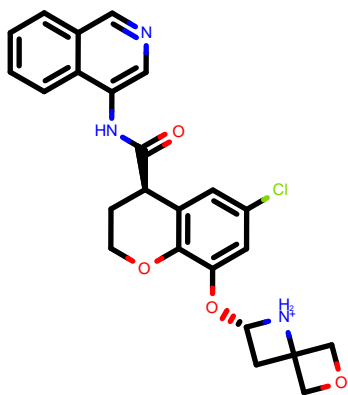
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCCC#N

RUN: RUN5767

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.30

DAR-DIA-23e5a6a0-3_2



CID: DAR-DIA-23e5a6a0-3_2

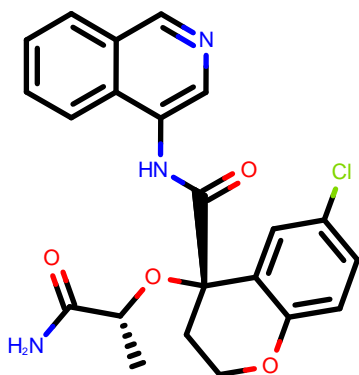
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOCc4c3cc(cc4O)[C@H]5CC6([NH2+][5])COC6Cl

RUN: RUN355

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.38

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

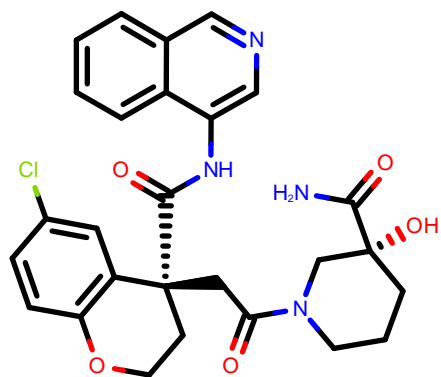
SMILES: C[C@H](C(=O)N)O[C@]1(C)C(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN5740

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.21

EN300-210553_1_1_1



CID: EN300-210553_1_1_1

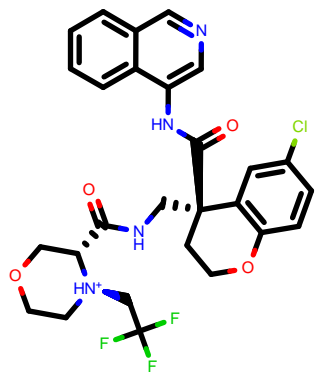
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]6(C)C(=O)N5O

RUN: RUN5207

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.51

EDJ-MED-4c7486ba-7_2



CID: EDJ-MED-4c7486ba-7_2

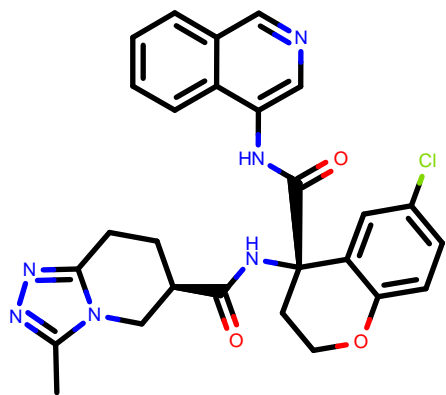
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COC6([5])COC6(F)F

RUN: RUN1843

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.38

EN300-50561_1_1_1



CID: EN300-50561_1_1_1

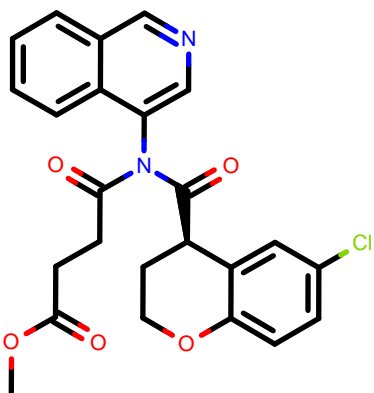
SMILES: Cc1nnc2n1C[C@@H](CC2)C(=O)N(C@)3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccc6

RUN: RUN4979

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.26

DAR-DIA-5ff57136-9_1_1



CID: DAR-DIA-5ff57136-9_1_1

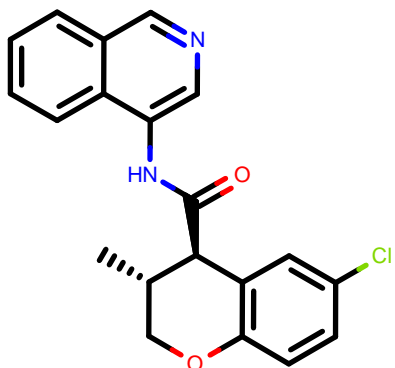
SMILES: COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN4631

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.34

EDJ-MED-e4b030d8-11_1_1



CID: EDJ-MED-e4b030d8-11_1_1

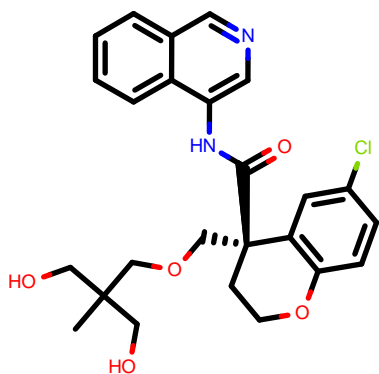
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN5837

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.05

EN300-218116_2_1_1



CID: EN300-218116_2_1_1

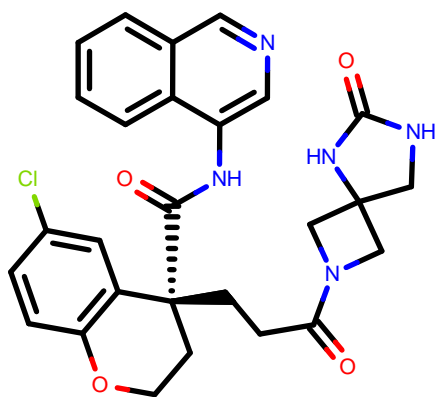
SMILES: CC(CO)(CO)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3455

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-1605226_2_1_1



CID: EN300-1605226_2_1_1

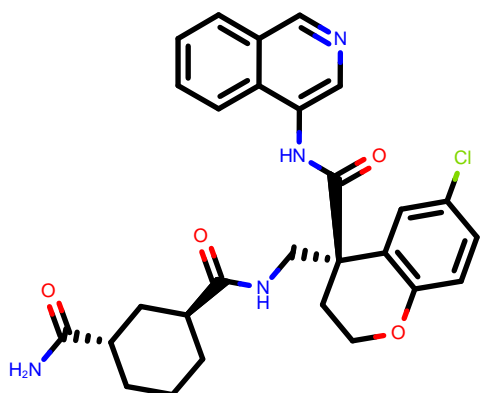
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC6(C5)CNC1=O)N6

RUN: RUN6161

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.25

EN300-90142_2_2_1



CID: EN300-90142_2_2_1

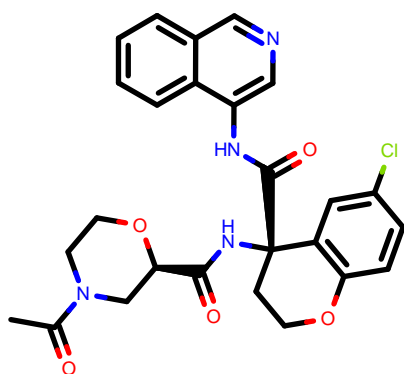
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC1=O)C@H)5CC[C@@]6H)C5)C1=O)N

RUN: RUN7181

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.33

EN300-100689_1_2_1



CID: EN300-100689_1_2_1

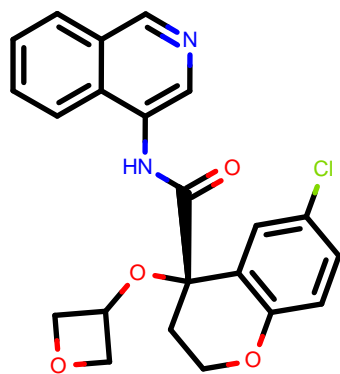
SMILES: CC(=O)N1CCO[C@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5807

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-317082_1_1_1



CID: EN300-317082_1_1_1

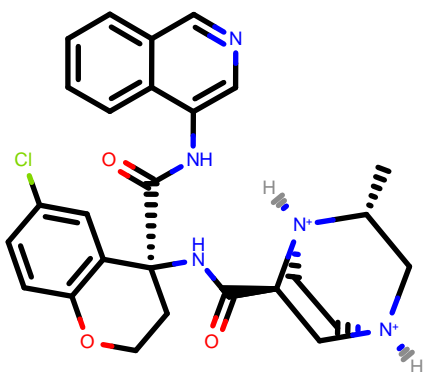
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC5COC5

RUN: RUN7281

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.19

EN300-120562_1_1_1



CID: EN300-120562_1_1_1

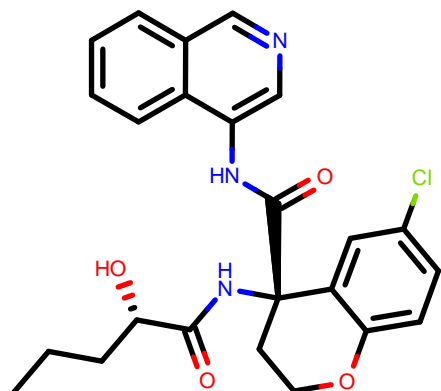
SMILES: C[C@@H]1CN[C@@]2CCN[C@H]1C[C@@H](C2)C(=O)N[C@@]3(CCOc4ccc(cc4)C)C(=O)Nc5ccc6c5ccc6

RUN: RUN7502

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-219531_1_1_1



CID: EN300-219531_1_1_1

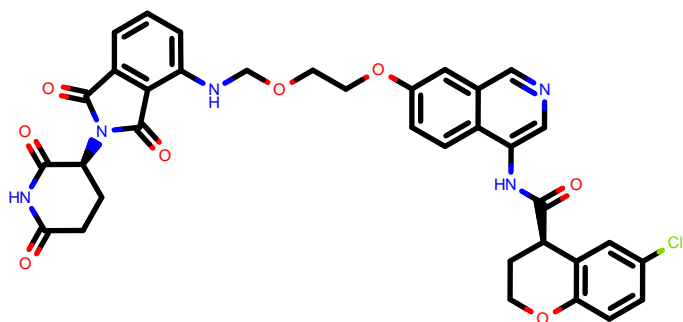
SMILES: CCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN3674

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.34

DAR-DIA-9e4459de-13_5



CID: DAR-DIA-9e4459de-13_5

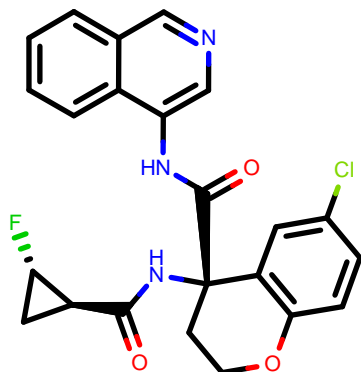
SMILES: c1cc2c(c1)NCOCCOc3ccc4c(c3)ncnc4N[C@@]5(C[C@@H]5COC6c6cc(cc6)Cl)c1c(c2)C[C@@H](C)C(=O)Nc7ccc8c7ccc8

RUN: RUN1363

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.39

EN300-97300_1_2_1



CID: EN300-97300_1_2_1

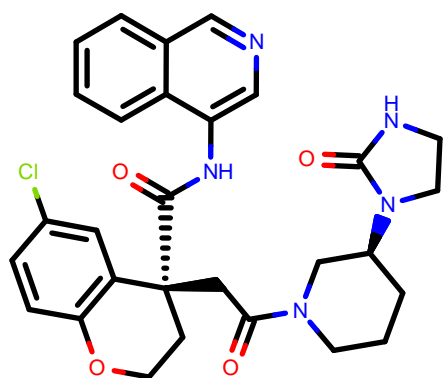
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C[C@@]4C3cc(cc4)C)N[C@@]5(C)[C@@H]5C[C@@]6H5F

RUN: RUN6127

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.20

EN300-55087_1_1_1



CID: EN300-55087_1_1_1

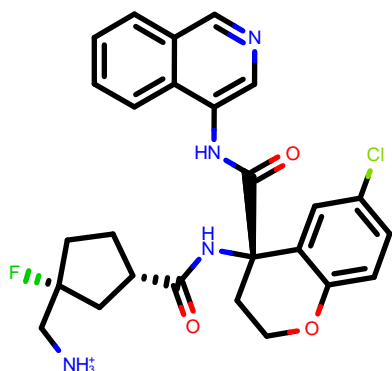
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](C(=O)N4C=CC=C4)C(=O)N5C=CC=C5C@@@6H[C@H](C5)N6CNC6=O

RUN: RUN6042

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EDG-MED-90036822-69_1



CID: EDG-MED-90036822-69_1

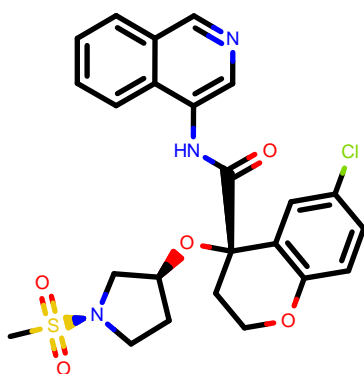
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](C(=O)N4C=CC=C4)C(=O)N5C=CC=C5C@@@6H[C@H](C5)N6CNC6=O

RUN: RUN1634

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-301690_1_1_1



CID: EN300-301690_1_1_1

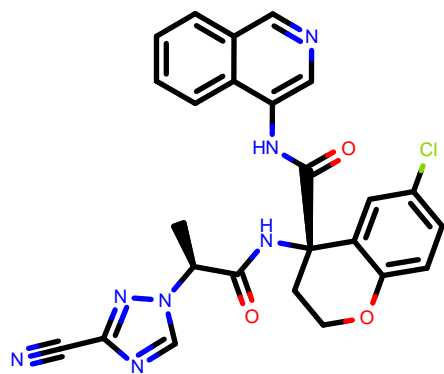
SMILES: CS(=O)(=O)N[C@@H]1CC[C@@H]2[C@H](C1)O[C@@H]2(C(=O)N3C=CC=C3)C(=O)N4C=CC=C4C@@@5H

RUN: RUN6861

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.30

EN300-198515_1_1_1



CID: EN300-198515_1_1_1

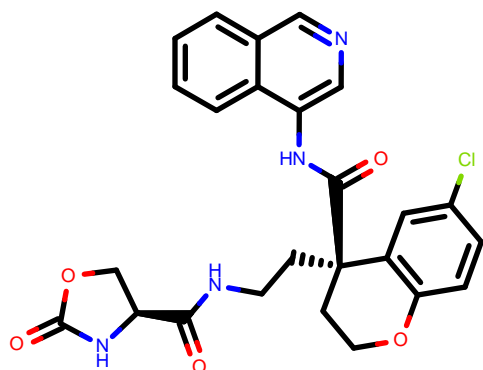
SMILES: C#N[C@@H]1C=CN=C1C(=O)N[C@@H]2[C@H](C1)O[C@@H]2(C(=O)N3C=CC=C3)C(=O)N4C=CC=C4C@@@5H

RUN: RUN2856

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.25

EN300-201346_3_1_1



CID: EN300-201346_3_1_1

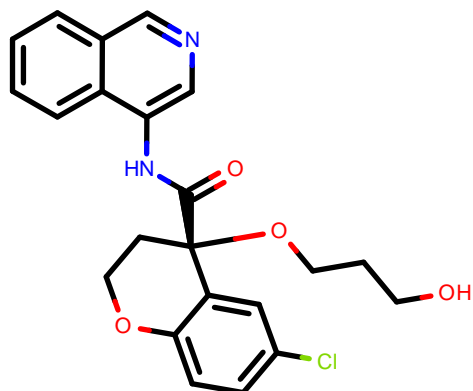
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5COC(=O)N5

RUN: RUN4388

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.26

EN300-221518_1_1_1



CID: EN300-221518_1_1_1

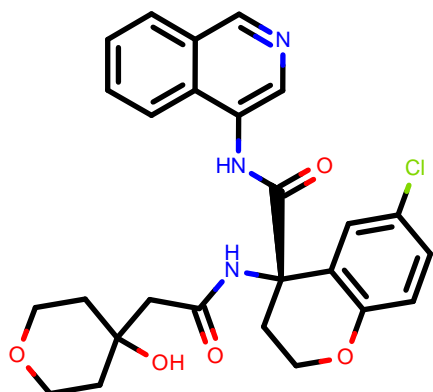
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCCO

RUN: RUN5339

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.18

EN300-151423_1_1_1



CID: EN300-151423_1_1_1

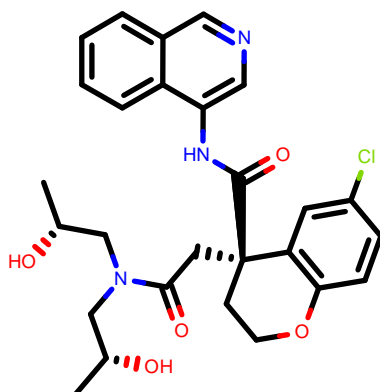
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5(COCCOC5)O

RUN: RUN4516

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.28

EN300-722418_1_2_1



CID: EN300-722418_1_2_1

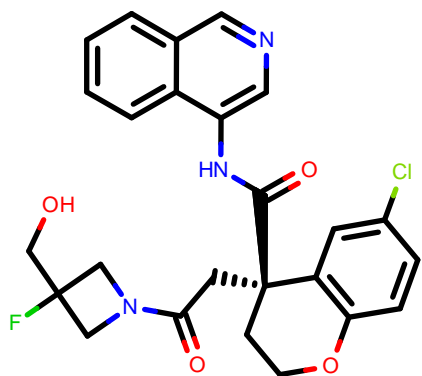
SMILES: C[C@H](CN(C[C@@H](C)O)C(=O)C[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5522

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.44

EN300-204507_1_1_1



CID: EN300-204507_1_1_1

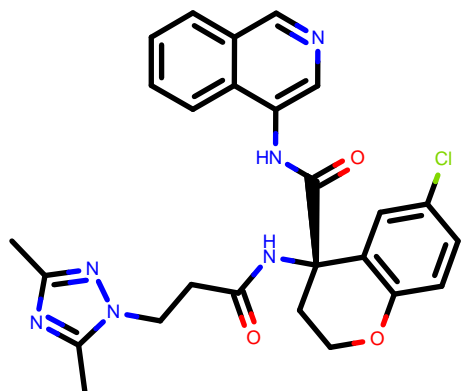
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F

RUN: RUN6947

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-41366_1_1_1



CID: EN300-41366_1_1_1

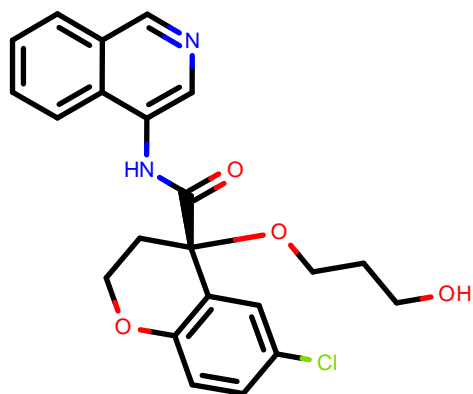
SMILES: Cc1nc(n1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5C

RUN: RUN4234

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-221518_1_1_1



CID: EN300-221518_1_1_1

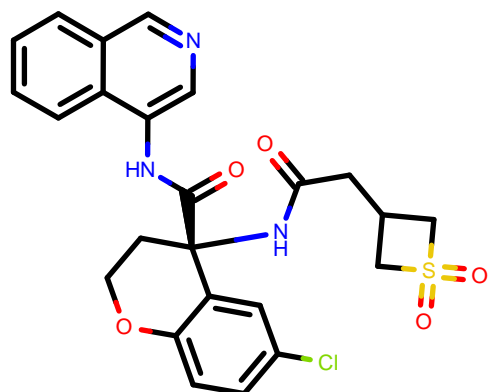
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO

RUN: RUN5155

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-256583_1_1_1



CID: EN300-256583_1_1_1

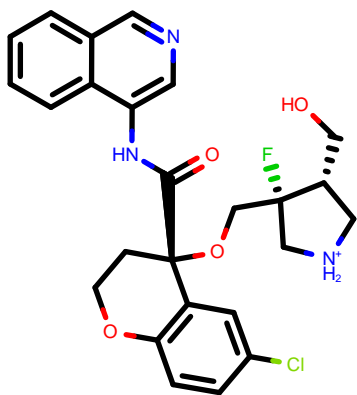
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5CS(=O)=O5

RUN: RUN4702

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-55_3



CID: ED_-GRI-5b13fbe2-55_3

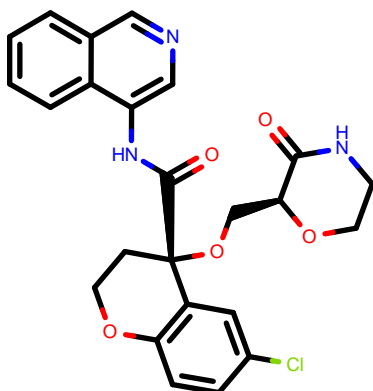
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5(C[NH2+])C[C@H]5COF

RUN: RUN1491

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.33

EN300-1706036_1_2_1



CID: EN300-1706036_1_2_1

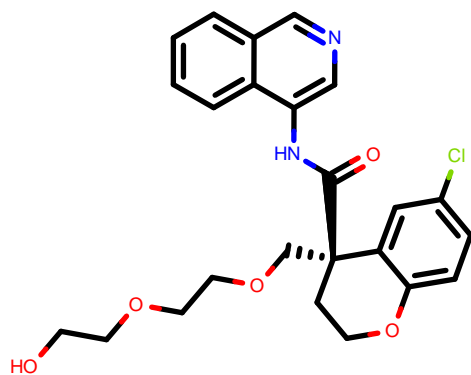
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C(=O)NCCO5

RUN: RUN4519

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-52467_2_1_1



CID: EN300-52467_2_1_1

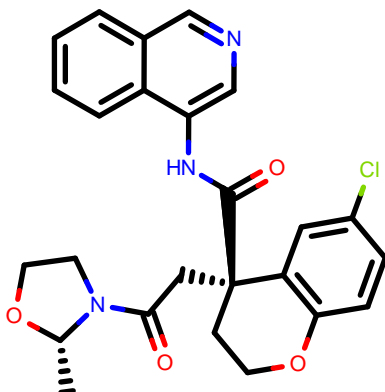
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCOCCO

RUN: RUN6299

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.24

EDG-MED-ba1ac7b9-7_4



CID: EDG-MED-ba1ac7b9-7_4

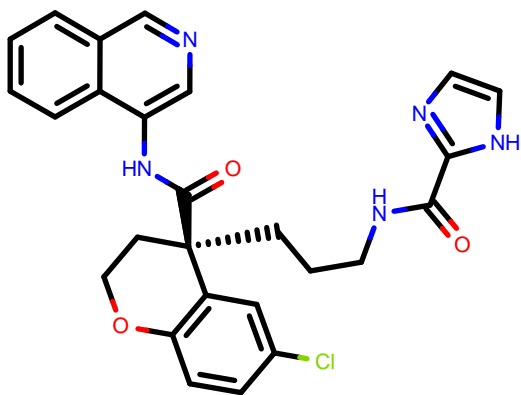
SMILES: C[C@H]1N(CCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN2463

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.25

EN300-315836_4_1_1



CID: EN300-315836_4_1_1

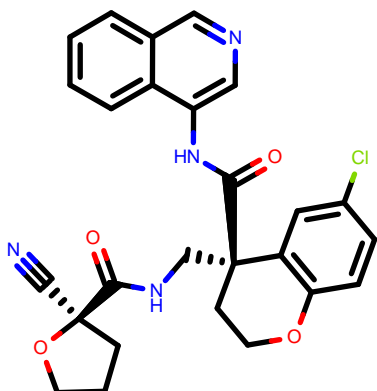
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5[nH]cn5

RUN: RUN5610

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.29

EN300-3710141_2_2_1



CID: EN300-3710141_2_2_1

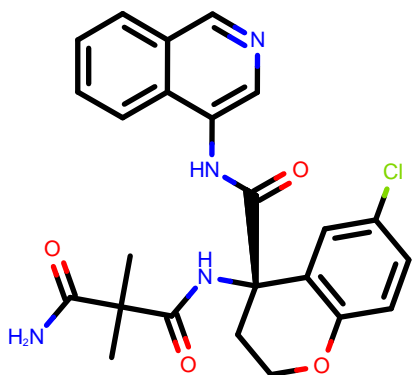
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@]5(CCCO5)C#N

RUN: RUN3235

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-182913_1_1_1



CID: EN300-182913_1_1_1

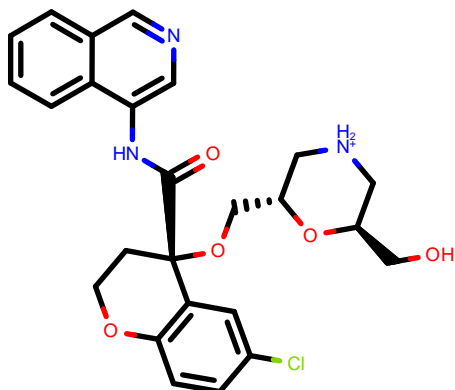
SMILES: CC(C)(C(=O)N)C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN4686

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.24

ED_-GRI-5b13fbe2-22_1



CID: ED_-GRI-5b13fbe2-22_1

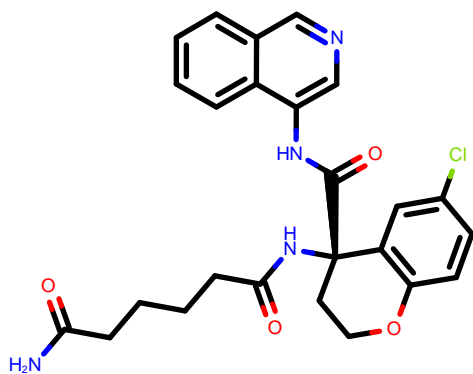
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@]5C[NH2+]C[C@H](O5)CO

RUN: RUN1405

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.38

EN300-142412_1_1_1



CID: EN300-142412_1_1_1

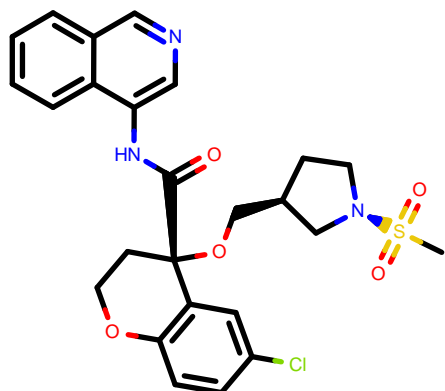
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN5294

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.28

EN300-261986_1_1_1



CID: EN300-261986_1_1_1

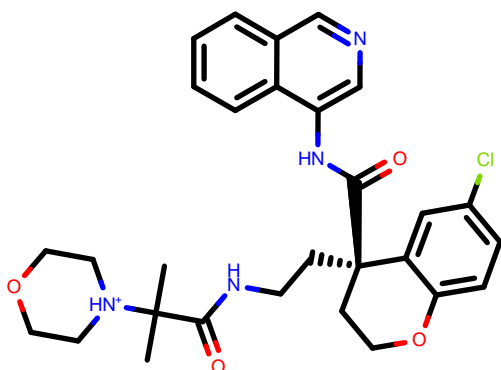
SMILES: CS(=O)(=O)N@1CC[C@@H](C1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3793

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.40

EN300-64247_3_1_1



CID: EN300-64247_3_1_1

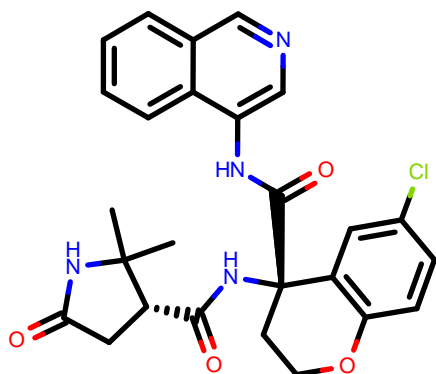
SMILES: CC(C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)[NH+]5COCOC5

RUN: RUN4542

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.46

EN300-1694056_1_1_1



CID: EN300-1694056_1_1_1

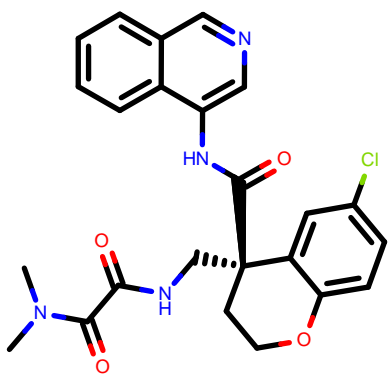
SMILES: CC1([C@@H](CC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)C

RUN: RUN3420

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.26

EN300-118647_2_1_1



CID: EN300-118647_2_1_1

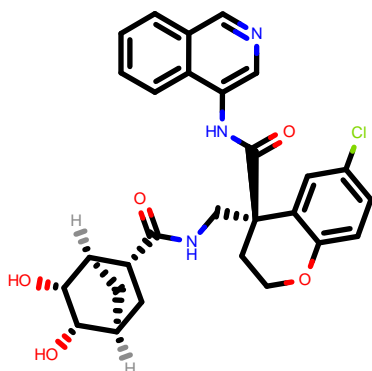
SMILES: CN(C)C(=O)C(=O)NC[C@]1(C)C(CO)C2=C1C(=O)Nc3ccc4c3cccc4

RUN: RUN6780

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-6744028_2_7_1



CID: EN300-6744028_2_7_1

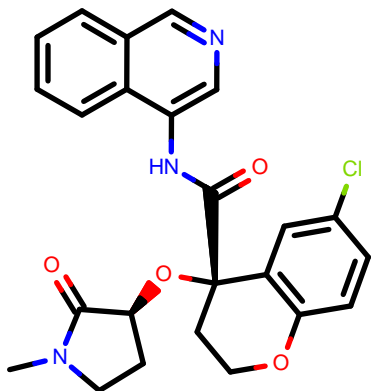
SMILES: c1ccc2c(c1)ccc2NC(=O)C[C@@]3(C)C(CO)C4=CC(=O)C(C)C(=O)Nc5ccc6c4cccc6

RUN: RUN7578

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.26

EN300-98648_1_1_1



CID: EN300-98648_1_1_1

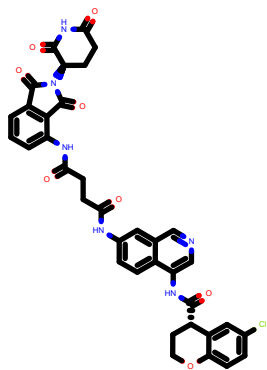
SMILES: CN1CC[C@@H](C1=O)O[C@@]2(C)C(CO)C3=CC(=O)C(=O)Nc4ccc5c4cccc5

RUN: RUN5414

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.20

DAR-DIA-9e4459de-15_11



CID: DAR-DIA-9e4459de-15_11

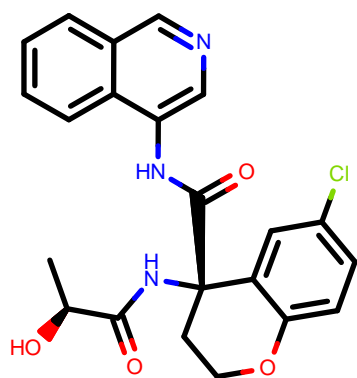
SMILES: c1ccc2c(c1)NC(=O)C(CO)C3=CC(=O)C(=O)Nc4ccc5c4cccc5

RUN: RUN1343

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.71

EN300-19542_1_1_1



CID: EN300-19542_1_1_1

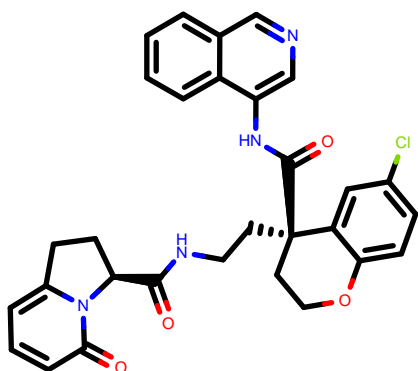
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN5166

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.21

EN300-332002_3_1_1



CID: EN300-332002_3_1_1

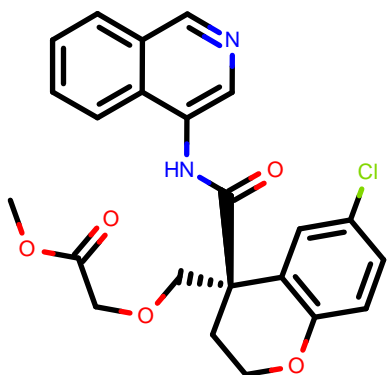
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(C)COC6c5c(-)Occc6

RUN: RUN6439

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.35

EN300-19700_2_1_1



CID: EN300-19700_2_1_1

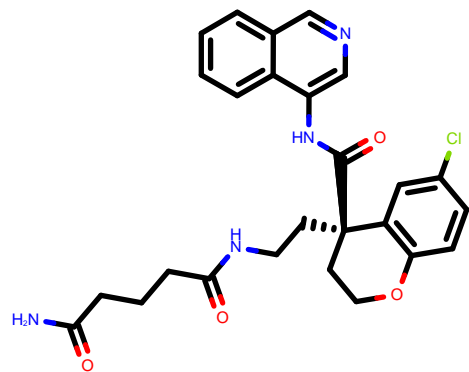
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4765

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.19

EN300-59478_3_1_1



CID: EN300-59478_3_1_1

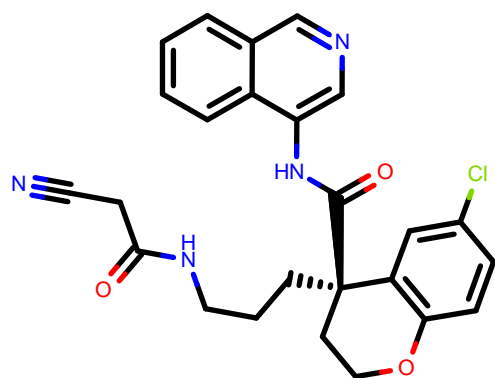
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCC(=O)N

RUN: RUN7372

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.41

EN300-19926_4_1_1



CID: EN300-19926_4_1_1

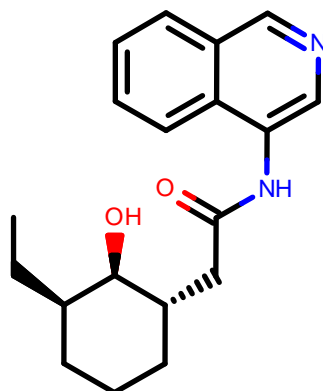
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCN(C=O)CC#N

RUN: RUN3008

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.29

MAK-UNK-c749d764-2_3



CID: MAK-UNK-c749d764-2_3

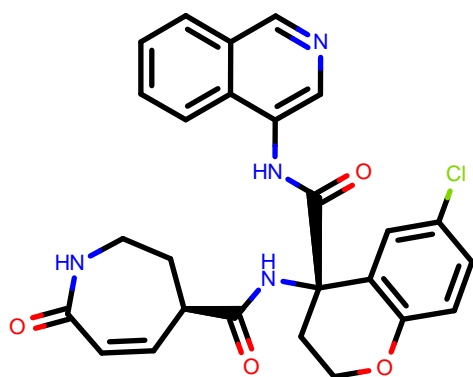
SMILES: CC[C@@H]1CCC[C@H]1([C@@H]1O)CC(=O)Nc2ncnc3c2ccc3

RUN: RUN808

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.32

EN300-152337_1_2_1



CID: EN300-152337_1_2_1

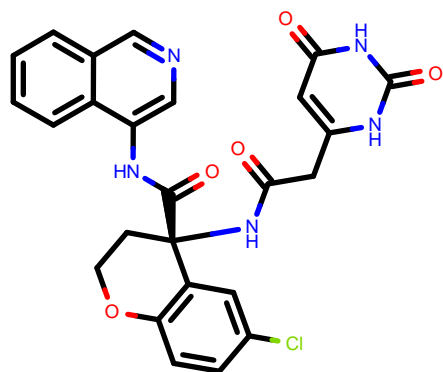
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCN5

RUN: RUN3953

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.26

EN300-11441_1_1_1



CID: EN300-11441_1_1_1

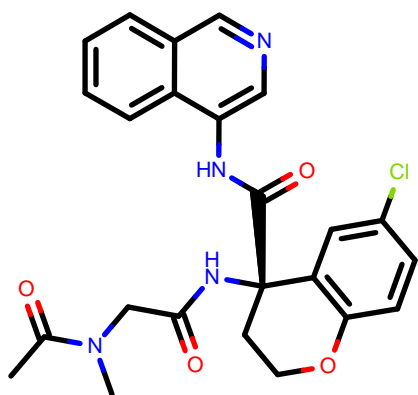
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5cc(=O)[nH]c(=O)[nH]5

RUN: RUN5706

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.25

EN300-33657_1_1_1



CID: EN300-33657_1_1_1

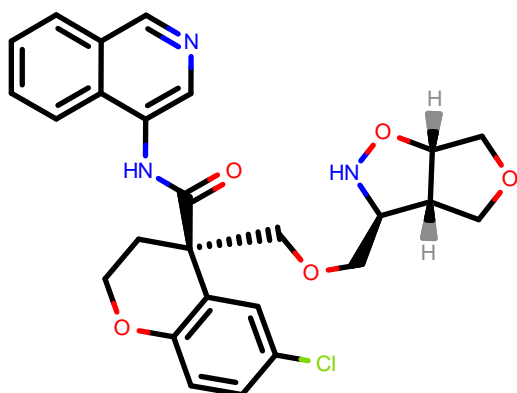
SMILES: CC(=O)N(C)CC(=O)N[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5763

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.26

EN300-7436306_2_1_1



CID: EN300-7436306_2_1_1

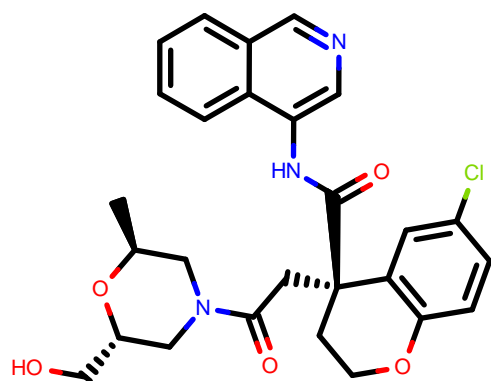
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](Cl)C(COC3c4cc(O)cc3)C(=O)N[C@@H]5C[C@H](C)O5

RUN: RUN3893

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.28

EN300-157776_1_2_1



CID: EN300-157776_1_2_1

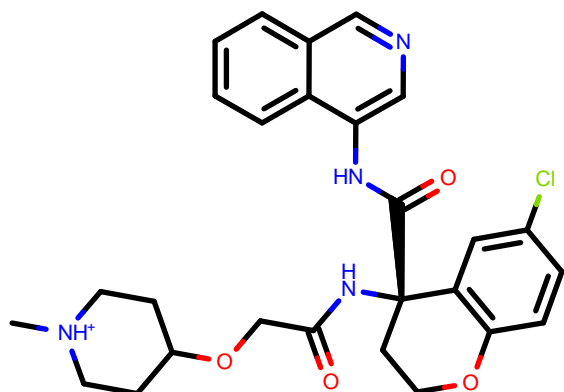
SMILES: C[C@@H]1CN[C@@H](O1)C(=O)C[C@@]2(C)C(COC3c2cc(O)cc3)C(=O)Nc4ncc5c4cccc5

RUN: RUN7139

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.38

EN300-237224_1_1_1



CID: EN300-237224_1_1_1

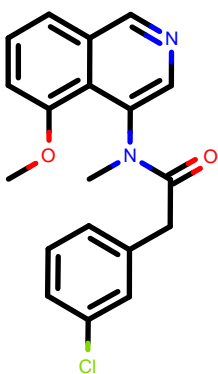
SMILES: C[NH+]1CCC(CC1)OCC(=O)N[C@@]2(C)C(COC3c2cc(O)cc3)C(=O)Nc4ncc5c4cccc5

RUN: RUN5755

DDG (kcal/mol): -0.81

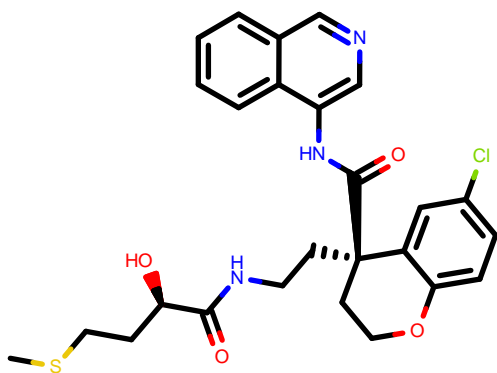
dDDG (kcal/mol): 0.34

MIC-UNK-67d4a29a-4_1



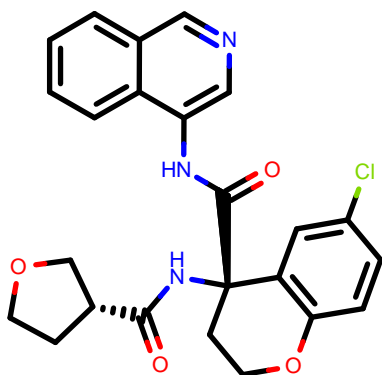
CID:	MIC-UNK-67d4a29a-4_1
SMILES:	<chem>CN(c1cncc2c1c(ccc2)OC)C(=O)Cc3cccc(c3)Cl</chem>
RUN:	RUN993
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.26

EN300-103144_3_2_1



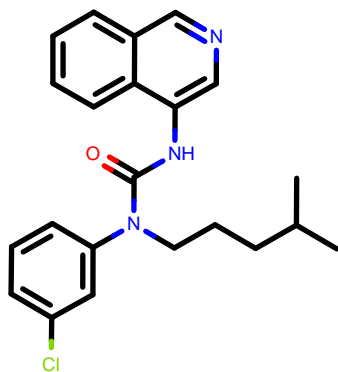
CID:	EN300-103144_3_2_1
SMILES:	<chem>CSCC[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4)O</chem>
RUN:	RUN7216
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.34

EN300-697519_1_1_1



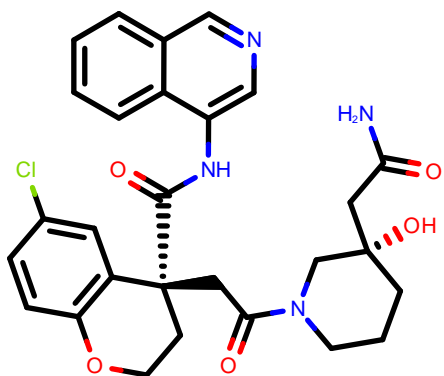
CID:	EN300-697519_1_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5COCOC5</chem>
RUN:	RUN5736
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.23

MIC-UNK-cdc2493e-19_1



CID:	MIC-UNK-cdc2493e-19_1
SMILES:	<chem>CC(C)CCCN(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN509
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.39

EN300-259060_1_1_1



CID: EN300-259060_1_1_1

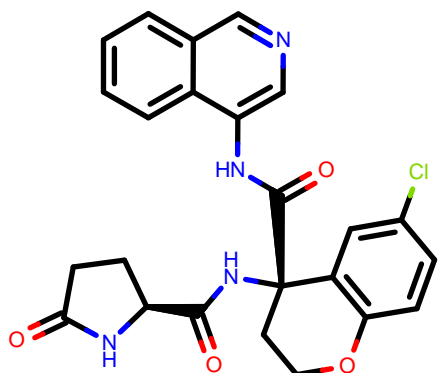
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COC(=O)C(C)CC(=O)N5CCC[C@@]3(C)C5(CC(=O)N)O

RUN: RUN7764

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.40

EN300-72896_1_1_1



CID: EN300-72896_1_1_1

SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COC(=O)C(C)C)NC(=O)[C@@]3[C@@]4H5CCC(=O)N5

RUN: RUN5397

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.21

CID: MIC-UNK-5a93dd5f-1_2

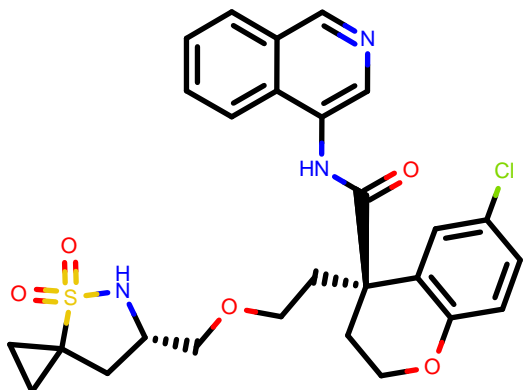
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COC(=O)C(C)C)NH+H4C[C@@]3[C@@]4H5CCC[C@@]3H5C4

RUN: RUN635

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.43

EN300-6504697_3_1_1



CID: EN300-6504697_3_1_1

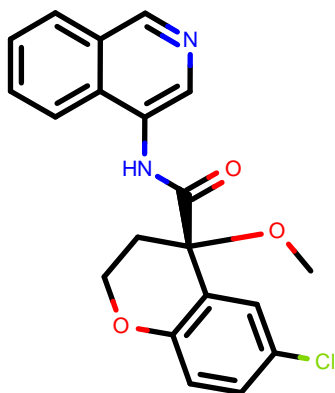
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COC(=O)C(C)C)COC(C)C[C@@]3[C@@]4H5COC(C)S(=O)(=O)N5

RUN: RUN6063

DDG (kcal/mol): -0.81

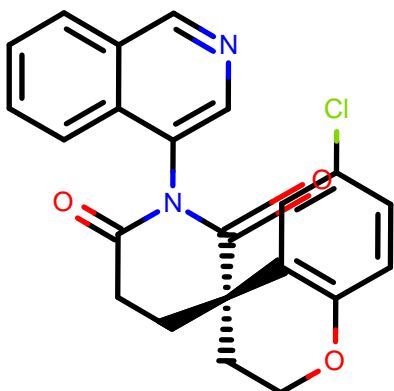
dDDG (kcal/mol): 0.31

EDJ-MED-d08626de-2_1



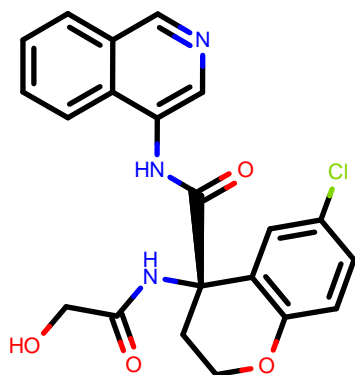
CID:	EDJ-MED-d08626de-2_1
SMILES:	<chem>CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN2192
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.12

VLA-UCB-05e51b3f-6_1



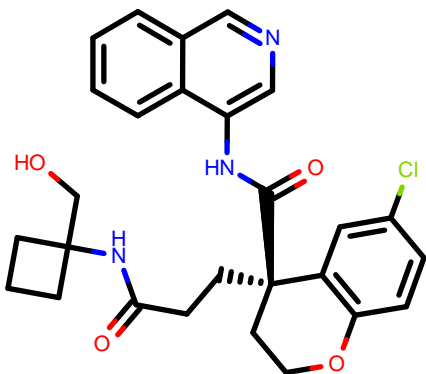
CID:	VLA-UCB-05e51b3f-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)CC[C@]4(C3=O)CCOC5c4cc(cc5)Cl</chem>
RUN:	RUN239
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.25

EDG-MED-90036822-13_1



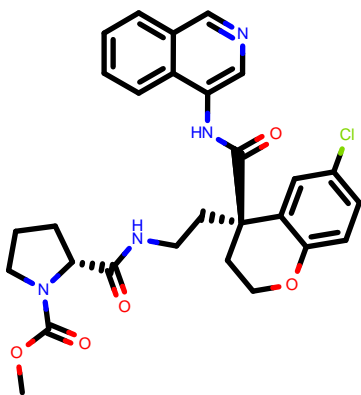
CID:	EDG-MED-90036822-13_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO</chem>
RUN:	RUN1522
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.16

EN300-1723511_2_1_1



CID:	EN300-1723511_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CCC5)CO</chem>
RUN:	RUN4804
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.26

EN300-66845_3_1_1



CID: EN300-66845_3_1_1

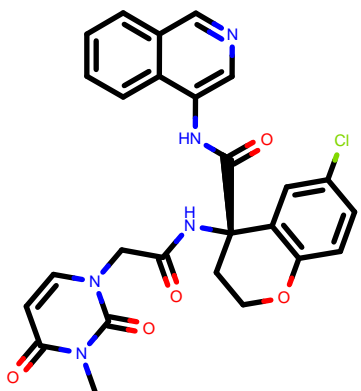
SMILES: COC(=O)N1CCC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6534

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.32

EN300-36690_1_1_1



CID: EN300-36690_1_1_1

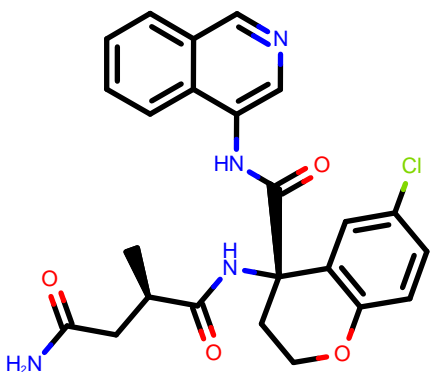
SMILES: Cn1c(=O)ccn(c1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3805

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.28

EN300-202757_1_2_1



CID: EN300-202757_1_2_1

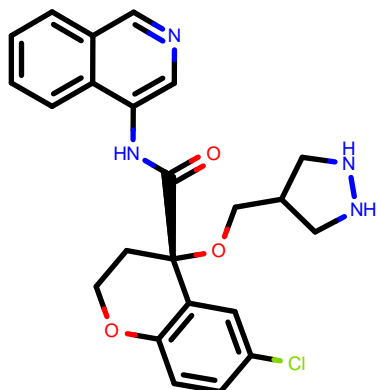
SMILES: C[C@H](CC(=O)N)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4604

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.32

ED_-GRI-5b13fbe2-53_1



CID: ED_-GRI-5b13fbe2-53_1

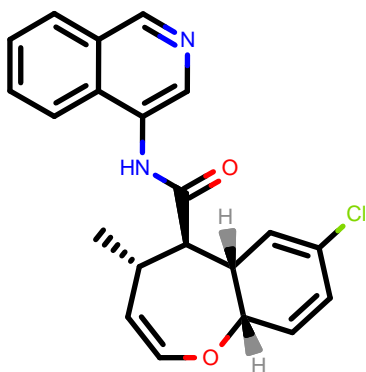
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5c[nH]nc5

RUN: RUN1438

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.21

DAR-DIA-0d514e7d-31_8



CID: DAR-DIA-0d514e7d-31_8

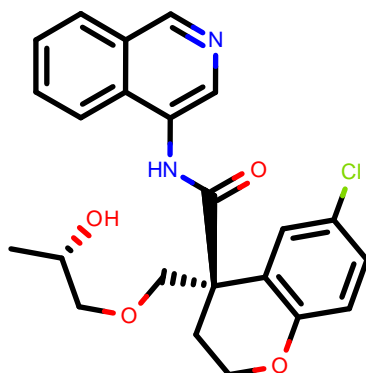
SMILES: C[C@H]1CCO[C@H]2C=CC(=C[C@H]2[C@@H]1C(=O)Nc3ccc4c3ccc4)Cl

RUN: RUN750

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.23

EN300-185378_2_1_1



CID: EN300-185378_2_1_1

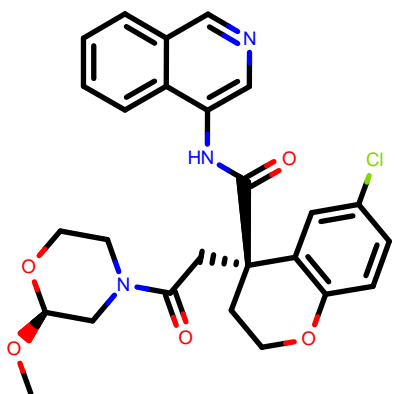
SMILES: C[C@@H](COC[C@]1(C)C(CO)c2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN4767

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.24

EN300-108507_1_1_1



CID: EN300-108507_1_1_1

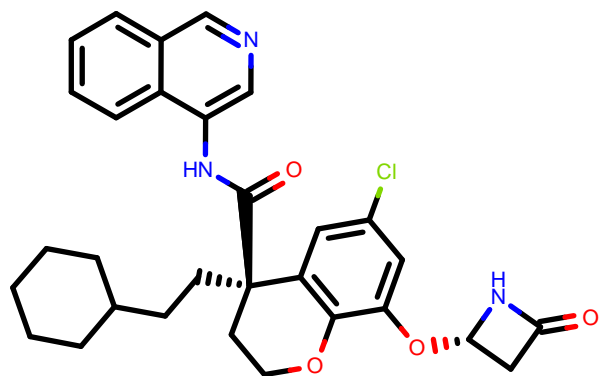
SMILES: CO[C@@H]1CN(CCO1)C(=O)C[C@]2(C)C(CCO)c3cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5819

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.31

VLA-UCB-50c39ae8-9_2



CID: VLA-UCB-50c39ae8-9_2

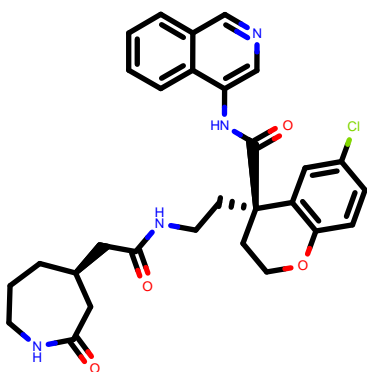
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)c4ccc(cc4O)[C@H]5CC(=O)N5)Cl)CC6CCCC6

RUN: RUN366

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.40

EN300-195590_3_1_1



CID: EN300-195590_3_1_1

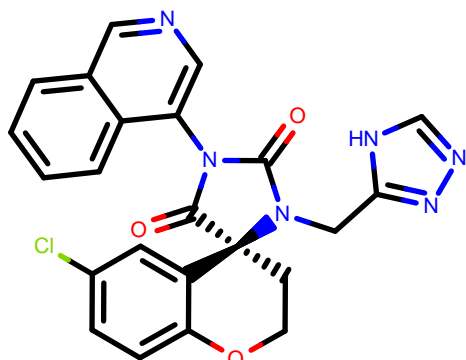
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5H5CCCCNC(=O)C5

RUN: RUN3991

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.35

VLA-UNK-f702bf1c-3_1



CID: VLA-UNK-f702bf1c-3_1

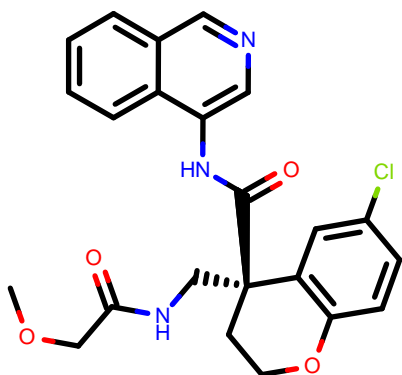
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(COCc5c4cc(cc5)Cl)N(C3=O)C6[nH]n6

RUN: RUN2111

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.30

EN300-20233_2_1_1



CID: EN300-20233_2_1_1

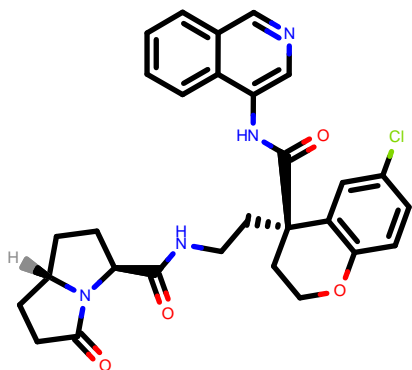
SMILES: COCC(=O)NC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6974

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.21

EN300-6479181_3_1_1



CID: EN300-6479181_3_1_1

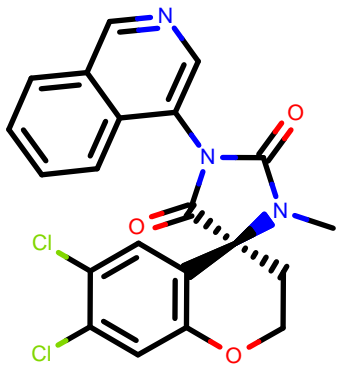
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5H5CCCC[C@@]6N5C(=O)C6

RUN: RUN6444

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.39

VLA-UNK-56836b69-3_1



CID: VLA-UNK-56836b69-3_1

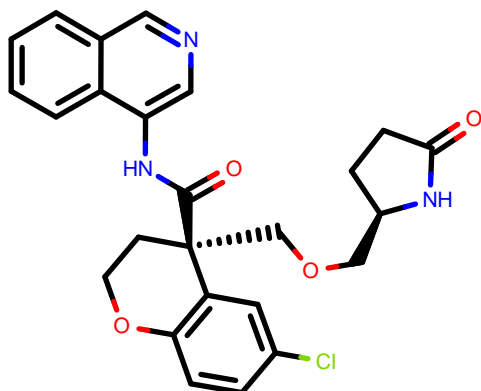
SMILES: CN1C(=O)N(C(=O)[C@@]12CCOCc3c2cc(c(c3)Cl)Cl)c4ncc5c4cccc5

RUN: RUN2098

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.24

EN300-195756_2_2_1



CID: EN300-195756_2_2_1

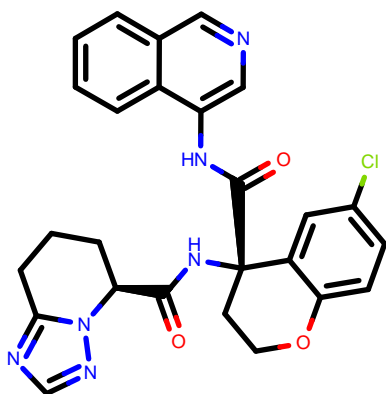
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CC(=O)N5

RUN: RUN5080

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.28

EN300-1273016_1_1_1



CID: EN300-1273016_1_1_1

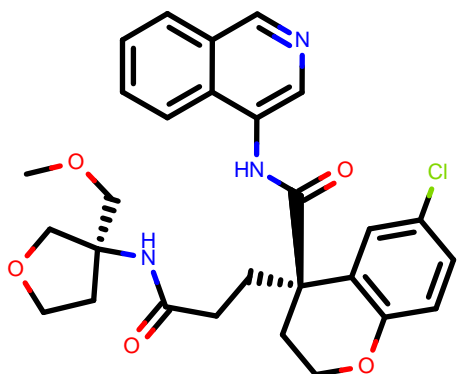
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5COCc6n5n6

RUN: RUN3339

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.24

EN300-250501_2_1_1



CID: EN300-250501_2_1_1

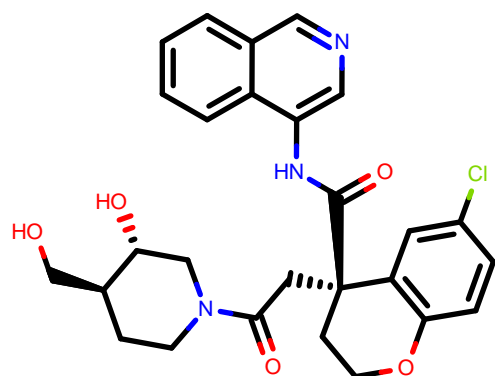
SMILES: COC[C@@]1(COC1)NC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5926

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.29

EN300-95639_1_2_1



CID: EN300-95639_1_2_1

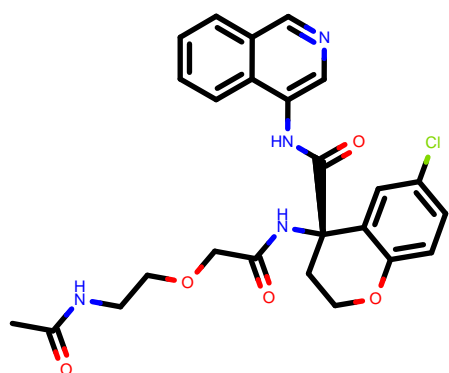
SMILES: c1ccc2c(c1)ncnc2N[C@@H](C(=O)N[C@@H]1CCOCc2ccccc2O)C(=O)N[C@@H]3CCOC4C(=O)N[C@@H]3C(=O)C

RUN: RUN3763

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.34

EN300-126555_1_1_1



CID: EN300-126555_1_1_1

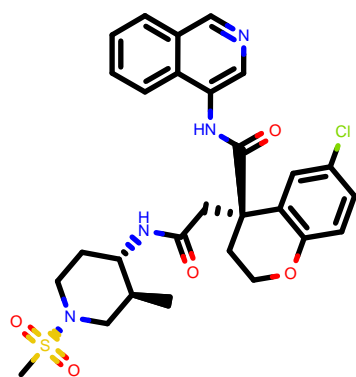
SMILES: CC(=O)NCCOCC(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4773

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.32

ALP-POS-2da19ca7-7_2



CID: ALP-POS-2da19ca7-7_2

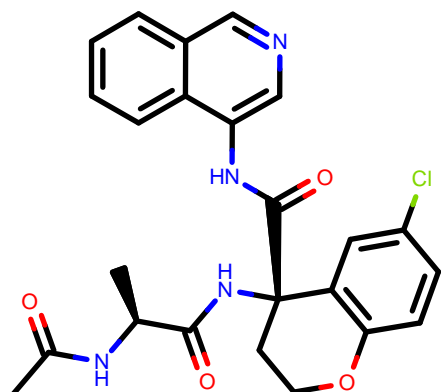
SMILES: C[C@@H]1CN[C@@H]1CC(=O)N[C@@H]2(C(=O)N[C@@H]3CCOC4C(=O)N[C@@H]3C(=O)C)C(=O)N[C@@H]2C(=O)C

RUN: RUN2240

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.39

EN300-18569_1_1_1



CID: EN300-18569_1_1_1

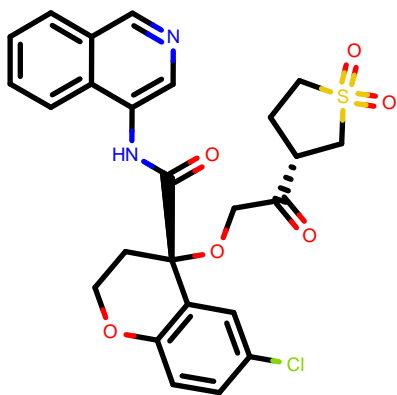
SMILES: C[C@@H]1CN[C@@H]1CC(=O)N[C@@H]2(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4N[C@@H]2C(=O)C

RUN: RUN6152

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.24

CHO-MSK-5891c1ff-5_1



CID: CHO-MSK-5891c1ff-5_1

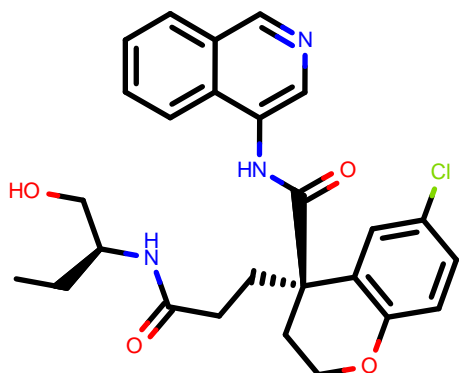
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)C@H]5CCS(=O)(=O)C5

RUN: RUN1797

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.34

EN300-157897_2_1_1



CID: EN300-157897_2_1_1

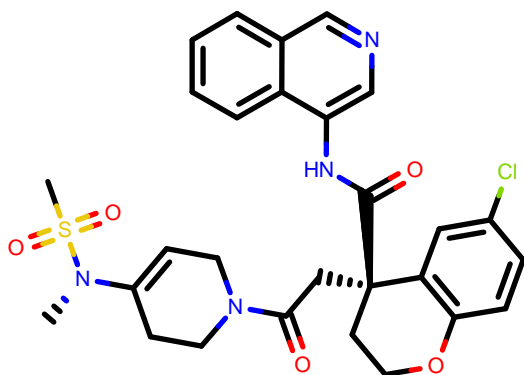
SMILES: CC[C@@H](CO)NC(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN7455

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.39

KAD-UNI-80f122c8-5_4



CID: KAD-UNI-80f122c8-5_4

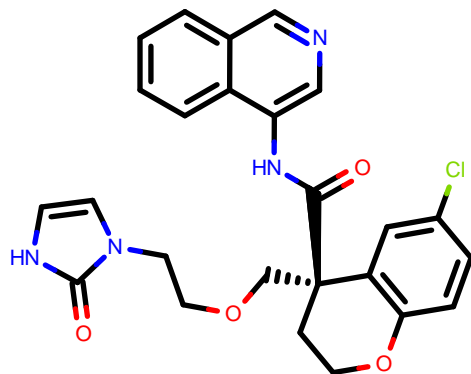
SMILES: CN@]1C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5S(=O)(=O)C

RUN: RUN2212

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.29

EN300-214800_2_1_1



CID: EN300-214800_2_1_1

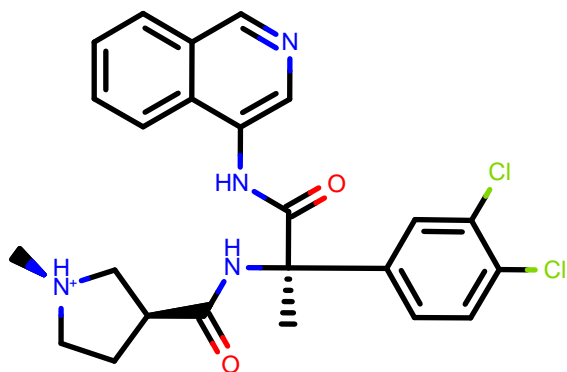
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCN5CCNC5=O

RUN: RUN4389

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.24

MAT-POS-e9e99895-13_7



CID: MAT-POS-e9e99895-13_7

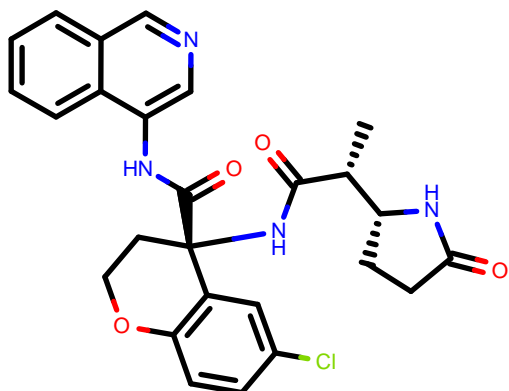
SMILES: C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2ccc3c2ccc3)NC(=O)[C@H]4CC[N@H]4C4C

RUN: RUN2170

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.52

EN300-249421_1_4_1



CID: EN300-249421_1_4_1

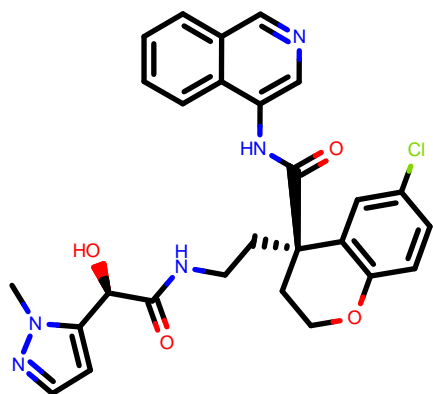
SMILES: C[C@H]([C@H]1CCC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3229

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.25

EN300-6473273_3_2_1



CID: EN300-6473273_3_2_1

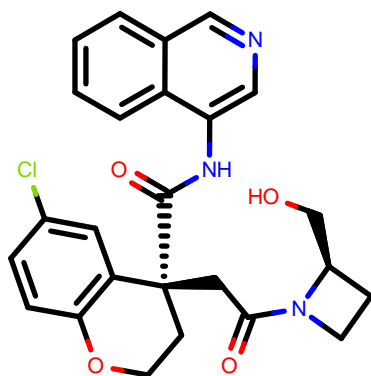
SMILES: Cn1c(cn1)[C@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN5024

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.39

EDG-MED-ba1ac7b9-2_1



CID: EDG-MED-ba1ac7b9-2_1

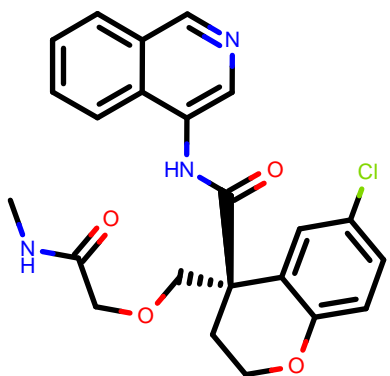
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO

RUN: RUN2464

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.29

EN300-2977549_2_1_1



CID: EN300-2977549_2_1_1

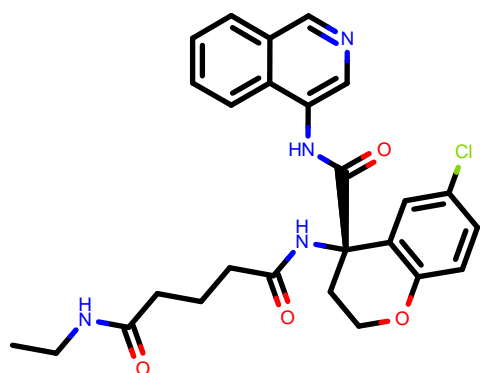
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5595

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.21

EN300-68635_1_1_1



CID: EN300-68635_1_1_1

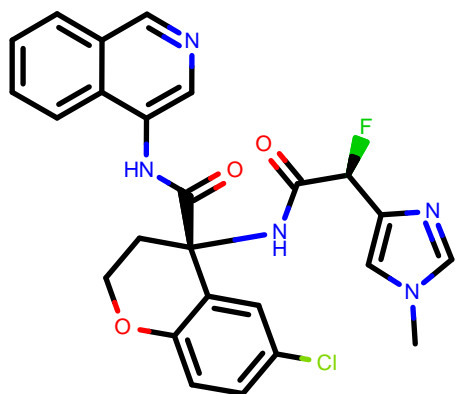
SMILES: CCNC(=O)CCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5209

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.28

EDG-MED-90036822-25_1



CID: EDG-MED-90036822-25_1

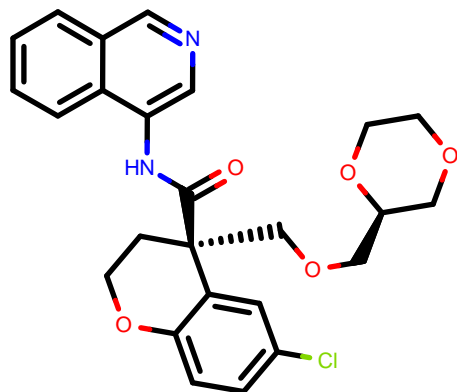
SMILES: Cn1cc(nc1)[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)F

RUN: RUN1580

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.26

EN300-139167_2_1_1



CID: EN300-139167_2_1_1

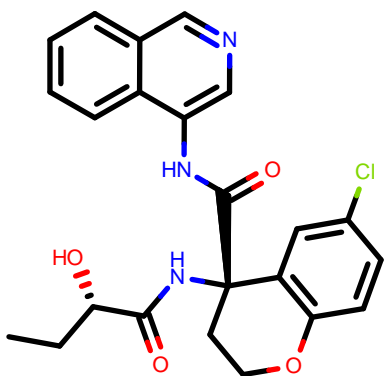
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5H5COCOC5

RUN: RUN4847

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.23

EN300-181492_1_1_1



CID: EN300-181492_1_1_1

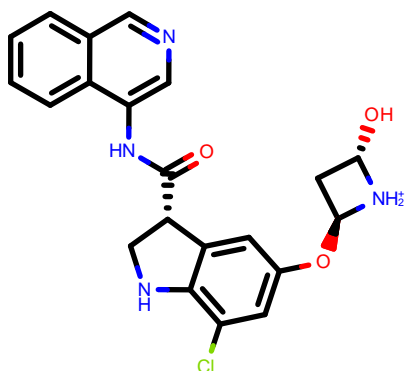
SMILES: C=C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5318

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.27

FRA-DIA-b66f7109-1_2



CID: FRA-DIA-b66f7109-1_2

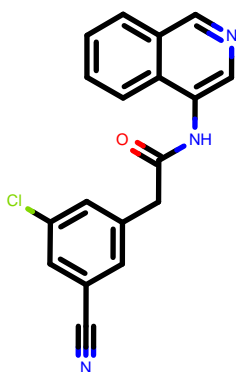
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@H]3CNc4c3cc(cc4Cl)O[C@H]5CC(=O)N5

RUN: RUN328

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.36

MAT-POS-cc05818f-1_1



CID: MAT-POS-cc05818f-1_1

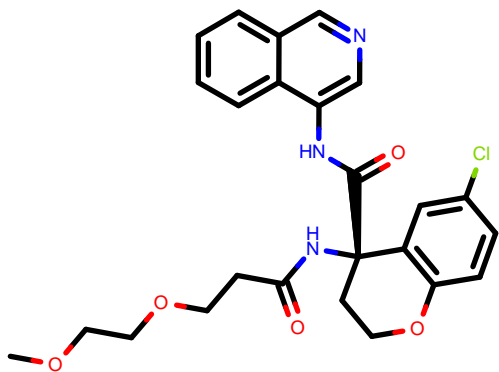
SMILES: c1ccc2c(c1)cnc2NC(=O)Cc3cc(cc(c3)Cl)C#N

RUN: RUN2003

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.28

EN300-55250_1_1_1



CID: EN300-55250_1_1_1

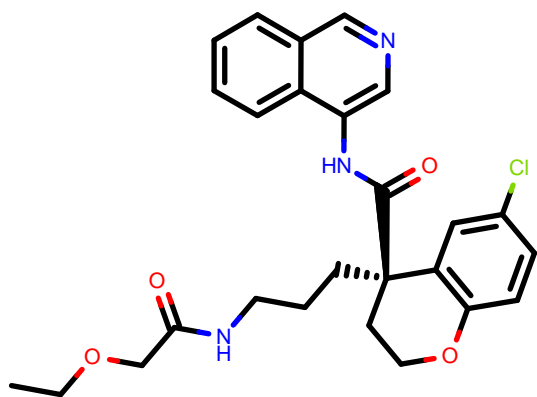
SMILES: COCCOCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5936

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.24

EN300-21303_4_1_1



CID: EN300-21303_4_1_1

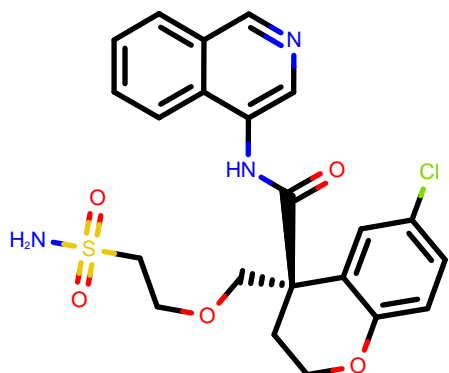
SMILES: CCOCC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6209

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-270710_2_1_1



CID: EN300-270710_2_1_1

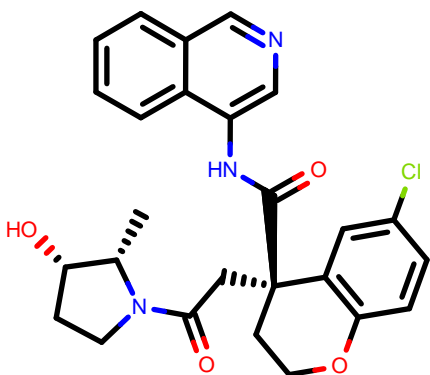
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N

RUN: RUN4387

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.25

EN300-2008120_1_1_1



CID: EN300-2008120_1_1_1

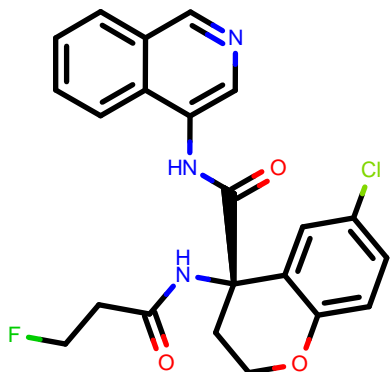
SMILES: C[C@H]1[C@H](CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN5270

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.36

EDG-MED-90036822-100_1



CID: EDG-MED-90036822-100_1

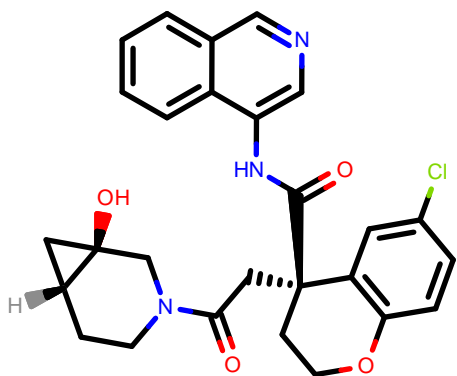
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCF

RUN: RUN1668

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.20

EN300-1267093_1_1_1



CID: EN300-1267093_1_1_1

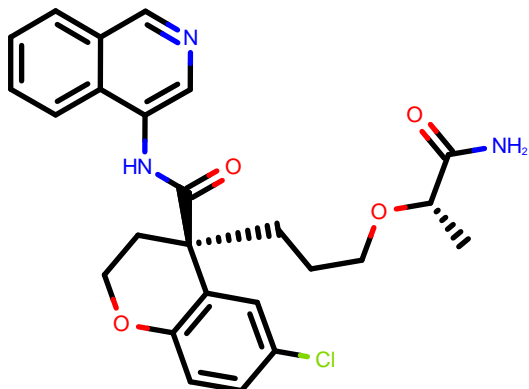
SMILES: c1cc2c(c1)nc2N(C(=O)C@H)(C@H)(C(=O)C1=O)N5CC1C@H)(C1C@H)C5=O

RUN: RUN4650

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.25

EN300-17381_4_1_1



CID: EN300-17381_4_1_1

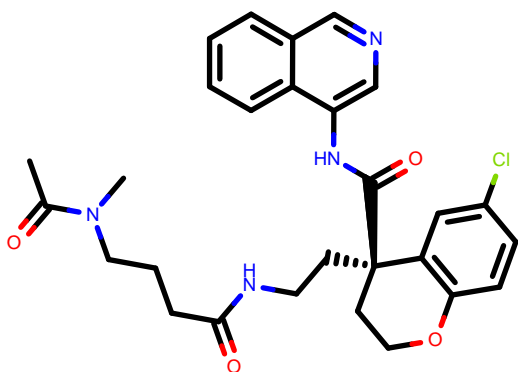
SMILES: C[C@@H](C(=O)N)OCCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN5240

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-128750_3_1_1



CID: EN300-128750_3_1_1

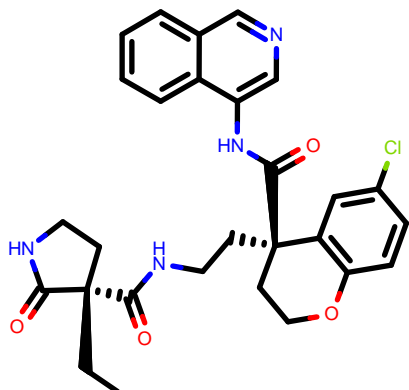
SMILES: CC(=O)N(C)OCCC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN5299

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.31

EN300-304135_3_1_1



CID: EN300-304135_3_1_1

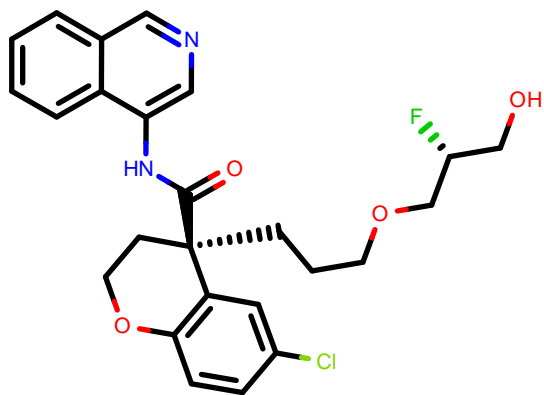
SMILES: CC[C@H]1(CCN(C1=O)C(=O)NCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN3661

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.35

EN300-1600517_4_1_1



CID: EN300-1600517_4_1_1

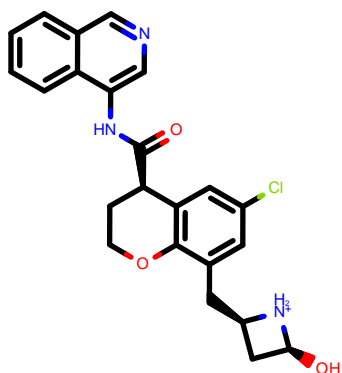
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCOC[C@@H](CO)F

RUN: RUN7070

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.48

DAR-DIA-6a508060-5_1_1



CID: DAR-DIA-6a508060-5_1_1

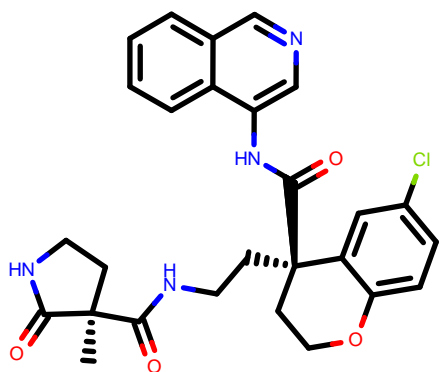
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)C@H]5C[C@@H]([NH2+])O)Cl

RUN: RUN4913

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-207959_3_2_1



CID: EN300-207959_3_2_1

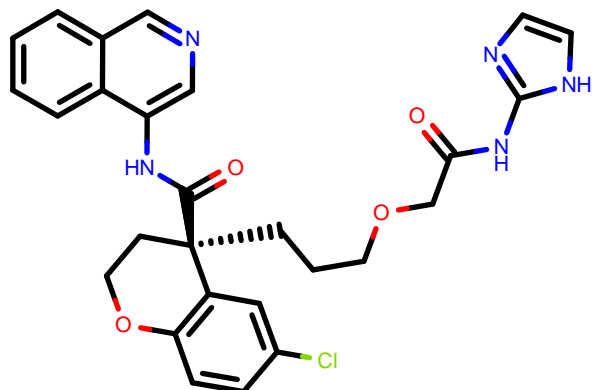
SMILES: C[C@@]1(C)CNC1=O[C@@]2(C)NCC[C@@]2(CCOc3c2cc(cc3C)C)C(=O)Nc4ncnc5c4ccoc5

RUN: RUN4211

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.36

EN300-331993_4_1_1



CID: EN300-331993_4_1_1

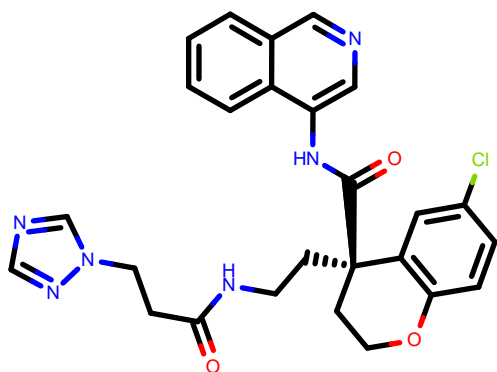
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCOC(=O)Nc5[nH]cn5

RUN: RUN6628

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.24

EN300-26147_3_1_1



CID: EN300-26147_3_1_1

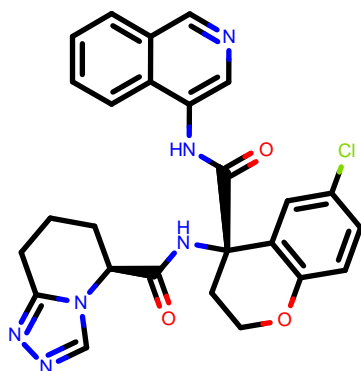
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5cnm5

RUN: RUN4310

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.42

EN300-6478631_1_1_1



CID: EN300-6478631_1_1_1

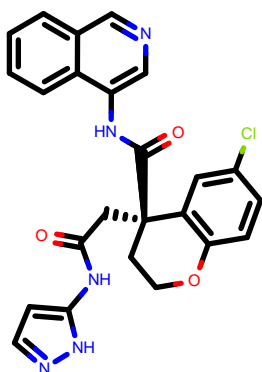
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5COCc6n5nm6

RUN: RUN4180

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

JAG-UCB-706446eb-6_1_1



CID: JAG-UCB-706446eb-6_1_1

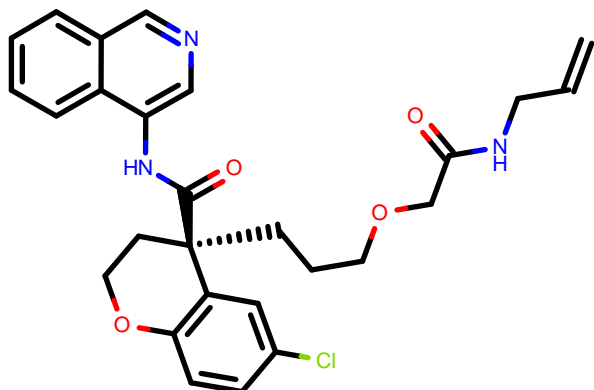
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5cn[nH]5

RUN: RUN6284

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

EN300-17184_4_1_1



CID: EN300-17184_4_1_1

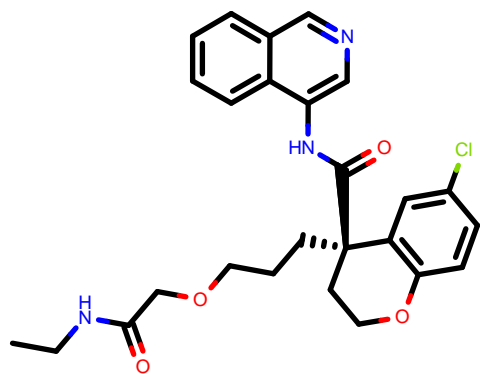
SMILES: C=CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN5250

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.29

EN300-7003350_4_1_1



CID: EN300-7003350_4_1_1

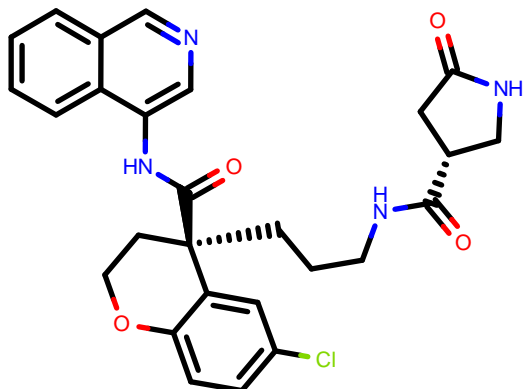
SMILES: CCNC(=O)COCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN6944

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.26

EN300-59487_4_1_1



CID: EN300-59487_4_1_1

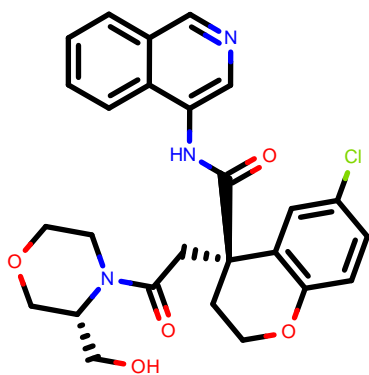
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@]5CNC(=O)NC5

RUN: RUN7755

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.37

EN300-154201_1_2_1



CID: EN300-154201_1_2_1

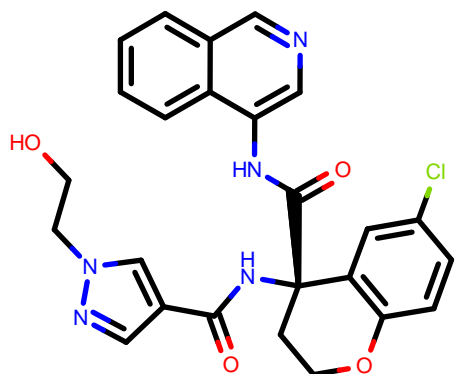
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@]5C(O)

RUN: RUN4859

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.36

EN300-761209_1_1_1



CID: EN300-761209_1_1_1

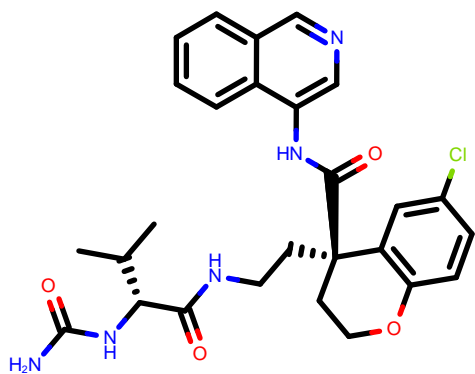
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn(c5)CCO

RUN: RUN5941

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.22

EN300-2972220_3_1_1



CID: EN300-2972220_3_1_1

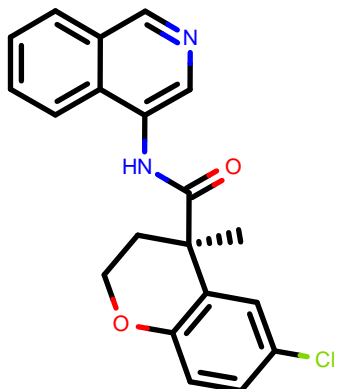
SMILES: CC(C)[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N

RUN: RUN6160

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.32

EDJ-MED-e4b030d8-13_1



CID: EDJ-MED-e4b030d8-13_1

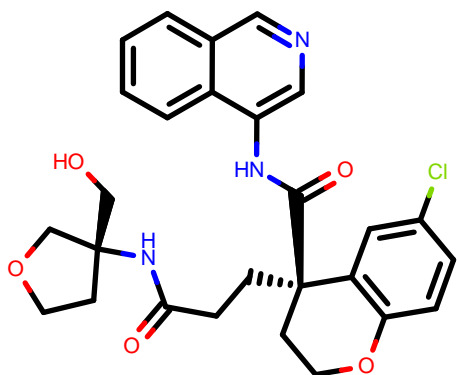
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN222

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.10

EN300-133788_2_1_1



CID: EN300-133788_2_1_1

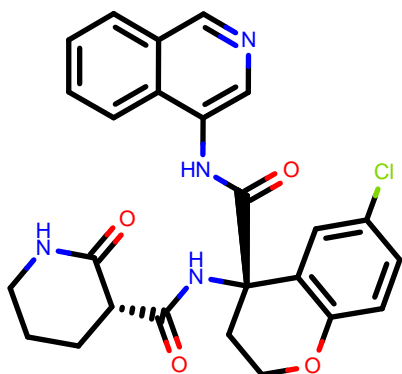
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]5(CCOCC5)CO

RUN: RUN7239

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.35

EN300-82616_1_1_1



CID: EN300-82616_1_1_1

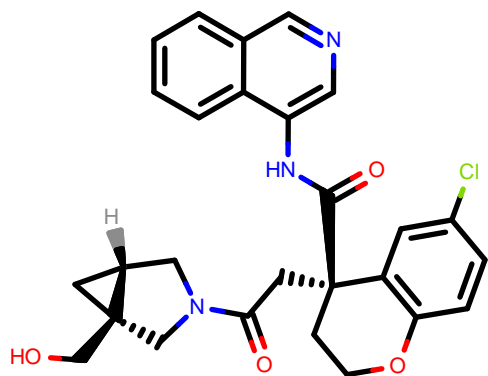
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCCN5)O

RUN: RUN3647

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.27

EN300-154179_1_4_1



CID: EN300-154179_1_4_1

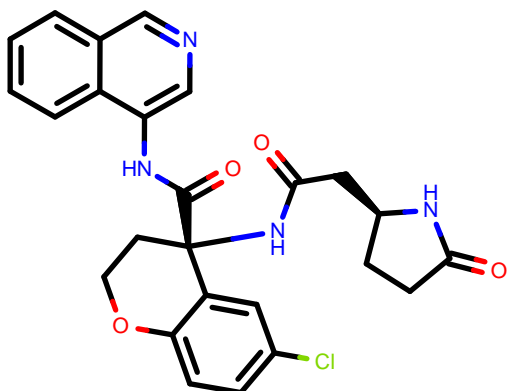
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@]8(C)C5)CO

RUN: RUN4220

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.30

EN300-68203_1_1_1



CID: EN300-68203_1_1_1

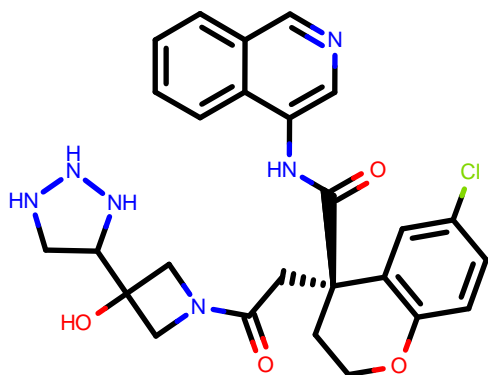
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@]8H5CCC(=O)N5

RUN: RUN7623

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.18

EN300-384234_1_1_1



CID: EN300-384234_1_1_1

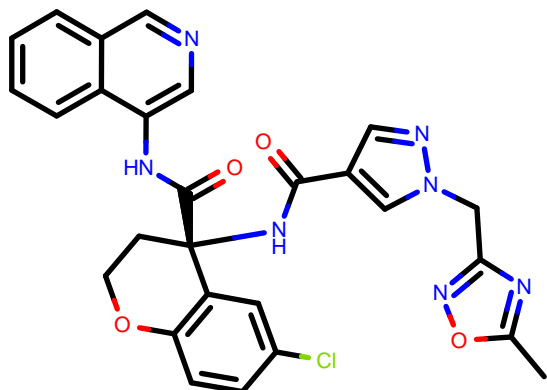
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cn[nH]n6)O

RUN: RUN6758

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.35

EN300-131219_1_1_1



CID: EN300-131219_1_1_1

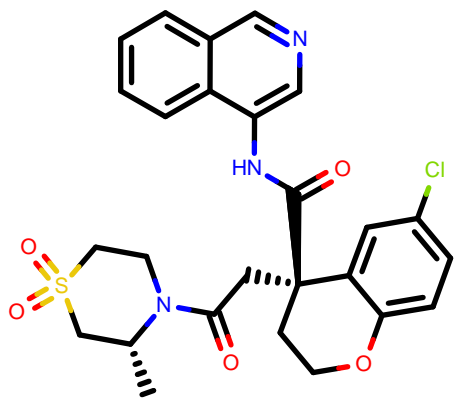
SMILES: Cc1nc(nc1)Cn2cc(cn2)C(=O)N[C@@3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncnc6c5ccc6

RUN: RUN4024

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.28

EN300-6497238_1_1_1



CID: EN300-6497238_1_1_1

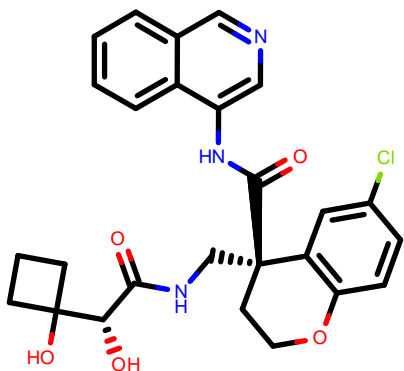
SMILES: C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5905

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.38

EN300-1073320_2_1_1



CID: EN300-1073320_2_1_1

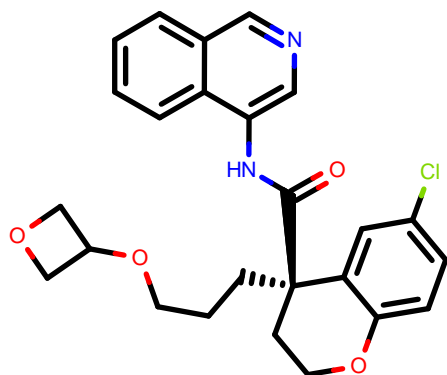
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN6663

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.39

EN300-317082_4_1_1



CID: EN300-317082_4_1_1

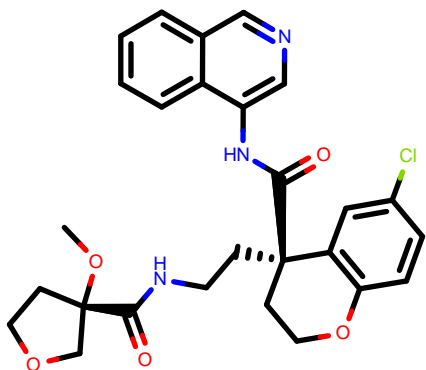
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC5COC5

RUN: RUN4740

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.31

EN300-174668_3_2_1



CID: EN300-174668_3_2_1

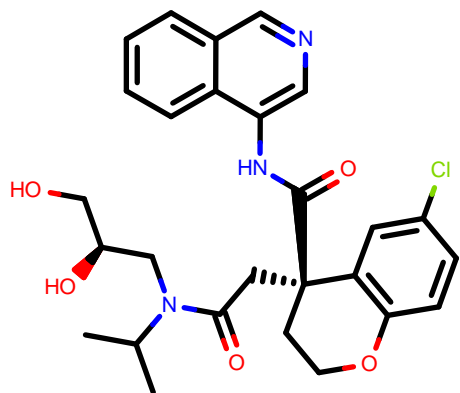
SMILES: CO[C@@]1(CCOc1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4420

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.42

EN300-138953_1_2_1



CID: EN300-138953_1_2_1

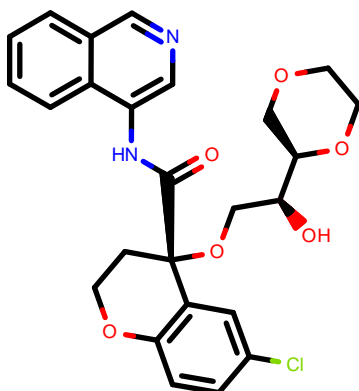
SMILES: CC(C)N(C)C@H](CO)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN5771

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.50

EN300-6238494_1_2_1



CID: EN300-6238494_1_2_1

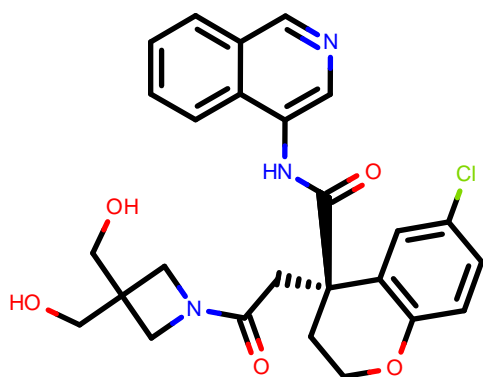
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]H([C@@H]5COCCO5)O

RUN: RUN5077

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.33

EN300-396146_1_1_1



CID: EN300-396146_1_1_1

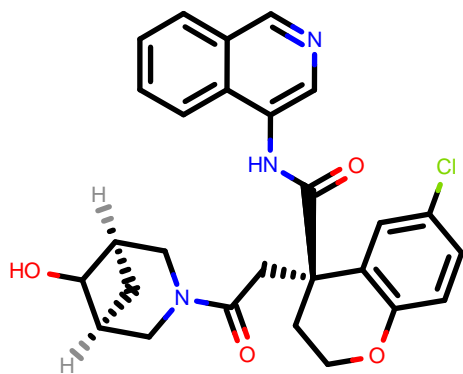
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)CO

RUN: RUN6693

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.29

EN300-90206_1_1_1



CID: EN300-90206_1_1_1

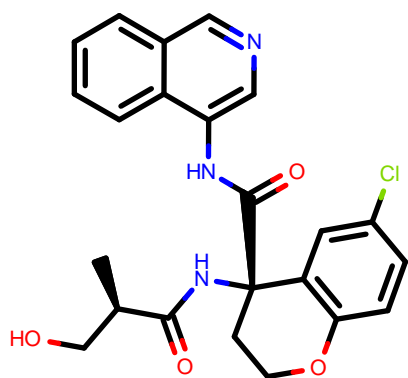
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@@H](C5)O6

RUN: RUN3861

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.25

EN300-55072_1_2_1



CID: EN300-55072_1_2_1

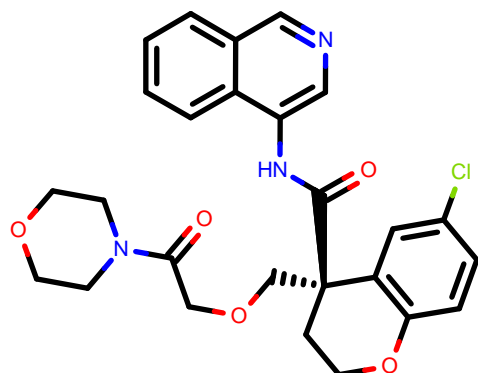
SMILES: C[C@H](CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN5346

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-1241327_2_1_1



CID: EN300-1241327_2_1_1

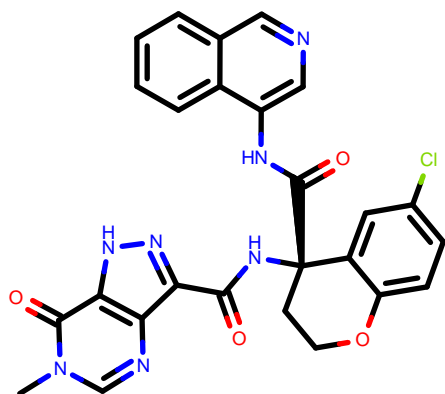
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CCOCC5

RUN: RUN5543

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.31

EN300-7355979_1_1_1



CID: EN300-7355979_1_1_1

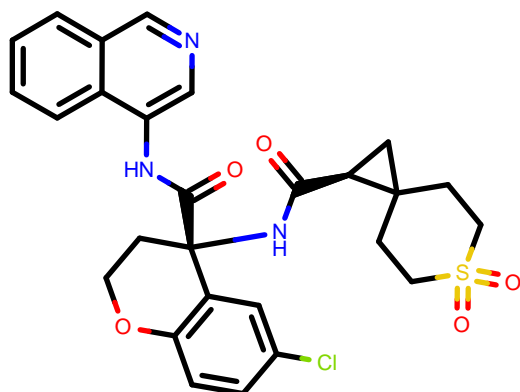
SMILES: Cn1cnc2c(c1=O)[nH]nc2C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6

RUN: RUN7629

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.24

EN300-141809_1_2_1



CID: EN300-141809_1_2_1

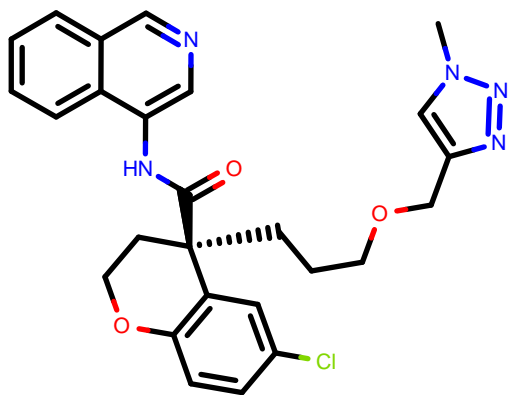
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C(=O)O)S(=O)(=O)C5=CC=CC=C5

RUN: RUN7591

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.34

EN300-120282_4_1_1



CID: EN300-120282_4_1_1

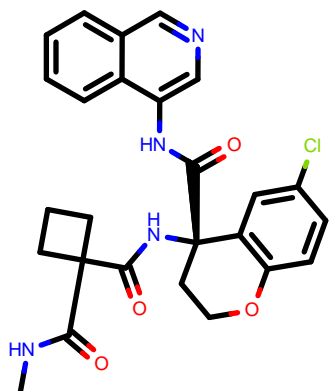
SMILES: Cn1cc(nn1)COC[C@]2(C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN5527

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.33

EN300-70064_1_1_1



CID: EN300-70064_1_1_1

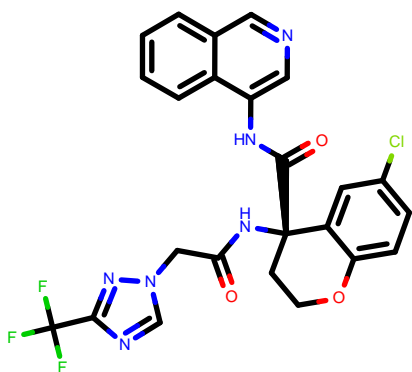
SMILES: CNC(=O)C1(CCC1)C(=O)N[C@]2(C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN4195

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.24

ALP-UNI-dbbfd3db-7_1



CID: ALP-UNI-dbbfd3db-7_1

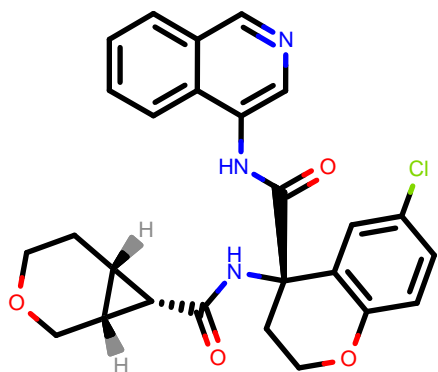
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN2636

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.29

EN300-1644723_1_6_1



CID: EN300-1644723_1_6_1

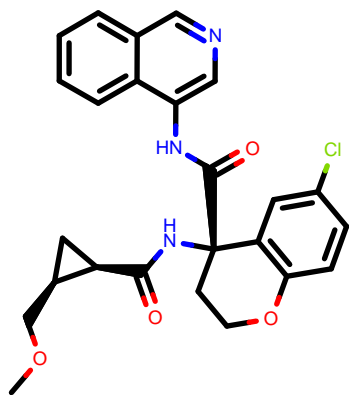
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN4583

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.31

EN300-705381_1_1_1



CID: EN300-705381_1_1_1

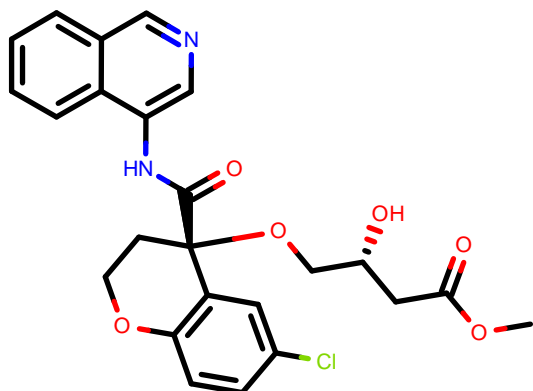
SMILES: COC[C@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5787

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.21

EN300-73662_1_1_1



CID: EN300-73662_1_1_1

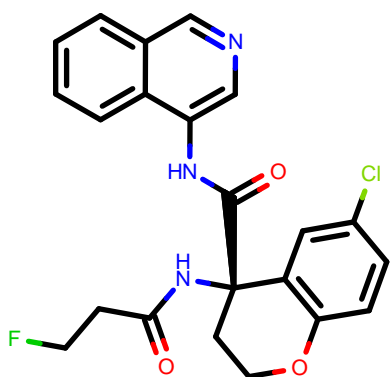
SMILES: COc(=O)C[C@H]1C[C@@]1(CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)O

RUN: RUN5783

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.36

EN300-97758_1_1_1



CID: EN300-97758_1_1_1

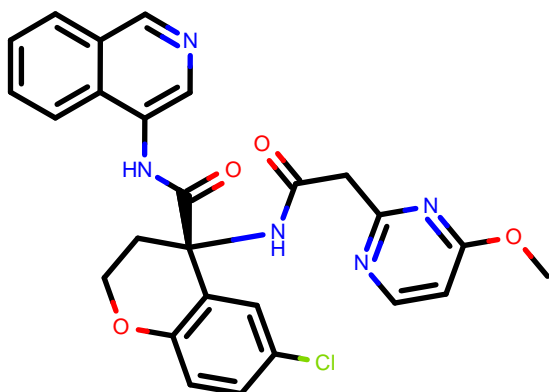
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCF

RUN: RUN5265

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.18

EN300-6480588_1_1_1



CID: EN300-6480588_1_1_1

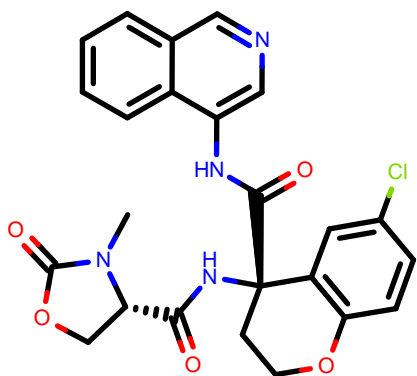
SMILES: COc1ccnc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5725

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.35

EN300-332838_1_1_1



CID: EN300-332838_1_1_1

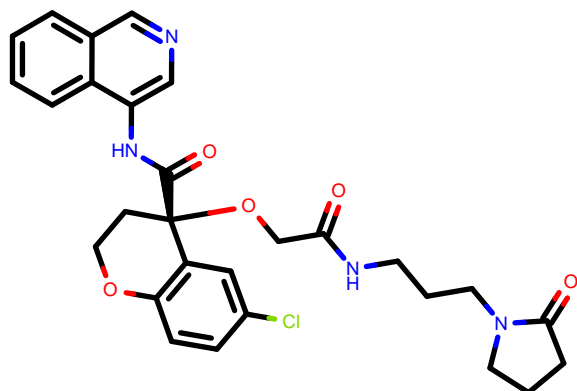
SMILES: CN1[C@@H](COC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN4609

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.26

EN300-08259_1_1_1



CID: EN300-08259_1_1_1

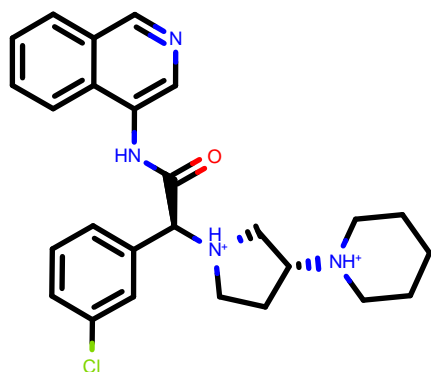
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCN5CCCC5=O

RUN: RUN5719

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.40

MIC-UNK-5a93dd5f-12_6



CID: MIC-UNK-5a93dd5f-12_6

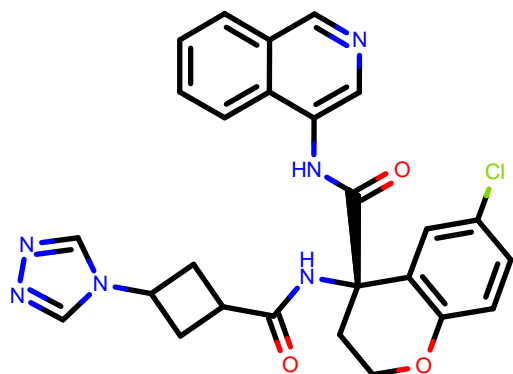
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H](c3ccccc3)C1N@@@4CC[C@@H](C4)[NH+]5CCCCC5

RUN: RUN717

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.42

EN300-7463161_1_1_1



CID: EN300-7463161_1_1_1

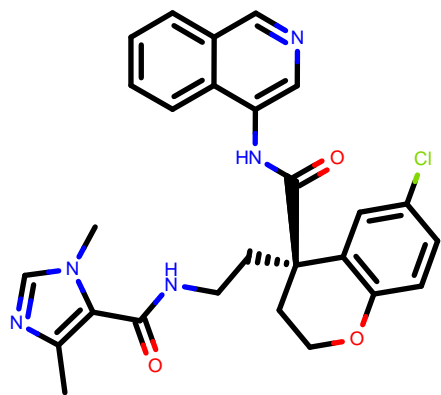
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5(C5)C5C(C5)n6cnnc6

RUN: RUN3961

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.29

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

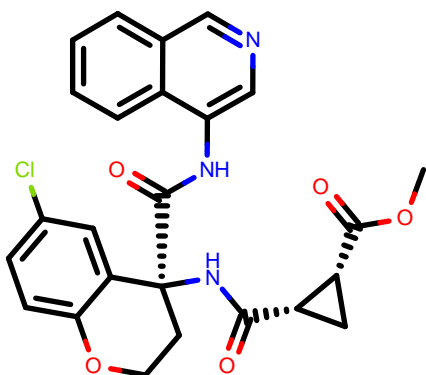
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7355

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.36

EN300-66764_1_1_1



CID: EN300-66764_1_1_1

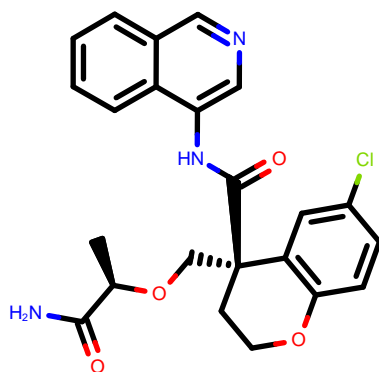
SMILES: COC(=O)[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6902

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.22

EN300-17381_2_2_1



CID: EN300-17381_2_2_1

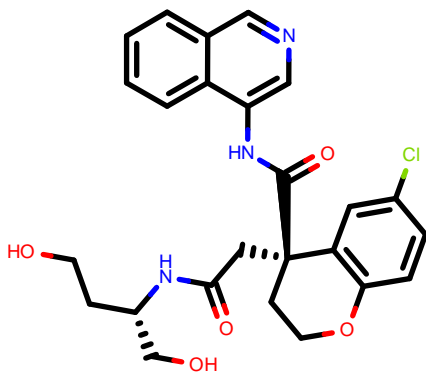
SMILES: C[C@H](C(=O)N)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7280

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-195790_1_1_1



CID: EN300-195790_1_1_1

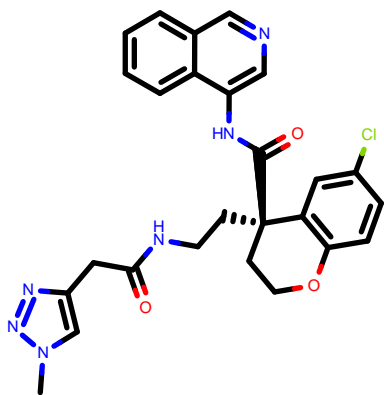
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)CO

RUN: RUN7483

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.29

KAD-UNI-8a629cb0-47_1



CID: KAD-UNI-8a629cb0-47_1

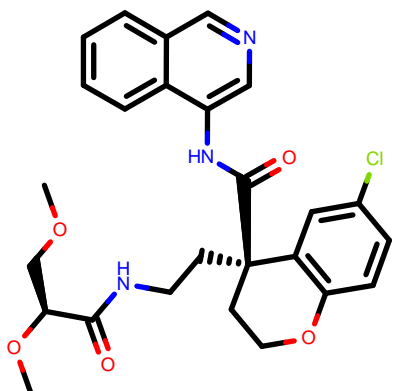
SMILES: Cn1cc(nn1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2028

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.32

EN300-305282_3_1_1



CID: EN300-305282_3_1_1

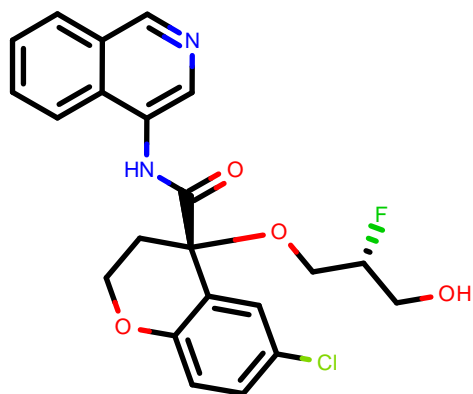
SMILES: COC[C@@H](C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC

RUN: RUN7686

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.36

EN300-1600517_1_1_1



CID: EN300-1600517_1_1_1

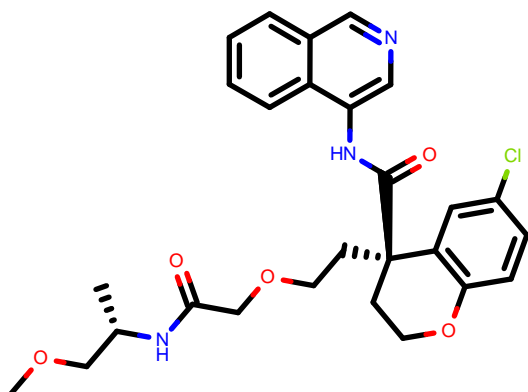
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC[C@@H](CO)F

RUN: RUN5711

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

EN300-02067_3_1_1



CID: EN300-02067_3_1_1

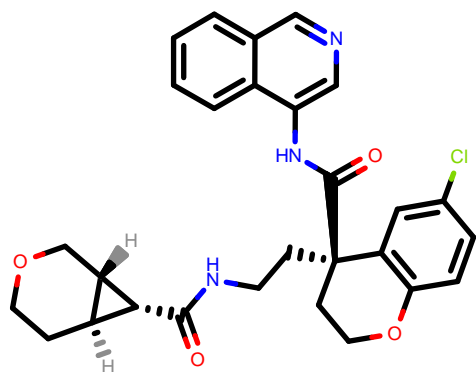
SMILES: C[C@@H](CO)NC(=O)COC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6625

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.35

KAD-UNI-8a629cb0-34_1



CID: KAD-UNI-8a629cb0-34_1

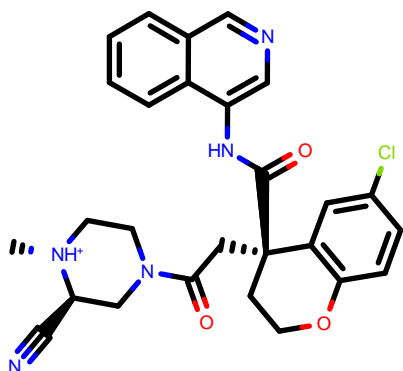
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@@]5H5C[C@@]H5C[C@@]H5COCC6

RUN: RUN1990

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-14_8



CID: EDG-MED-ba1ac7b9-14_8

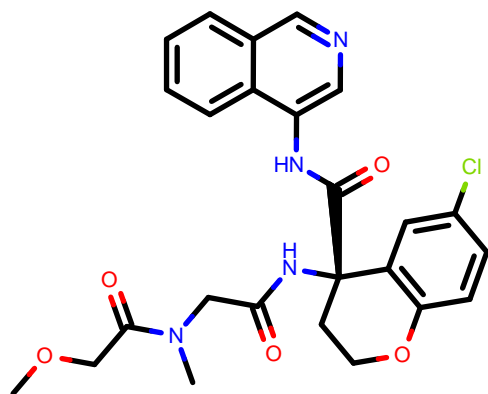
SMILES: C1N[C@@]1CCN(C[C@@]2(C)C(=O)C[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2487

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.30

EN300-35612_1_1_1



CID: EN300-35612_1_1_1

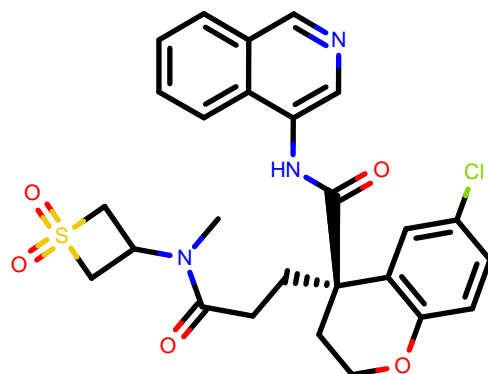
SMILES: CN(CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4)C(=O)COC

RUN: RUN6463

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.28

EN300-318341_2_1_1



CID: EN300-318341_2_1_1

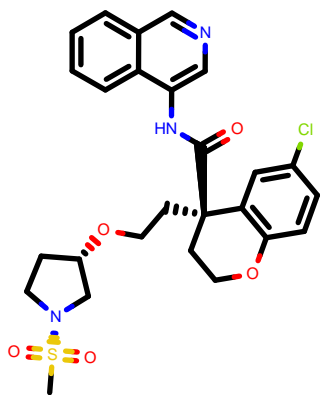
SMILES: CN(C1CS(=O)(=O)C1)C(=O)CC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN7770

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

KAD-UNI-8a629cb0-44_2



CID: KAD-UNI-8a629cb0-44_2

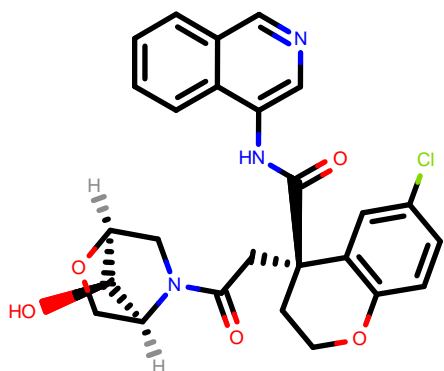
SMILES: CS(=O)(=O)[N@]1CC[C@@H](C1)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN1980

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.34

EN300-6493060_1_1_1



CID: EN300-6493060_1_1_1

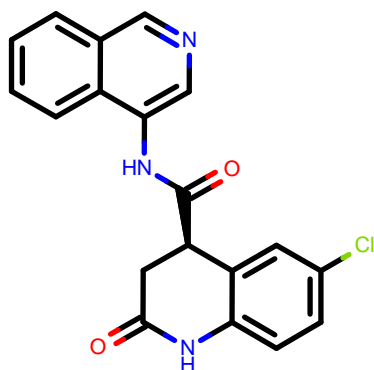
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)C[C@@]5N[C@@H]R[C@@H]3[C@@]5H5CO6/O

RUN: RUN7538

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.26

MIC-UNK-45817b9b-1_1



CID: MIC-UNK-45817b9b-1_1

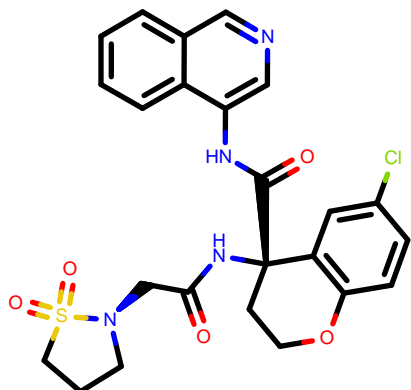
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4)Cl

RUN: RUN1166

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.29

EN300-43206_1_1_1



CID: EN300-43206_1_1_1

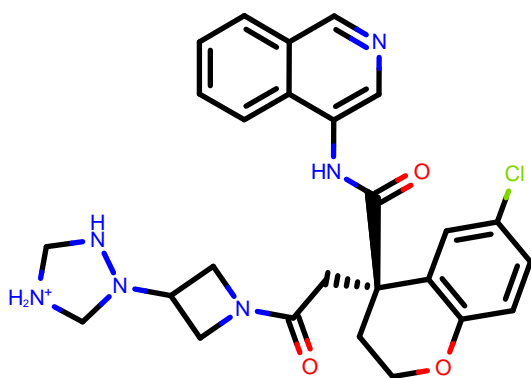
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[N@]5CCCC5(=O)=O

RUN: RUN3880

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.32

EN300-66518_1_1_1



CID: EN300-66518_1_1_1

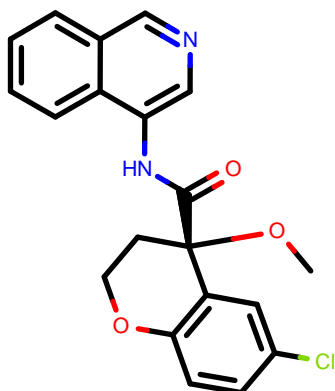
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)n6cnr6

RUN: RUN7541

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.27

PET-UNK-29afea89-2_1_1



CID: PET-UNK-29afea89-2_1_1

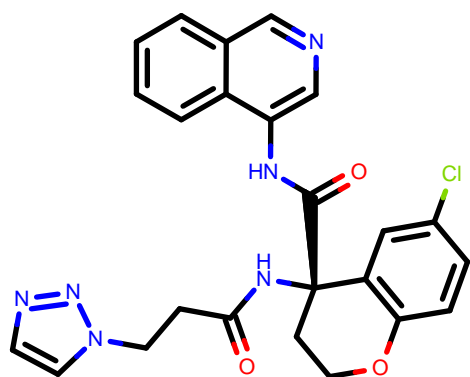
SMILES: CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN6744

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.13

EN300-28871_1_1_1



CID: EN300-28871_1_1_1

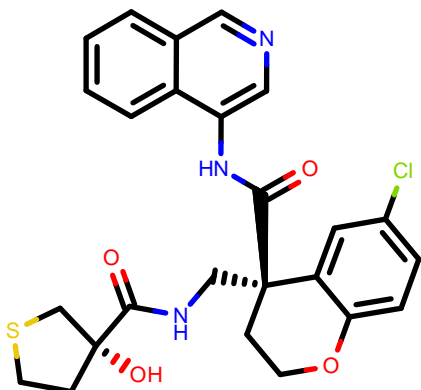
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5

RUN: RUN4159

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

EDJ-MED-40433386-7_1



CID: EDJ-MED-40433386-7_1

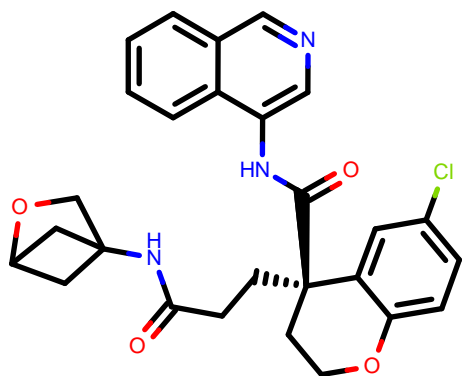
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@5(CSCS5)O

RUN: RUN2401

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.34

EN300-6734977_2_1_1



CID: EN300-6734977_2_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC56CC(C5)OC6

RUN:

RUN5757

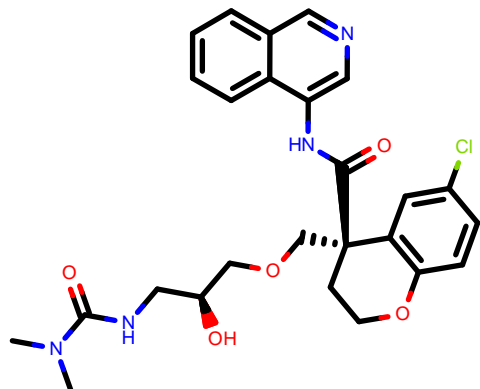
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.27

EN300-6501360_2_1_1



CID: EN300-6501360_2_1_1

SMILES:

CN(C)C(=O)NC[C@@H](COC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O

RUN:

RUN6644

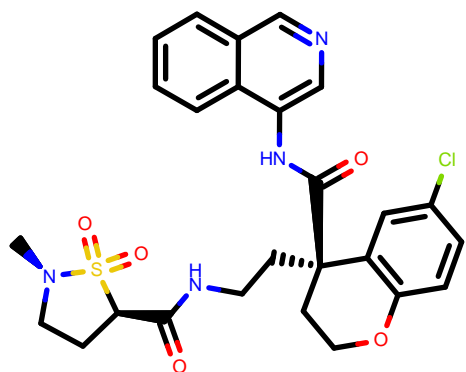
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.44

EN300-255496_3_1_1



CID: EN300-255496_3_1_1

SMILES:

C[N@@]1CC[C@@H](S1(=O)=O)C(=O)NC[C@@]2(COCc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN:

RUN4904

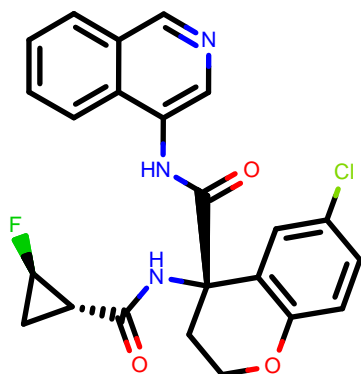
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.37

EN300-4698402_1_1_1



CID: EN300-4698402_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@H]5F

RUN:

RUN4871

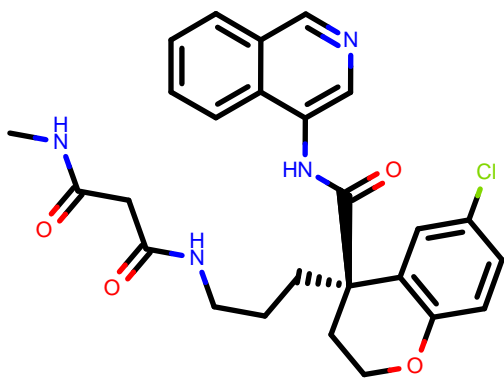
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.18

EN300-128463_4_1_1



CID: EN300-128463_4_1_1

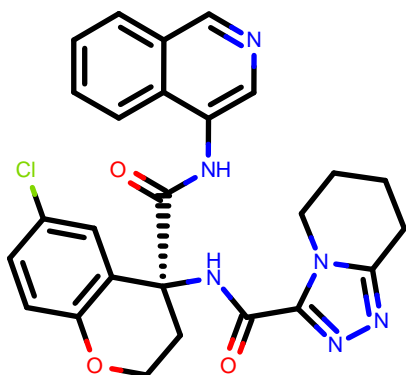
SMILES: CNC(=O)CC(=O)NCCC[C@]1(C)C(CO)c2c1cc(cc2)C(=O)Nc3cnc4c3cccc4

RUN: RUN3422

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.27

EN300-6746631_1_1_1



CID: EN300-6746631_1_1_1

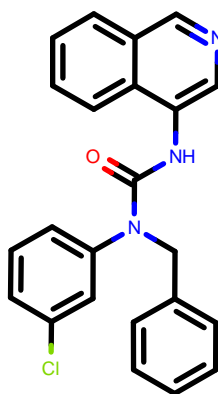
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CO)c4c3cc(cc4)C(=O)Nc5nc6n5CCCC6

RUN: RUN6998

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.26

MIC-UNK-bcd487e9-1_1



CID: MIC-UNK-bcd487e9-1_1

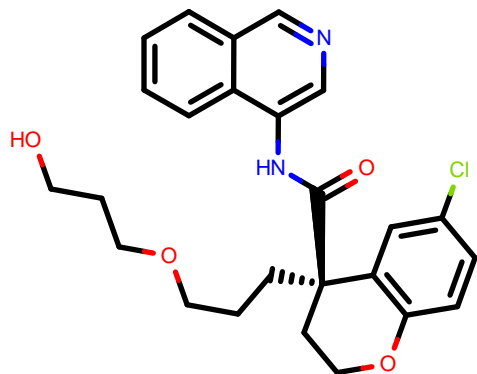
SMILES: c1ccc(cc1)CN(c2cccc(c2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN516

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.32

EN300-221518_4_1_1



CID: EN300-221518_4_1_1

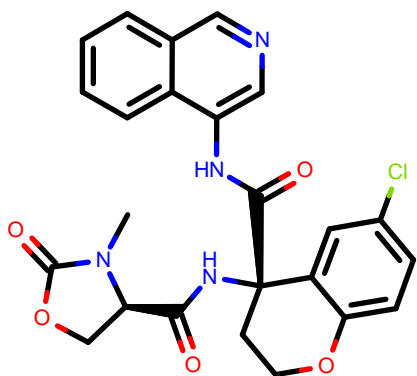
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CO)c4c3cc(cc4)C(=O)Nc5cnc6c5CCCCO

RUN: RUN7324

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.35

EN300-332838_1_2_1



CID: EN300-332838_1_2_1

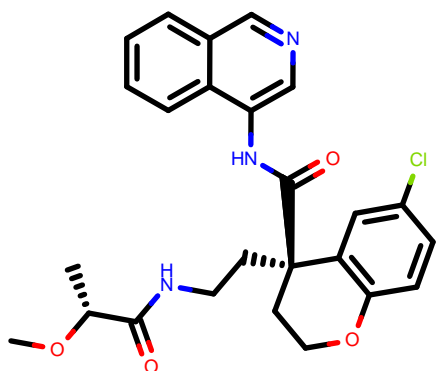
SMILES: CN1C@H](COC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN5338

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-51257_3_2_1



CID: EN300-51257_3_2_1

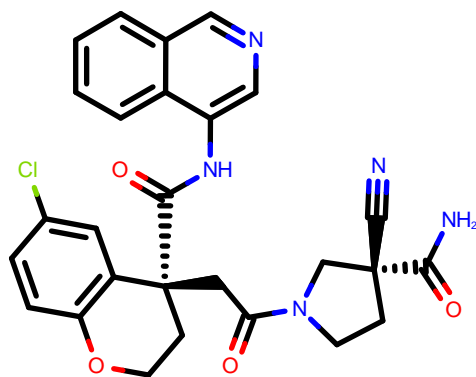
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN5745

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.28

EN300-1608992_1_1_1



CID: EN300-1608992_1_1_1

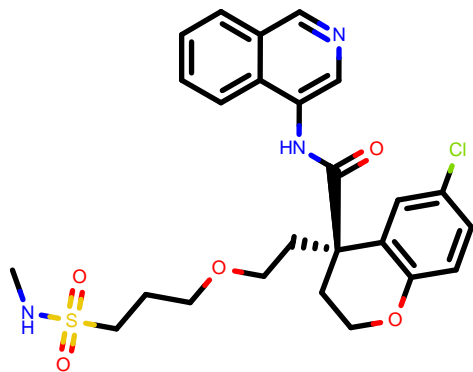
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3(C#N)C(=O)N

RUN: RUN4456

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.24

EN300-68875_3_1_1



CID: EN300-68875_3_1_1

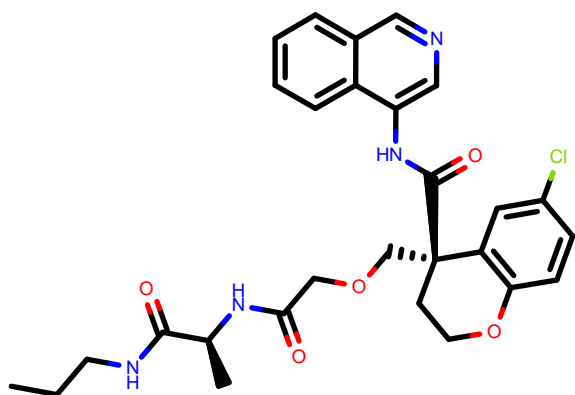
SMILES: CNS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6409

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.30

EN300-23214_2_2_1



CID: EN300-23214_2_2_1

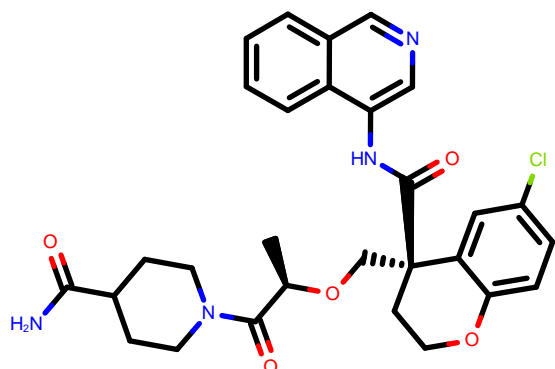
SMILES: CCCNC(=O)[C@H](C)NC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN3956

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.40

EN300-28113_2_2_1



CID: EN300-28113_2_2_1

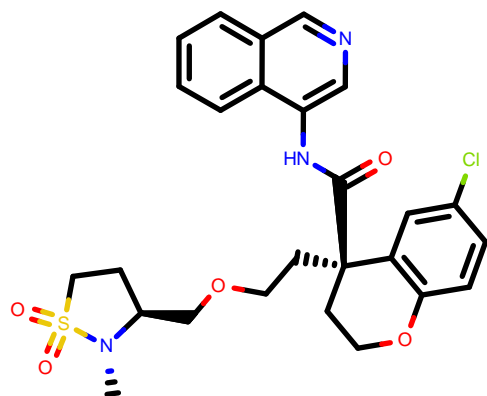
SMILES: C[C@H](C(=O)N1CCC(CC1)C(=O)N)OC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN6745

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.34

KAD-UNI-8a629cb0-38_1



CID: KAD-UNI-8a629cb0-38_1

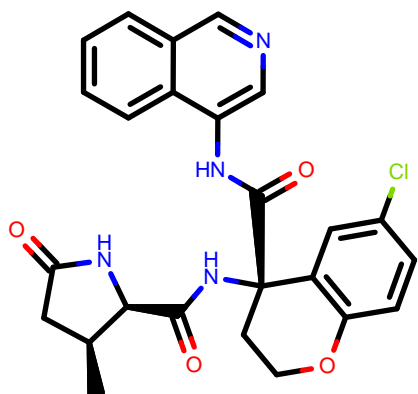
SMILES: C[N@@]1[C@@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2042

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.28

EN300-155362_1_4_1



CID: EN300-155362_1_4_1

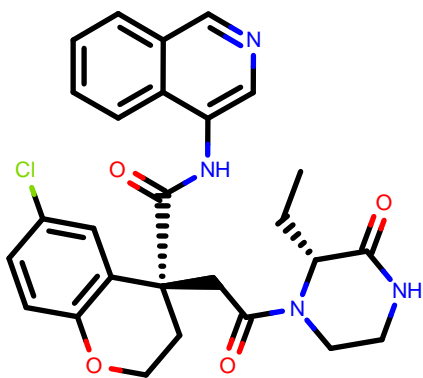
SMILES: C[C@H]1CC(=O)N[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4432

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.26

EN300-67439_1_1_1



CID: EN300-67439_1_1_1

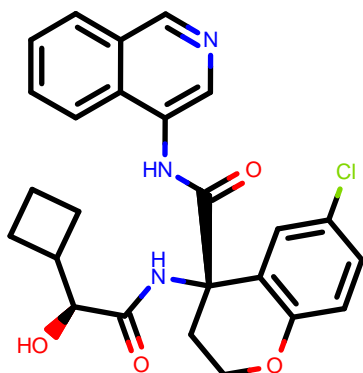
SMILES: CC[C@@H]1C(=O)NCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6067

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.27

EN300-249764_1_2_1



CID: EN300-249764_1_2_1

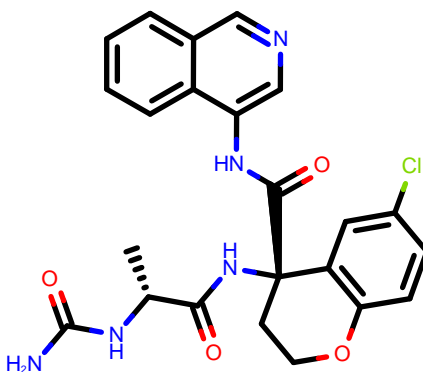
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@H](C)C5CC5O

RUN: RUN6658

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.23

EN300-00271_1_2_1



CID: EN300-00271_1_2_1

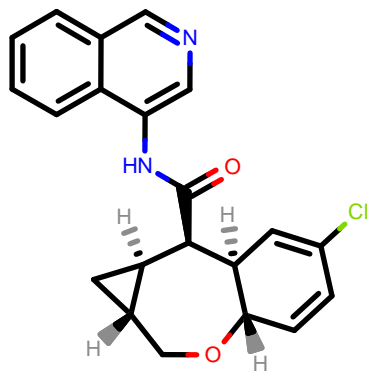
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)NC(=O)N

RUN: RUN4830

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.24

DAR-DIA-0d514e7d-32_5



CID: DAR-DIA-0d514e7d-32_5

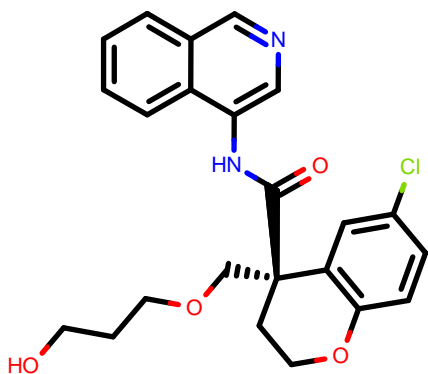
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H]4[C@@H]4C[C@@H]5[C@@H]3C=C(C=C5)Cl

RUN: RUN774

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.22

EN300-221518_2_1_1



CID: EN300-221518_2_1_1

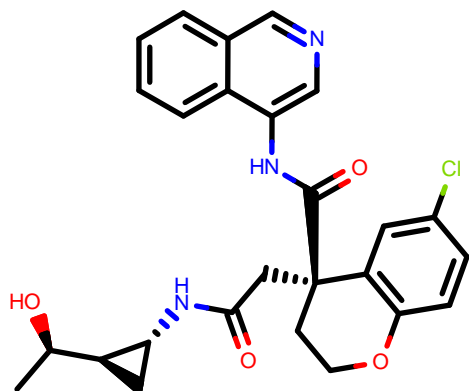
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COCCCO

RUN: RUN4390

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-7463275_1_2_1



CID: EN300-7463275_1_2_1

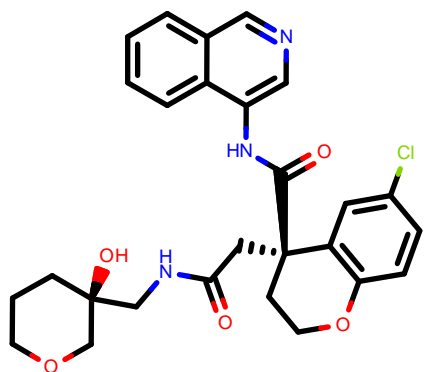
SMILES: C[C@H]1[C@@H]1[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5O

RUN: RUN5500

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-193679_1_2_1



CID: EN300-193679_1_2_1

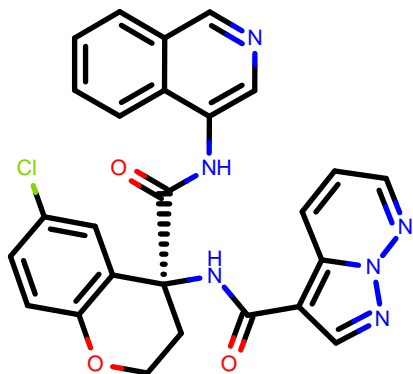
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCCOC5)O

RUN: RUN6173

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.39

EN300-114593_1_1_1



CID: EN300-114593_1_1_1

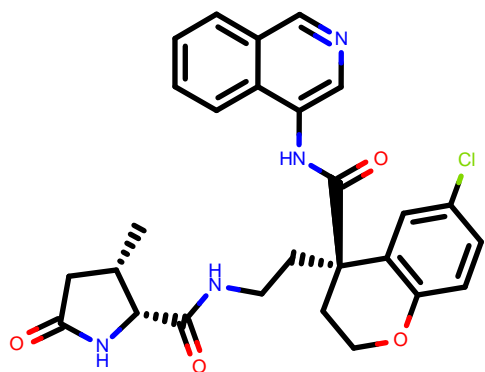
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5ccc6

RUN: RUN6036

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.22

EN300-155362_3_4_1



CID: EN300-155362_3_4_1

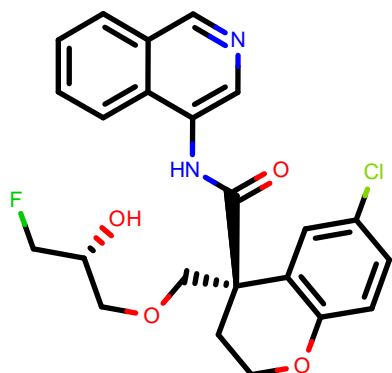
SMILES: C[C@H]1CC(=O)N[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4891

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.31

EN300-1968342_2_2_1



CID: EN300-1968342_2_2_1

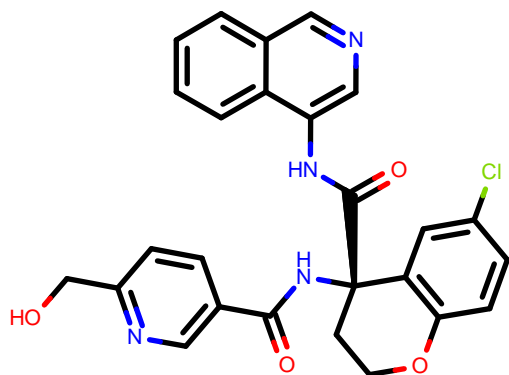
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN3951

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-146051_1_1_1



CID: EN300-146051_1_1_1

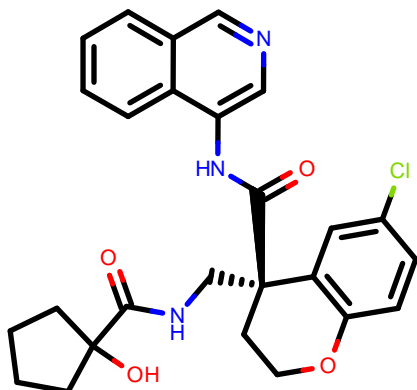
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(O)cc5

RUN: RUN4653

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.24

EN300-25960_2_1_1



CID: EN300-25960_2_1_1

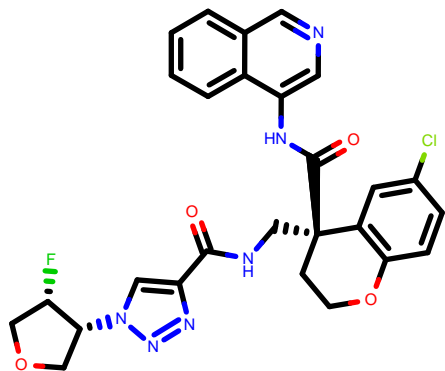
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCC5)O

RUN: RUN4139

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.41

EN300-6759512_2_1_1



CID: EN300-6759512_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(O)C)CNC1=Oe5cn(m5)[C@@H]6COC[C@H]6F

RUN:

RUN6110

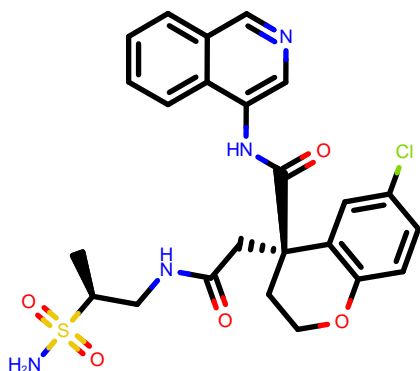
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.28

EN300-123623_1_1_1



CID: EN300-123623_1_1_1

SMILES:

C[C@@H](CNC(=O)[C@@H]1(CCOc2c1cc(O)C)C(=O)Nc3nc4c3cc(O)S(=O)(=O)N

RUN:

RUN5871

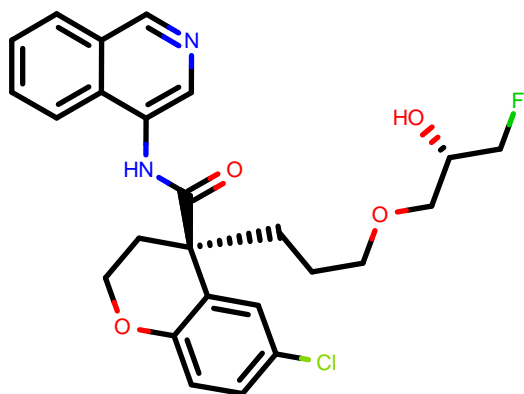
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.30

EN300-1968342_4_1_1



CID: EN300-1968342_4_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(O)C)CCOC[C@@H](C)F

RUN:

RUN7027

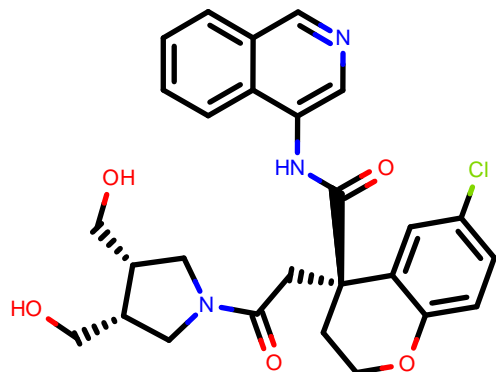
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.43

EN300-333677_1_1_1



CID: EN300-333677_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(O)C)CC(O)N[C@@H](C)C(O)CO

RUN:

RUN6957

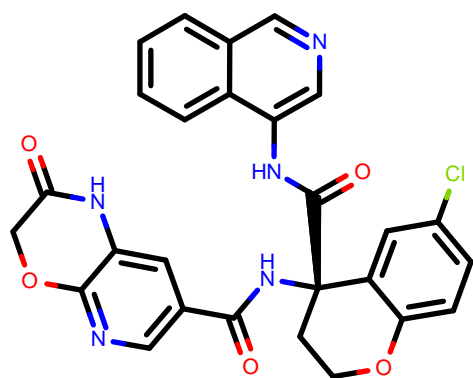
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.27

EN300-103979_1_1_1



CID: EN300-103979_1_1_1

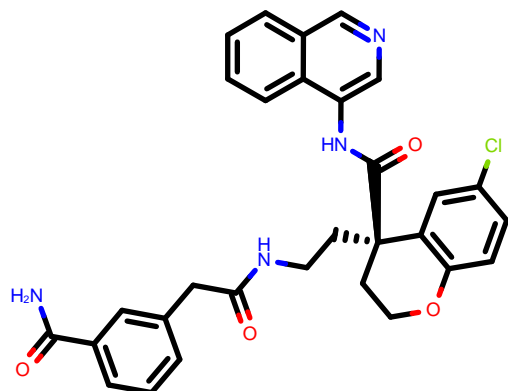
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c(nc5)OCC(=O)N6

RUN: RUN6691

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-1179673_3_1_1



CID: EN300-1179673_3_1_1

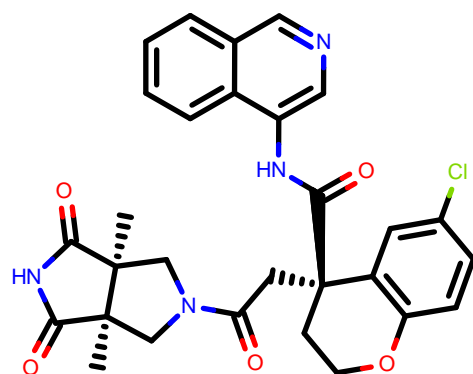
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5cccc(c5)C(=O)N

RUN: RUN6147

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.29

ALP-UNI-76695c4f-10_1



CID: ALP-UNI-76695c4f-10_1

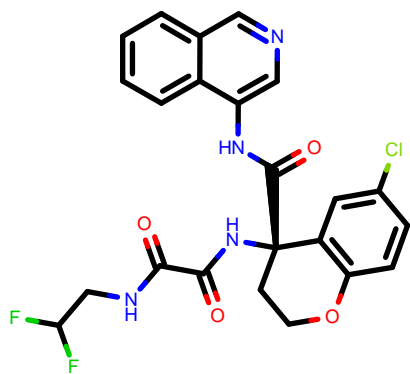
SMILES: C[C@@]12CN[C@@]1(C)C(=O)NC2=O(C)C(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)Nc5nc6c5ccccc6

RUN: RUN2023

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.39

EN300-128277_1_1_1



CID: EN300-128277_1_1_1

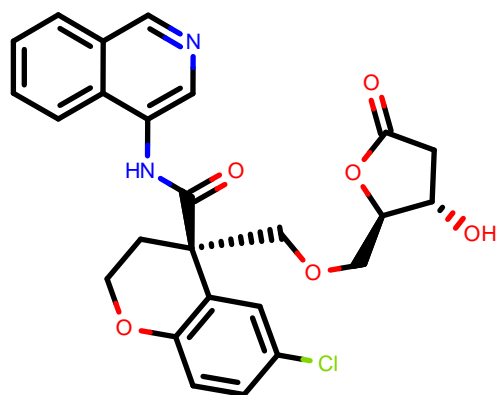
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NCC(F)F

RUN: RUN5264

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.28

EN300-6487407_2_1_1



CID: EN300-6487407_2_1_1

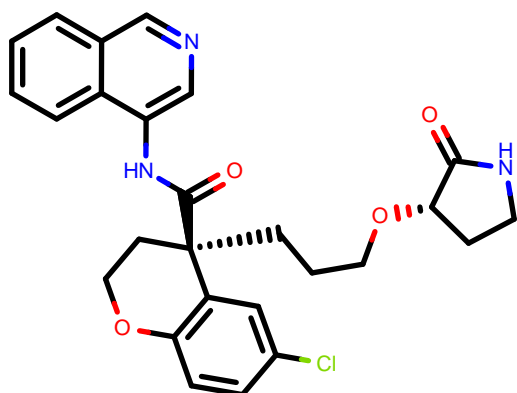
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]H5[C@H](CC(=O)O)O5

RUN: RUN7499

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.29

EN300-6736413_4_2_1



CID: EN300-6736413_4_2_1

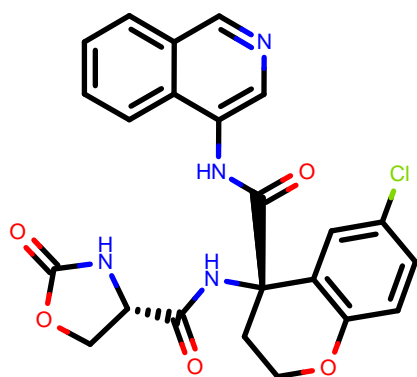
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@]H5CCNC5=O

RUN: RUN4982

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.31

EN300-126389_1_1_1



CID: EN300-126389_1_1_1

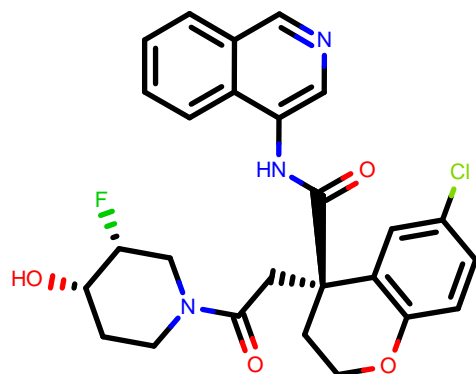
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]H5COC(=O)N5

RUN: RUN6114

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.21

EN300-741926_1_1_1



CID: EN300-741926_1_1_1

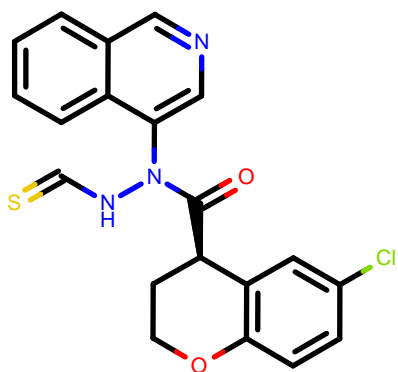
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N6C[C@@]H[C@@]H(C5)F5O

RUN: RUN5458

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.23

DAR-DIA-5ff57136-18_1_1



CID: DAR-DIA-5ff57136-18_1_1

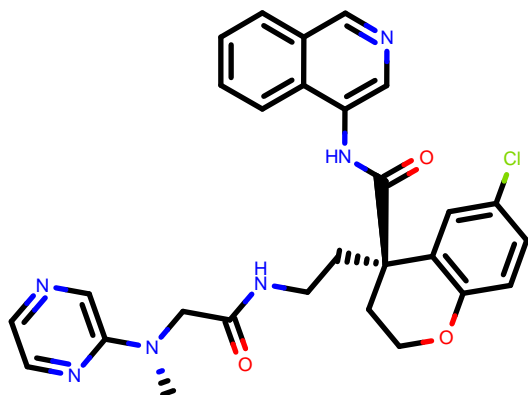
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)NC=S

RUN: RUN3501

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.12

EN300-36855_3_1_1



CID: EN300-36855_3_1_1

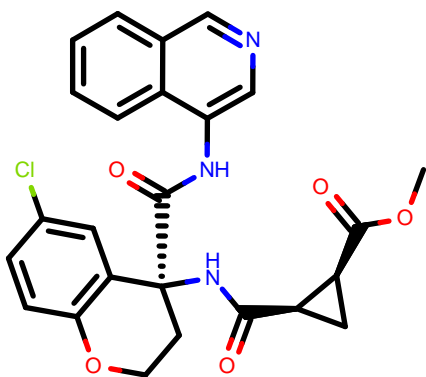
SMILES: CN(CC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)c5nccn5

RUN: RUN4007

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.29

EN300-66764_1_4_1



CID: EN300-66764_1_4_1

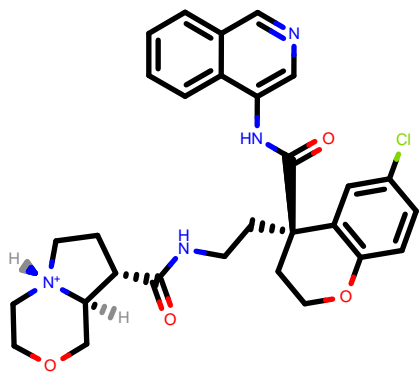
SMILES: COC(=O)[C@H]1[C@@H]2[C@H]1C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6144

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.29

EN300-1588613_3_2_1



CID: EN300-1588613_3_2_1

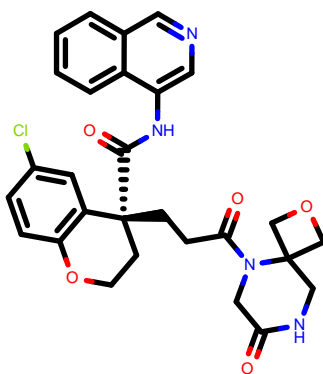
SMILES: c1ccc2c(c1)ncn2N(C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCN[C@@H]5

RUN: RUN6318

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.33

EN300-366278_2_1_1



CID: EN300-366278_2_1_1

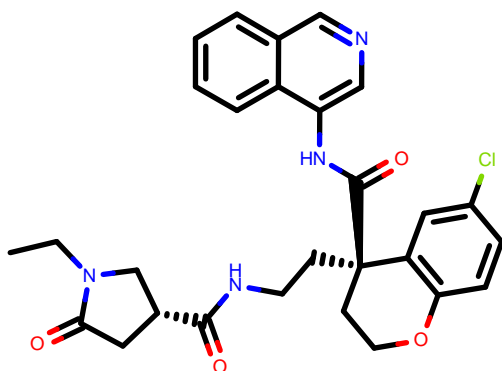
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC(=O)NCC56COC6

RUN: RUN6500

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.27

EN300-33478_3_1_1



CID: EN300-33478_3_1_1

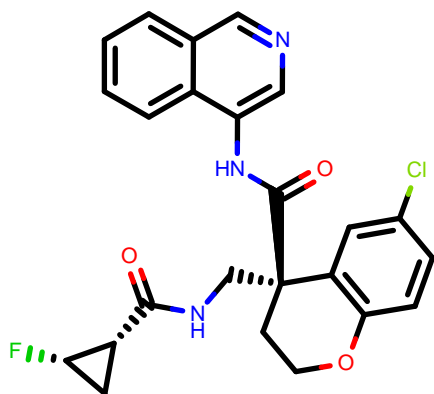
SMILES: CCN1C[C@@H](CC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN7415

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.35

EN300-1654606_2_1_1



CID: EN300-1654606_2_1_1

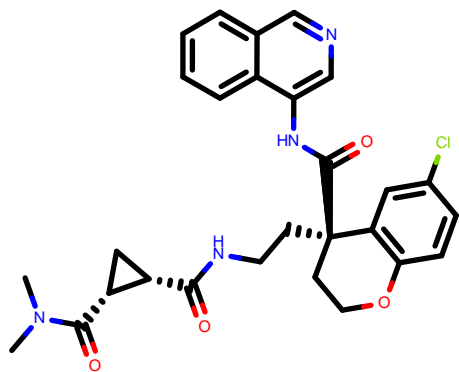
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN4102

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.23

EN300-253462_3_1_1



CID: EN300-253462_3_1_1

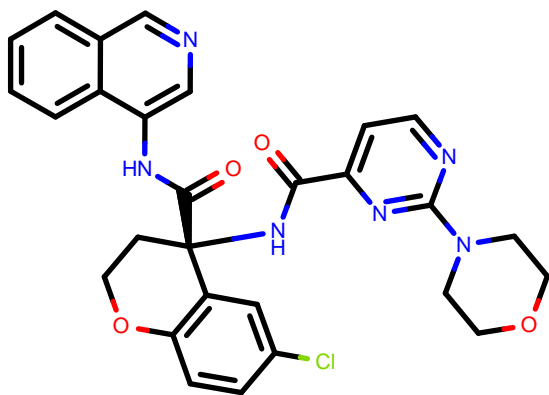
SMILES: CN(C)C(=O)[C@@H]1C[C@@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3917

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.37

EN300-312450_1_1_1



CID: EN300-312450_1_1_1

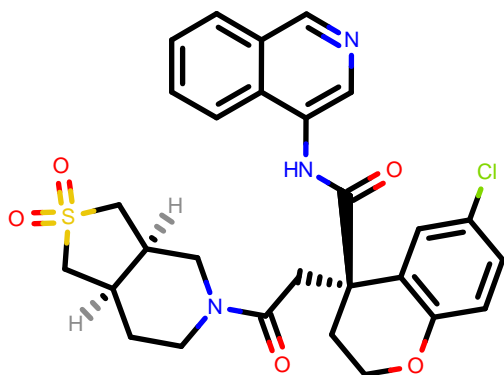
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)c5ccnc(n5)N6CCOCC6

RUN: RUN5071

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.30

EN300-365993_1_4_1



CID: EN300-365993_1_4_1

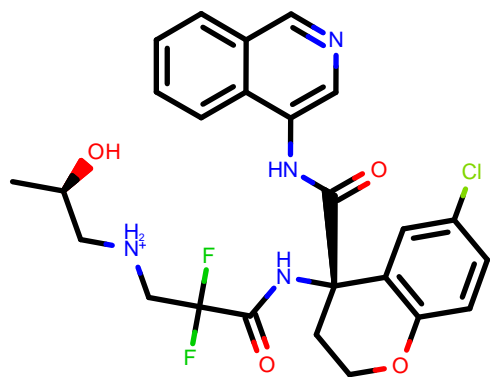
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)N5CC[C@@H]6CS(=O)(=O)C[C@@H]6C5

RUN: RUN3273

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.39

EDG-MED-90036822-38_2



CID: EDG-MED-90036822-38_2

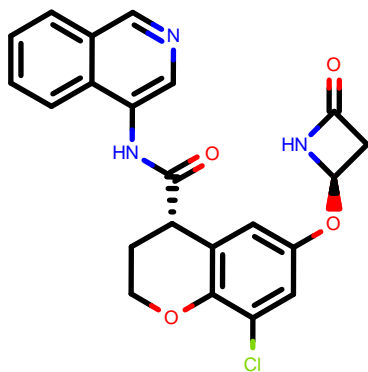
SMILES: C[C@H](CNCC(C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)Cl)C(=O)Nc3ncc4c3ccc4(F)F)O

RUN: RUN1665

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.36

FRA-DIA-b66f7109-3_1_1



CID: FRA-DIA-b66f7109-3_1_1

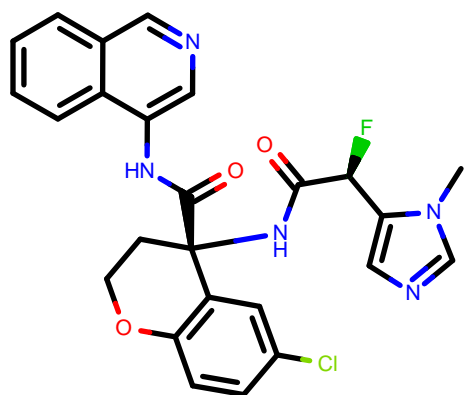
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOc4c3cc(cc4Cl)Cl)O[C@@H]5CC(=O)N5

RUN: RUN5111

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.30

EDG-MED-90036822-26_1



CID: EDG-MED-90036822-26_1

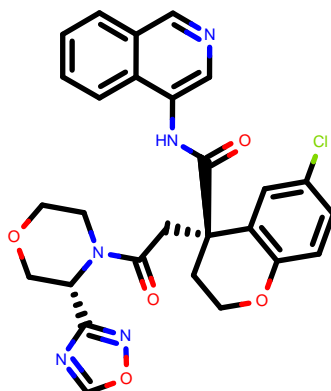
SMILES: Cn1cnc1[C@@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)F

RUN: RUN1584

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.28

EN300-122849_1_2_1



CID: EN300-122849_1_2_1

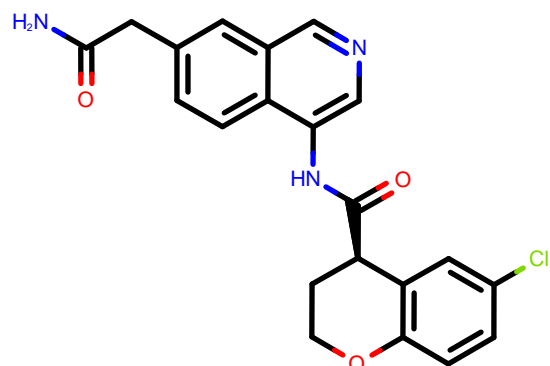
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5c6ncn6

RUN: RUN6643

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.26

MAK-UNK-8be7dca9-2_1_1



CID: MAK-UNK-8be7dca9-2_1_1

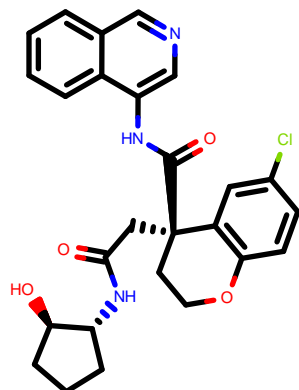
SMILES: c1cc2c(cc1CC(=O)N)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN7761

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.08

EN300-60314_1_1_1



CID: EN300-60314_1_1_1

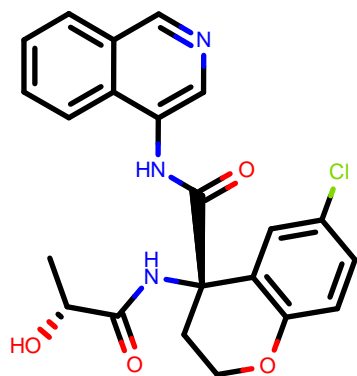
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5C[C@H]5O

RUN: RUN6058

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.24

EDG-MED-90036822-29_1



CID: EDG-MED-90036822-29_1

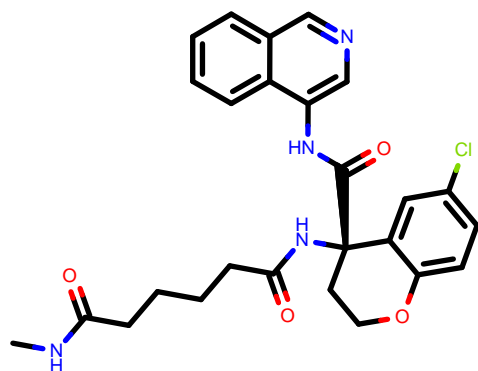
SMILES: C[C@H](C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN1536

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.21

EN300-154693_1_1_1



CID: EN300-154693_1_1_1

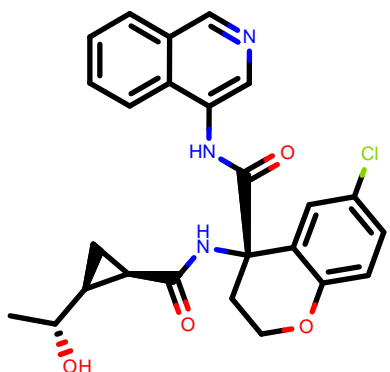
SMILES: CNC(=O)CCCCCC(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5907

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.27

EN300-6729572_1_8_1



CID: EN300-6729572_1_8_1

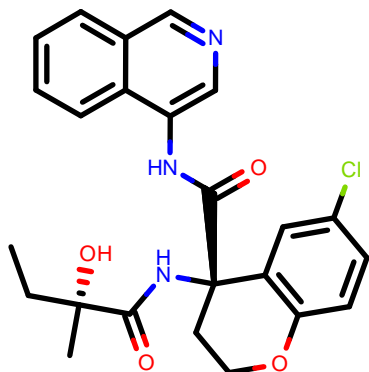
SMILES: C[C@H]([C@H]1[C@H]1C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN5925

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.23

EN300-104746_1_2_1



CID: EN300-104746_1_2_1

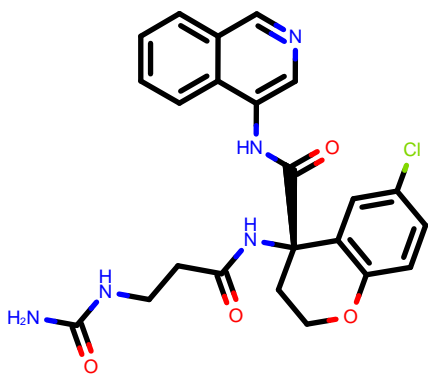
SMILES: CC[C@](C)(C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6669

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.24

EN300-10729_1_1_1



CID: EN300-10729_1_1_1

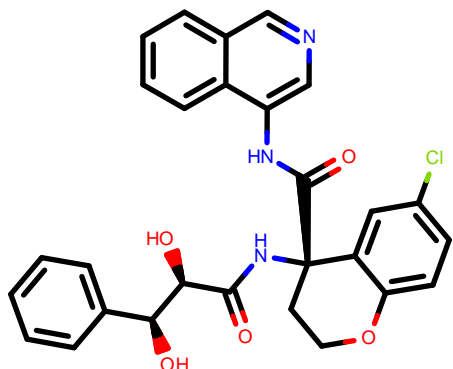
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)N

RUN: RUN5278

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.25

EN300-2923949_1_3_1



CID: EN300-2923949_1_3_1

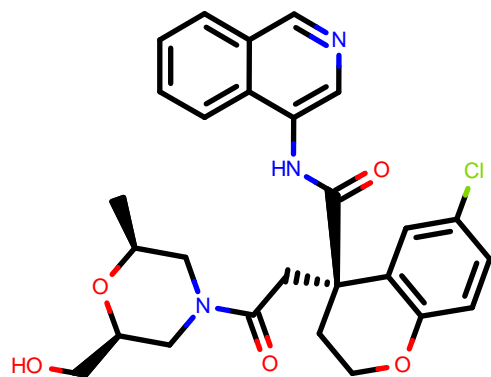
SMILES: c1ccc(cc1)[C@@H](C@H)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5O)O

RUN: RUN6305

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.30

EN300-157776_1_4_1



CID: EN300-157776_1_4_1

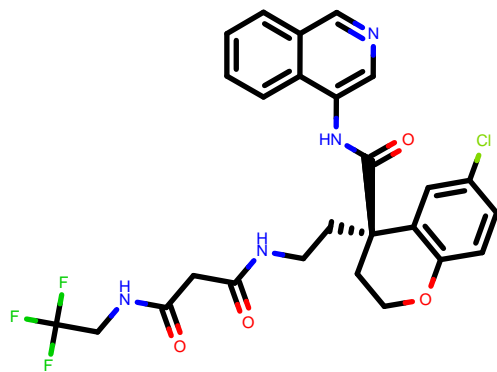
SMILES: C[C@@H]1CN[C@@H](O1)CO(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4202

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.37

EN300-128715_3_1_1



CID: EN300-128715_3_1_1

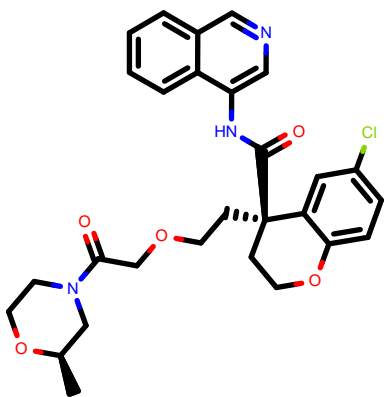
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(F)(F)F

RUN: RUN6400

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.29

EN300-25572_3_1_1



CID: EN300-25572_3_1_1

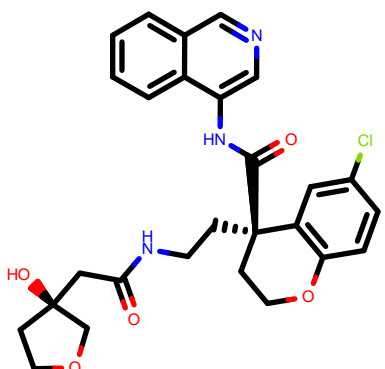
SMILES: C[C@@H]1CN(CCO1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5292

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.31

EN300-360157_3_2_1



CID: EN300-360157_3_2_1

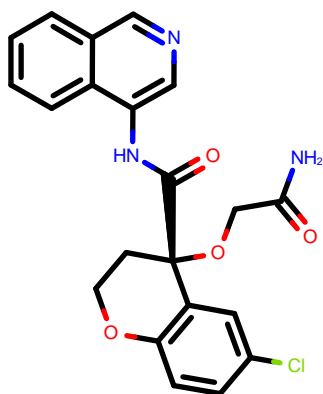
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@]5(CCOc5)O

RUN: RUN4426

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.32

EDG-MED-4c68219f-6_1



CID: EDG-MED-4c68219f-6_1

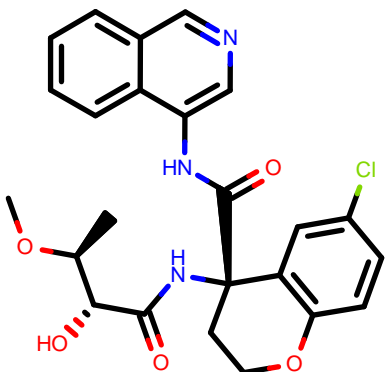
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N

RUN: RUN1498

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.17

EN300-220194_1_3_1



CID: EN300-220194_1_3_1

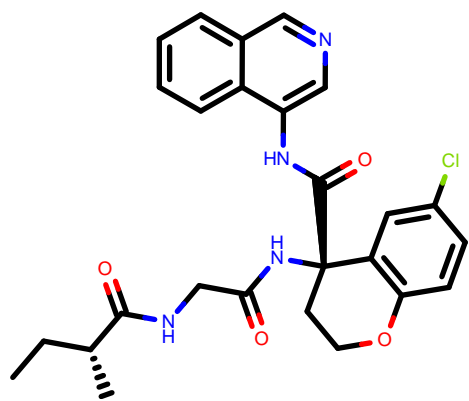
SMILES: C[C@@H]([C@H](C=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O)OC

RUN: RUN5162

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-51961_1_1_1



CID: EN300-51961_1_1_1

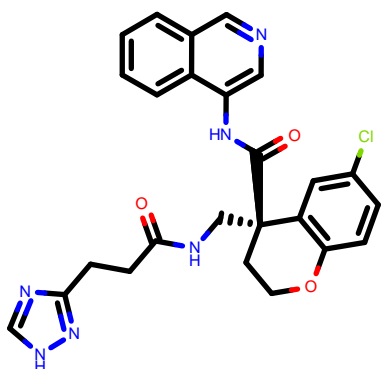
SMILES: CC[C@@H](C)C(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4188

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-101197_2_1_1



CID: EN300-101197_2_1_1

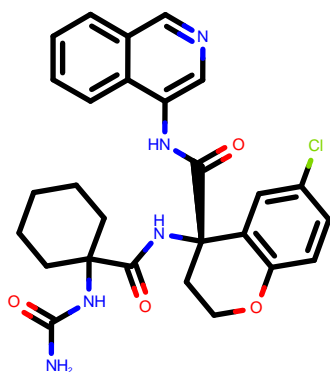
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCc5[nH]nns5

RUN: RUN4964

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.27

EN300-78368_1_1_1



CID: EN300-78368_1_1_1

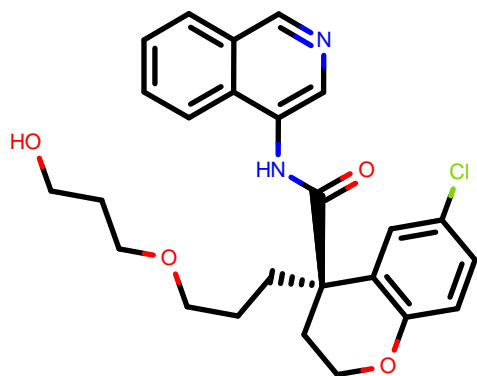
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCC5)NC(=O)N

RUN: RUN5704

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.33

EN300-221518_4_1_1



CID: EN300-221518_4_1_1

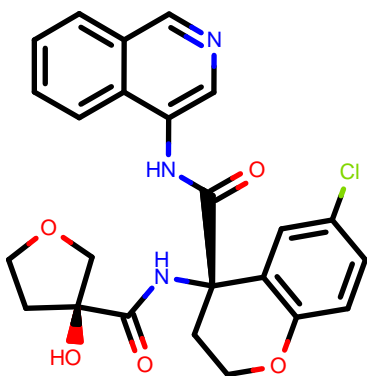
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN5952

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.27

EN300-148421_1_1_1



CID: EN300-148421_1_1_1

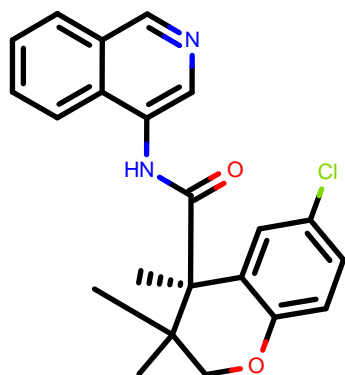
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOC5)O

RUN: RUN6009

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-30_1_1



CID: DAR-DIA-0d514e7d-30_1_1

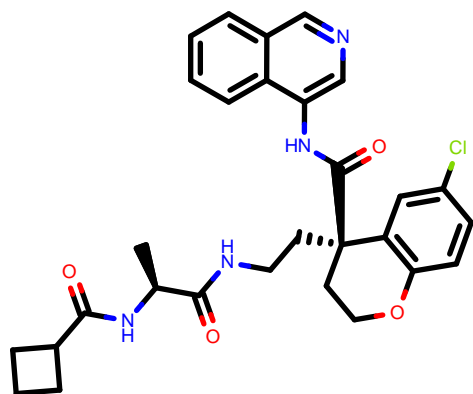
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5116

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-66082_3_1_1



CID: EN300-66082_3_1_1

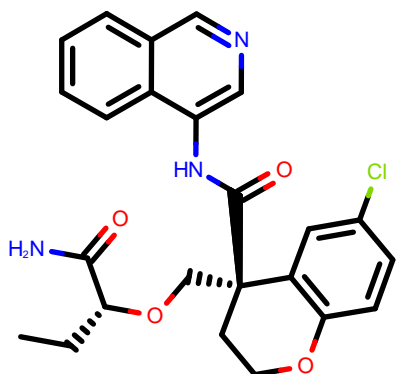
SMILES: C[C@@]H[C](=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCCC5

RUN: RUN5982

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.35

EN300-65839_2_2_1



CID: EN300-65839_2_2_1

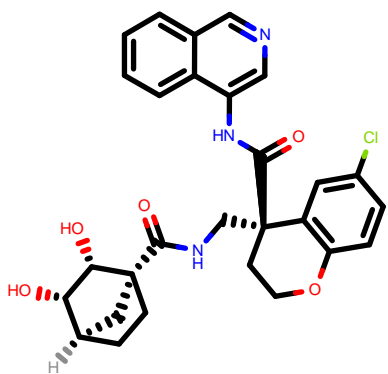
SMILES: CC[C@@]H[C](=O)N)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6195

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.25

EN300-7432302_2_1_1



CID: EN300-7432302_2_1_1

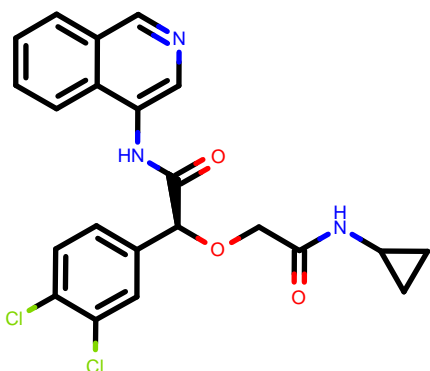
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)CNC1=O

RUN: RUN7399

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.25

MAT-POS-de59a476-6_2



CID: MAT-POS-de59a476-6_2

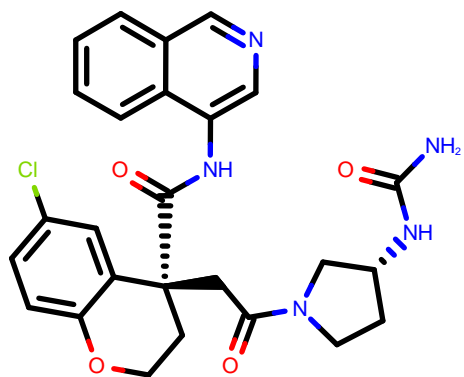
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)OCC(=O)NC4CC4

RUN: RUN2094

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.33

EN300-118869_1_2_1



CID: EN300-118869_1_2_1

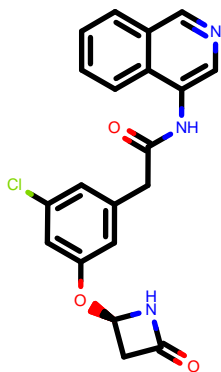
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC4=CC=CC=C4)CNC1=O

RUN: RUN7333

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.28

MAT-POS-3b92565d-3_1



CID: MAT-POS-3b92565d-3_1

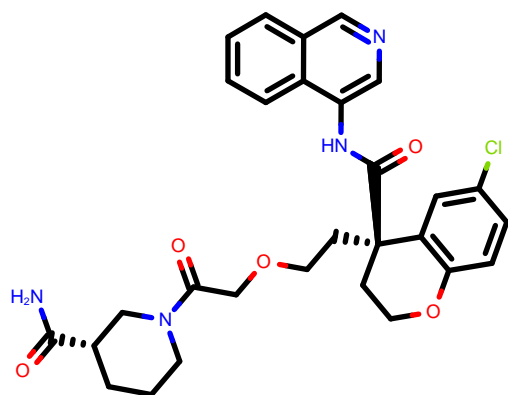
SMILES: c1ccc2c(c1)ncnc2NC(=O)Cc3ccc(cc3)Cl)OCC(=O)NC4CC4

RUN: RUN51

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.46

EN300-22880_3_1_1



CID: EN300-22880_3_1_1

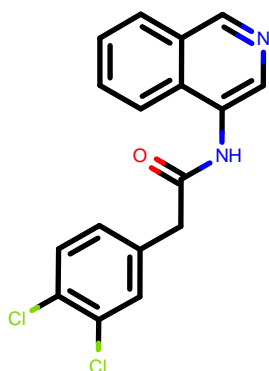
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@O]c4cc3c(c4)C(=O)C(=O)N5CCCC5C@H](C)Cl=O

RUN: RUN6417

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.40

MAT-POS-23a8a11a-1_1



CID: MAT-POS-23a8a11a-1_1

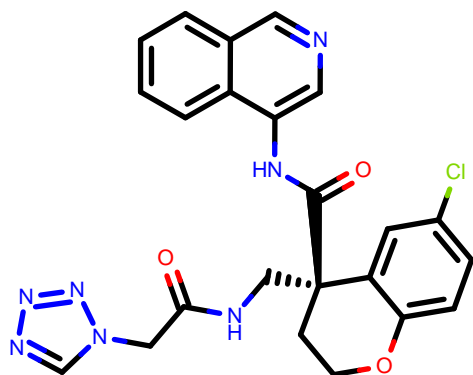
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3ccc(c(c3)Cl)Cl

RUN: RUN1247

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.28

EN300-20980_2_1_1



CID: EN300-20980_2_1_1

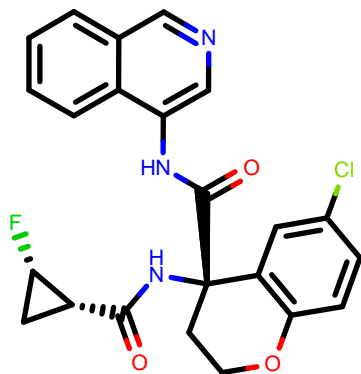
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4cc3c(c4)C(=O)C(=O)N5C=NN=C5

RUN: RUN5259

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.29

EN300-97300_1_1_1



CID: EN300-97300_1_1_1

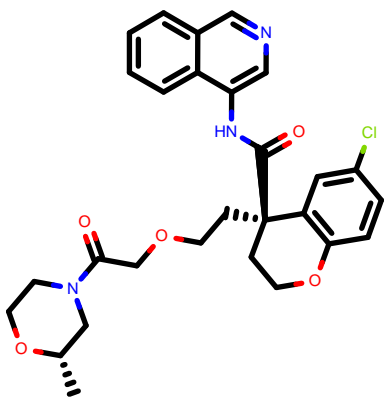
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4cc3c(c4)C(=O)N(C)C(=O)C5CC5F

RUN: RUN5483

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.20

EN300-25572_3_2_1



CID: EN300-25572_3_2_1

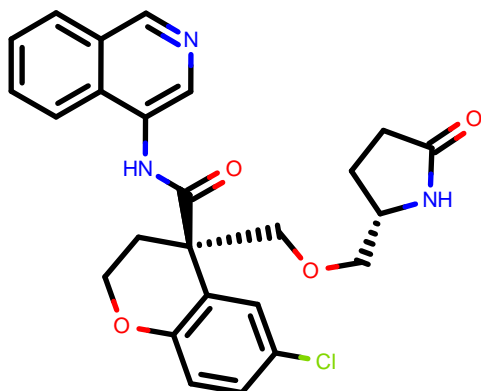
SMILES: C[C@H]1CN(CCO1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6634

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.29

EN300-195756_2_1_1



CID: EN300-195756_2_1_1

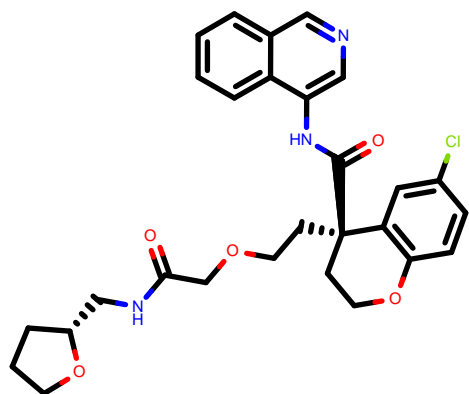
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]H5CCCC(=O)N5

RUN: RUN6049

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-01527_3_2_1



CID: EN300-01527_3_2_1

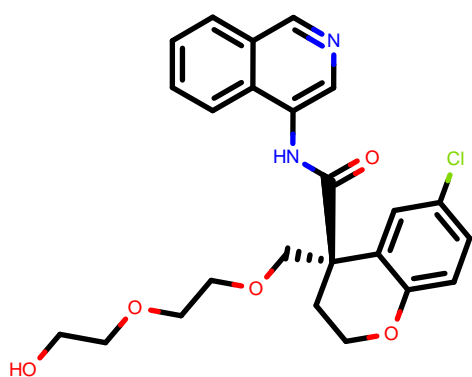
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@@]H5CCCCO5

RUN: RUN4512

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.32

EN300-52467_2_1_1



CID: EN300-52467_2_1_1

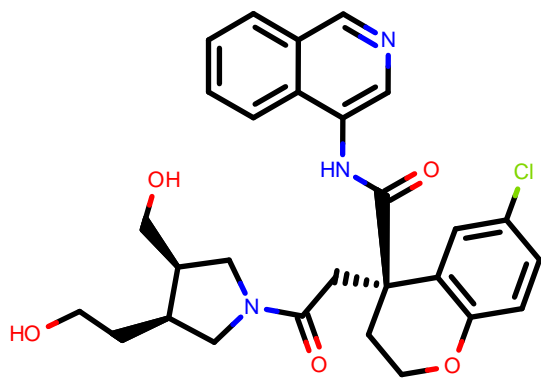
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)CO

RUN: RUN6816

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.25

EN300-1425608_1_4_1



CID: EN300-1425608_1_4_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4cc3cc4C)CC(=O)N5C[C@H](C)C5CO)CCO

RUN:

RUN5567

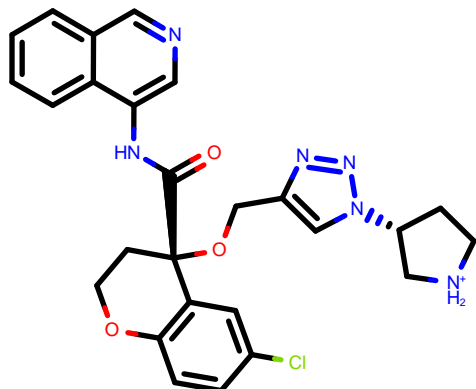
DDG (kcal/mol):

-0.70

dDDG (kcal/mol):

0.30

ED_-GRI-5b13fbe2-61_1



CID: ED_-GRI-5b13fbe2-61_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4cc3cc4C)OCc5cn(mn5)[C@@]6C[NH2+]C6

RUN:

RUN1462

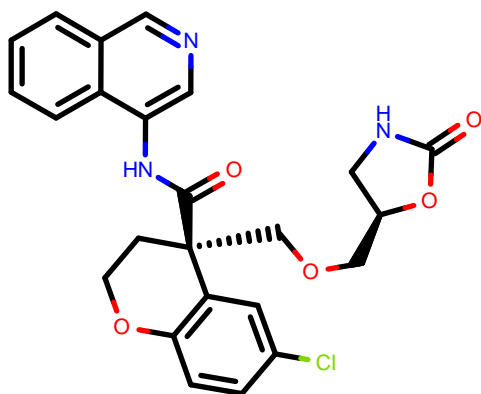
DDG (kcal/mol):

-0.70

dDDG (kcal/mol):

0.27

EN300-203293_2_2_1



CID: EN300-203293_2_2_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4cc3cc4C)COC[C@H]5CNC(=O)O5

RUN:

RUN4794

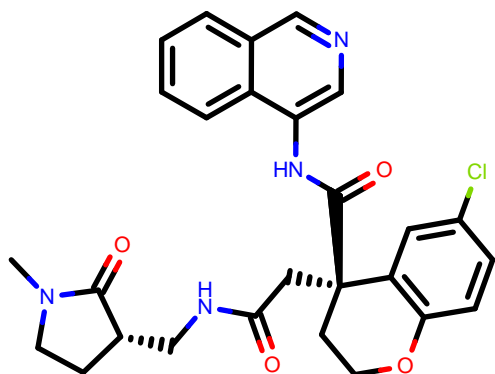
DDG (kcal/mol):

-0.70

dDDG (kcal/mol):

0.30

EN300-1264816_1_2_1



CID: EN300-1264816_1_2_1

SMILES:

CN1CC[C@H](C1=O)CNC(=O)C[C@@]2(CCOc3cc2cc3C)C(=O)N4nccoc5c4ccc5

RUN:

RUN7226

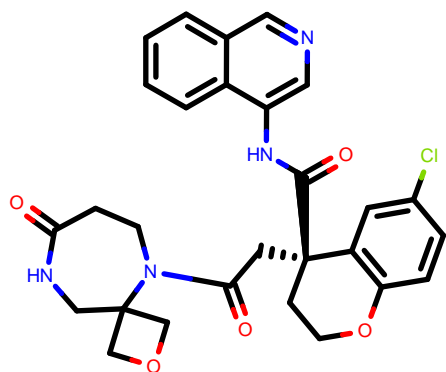
DDG (kcal/mol):

-0.70

dDDG (kcal/mol):

0.30

EN300-367589_1_1_1



CID: EN300-367589_1_1_1

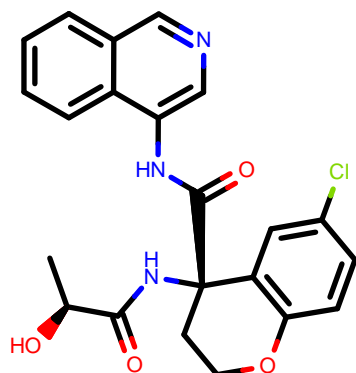
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(=O)NCC56COC6

RUN: RUN3298

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.29

EDG-MED-90036822-28_1



CID: EDG-MED-90036822-28_1

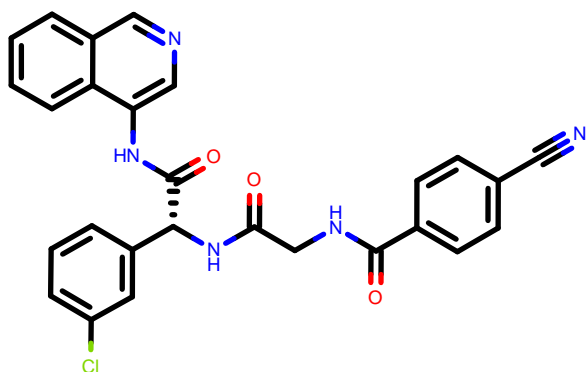
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)O

RUN: RUN1543

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.21

EDJ-MED-ee07cf00-5_1



CID: EDJ-MED-ee07cf00-5_1

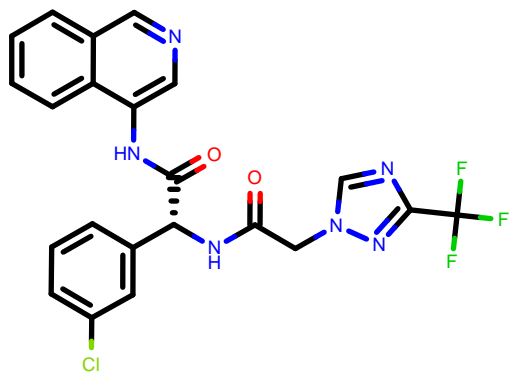
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)CNC(=O)c4ccc(cc4)C#N

RUN: RUN2664

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.58

EDJ-MED-ee07cf00-10_1



CID: EDJ-MED-ee07cf00-10_1

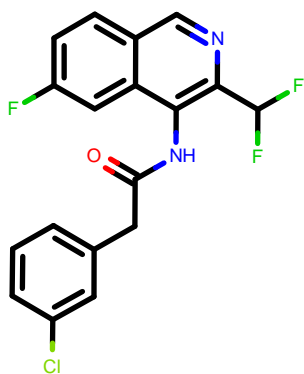
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4ncnc4C(F)(F)F

RUN: RUN2669

DDG (kcal/mol): -0.69

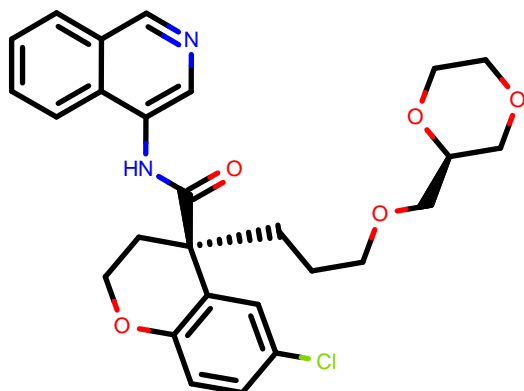
dDDG (kcal/mol): 0.39

JOH-UNI-6fede743-5_1



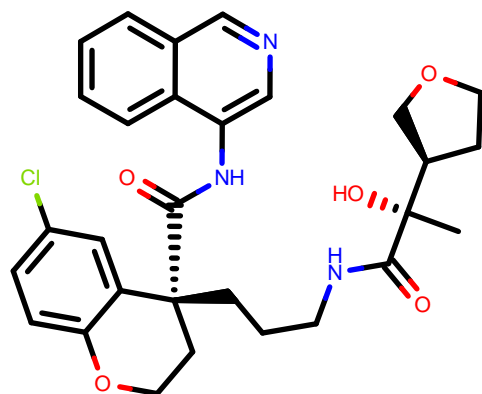
CID:	JOH-UNI-6fede743-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cc(ccc3cnc2C(F)F)F</chem>
RUN:	RUN1071
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.39

EN300-139167_4_1_1



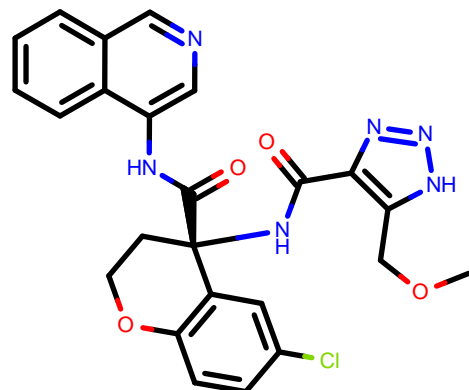
CID:	EN300-139167_4_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCCO5</chem>
RUN:	RUN4569
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.34

EN300-217494_4_2_1



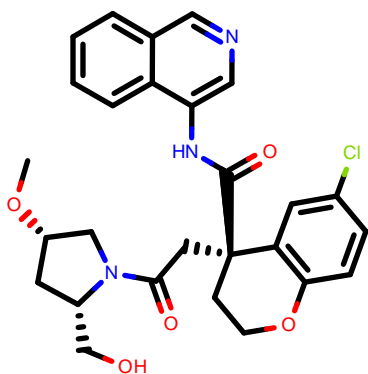
CID:	EN300-217494_4_2_1
SMILES:	<chem>CC@@H1CCOC1)(C(=O)NCCC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O</chem>
RUN:	RUN6589
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.37

EN300-785910_1_1_1



CID:	EN300-785910_1_1_1
SMILES:	<chem>COCc1c(n[nH]n1)C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5</chem>
RUN:	RUN4998
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.26

EN300-244713_1_1_1



CID: EN300-244713_1_1_1

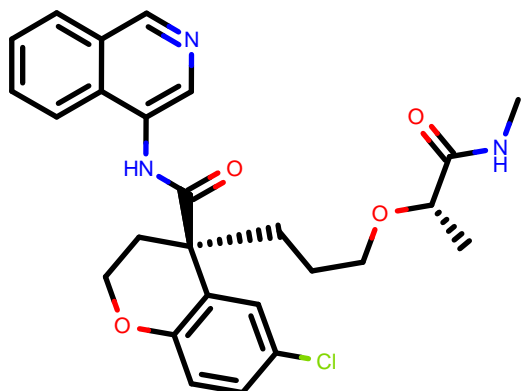
SMILES: CO[C@@H]1C[C@H](N(C1)C(=O)C[C@]2(CCOC3C2C(C3)C)C(=O)Nc4cnc5c4ccc5)CO

RUN: RUN5831

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.31

EN300-211482_4_1_1



CID: EN300-211482_4_1_1

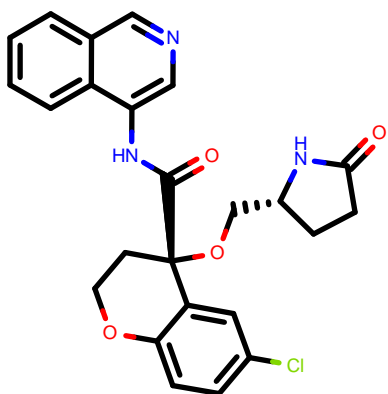
SMILES: C[C@@H](C(=O)N)OCC[C@@]1(CCOC2C1C(C2)C)C(=O)Nc3cnc4c3ccc4

RUN: RUN7528

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.46

EN300-195756_1_2_1



CID: EN300-195756_1_2_1

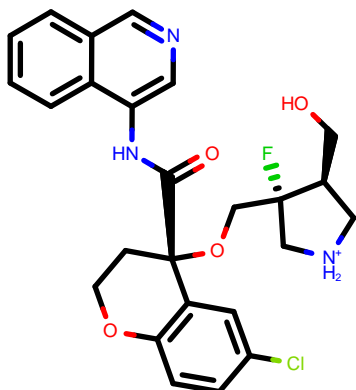
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5CCCC(=O)N5

RUN: RUN7478

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-55_1



CID: ED_-GRI-5b13fbe2-55_1

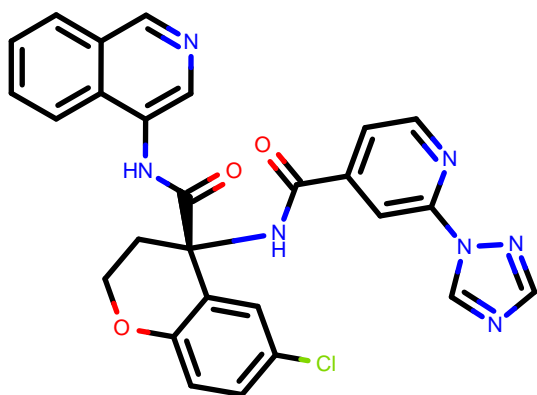
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@]5(C[NH2+])C[C@H]5COF

RUN: RUN1482

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.37

EN300-58433_1_1_1



CID: EN300-58433_1_1_1

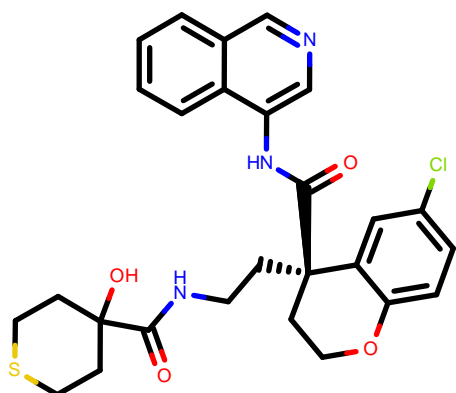
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cncc(c5)n6cnnc6

RUN: RUN6645

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.37

EN300-122340_3_1_1



CID: EN300-122340_3_1_1

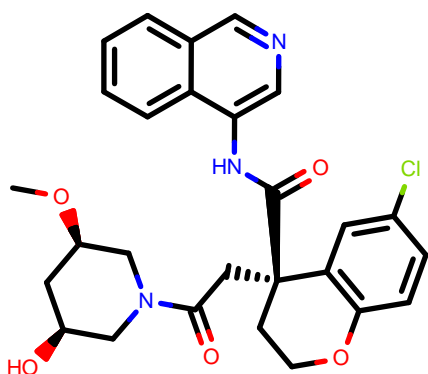
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCSC5)O

RUN: RUN7050

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.34

EN300-6763507_1_1_1



CID: EN300-6763507_1_1_1

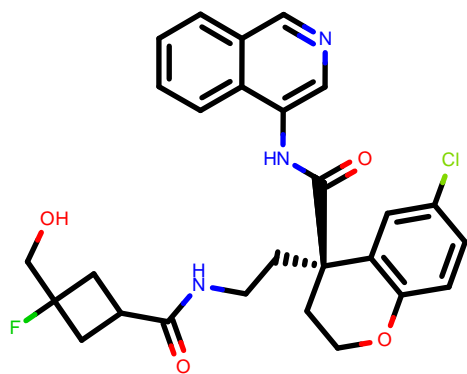
SMILES: CO[C@@]1H[C@@]2H[C@N](C1)C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N4cnc5cc4ccc5)O

RUN: RUN4394

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

EN300-6746918_3_1_1



CID: EN300-6746918_3_1_1

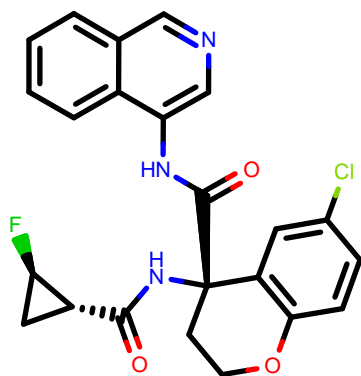
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5CC(C5)(CO)F

RUN: RUN4147

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.36

EN300-97300_1_3_1



CID: EN300-97300_1_3_1

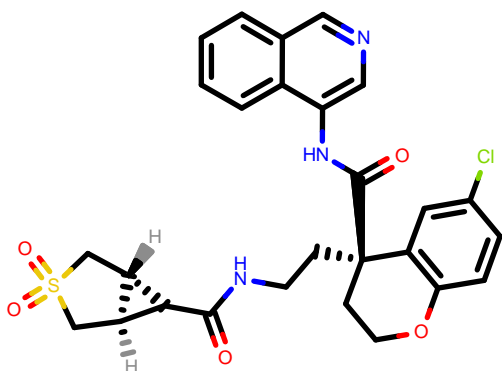
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)[C@@]3[C@@]H5C[C@@]H5F

RUN: RUN4800

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.17

KAD-UNI-8a629cb0-32_1



CID: KAD-UNI-8a629cb0-32_1

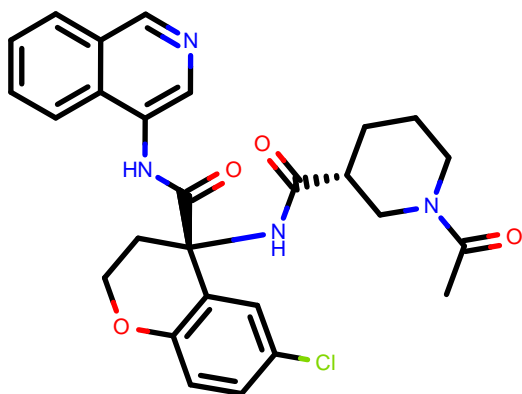
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)CCS(=O)(=O)C

RUN: RUN1970

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.29

EN300-14752_1_2_1



CID: EN300-14752_1_2_1

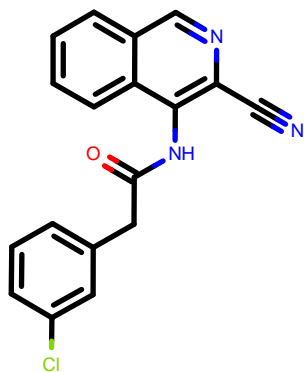
SMILES: CC(=O)N1CCCC[C@@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccc5occcc5

RUN: RUN4082

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

JOH-UNI-3fc3434e-8_1



CID: JOH-UNI-3fc3434e-8_1

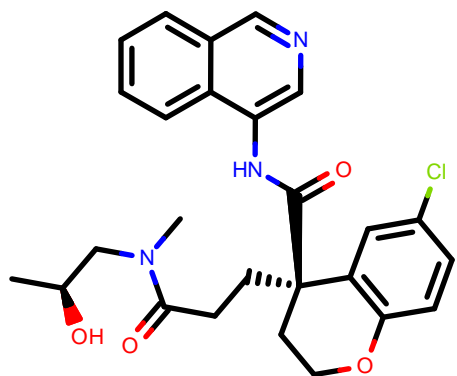
SMILES: c1ccc2c(c1)cnc(c2NC(=O)Cc3cccc(c3)Cl)C#N

RUN: RUN1742

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.29

EN300-210254_2_1_1



CID: EN300-210254_2_1_1

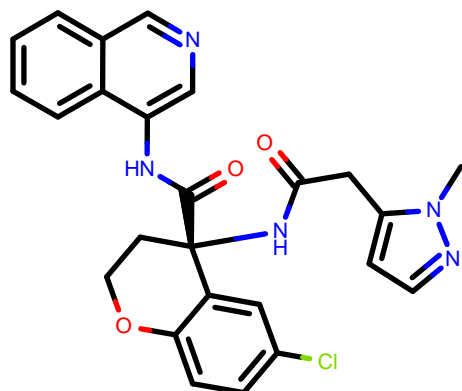
SMILES: C[C@@H](CN(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5574

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-114805_1_1_1



CID: EN300-114805_1_1_1

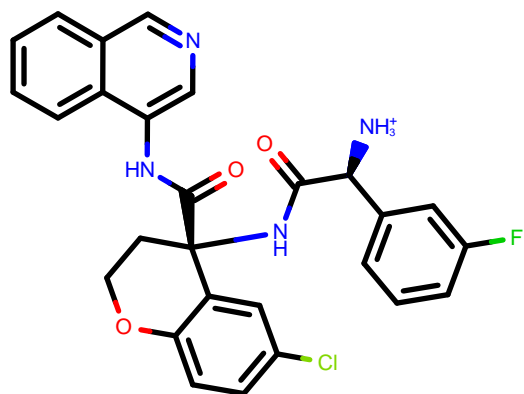
SMILES: Cn1c(ccn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3715

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.21

EDG-MED-90036822-91_2



CID: EDG-MED-90036822-91_2

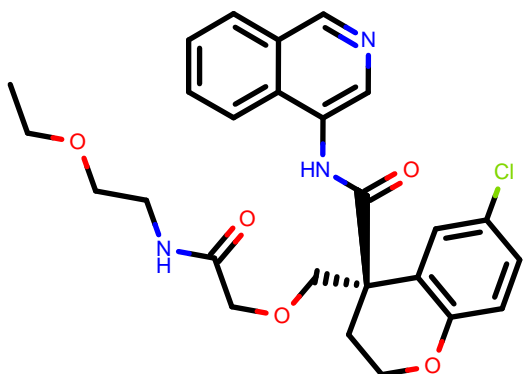
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C)C(=O)[C@H](c5cccc(c5)F)N[H3+]

RUN: RUN1655

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.28

EN300-103187_2_1_1



CID: EN300-103187_2_1_1

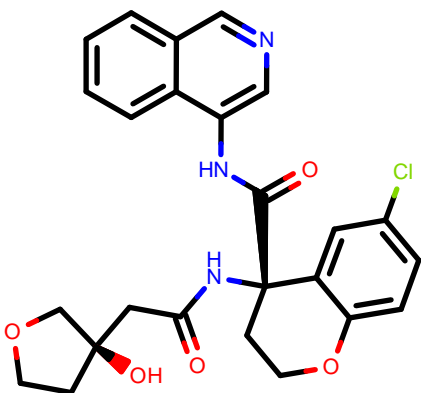
SMILES: CCOCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7232

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.30

EN300-360157_1_1_1



CID: EN300-360157_1_1_1

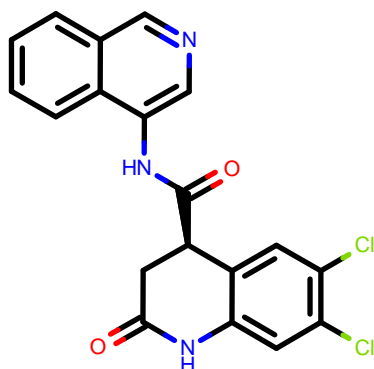
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCOCS)O

RUN: RUN5316

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.28

VLA-UNK-56836b69-1_1



CID: VLA-UNK-56836b69-1_1

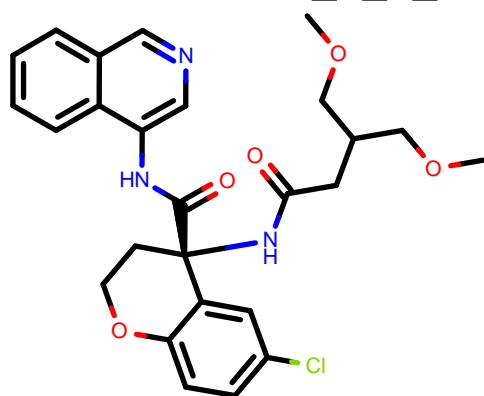
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(c(c4)Cl)Cl

RUN: RUN2127

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.38

EN300-7102031_1_1_1



CID: EN300-7102031_1_1_1

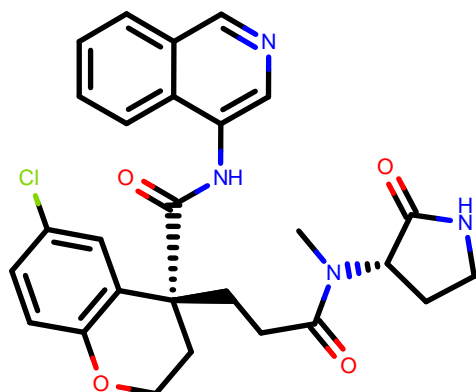
SMILES: COCC(CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)COC

RUN: RUN4915

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.33

EN300-120119_2_2_1



CID: EN300-120119_2_2_1

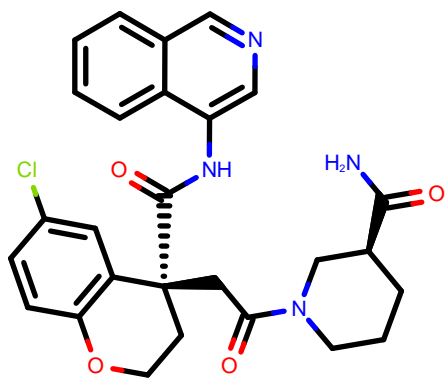
SMILES: CN([C@@H]1CCNC1=O)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN7552

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.22

EN300-18610_1_1_1



CID: EN300-18610_1_1_1

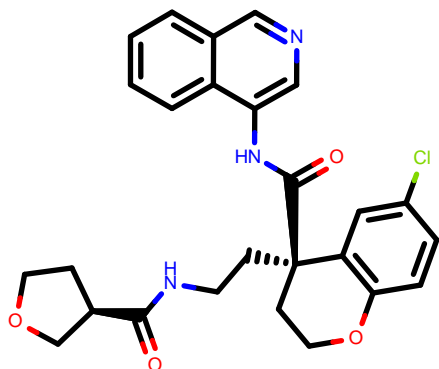
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COCc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)C(=O)N

RUN: RUN4085

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.45

EN300-53423_3_1_1



CID: EN300-53423_3_1_1

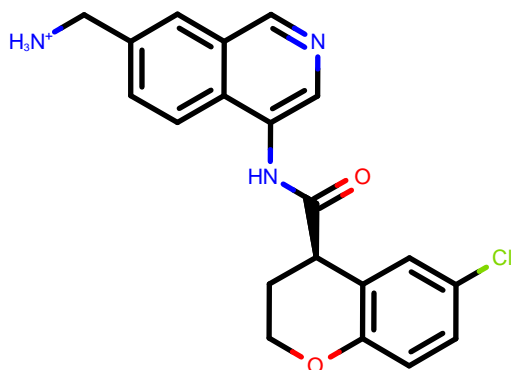
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COCc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCOC5

RUN: RUN4700

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.29

MAK-UNK-8be7dca9-5_1_1



CID: MAK-UNK-8be7dca9-5_1_1

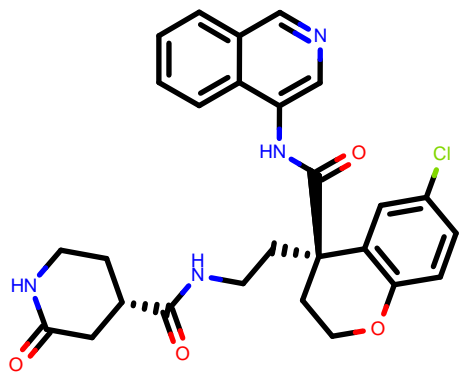
SMILES: c1cc2c(cc1C[NH3+])ncnc2NC(=O)[C@@]3[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN5450

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.11

EN300-107493_3_2_1



CID: EN300-107493_3_2_1

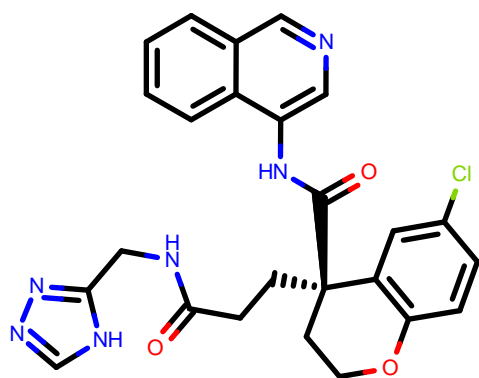
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COCc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCNC(=O)C5

RUN: RUN6343

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.27

EN300-43972_2_1_1



CID: EN300-43972_2_1_1

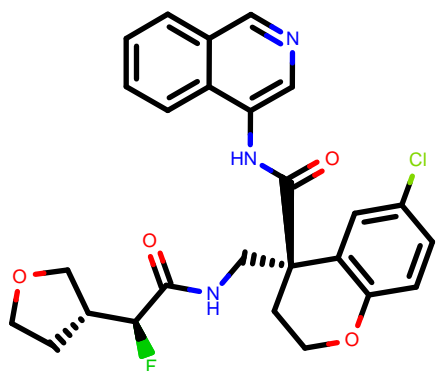
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCc5[nH]nns5

RUN: RUN7733

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.30

EN300-783124_2_2_1



CID: EN300-783124_2_2_1

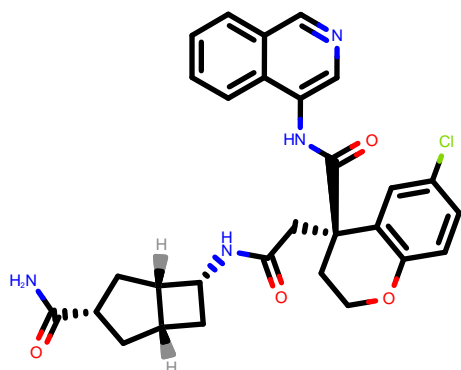
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]([C@@]5COCOC5)F

RUN: RUN6260

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.20

ALP-UNI-3496895b-15_3



CID: ALP-UNI-3496895b-15_3

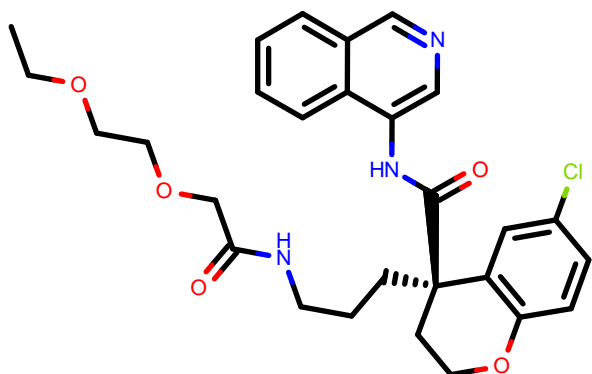
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(O)NC@@H5C[C@@H]6[C@H](C6)Cl<N

RUN: RUN2376

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.31

EN300-54304_4_1_1



CID: EN300-54304_4_1_1

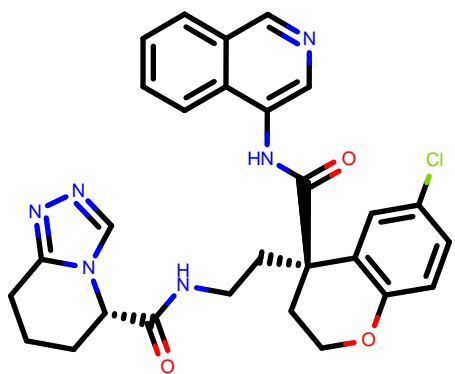
SMILES: CCOCCOCC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6742

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.36

EN300-6478631_3_1_1



CID: EN300-6478631_3_1_1

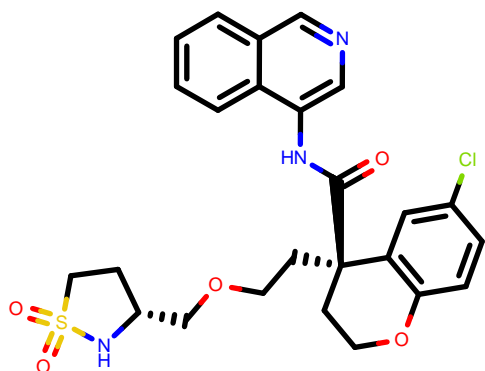
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCCn6

RUN: RUN3280

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.34

EN300-1699871_3_2_1



CID: EN300-1699871_3_2_1

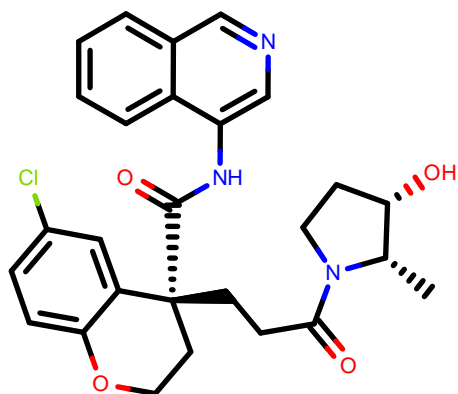
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)N5

RUN: RUN6321

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-2008120_2_1_1



CID: EN300-2008120_2_1_1

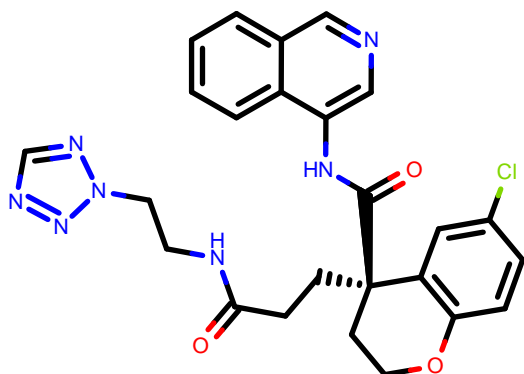
SMILES: C[C@@H]1[C@@H](CCN1C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN6647

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-107823_2_1_1



CID: EN300-107823_2_1_1

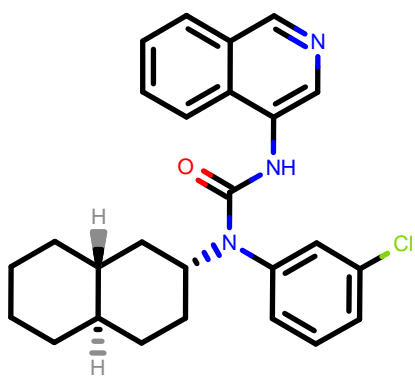
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCn5

RUN: RUN6090

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.25

MIC-UNK-cdc2493e-8_3



CID: MIC-UNK-cdc2493e-8_3

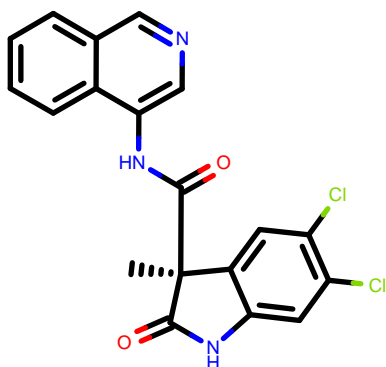
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C@@H4CC[C@@H]5CCCC[C@@H]5C4

RUN: RUN474

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.32

EDJ-MED-9e38fd34-4_1



CID: EDJ-MED-9e38fd34-4_1

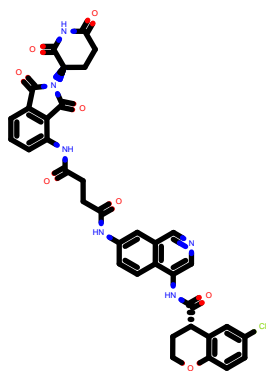
SMILES: C[C@@@]1(c2cc(c(cc2NC1=O)Cl)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN2177

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

DAR-DIA-9e4459de-15_9



CID: DAR-DIA-9e4459de-15_9

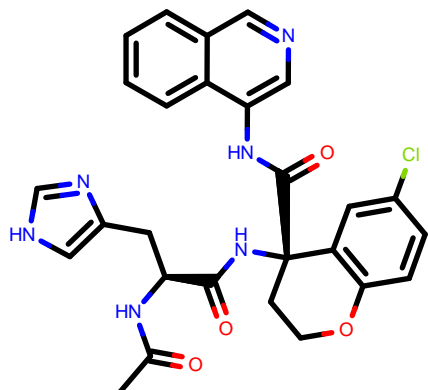
SMILES: c1cc2c(c1)NC(=O)CC(=O)Nc3cccc(c3)NC(=O)C@H4CCOCc5c6c5c(c6)Cl)c7c(c2O)C@H]7CC(=O)NC7=O)O

RUN: RUN1337

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.75

EN300-196320_1_1_1



CID: EN300-196320_1_1_1

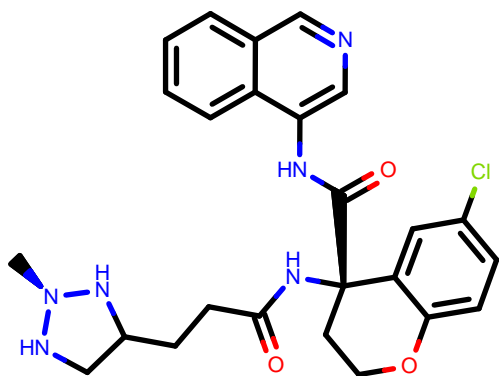
SMILES: CC(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6611

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-244744_1_1_1



CID: EN300-244744_1_1_1

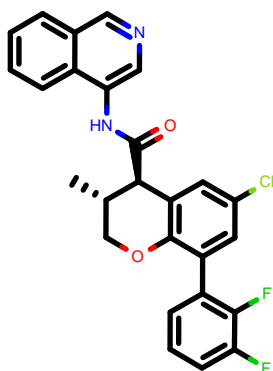
SMILES: Cn1ncc(n1)CCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3938

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.25

DAR-DIA-0d514e7d-14_1_1



CID: DAR-DIA-0d514e7d-14_1_1

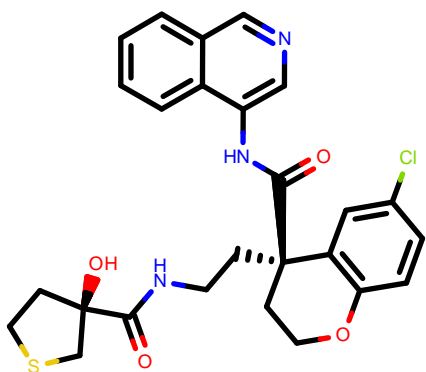
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5ccoc(c5)F

RUN: RUN7282

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.20

EN300-122656_3_2_1



CID: EN300-122656_3_2_1

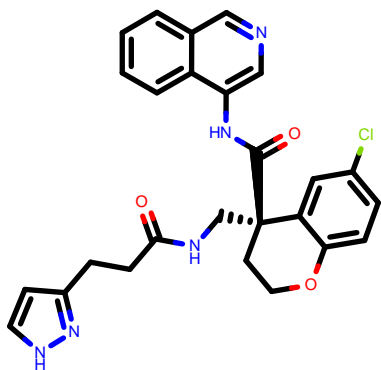
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCSC5)O

RUN: RUN4125

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.43

EN300-1664603_2_1_1



CID: EN300-1664603_2_1_1

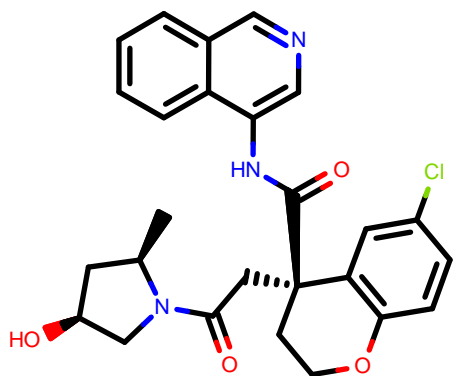
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CC5ccn[nH]5

RUN: RUN7112

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-173562_1_1_1



CID: EN300-173562_1_1_1

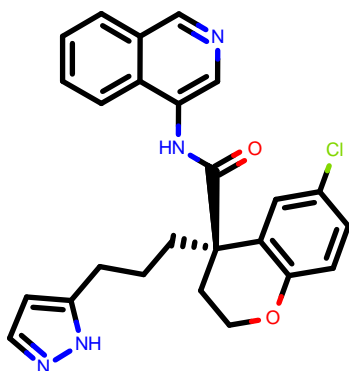
SMILES: C[C@@H]1C[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5)O

RUN: RUN4395

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

VLA-UCB-34f3ed0c-10_1



CID: VLA-UCB-34f3ed0c-10_1

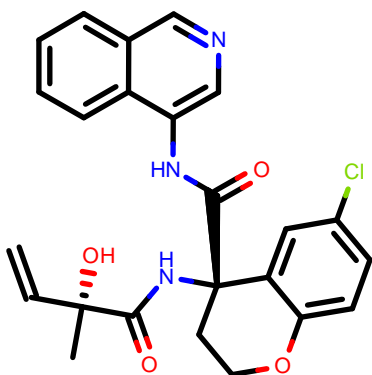
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5cn[nH]5

RUN: RUN570

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.28

EN300-248888_1_1_1



CID: EN300-248888_1_1_1

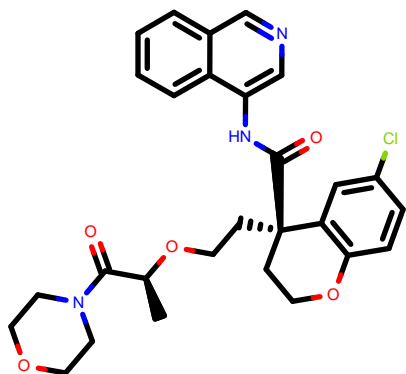
SMILES: C[C@@](C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccc4)O

RUN: RUN5908

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

EN300-05754_3_1_1



CID: EN300-05754_3_1_1

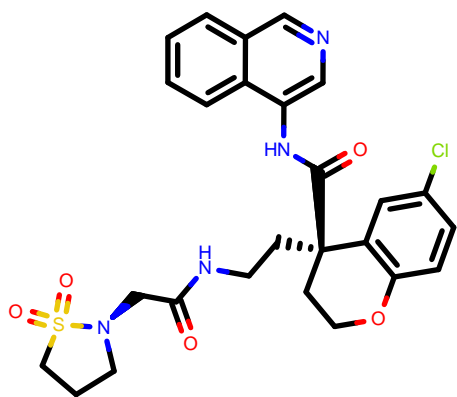
SMILES: C[C@@H](C(=O)N1CCOCC1)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN4421

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.38

EN300-43206_3_1_1



CID: EN300-43206_3_1_1

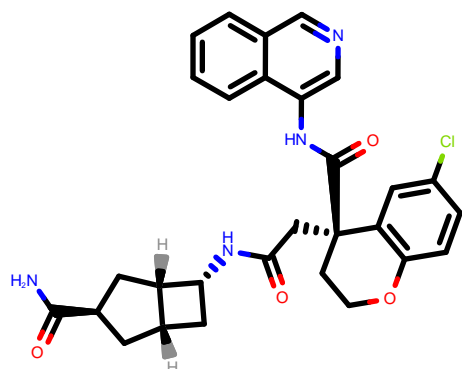
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[N@]5CCCS5(=O)=O

RUN: RUN5472

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.34

EN300-1268016_1_3_1



CID: EN300-1268016_1_3_1

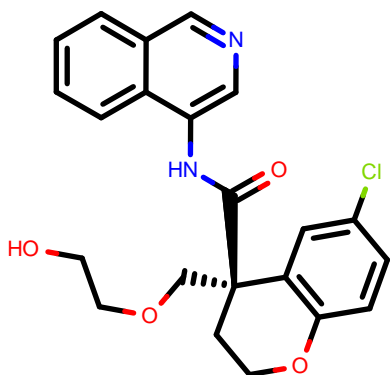
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[C@@]5H5C[C@@H]6[C@@]5H5C[C@@H]6Cl=O

RUN: RUN5654

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.34

EN300-21258_2_1_1



CID: EN300-21258_2_1_1

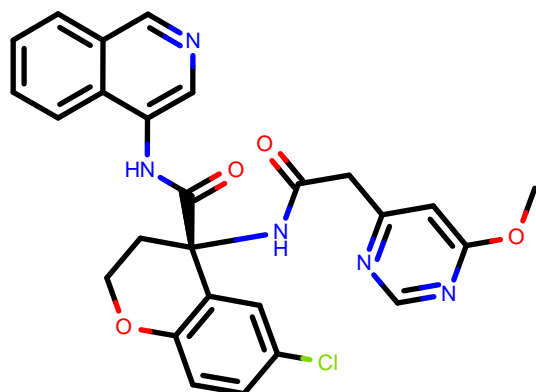
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCO

RUN: RUN6798

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.18

EN300-7444950_1_1_1



CID: EN300-7444950_1_1_1

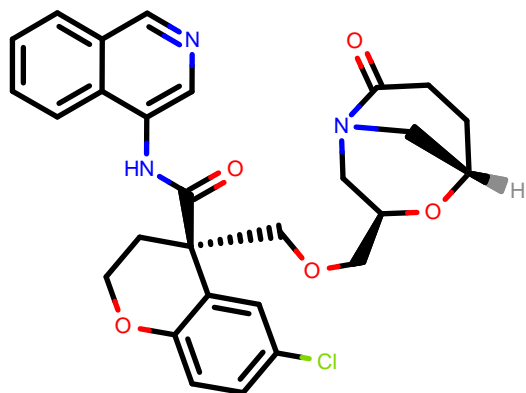
SMILES: COc1cc(ncn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4311

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.34

LEE-CAM-7ab9b158-4_3



CID: LEE-CAM-7ab9b158-4_3

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)COC(C@@H)5CN6CQC@@H)O5CCC6=O

RUN:

RUN2079

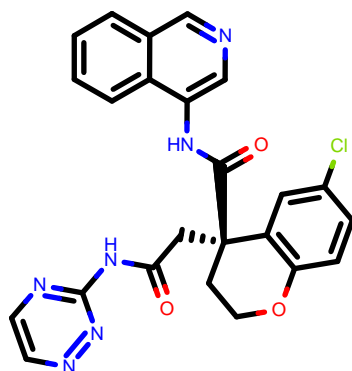
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.46

CHO-MSK-a31cca77-3_1



CID: CHO-MSK-a31cca77-3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CC(=O)Nc5ncnn5

RUN:

RUN2054

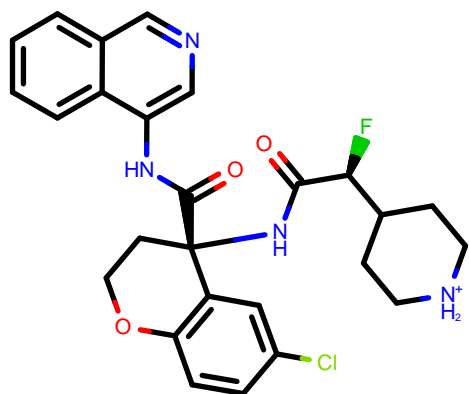
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.25

EDG-MED-90036822-95_2



CID: EDG-MED-90036822-95_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@H)C5CC[NH2+](C)C5)F

RUN:

RUN1675

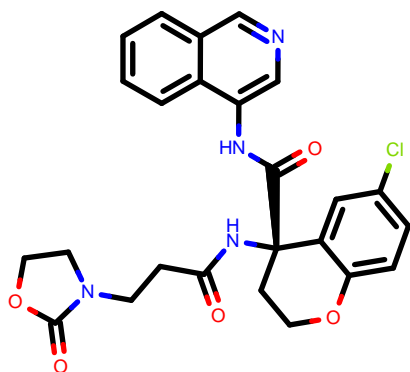
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.26

EN300-53918_1_1_1



CID: EN300-53918_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)CCN5CCOC5=O

RUN:

RUN6001

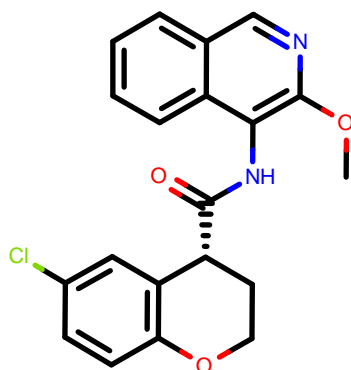
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.25

JOH-UNI-f51e3bbc-4_1_1



CID: JOH-UNI-f51e3bbc-4_1_1

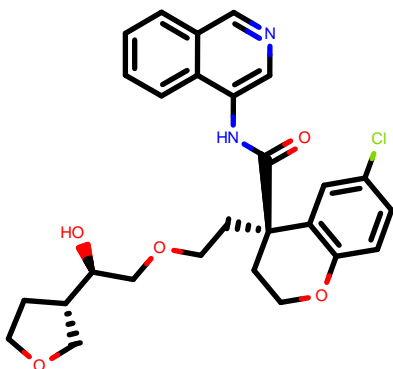
SMILES: COc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN5576

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.12

EN300-1911992_3_3_1



CID: EN300-1911992_3_3_1

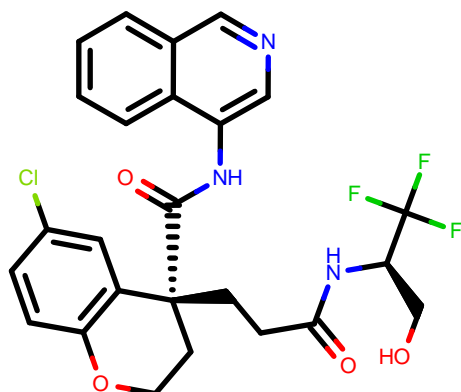
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](C@H)5COCOC5O

RUN: RUN6212

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.36

EN300-296237_2_2_1



CID: EN300-296237_2_2_1

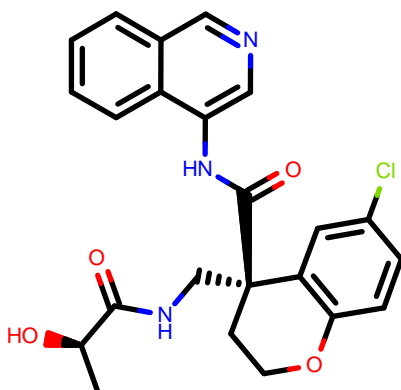
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CO)C(F)(F)F

RUN: RUN7068

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.50

EN300-19542_2_2_1



CID: EN300-19542_2_2_1

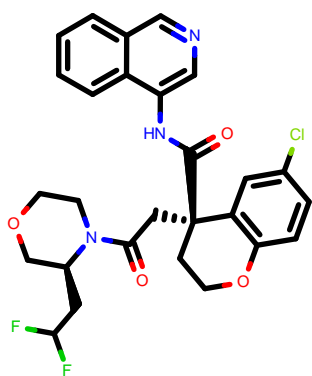
SMILES: C[C@@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6504

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.25

EDG-MED-ba1ac7b9-20_1



CID: EDG-MED-ba1ac7b9-20_1

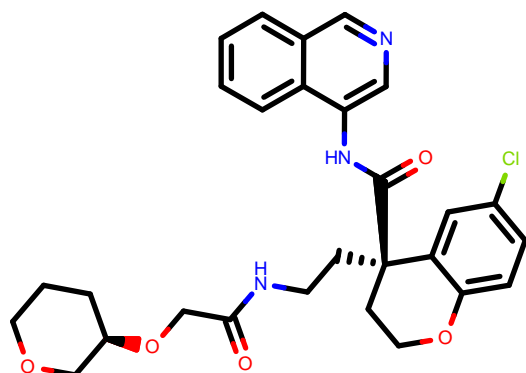
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5C(F)F

RUN: RUN2569

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.24

EN300-1627945_3_1_1



CID: EN300-1627945_3_1_1

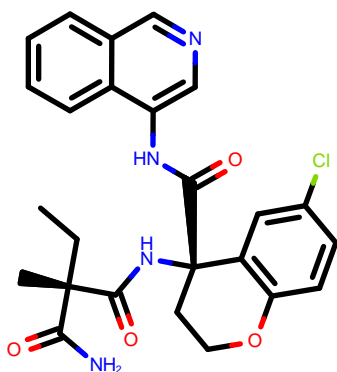
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN5059

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.24

EN300-2908024_1_1_1



CID: EN300-2908024_1_1_1

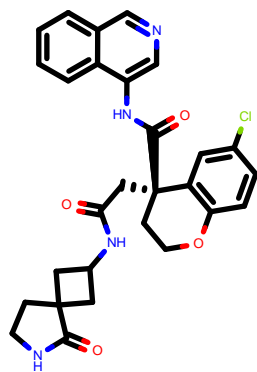
SMILES: CC(C@@]1(C)C(=O)N[C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5820

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.26

EN300-743350_1_1_1



CID: EN300-743350_1_1_1

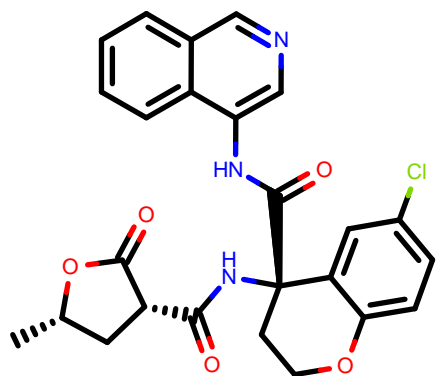
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6C(C5)CCNCC6=O

RUN: RUN6111

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.28

EN300-7444533_1_4_1



CID: EN300-7444533_1_4_1

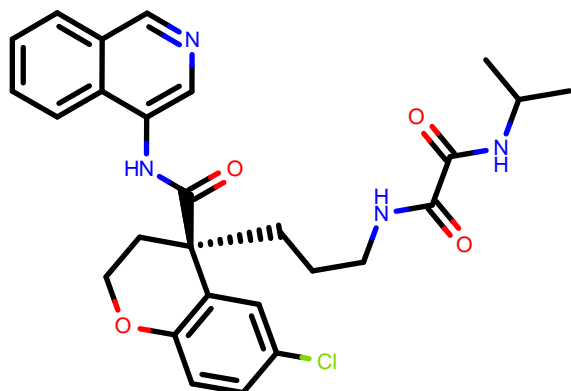
SMILES: C[C@H]1C[C@H](C(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5202

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.21

EN300-1262640_4_1_1



CID: EN300-1262640_4_1_1

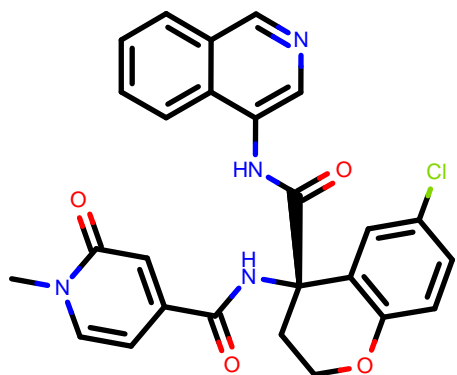
SMILES: CC(C)N[C(=O)C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5427

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.31

EN300-30480_1_1_1



CID: EN300-30480_1_1_1

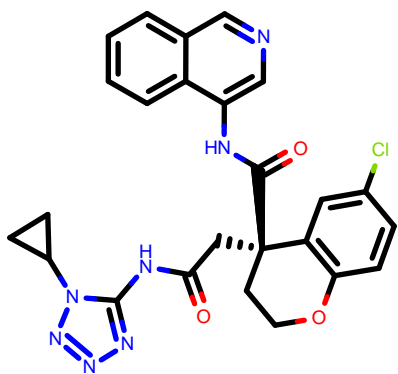
SMILES: Cn1ccc(cc1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6061

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.24

EDJ-MED-d203f206-11_1



CID: EDJ-MED-d203f206-11_1

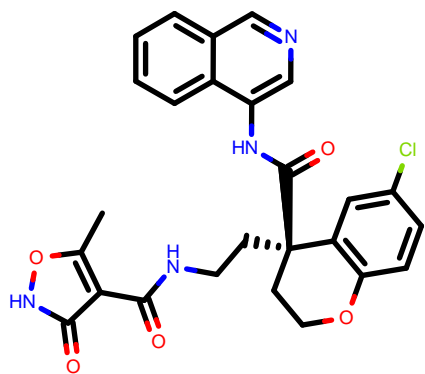
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnnn5C6C6

RUN: RUN2396

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.27

EN300-110423_3_1_1



CID: EN300-110423_3_1_1

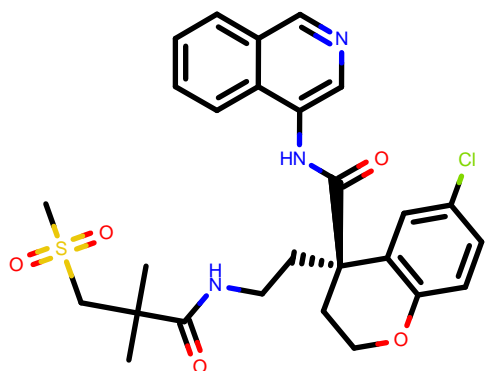
SMILES: Cc1c(c(=O)[nH]o1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4893

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.30

EN300-188217_3_1_1



CID: EN300-188217_3_1_1

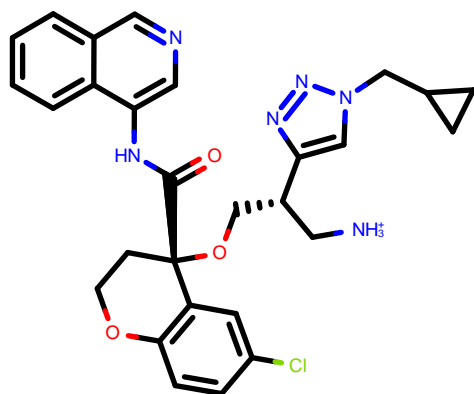
SMILES: CC(C)(CS(=O)(=O)C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN3248

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.48

ED_-GRI-5b13fbe2-49_1



CID: ED_-GRI-5b13fbe2-49_1

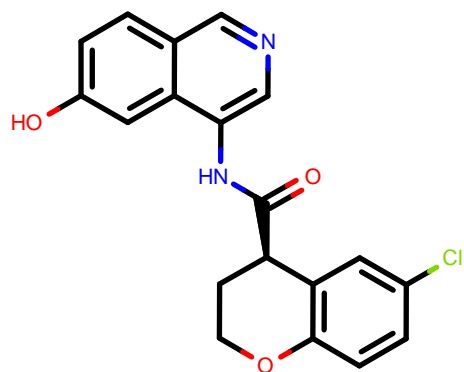
SMILES: c1ccc2c(1)ncnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)OC[C@]5H[C@@H]3CN5c6cnc6

RUN: RUN1526

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.37

BEN-DND-c852c98b-4_1_1



CID: BEN-DND-c852c98b-4_1_1

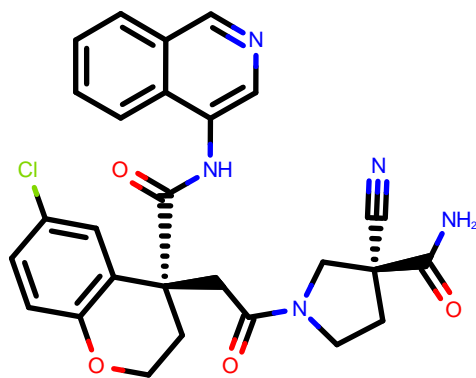
SMILES: c1cc2cnc(c2cc1O)NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C

RUN: RUN6535

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.04

EN300-1608992_1_2_1



CID: EN300-1608992_1_2_1

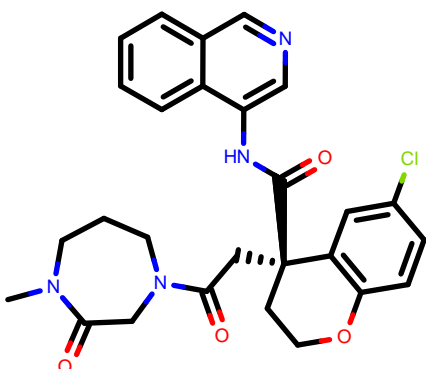
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@](C5)(C#N)C(=O)N

RUN: RUN6187

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.30

EN300-160143_1_1_1



CID: EN300-160143_1_1_1

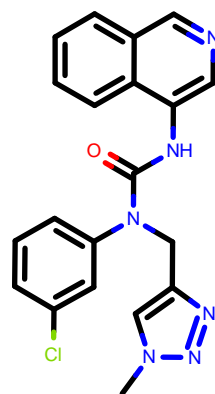
SMILES: CN1CCN(CC1=O)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3975

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

MIC-UNK-bcd487e9-9_1



CID: MIC-UNK-bcd487e9-9_1

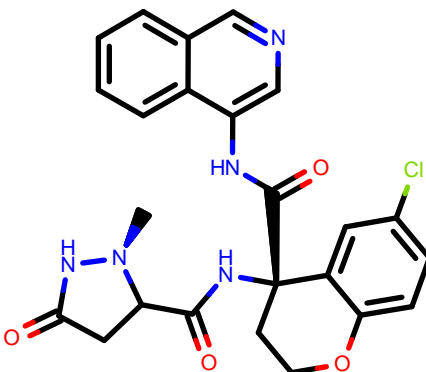
SMILES: Cn1cc(nn1)CN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN498

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.39

EN300-248352_1_1_1



CID: EN300-248352_1_1_1

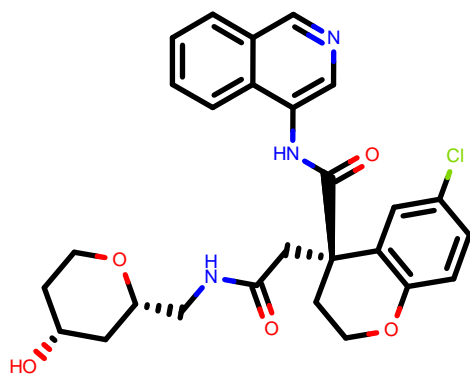
SMILES: Cn1c(cc(=O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3668

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.21

EN300-1708899_1_1_1



CID: EN300-1708899_1_1_1

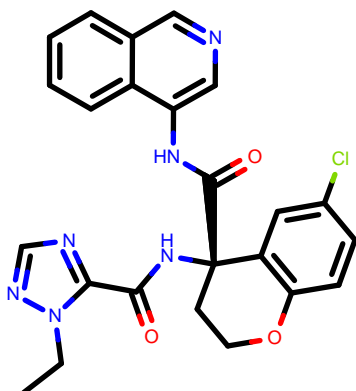
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@H3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H]5C[C@@H]3CCO5O

RUN: RUN7638

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.28

EN300-6494693_1_1_1



CID: EN300-6494693_1_1_1

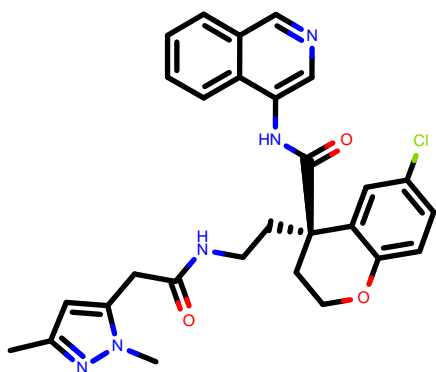
SMILES: CCn1c(ncn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN2757

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.21

EN300-6499639_3_1_1



CID: EN300-6499639_3_1_1

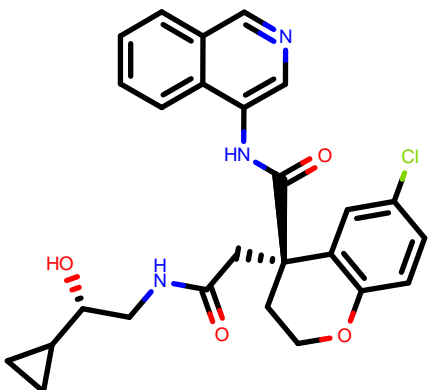
SMILES: Cc1cc(n(n1)C)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN5323

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.33

EN300-67533_1_2_1



CID: EN300-67533_1_2_1

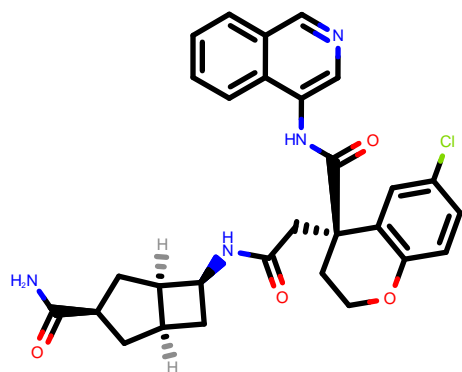
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@H3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H]5C5CC5O

RUN: RUN4009

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

EN300-1268016_1_6_1



CID: EN300-1268016_1_6_1

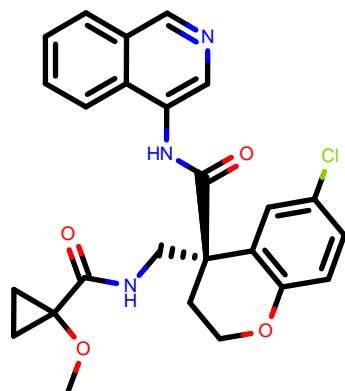
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@O]c4cc3oc4C(C)C(=O)N[C@@H]5[C@@H](C)C(=O)N

RUN: RUN5313

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.40

EN300-182124_2_1_1



CID: EN300-182124_2_1_1

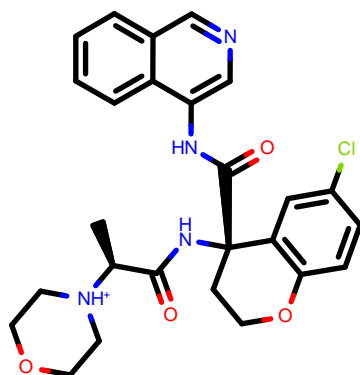
SMILES: COC1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4843

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.26

EN300-41473_1_1_1



CID: EN300-41473_1_1_1

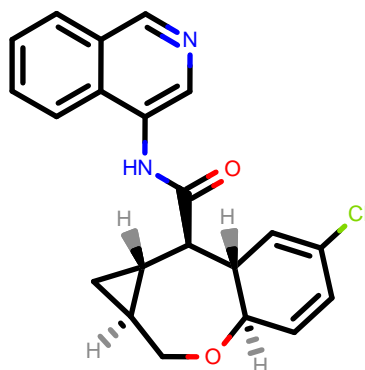
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4)[NH+]5CCOCC5

RUN: RUN4444

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.35

DAR-DIA-0d514e7d-32_27



CID: DAR-DIA-0d514e7d-32_27

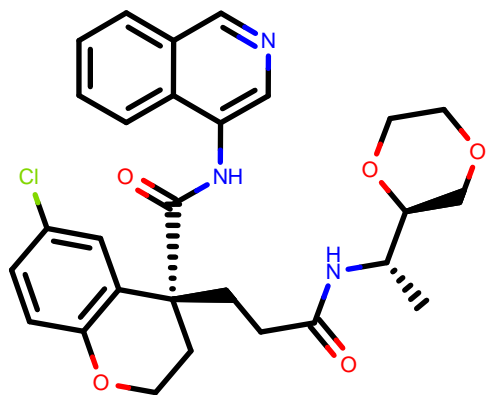
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@H]3[C@@H]4[C@@]3[C@@H]4C(C)C(=O)N[C@@H]5[C@@H]3C(=C=C5)C1

RUN: RUN810

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.24

EN300-6736515_2_1_1



CID: EN300-6736515_2_1_1

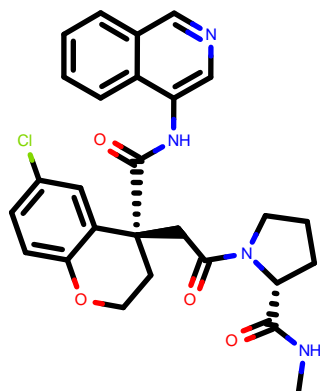
SMILES: C[C@@H]([C@@H]1COCCO1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc5

RUN: RUN7260

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

EN300-55355_1_2_1



CID: EN300-55355_1_2_1

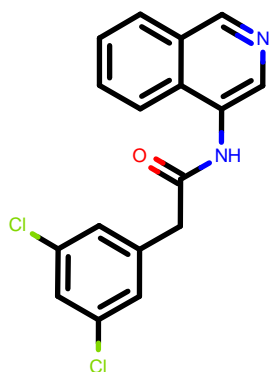
SMILES: CNC(=O)[C@H]1CCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc5

RUN: RUN7052

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

MAT-POS-fce787c2-2_1



CID: MAT-POS-fce787c2-2_1

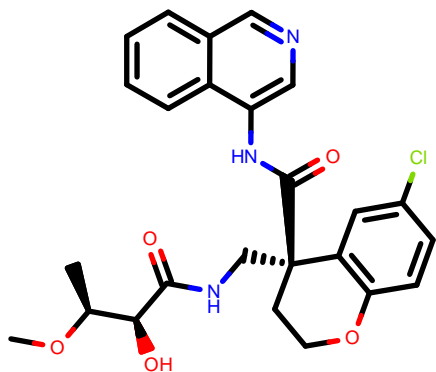
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Cl

RUN: RUN1939

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.23

EN300-220194_2_1_1



CID: EN300-220194_2_1_1

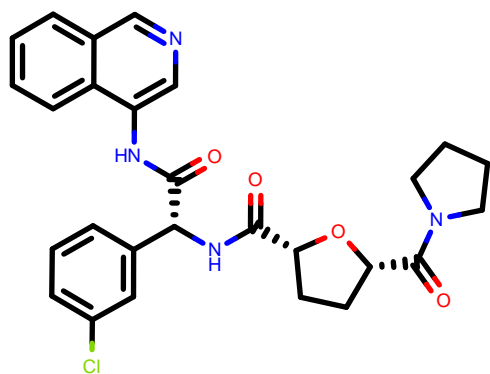
SMILES: C[C@@H]([C@@H]([C@H]1COCCO1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc4)O)OC

RUN: RUN6556

DDG (kcal/mol): -0.65

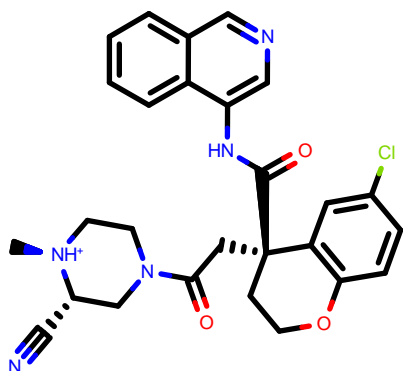
dDDG (kcal/mol): 0.32

EDJ-MED-ee07cf00-11_7



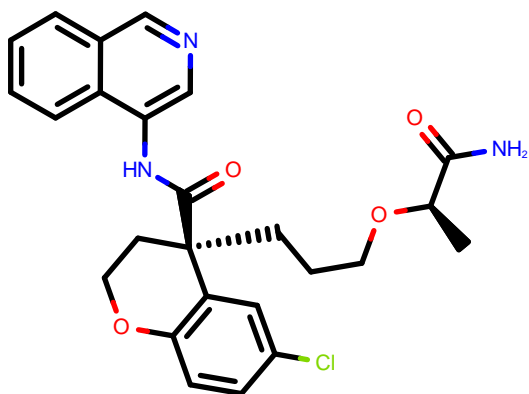
CID:	EDJ-MED-ee07cf00-11_7
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3cccc(c3)C)N[C@@H](C)C(=O)N4CCCC4</chem>
RUN:	RUN2663
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.52

EDG-MED-ba1ac7b9-14_6



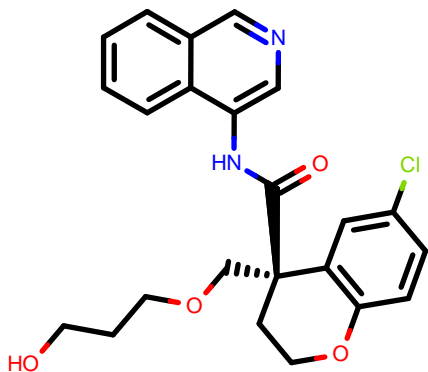
CID:	EDG-MED-ba1ac7b9-14_6
SMILES:	<chem>C[N@H]1CCN(C[C@@H]1C#N)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5</chem>
RUN:	RUN2510
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.28

EN300-17381_4_2_1



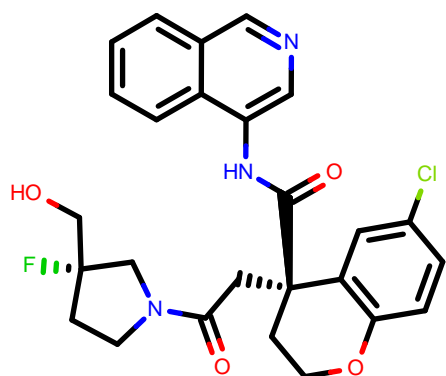
CID:	EN300-17381_4_2_1
SMILES:	<chem>C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN4840
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.30

EN300-221518_2_1_1



CID:	EN300-221518_2_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO</chem>
RUN:	RUN4598
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.26

EN300-203118_1_2_1



CID: EN300-203118_1_2_1

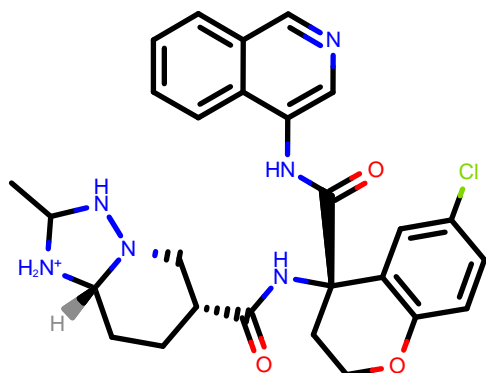
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@](C5)(CO)F

RUN: RUN5664

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.28

ALP-UNI-dbbfd3db-4_1



CID: ALP-UNI-dbbfd3db-4_1

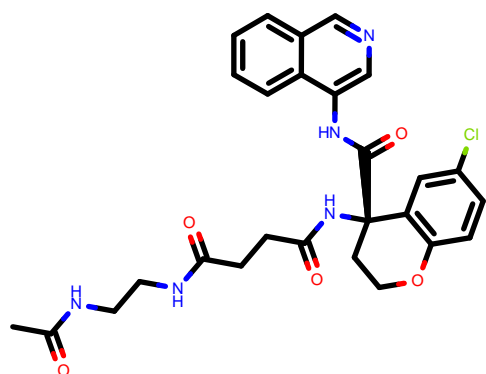
SMILES: Cc1nc2n(m1)C[C@@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN2600

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.26

EN300-73507_1_1_1



CID: EN300-73507_1_1_1

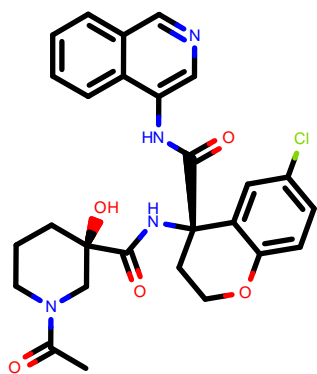
SMILES: CC(=O)NCCNC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4

RUN: RUN5896

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.30

EN300-210552_1_1_1



CID: EN300-210552_1_1_1

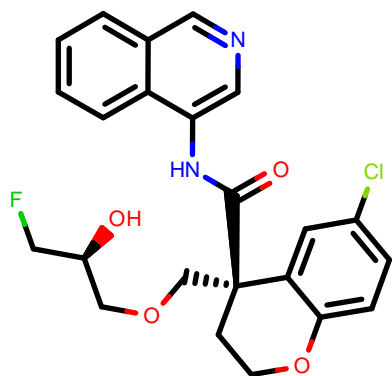
SMILES: CC(=O)N1CCC[C@](C1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O

RUN: RUN5879

DDG (kcal/mol): -0.64

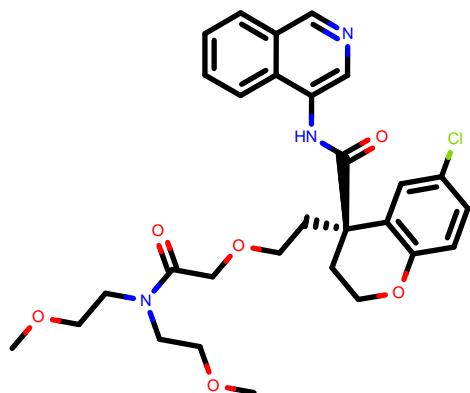
dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-4_1



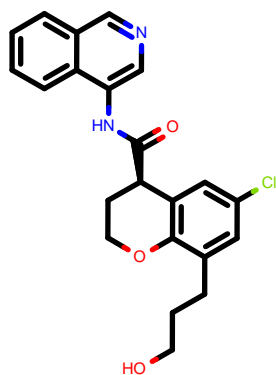
CID:	EDJ-MED-fcba3f31-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O</chem>
RUN:	RUN2384
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.31

EN300-04491_3_1_1



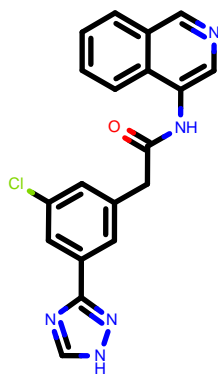
CID:	EN300-04491_3_1_1
SMILES:	<chem>COCCN(CCOC)C(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4</chem>
RUN:	RUN6251
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.50

LAU-MED-88a3970a-5_1



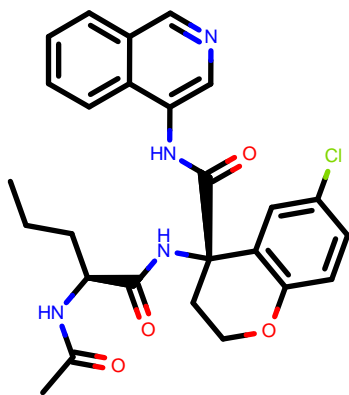
CID:	LAU-MED-88a3970a-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4CCCO)Cl</chem>
RUN:	RUN1339
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.19

MAT-POS-281d2ee9-2_1



CID:	MAT-POS-281d2ee9-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)c4[nH]n4</chem>
RUN:	RUN1721
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.31

EN300-43047_1_1_1



CID: EN300-43047_1_1_1

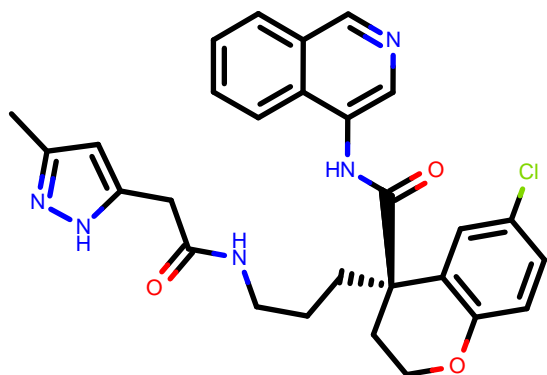
SMILES: CC(=O)N[C@@H](CC=C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6738

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.26

EN300-105110_4_1_1



CID: EN300-105110_4_1_1

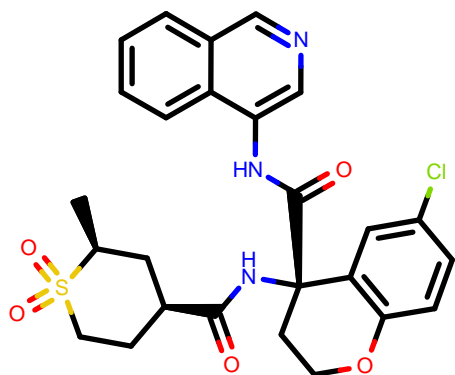
SMILES: Cc1cc(n[nH]1)CC(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4791

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.32

EN300-6082676_1_4_1



CID: EN300-6082676_1_4_1

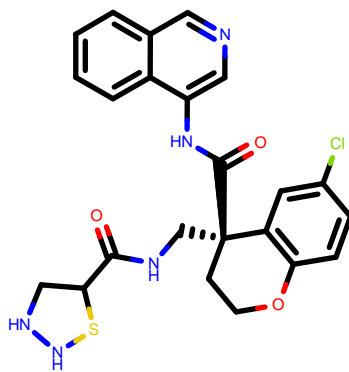
SMILES: C[C@H]1[C@@H](CCS1(=O)=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4755

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.23

EN300-42269_2_1_1



CID: EN300-42269_2_1_1

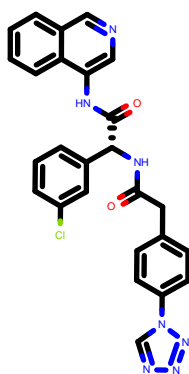
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnns5

RUN: RUN6340

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.28

EDJ-MED-ee07cf00-15_1



CID: EDJ-MED-ee07cf00-15_1

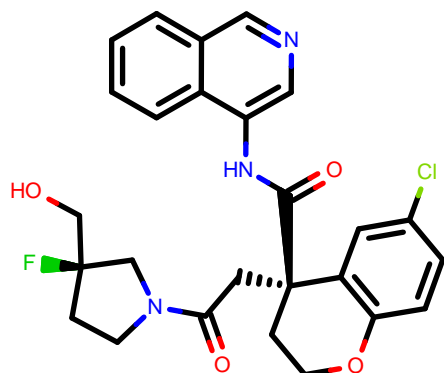
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](c3cccc(c3)C)NC(=O)C4ccc(cc4)n5cnnn5

RUN: RUN2678

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.45

EN300-203118_1_1_1



CID: EN300-203118_1_1_1

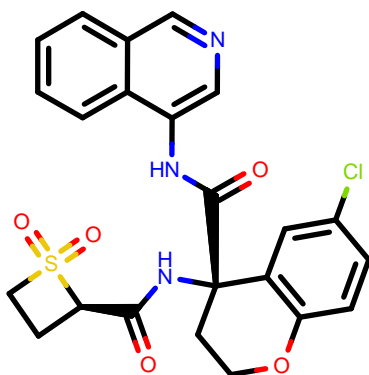
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3(C5)COF

RUN: RUN4324

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.28

EN300-1387104_1_2_1



CID: EN300-1387104_1_2_1

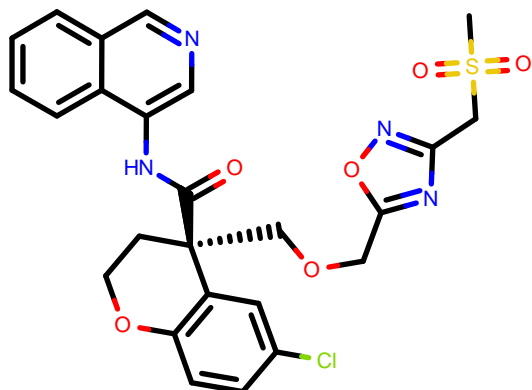
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCS5(=O)=O

RUN: RUN3053

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.29

EN300-94900_2_1_1



CID: EN300-94900_2_1_1

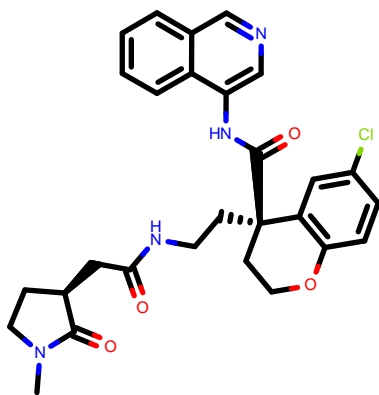
SMILES: CS(=O)(=O)C1cnc(on1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5016

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.45

EN300-378722_3_2_1



CID: EN300-378722_3_2_1

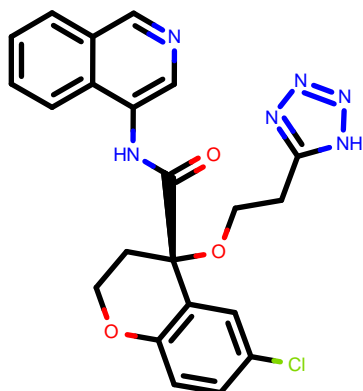
SMILES: CN1CC[C@H](C1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6302

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.32

ED_-GRI-5b13fbe2-56_1



CID: ED_-GRI-5b13fbe2-56_1

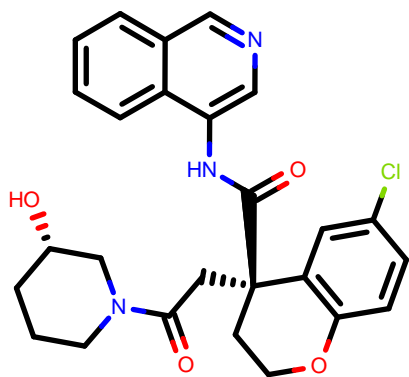
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CCc5n[n-]nn5

RUN: RUN1427

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.25

EN300-188582_1_1_1



CID: EN300-188582_1_1_1

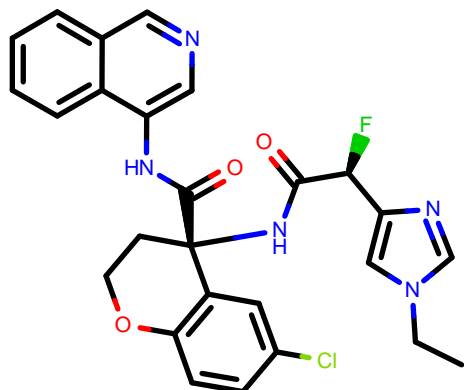
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CC[C@]([H])(C5)O

RUN: RUN4759

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

EDG-MED-90036822-53_1



CID: EDG-MED-90036822-53_1

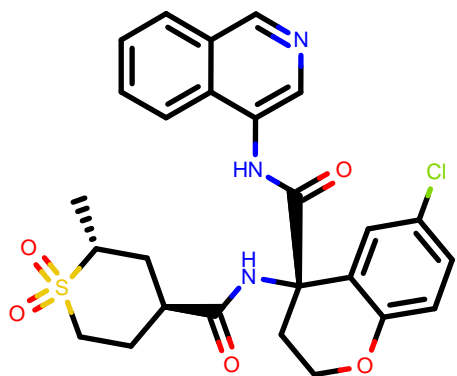
SMILES: Cc1cc(nc1)[C@@]([H])(C(=O)N[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5)F

RUN: RUN1651

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

EN300-6082676_1_3_1



CID: EN300-6082676_1_3_1

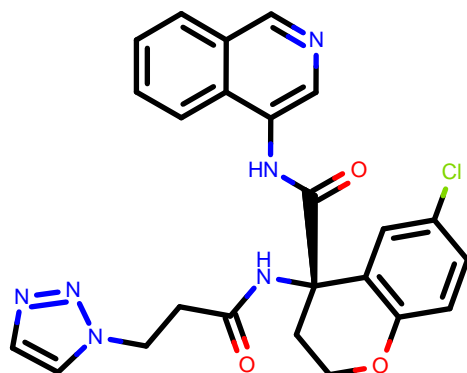
SMILES: C[C@@H]1C[C@H](CCS1(=O)=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7517

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.29

EN300-28871_1_1_1



CID: EN300-28871_1_1_1

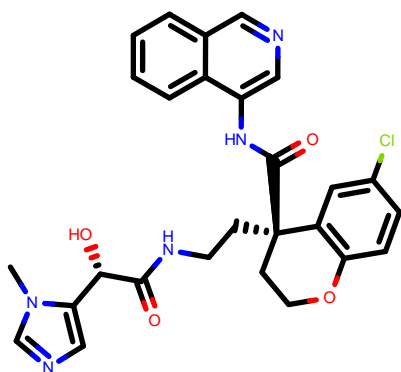
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5

RUN: RUN3566

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.25

EN300-190283_3_1_1



CID: EN300-190283_3_1_1

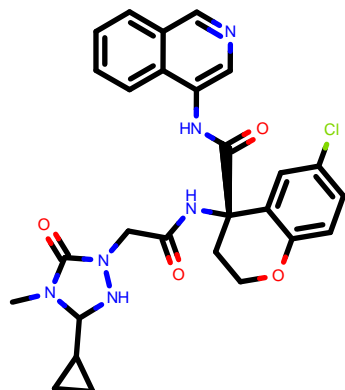
SMILES: Cn1cnc1[C@@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN4486

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.45

EN300-6478432_1_1_1



CID: EN300-6478432_1_1_1

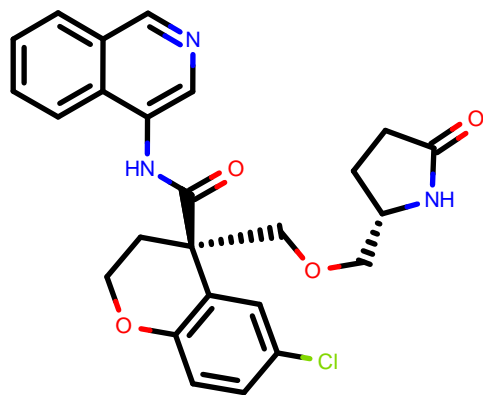
SMILES: Cn1c(nc1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C6C6

RUN: RUN5158

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.42

EN300-264301_2_1_1



CID: EN300-264301_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)COC[C@@H]5CC(=O)N5

RUN:

RUN6610

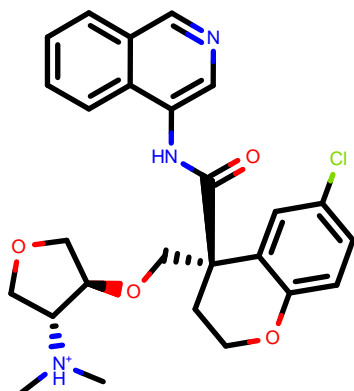
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.24

LEE-CAM-7ab9b158-1_7



CID: LEE-CAM-7ab9b158-1_7

SMILES:

C[NH+](C)[C@@H]1COC[C@H]1OC[C@]2(CCOc3c2cc(cc3)O)C(=O)Nc4ncnc5c4cccc5

RUN:

RUN2044

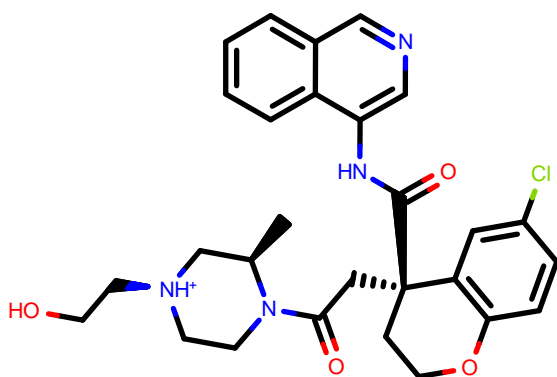
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.37

EDG-MED-ba1ac7b9-27_5



CID: EDG-MED-ba1ac7b9-27_5

SMILES:

C[C@@H]1CN[C@@H]2(CCN1C)O[C@@]3(CCOc4c2ccc3O)C(=O)Nc4ncnc5c4cccc5COO

RUN:

RUN2553

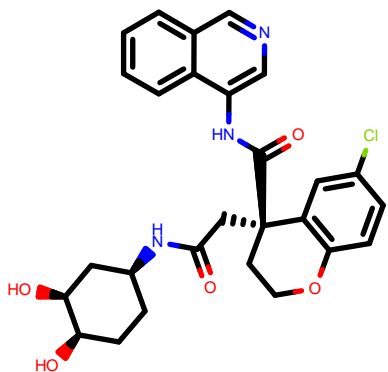
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.63

EN300-741822_1_2_1



CID: EN300-741822_1_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3ccc4)C(=O)N[C@@H]5C[C@@H]6[C@@H](C5)O

RUN:

RUN5507

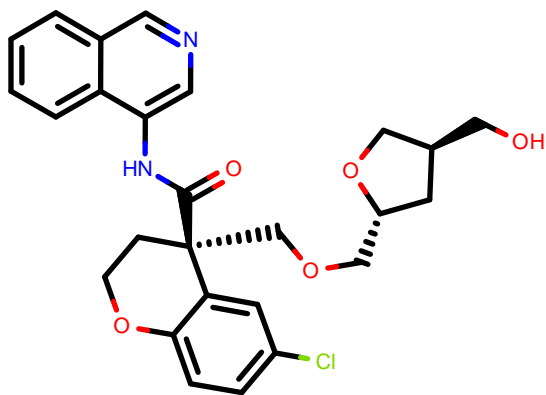
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.24

EN300-6494158_2_2_1



CID: EN300-6494158_2_2_1

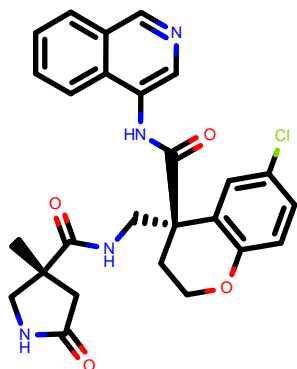
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C[C@@H](CO)C5

RUN: RUN6025

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-132157_2_2_1



CID: EN300-132157_2_2_1

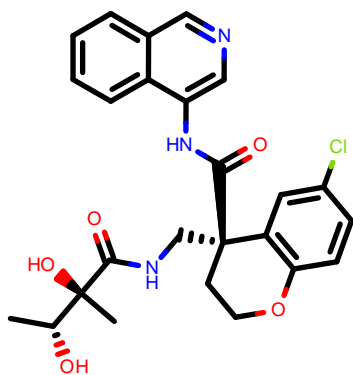
SMILES: C[C@]1(C(=O)NC1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4111

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-202922_2_2_1



CID: EN300-202922_2_2_1

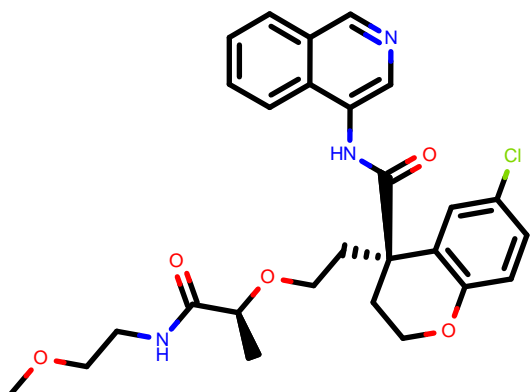
SMILES: C[C@H]([C@@](C)(C)(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN6079

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.29

EN300-23317_3_1_1



CID: EN300-23317_3_1_1

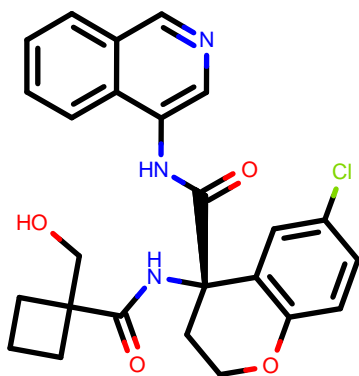
SMILES: C[C@@H](C(=O)NCCOC)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5994

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.41

EN300-149975_1_1_1



CID: EN300-149975_1_1_1

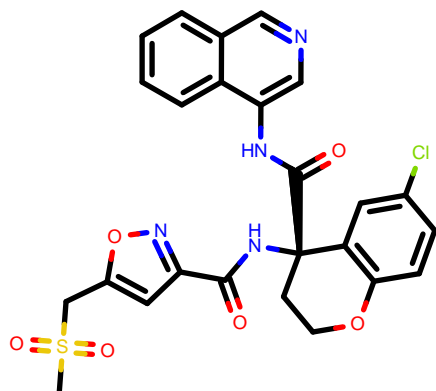
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)CO

RUN: RUN3549

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.25

EN300-1987964_1_1_1



CID: EN300-1987964_1_1_1

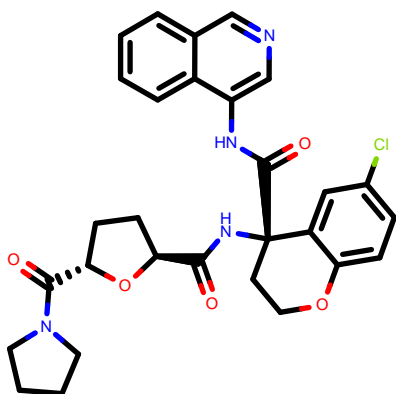
SMILES: CS(=O)(=O)Cc1cc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccs5

RUN: RUN5749

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.37

ALP-UNI-dbbfd3db-6_3



CID: ALP-UNI-dbbfd3db-6_3

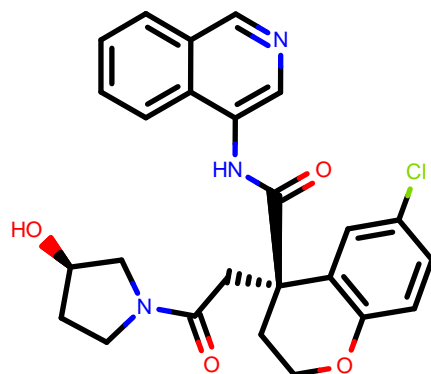
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4(C)N[C@@]4(O)C5(C)CC5

RUN: RUN2616

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-295515_1_2_1



CID: EN300-295515_1_2_1

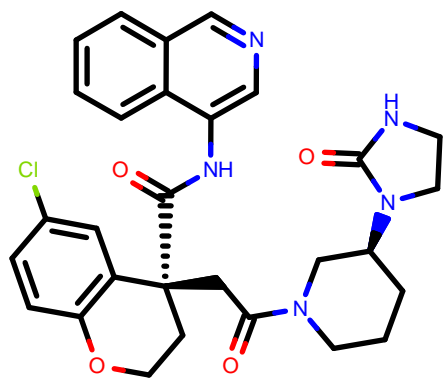
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C5)O

RUN: RUN6156

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.28

EN300-55087_1_1_1



CID: EN300-55087_1_1_1

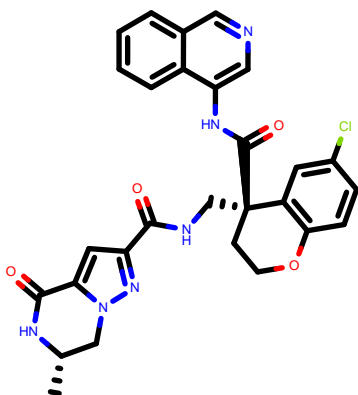
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H]5C6NCCN6=O

RUN: RUN6452

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.35

EN300-265285_2_2_1



CID: EN300-265285_2_2_1

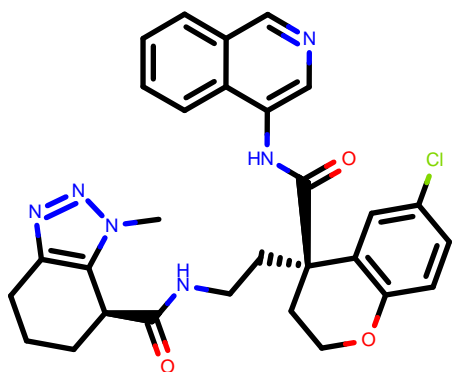
SMILES: C[C@H]1Cn2c(ccn2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5nc6c65ccoc6)C(=O)N1

RUN: RUN4205

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

EN300-1664865_3_1_1



CID: EN300-1664865_3_1_1

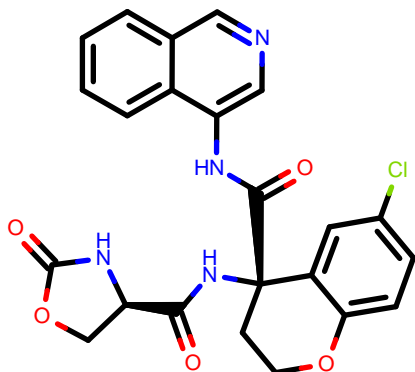
SMILES: Cn1c2c(n1)C[C@]3(CO)NCC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5nc6c65ccoc6

RUN: RUN3479

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.35

EN300-305996_1_1_1



CID: EN300-305996_1_1_1

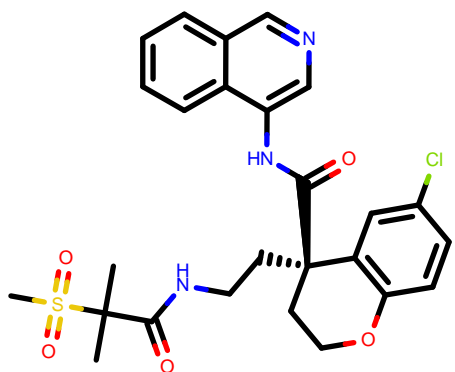
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5COC(=O)N5

RUN: RUN6808

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.22

EN300-76205_3_1_1



CID: EN300-76205_3_1_1

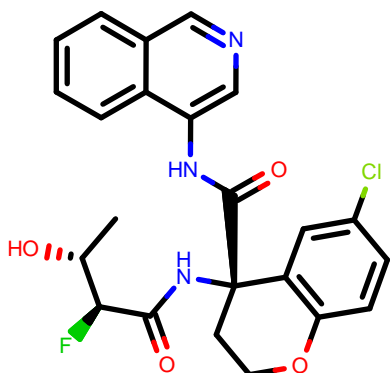
SMILES: CC(C)(C=O)NCC[C@@]1(C)C(=O)NCC[C@@]1(C)C(=O)Nc3ccc4c3ccc4S(=O)(=O)C

RUN: RUN3984

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.46

EDG-MED-90036822-37_2



CID: EDG-MED-90036822-37_2

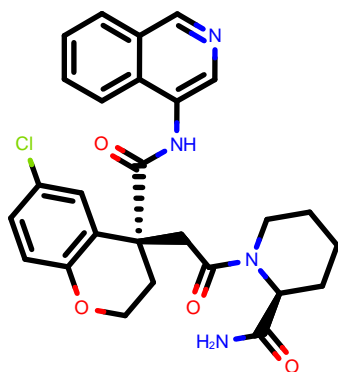
SMILES: C[C@H]([C@@H](C(=O)N[C@@]1(C)C(=O)NCC[C@@]1(C)C(=O)Nc3ccc4c3ccc4F)O

RUN: RUN1589

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.20

EN300-34542_1_2_1



CID: EN300-34542_1_2_1

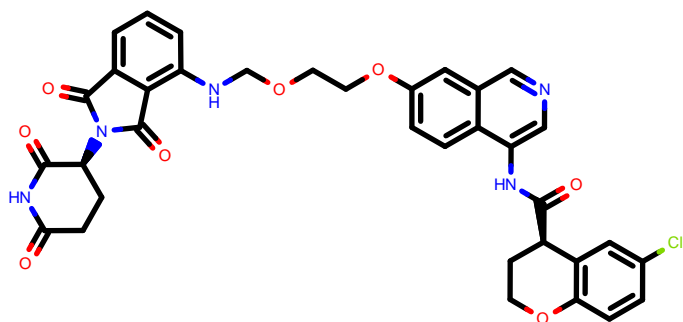
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(=O)NCC[C@@]3(C)C(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN4062

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.35

DAR-DIA-9e4459de-13_8



CID: DAR-DIA-9e4459de-13_8

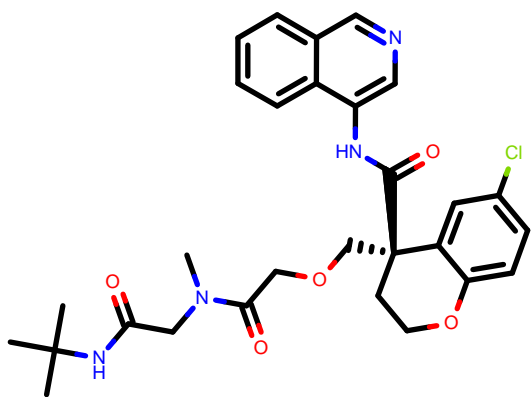
SMILES: c1ccc2c(c1)NC(=O)C3CC4=C(C3)NCC[C@@]4(C)C(=O)Nc5ccc6c5ccc6C(=O)Nc7ccc8c7ccc8NC(=O)N

RUN: RUN1331

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.34

EN300-23019_2_1_1



CID: EN300-23019_2_1_1

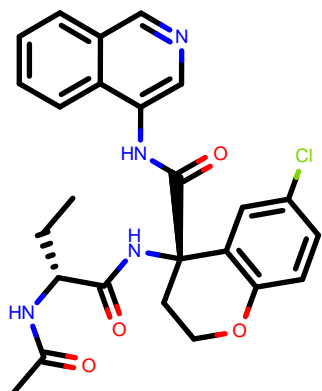
SMILES: CC(C)(C)NC(=O)CN(C)C(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4

RUN: RUN6317

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.33

EN300-332601_1_2_1



CID: EN300-332601_1_2_1

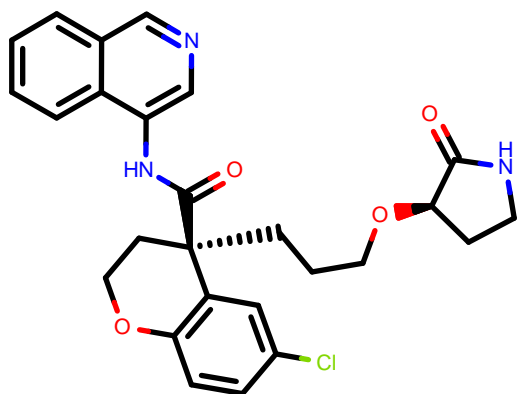
SMILES: CC[C@H](C)C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4)NC(=O)C

RUN: RUN3268

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.24

EN300-6736413_4_1_1



CID: EN300-6736413_4_1_1

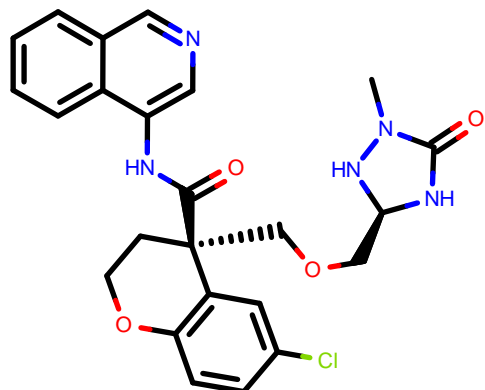
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN3792

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.32

EN300-124918_2_1_2



CID: EN300-124918_2_1_2

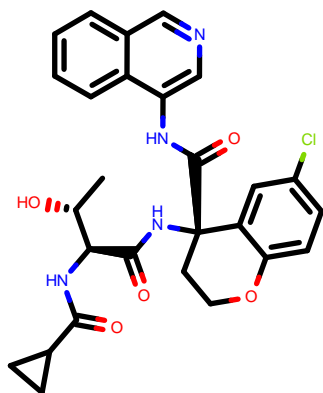
SMILES: CN1C(=O)N[C@@H]([NH2+])COC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN5728

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.27

EN300-96362_1_2_1



CID: EN300-96362_1_2_1

SMILES:

C1C@H][C@@H](C1=O)NC@@1(CCOc2c1cc(c2)Cl)C(=O)Nc3ccc4c3ccc4NC(=O)C5CC5O

RUN:

RUN6104

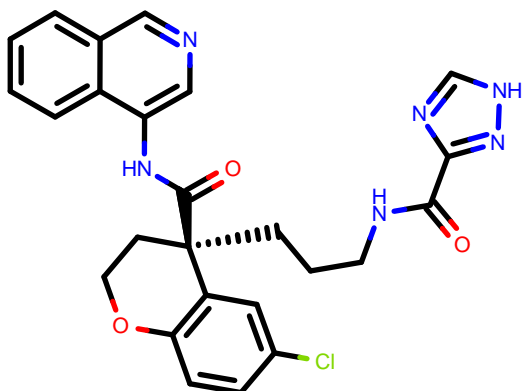
DDG (kcal/mol):

-0.62

dDDG (kcal/mol):

0.33

EN300-100741_4_1_1



CID: EN300-100741_4_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5[nH]nns5

RUN:

RUN7184

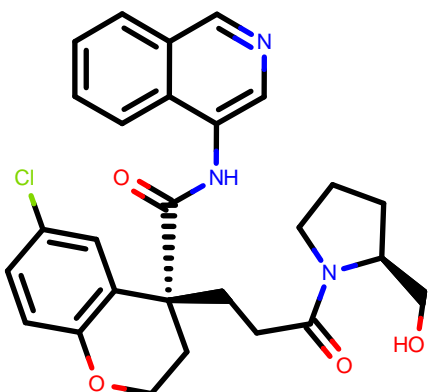
DDG (kcal/mol):

-0.62

dDDG (kcal/mol):

0.31

EN300-70033_2_1_1



CID: EN300-70033_2_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@H]5CO

RUN:

RUN7000

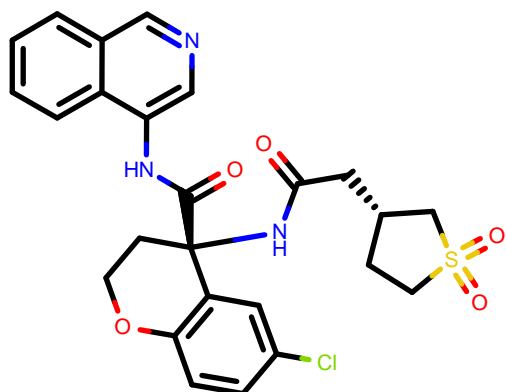
DDG (kcal/mol):

-0.62

dDDG (kcal/mol):

0.26

EN300-14006_1_2_1



CID: EN300-14006_1_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5SCS(=O)(=O)C5

RUN:

RUN5127

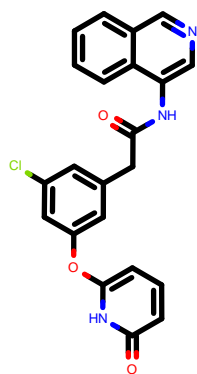
DDG (kcal/mol):

-0.62

dDDG (kcal/mol):

0.33

MAT-POS-9ff17035-2_1



CID: MAT-POS-9ff17035-2_1

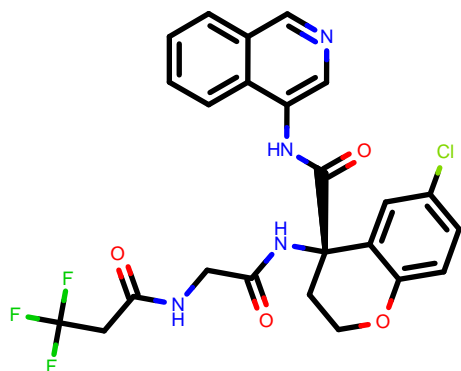
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Oc4cccc(=O)[nH]4

RUN: RUN101

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.40

EN300-43939_1_1_1



CID: EN300-43939_1_1_1

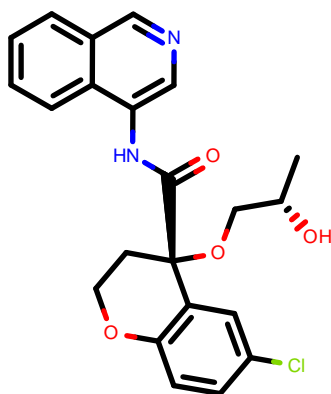
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)CC(F)(F)F

RUN: RUN4034

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.28

EN300-185378_1_1_1



CID: EN300-185378_1_1_1

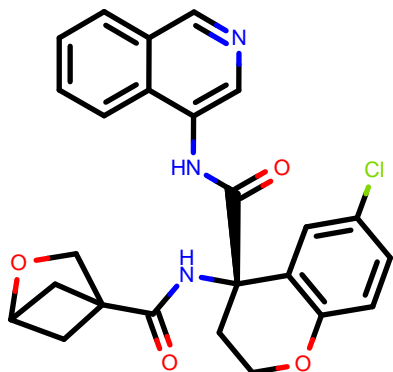
SMILES: C[C@@H](CO[C@]1)1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)O

RUN: RUN7459

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.31

EN300-1604607_1_1_1



CID: EN300-1604607_1_1_1

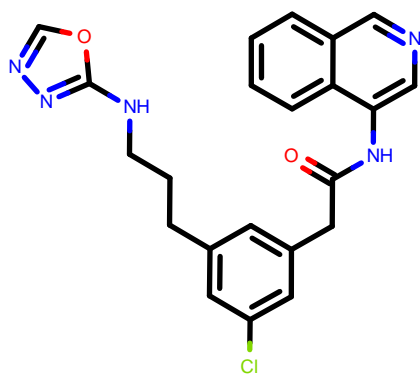
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(C5)OC6

RUN: RUN3837

DDG (kcal/mol): -0.62

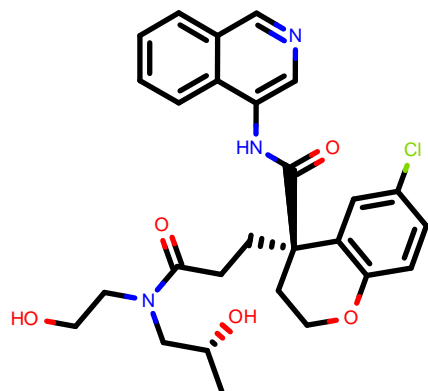
dDDG (kcal/mol): 0.27

PET-UNK-b87f07d0-4_1



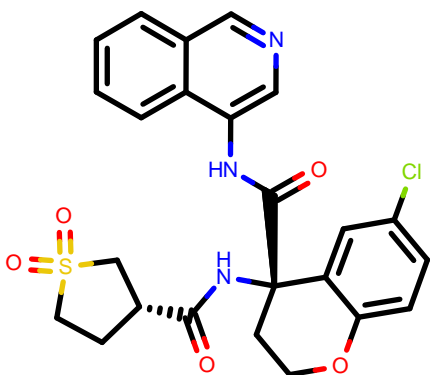
CID:	PET-UNK-b87f07d0-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CCCNc4nnc4</chem>
RUN:	RUN1736
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.51

EN300-214038_2_2_1



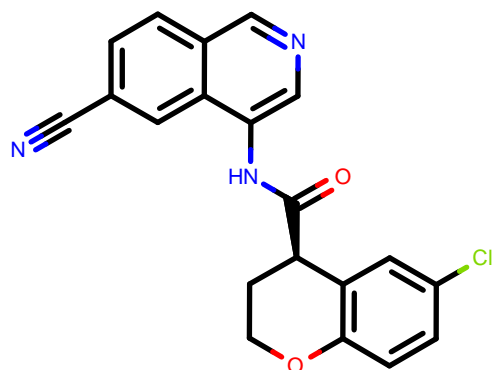
CID:	EN300-214038_2_2_1
SMILES:	<chem>C[C@H](CN(CC(O)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O</chem>
RUN:	RUN6925
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.27

EN300-14437_1_1_1



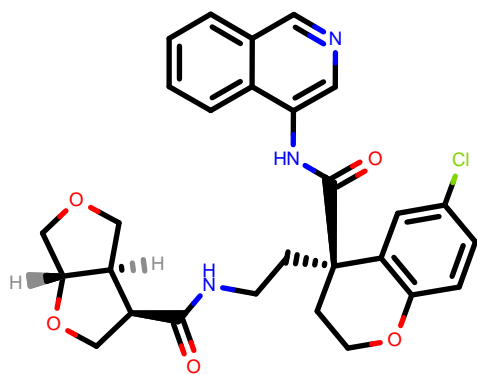
CID:	EN300-14437_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCS(=O)(=O)C5</chem>
RUN:	RUN7392
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.21

BEN-DND-c852c98b-1_1



CID:	BEN-DND-c852c98b-1_1
SMILES:	<chem>c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN1086
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.05

EN300-6482296_3_8_1



CID: EN300-6482296_3_8_1

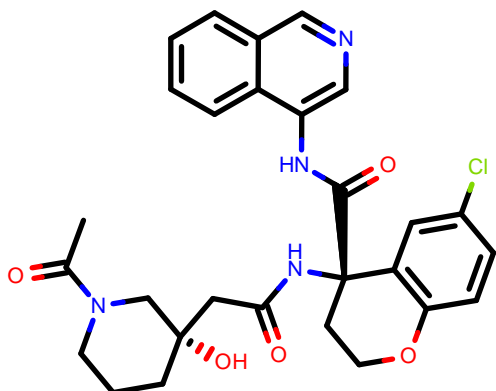
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@([C@@]3(CCOc4ccc(cc4)C)CN(C=O)C)C@H5CO[C@@H]6C@H5COO6

RUN: RUN3396

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.32

EN300-259063_1_1_1



CID: EN300-259063_1_1_1

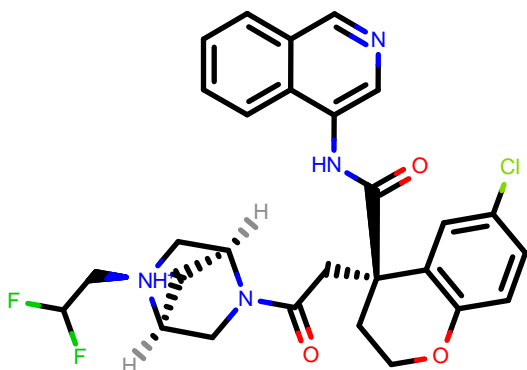
SMILES: CC(=O)N1CCC[C@@]([C1])(CC(=O)N[C@@]2(CCOc3ccc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN4284

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.34

EDG-MED-ba1ac7b9-23_1



CID: EDG-MED-ba1ac7b9-23_1

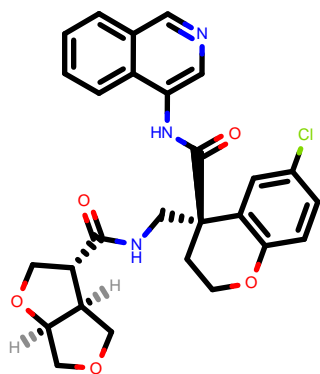
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@([C@@]3(CCOc4ccc(cc4)C)CC(=O)N5C[C@@H]6C[C@H]5[C@@]6)F

RUN: RUN2596

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.27

EN300-6482296_2_4_1



CID: EN300-6482296_2_4_1

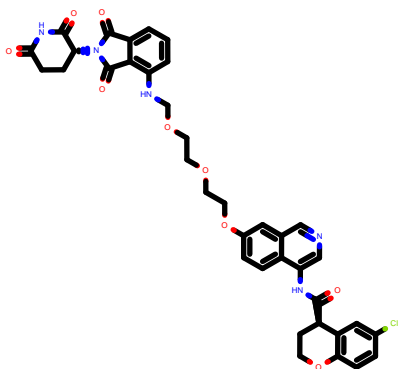
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@([C@@]3(CCOc4ccc(cc4)C)CN(C=O)C)C@H5CO[C@@H]6C@H5COO6

RUN: RUN6968

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.28

DAR-DIA-9e4459de-11_2



CID: DAR-DIA-9e4459de-11_2

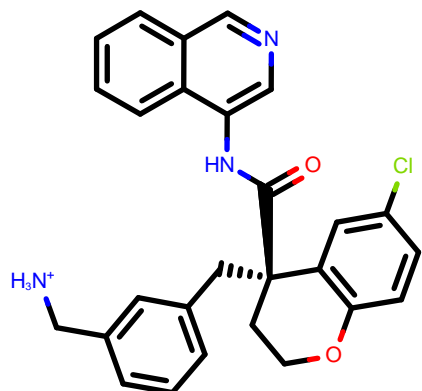
SMILES: c1ccc2c(c1)NCOCCCCOCC3CCO4C(C)CNC4NC(=O)[C@@H]5COCOC6C(CO)C(C)C6@H7C(C)C(=O)NC7=O

RUN: RUN1352

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.38

JAG-UCB-706446eb-8_1



CID: JAG-UCB-706446eb-8_1

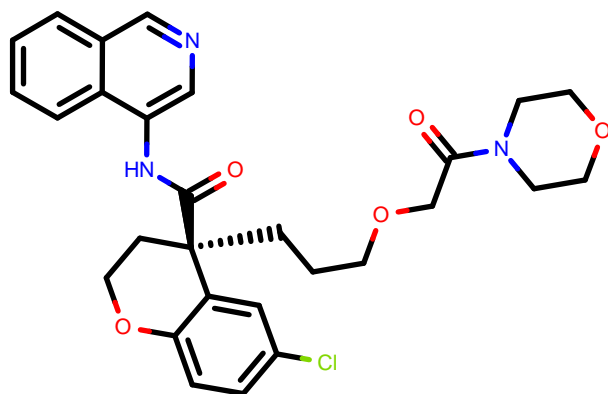
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COc4c3cc(cc4)Cl)Coc5ccccc5[NH3+]

RUN: RUN563

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.30

EN300-1241327_4_1_1



CID: EN300-1241327_4_1_1

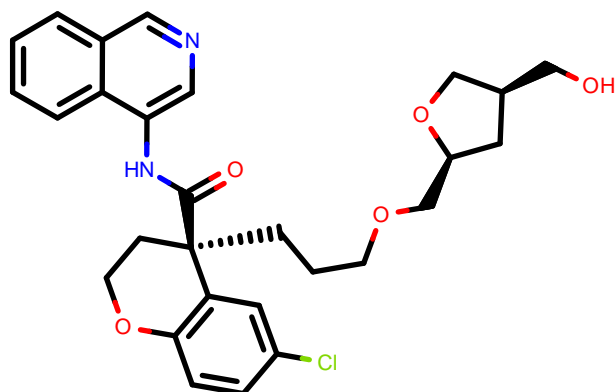
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COc4c3cc(cc4)Cl)CCCCOC(=O)N5CCOCC5

RUN: RUN5509

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.31

EN300-6494158_4_1_1



CID: EN300-6494158_4_1_1

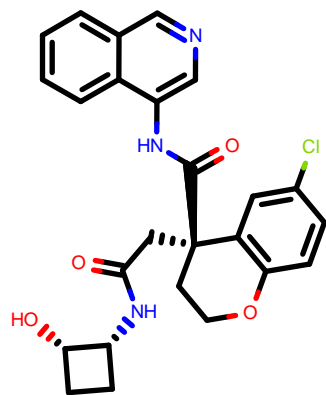
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COc4c3cc(cc4)Cl)CCOC[C@@H]5C[C@@H](CO)CO5

RUN: RUN6174

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.37

EN300-129424_1_1_1



CID: EN300-129424_1_1_1

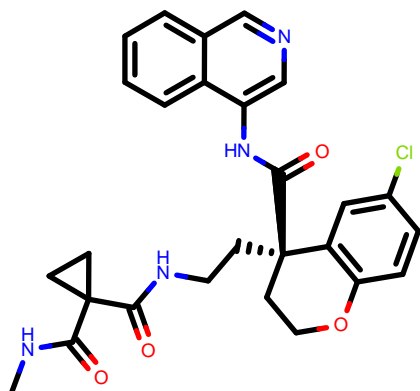
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5CC[C@@]H5O

RUN: RUN7339

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.23

EN300-66770_3_1_1



CID: EN300-66770_3_1_1

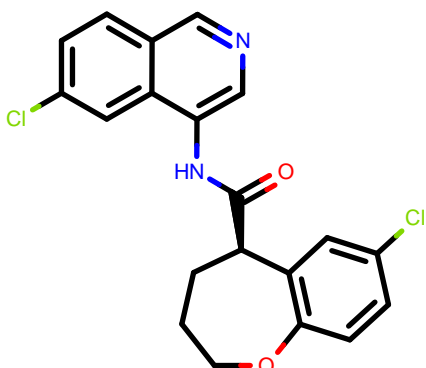
SMILES: CNC(=O)C1(CC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc55

RUN: RUN5453

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.27

ALF-EVA-5b152d2f-3_1



CID: ALF-EVA-5b152d2f-3_1

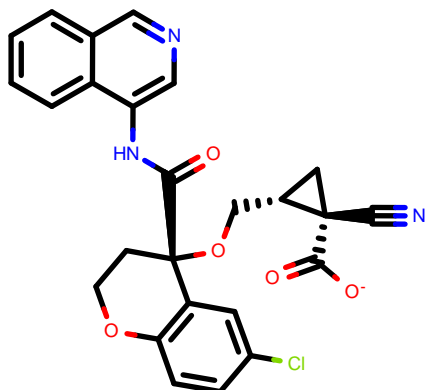
SMILES: c1cc2cnc(cc2cc1Cl)NC(=O)[C@@]H3CCCCOc4c3cc(cc4)Cl

RUN: RUN2174

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.20

ED_-GRI-5b13fbe2-50_3



CID: ED_-GRI-5b13fbe2-50_3

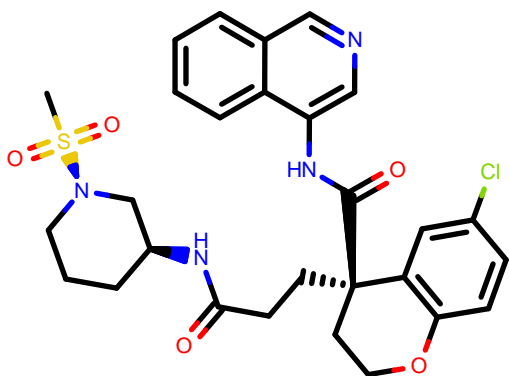
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)OC[C@@]H5C[C@@]5(C#N)C(=O)[O-]

RUN: RUN1447

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.41

EN300-54922_2_1_1



CID: EN300-54922_2_1_1

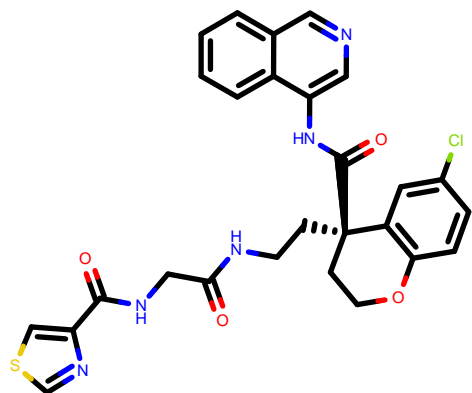
SMILES: CS(=O)(=O)N@1CCCC@1[C@@H](C1=NC(=O)C=C2(COC3C2C(=O)C)C1=O)Nc4nc5c4ccc5

RUN: RUN5592

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.31

EN300-182084_3_1_1



CID: EN300-182084_3_1_1

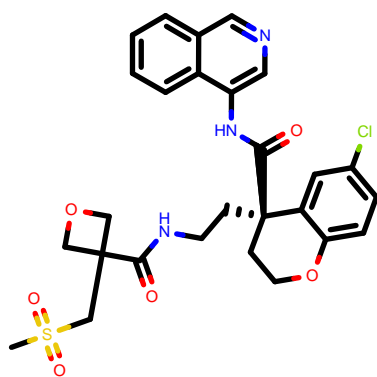
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C@H)3(CCOC4C3C(=O)C)CCNC(=O)CNC(=O)c5csn5

RUN: RUN6386

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.33

EN300-262204_3_1_1



CID: EN300-262204_3_1_1

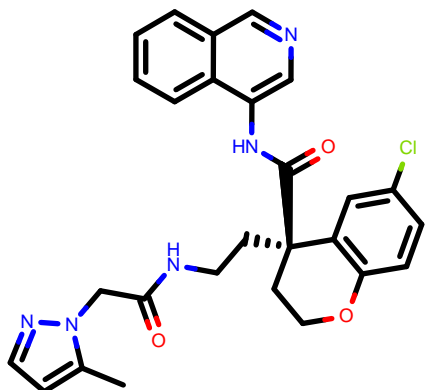
SMILES: CS(=O)(=O)CC1(COC1)C(=O)NCC[C@@H](COC2C3C(=O)C)C(=O)Nc4nc5c4ccc5

RUN: RUN3050

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.48

EN300-83558_3_1_1



CID: EN300-83558_3_1_1

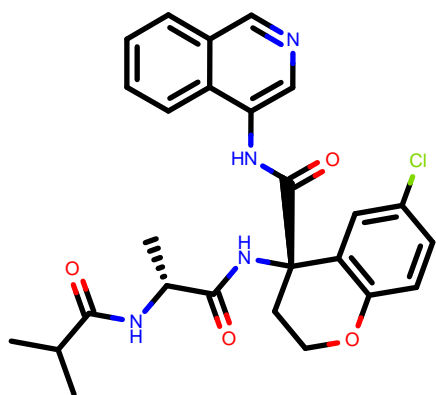
SMILES: Cc1cnn1CC(=O)NCC[C@@H](COC2C3C(=O)C)C(=O)Nc4nc5c4ccc5

RUN: RUN5536

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.25

EN300-31184_1_2_1



CID: EN300-31184_1_2_1

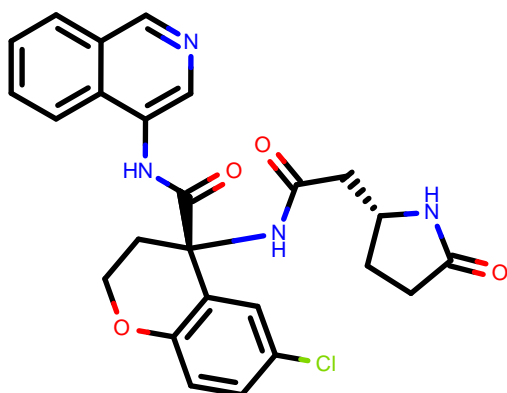
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)C(C)C

RUN: RUN3759

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.29

EN300-68203_1_2_1



CID: EN300-68203_1_2_1

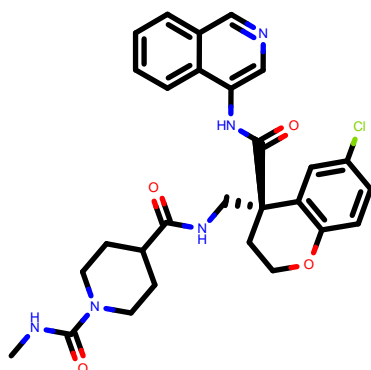
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCN(=O)N5

RUN: RUN4668

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

EN300-6478526_2_1_1



CID: EN300-6478526_2_1_1

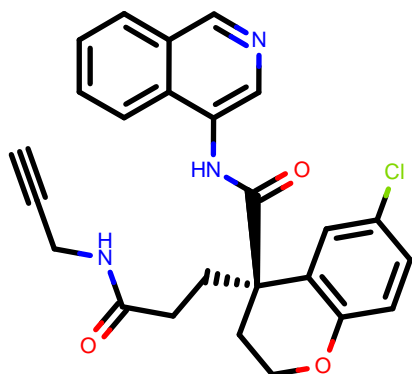
SMILES: CNC(=O)N1CCC(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7749

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-21409_2_1_1



CID: EN300-21409_2_1_1

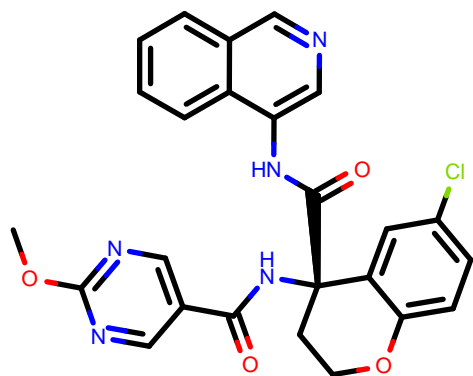
SMILES: C#CCNC(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6641

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

EN300-77543_1_1_1



CID: EN300-77543_1_1_1

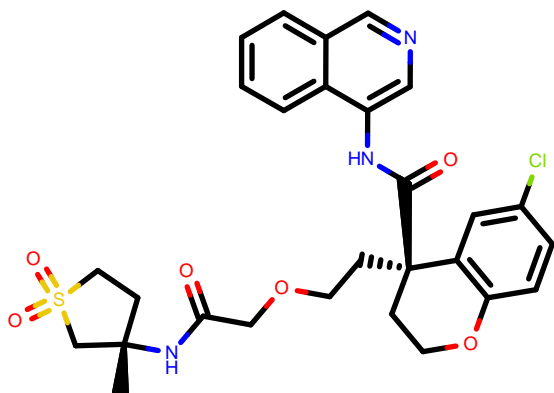
SMILES: COc1ncc(cn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6835

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.19

EN300-10414_3_1_1



CID: EN300-10414_3_1_1

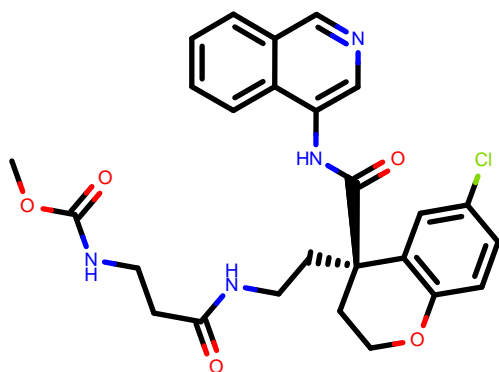
SMILES: C[C@@]1(CC(=O)C(=O)C1)NC(=O)COC[C@@]2(CCOC3c2cc(cc3)O)C(=O)Nc4cncc5c4cccc5

RUN: RUN5456

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.40

EN300-71558_3_1_1



CID: EN300-71558_3_1_1

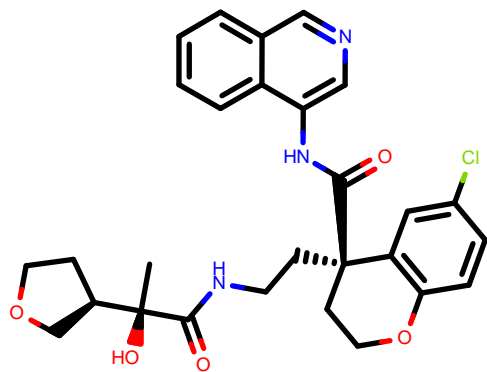
SMILES: COC(=O)NCCC(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4452

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-217494_3_1_1



CID: EN300-217494_3_1_1

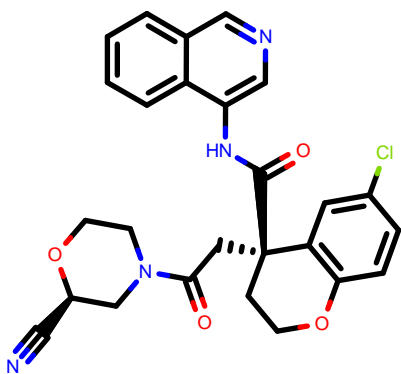
SMILES: C[C@@]1([C@@H]1CCOC1)C(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN4074

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.24

EDJ-MED-d203f206-25_1



CID: EDJ-MED-d203f206-25_1

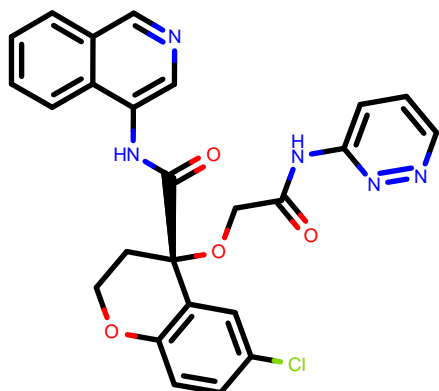
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)C#N

RUN: RUN2408

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.25

EN300-761618_1_1_1



CID: EN300-761618_1_1_1

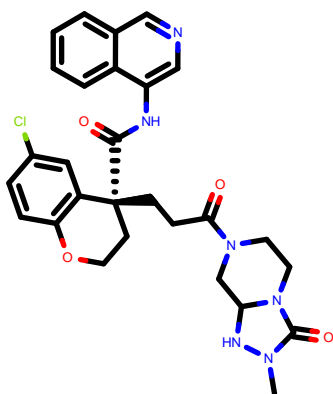
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5ccnnc5

RUN: RUN6037

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

EN300-814032_2_1_1



CID: EN300-814032_2_1_1

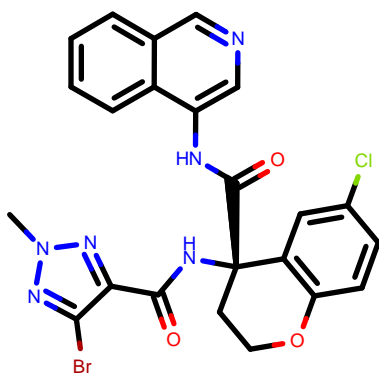
SMILES: Cn1c(=O)n2c(n1)CN(CC2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN6840

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-1439991_1_1_1



CID: EN300-1439991_1_1_1

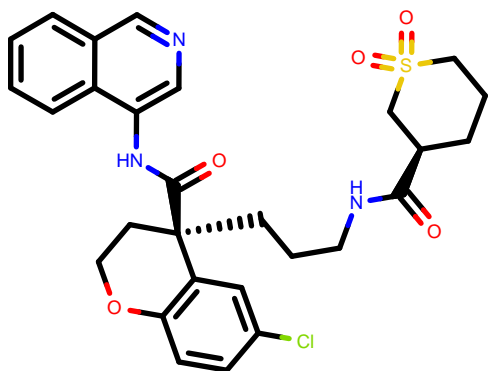
SMILES: Cn1nc(c(n1)Br)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3414

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.25

EN300-77778_4_1_1



CID: EN300-77778_4_1_1

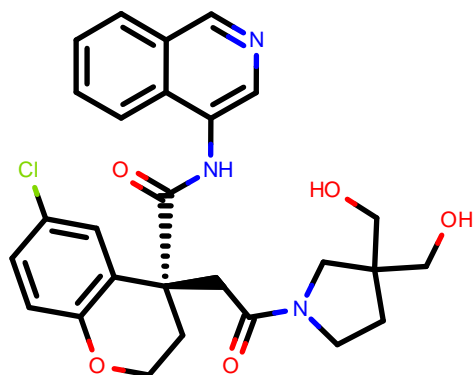
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCN(=O)C@@H5CCCC5(=O)C=O

RUN: RUN7562

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.42

EN300-306144_1_1_1



CID: EN300-306144_1_1_1

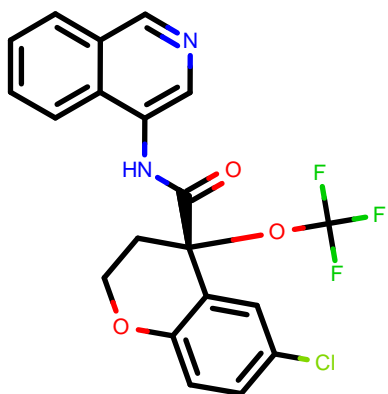
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(=O)C5

RUN: RUN6879

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.34

DAR-DIA-e7614d05-1_1



CID: DAR-DIA-e7614d05-1_1

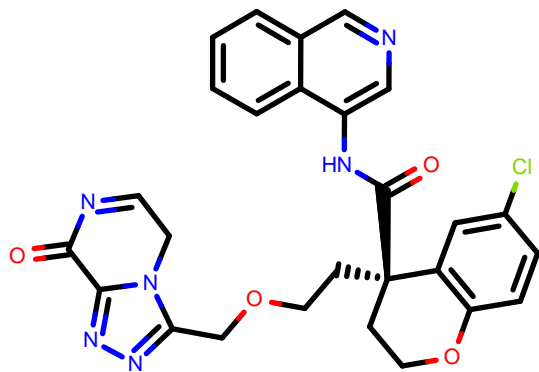
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(F)F

RUN: RUN2310

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.15

EN300-378316_3_1_1



CID: EN300-378316_3_1_1

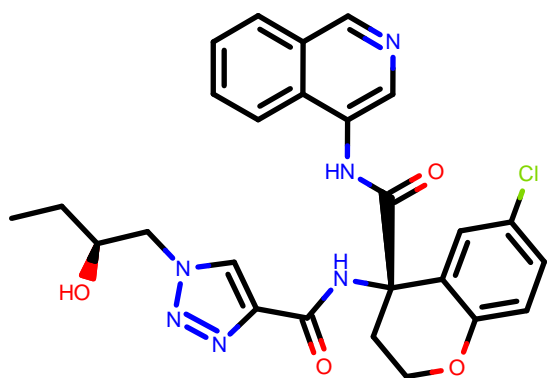
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]nc6[nH]c5=O

RUN: RUN4789

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.37

EN300-366050_1_1_1



CID: EN300-366050_1_1_1

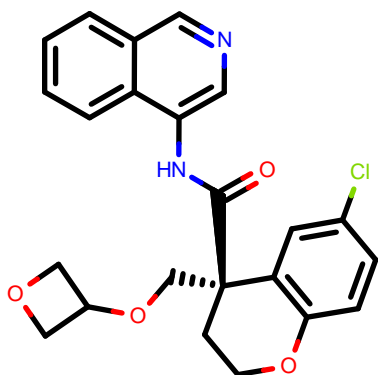
SMILES: CC[C@@H](Cn1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5)O

RUN: RUN5177

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.24

EN300-317082_2_1_1



CID: EN300-317082_2_1_1

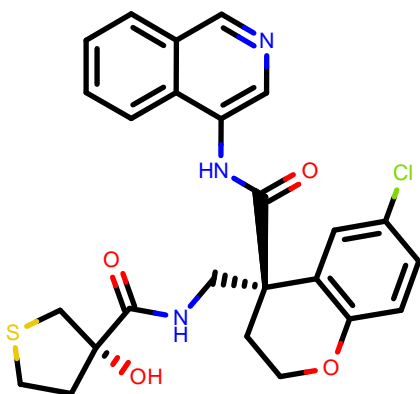
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC5OC5

RUN: RUN4699

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.21

EN300-122656_2_2_1



CID: EN300-122656_2_2_1

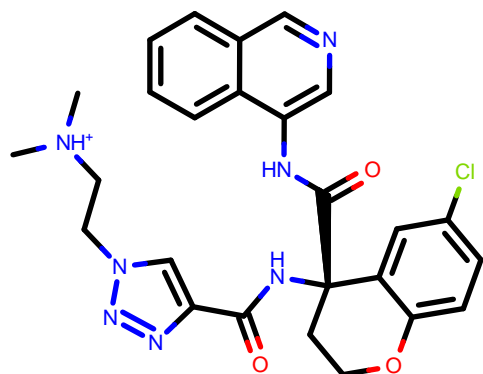
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCS5)O

RUN: RUN4171

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.43

EN300-7543132_1_1_1



CID: EN300-7543132_1_1_1

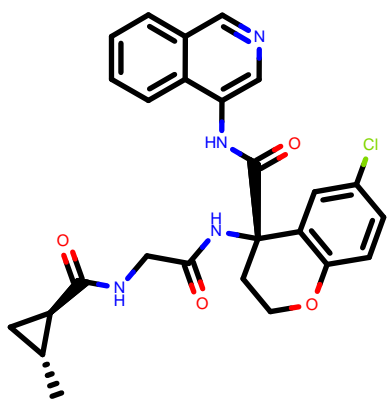
SMILES: C[NH+](C)CCn1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN7062

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.37

EN300-30768_1_3_1



CID: EN300-30768_1_3_1

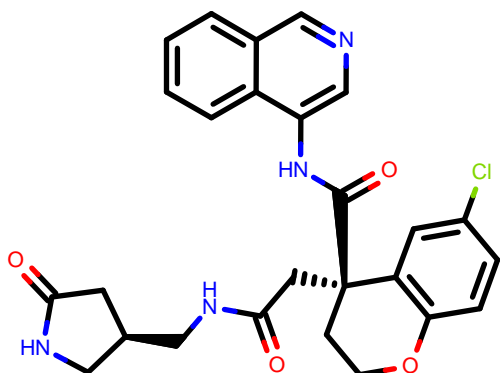
SMILES: C[C@@H]1C[C@H]1C(=O)NCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5174

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-238405_1_1_1



CID: EN300-238405_1_1_1

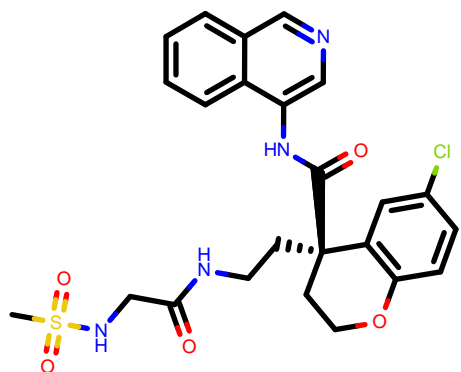
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5H5CC(=O)NC5

RUN: RUN7418

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-30419_3_1_1



CID: EN300-30419_3_1_1

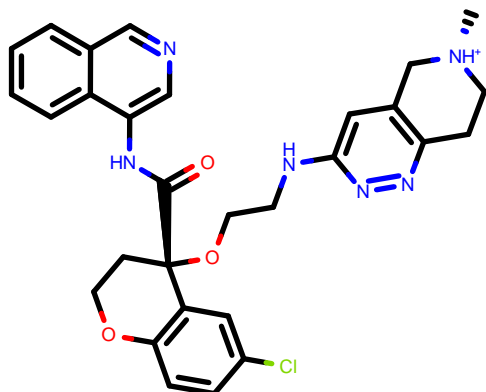
SMILES: CS(=O)(=O)NCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5360

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.39

ED_-GRI-5b13fbe2-67_1



CID: ED_-GRI-5b13fbe2-67_1

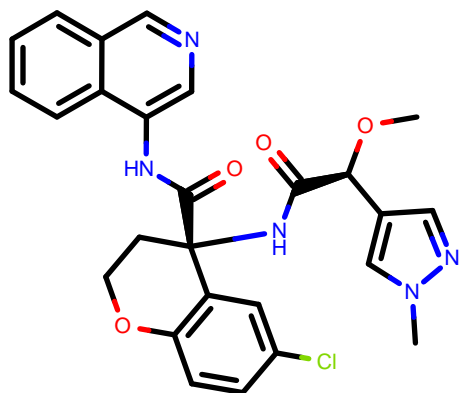
SMILES: C[NH+]1CCc2c(ccn2)NCCO[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)C1

RUN: RUN1481

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-198240_1_1_1



CID: EN300-198240_1_1_1

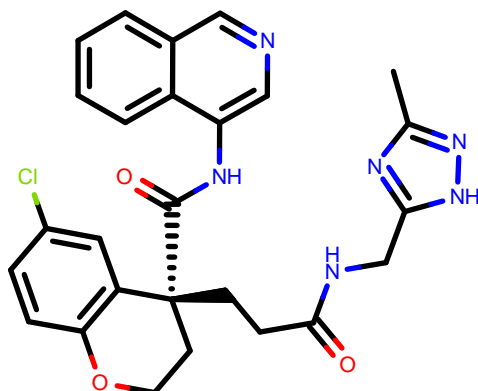
SMILES: Cn1cc(n1)[C@@H](C(=O)N[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5)OC

RUN: RUN3978

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.27

EN300-70487_2_1_1



CID: EN300-70487_2_1_1

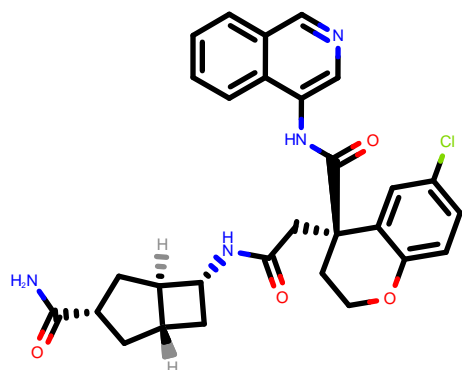
SMILES: Cc1[nH]nc(n1)CNC(=O)CC[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5412

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

ALP-UNI-3496895b-15_7



CID: ALP-UNI-3496895b-15_7

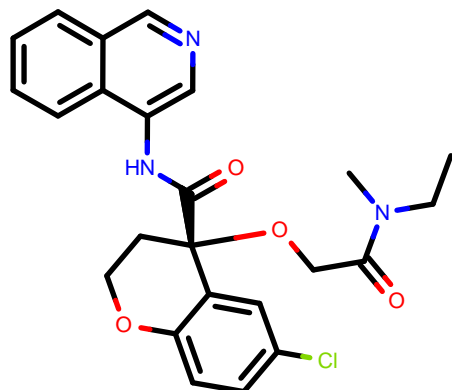
SMILES: c1ccc2c(e1)ncnc2N[C@@]3(C)CCOC4c3cc(c4)C[C@@]5(C)N[C@@]6HJ5[C@@]HJ6[C@@]HJ5[C@@]HJ6[C@@]HJ6[C@@]HJ6

RUN: RUN2347

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-1253122_1_1_1



CID: EN300-1253122_1_1_1

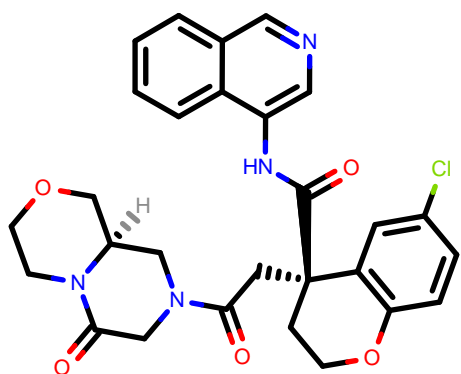
SMILES: CCN(C)C(=O)CO[C@]1(CCOC2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN4763

DDG (kcal/mol): -0.60

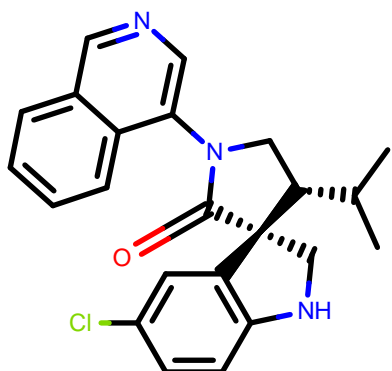
dDDG (kcal/mol): 0.23

EDJ-MED-d203f206-32_1



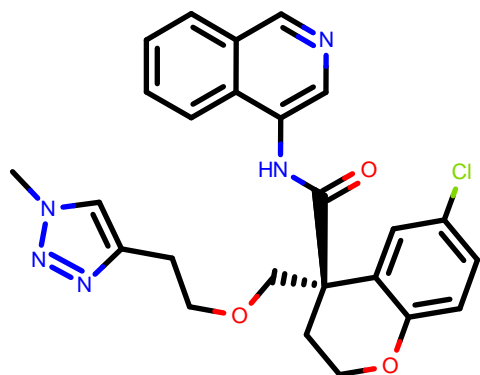
CID:	EDJ-MED-d203f206-32_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N(C=O)[C@@H](C)COC(=O)N1CCN(C)C1=O</chem>
RUN:	RUN2453
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.31

DAR-DIA-6be260fc-4_1



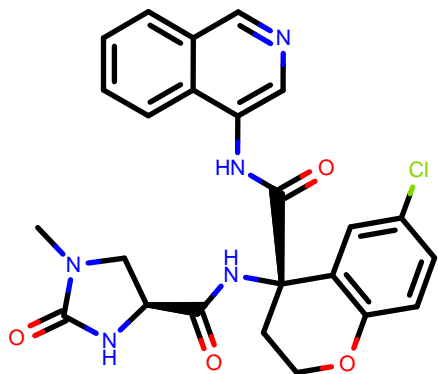
CID:	DAR-DIA-6be260fc-4_1
SMILES:	<chem>CC(C)[C@H]1CN(C(=O)[C@@H](C)COC(=O)N1)C1=CC=C(C=C1)Cl</chem>
RUN:	RUN1931
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.30

EN300-1600786_2_1_1



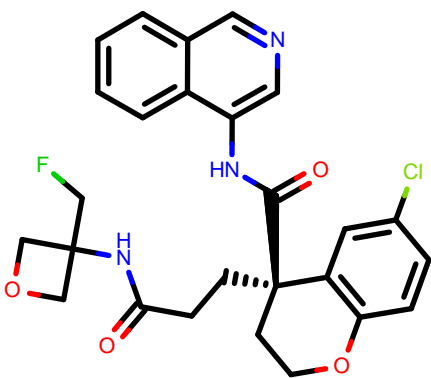
CID:	EN300-1600786_2_1_1
SMILES:	<chem>Cn1cc(nn1)CCOC[C@@H]2(COC(=O)N1CCN(C)C1=O)C(=O)Nc4ccc5c4cccc5</chem>
RUN:	RUN5164
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.28

EN300-255795_1_2_1



CID:	EN300-255795_1_2_1
SMILES:	<chem>CN1C[C@H](N1C(=O)C(=O)N)[C@@H]2(COC(=O)N1CCN(C)C1=O)C(=O)Nc4ccc5c4cccc5</chem>
RUN:	RUN6510
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.22

EN300-6970573_2_1_1



CID: EN300-6970573_2_1_1

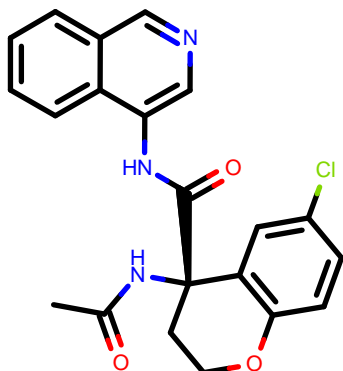
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(COC5)CF

RUN: RUN4132

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-18074_1_1_1



CID: EN300-18074_1_1_1

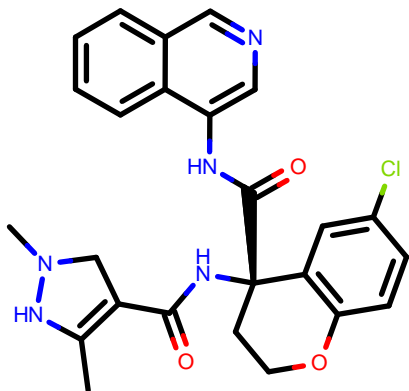
SMILES: CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7687

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.14

EN300-76584_1_1_1



CID: EN300-76584_1_1_1

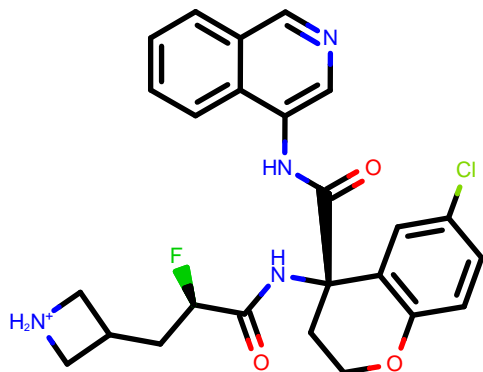
SMILES: Cc1c(cn(n1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6705

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.27

EDG-MED-90036822-81_1



CID: EDG-MED-90036822-81_1

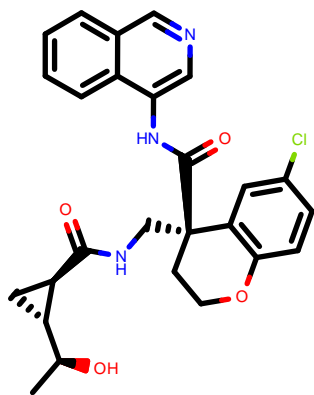
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H[CC5C[NH2+]]C5F

RUN: RUN1644

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.51

EN300-6729572_2_5_1



CID: EN300-6729572_2_5_1

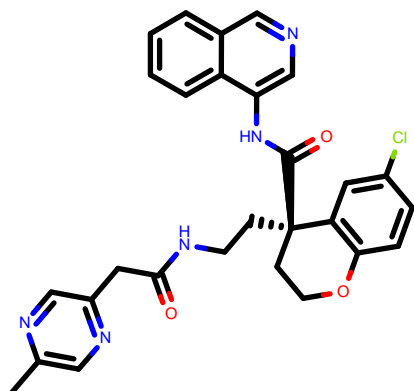
SMILES: C[C@@H]([C@@H]1C[C@H]1C(=O)NC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN6608

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.23

EN300-1709295_3_1_1



CID: EN300-1709295_3_1_1

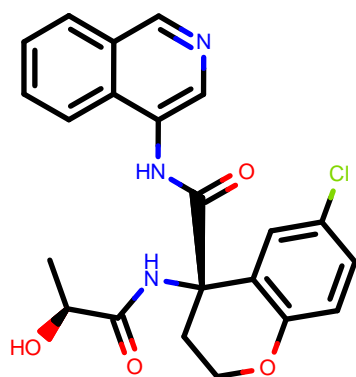
SMILES: Cc1cnc(en1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6580

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.32

EN300-91905_1_1_1



CID: EN300-91905_1_1_1

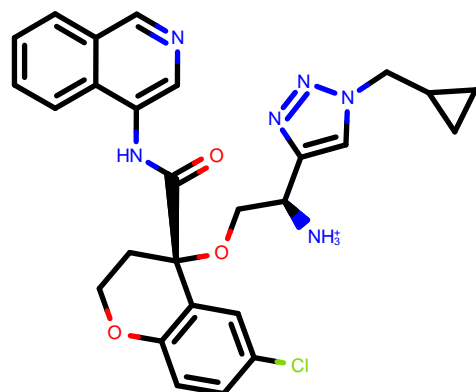
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6583

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.20

ED_-GRI-5b13fbe2-16_1



CID: ED_-GRI-5b13fbe2-16_1

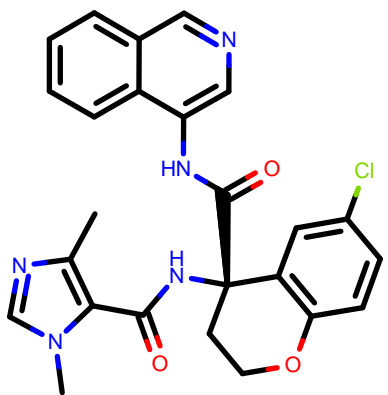
SMILES: c1ccc2c(c1)nncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H](c5cn[nH]5)N3

RUN: RUN1458

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.34

EN300-6498351_1_1_1



CID: EN300-6498351_1_1_1

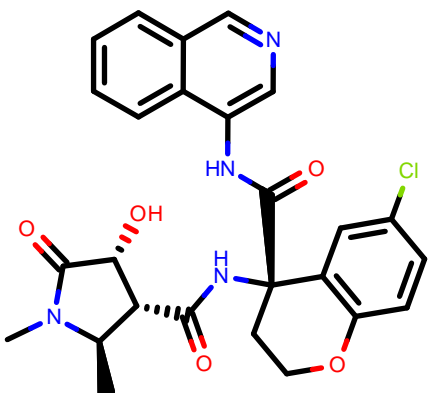
SMILES: Cc1c(n(en1)C)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3979

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.25

EN300-378828_1_1_1



CID: EN300-378828_1_1_1

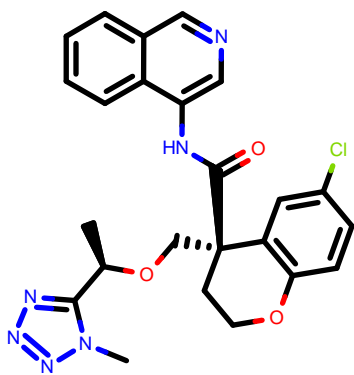
SMILES: C[C@H]1[C@H]([C@H]1C)O[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7725

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.27

EN300-173006_2_2_1



CID: EN300-173006_2_2_1

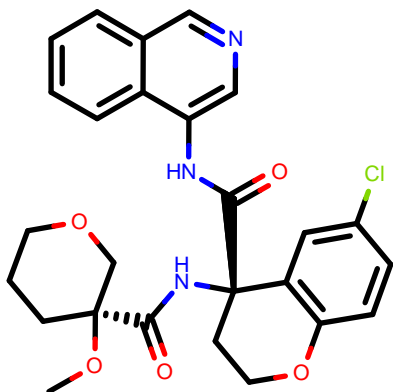
SMILES: C[C@H]1(c1nnn1C)OC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3911

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.29

EN300-1072199_1_2_1



CID: EN300-1072199_1_2_1

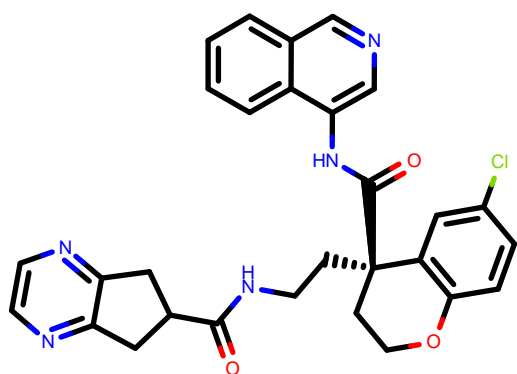
SMILES: CO[C@]1(CCCOC1)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2893

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.28

EN300-2011576_3_1_1



CID: EN300-2011576_3_1_1

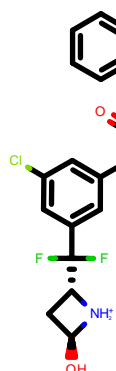
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5Cc6c(ncn6)C5

RUN: RUN4986

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.29

ALP-POS-fab80cf2-1_2



CID: ALP-POS-fab80cf2-1_2

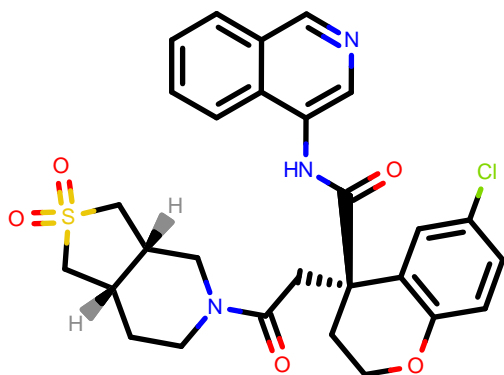
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(Cc3cc(cc(c3)Cl)C)C(C@H)4CC(=O)N4)(F)F

RUN: RUN1365

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.47

EN300-365993_1_1_1



CID: EN300-365993_1_1_1

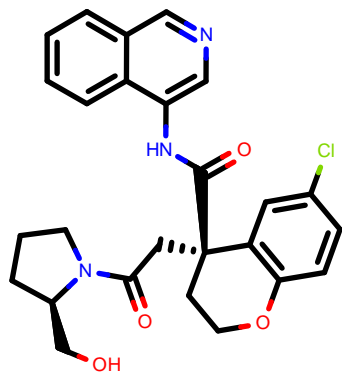
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C)C@H)C5S(=O)(=O)C6

RUN: RUN6242

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.42

EN300-378343_1_1_1



CID: EN300-378343_1_1_1

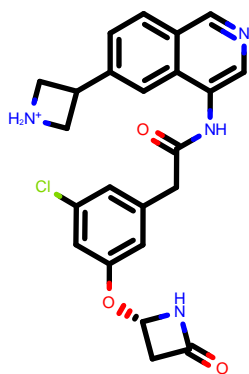
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC=C)C)C@H)5CO

RUN: RUN5959

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.23

ALF-EVA-0b412456-8_2



CID: ALF-EVA-0b412456-8_2

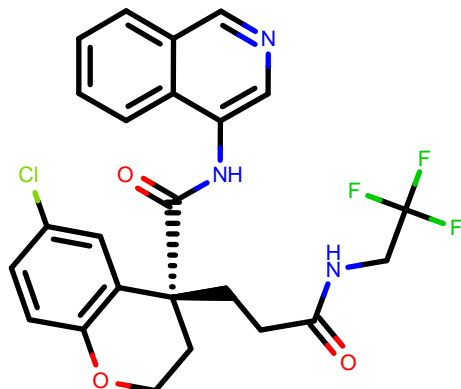
SMILES: c1cc2nccc(c2cc1C3C[NH2+])C3)NC(=O)Cc4cc(ccc4)Cl)O[C@H]5CC(=O)N5

RUN: RUN2568

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.43

JAG-UCB-706446eb-1_1



CID: JAG-UCB-706446eb-1_1

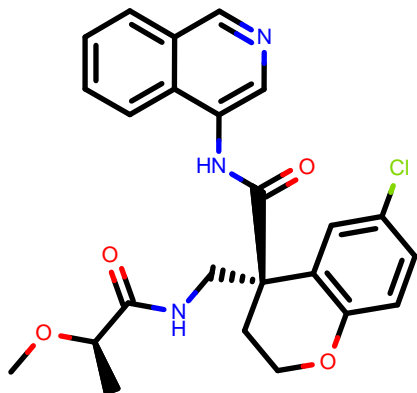
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CO)c4cc(cc4)Cl)CCC(=O)NCC(F)(F)F

RUN: RUN598

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.21

EN300-51257_2_2_1



CID: EN300-51257_2_2_1

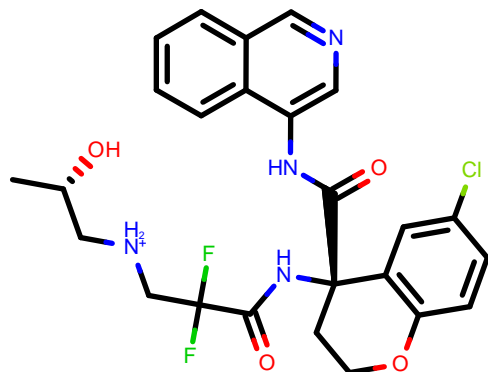
SMILES: C[C@H](C(=O)NCC[C@]1(C)C(CO)c2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)OC

RUN: RUN7593

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.17

EDG-MED-90036822-38_1



CID: EDG-MED-90036822-38_1

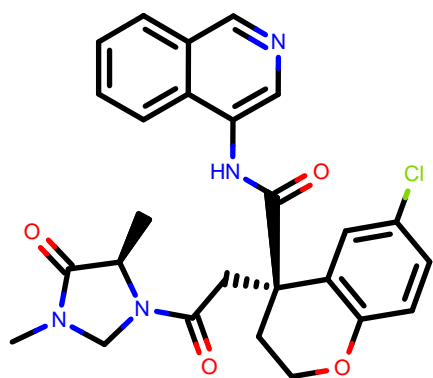
SMILES: C[C@@]1(C)C(CO)NCC(C(=O)NCC[C@]2(C)C(CO)c3cc(cc3)Cl)C(=O)Nc3nccc4c3ccc4)(F)F)O

RUN: RUN1664

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.41

EN300-261410_1_1_1



CID: EN300-261410_1_1_1

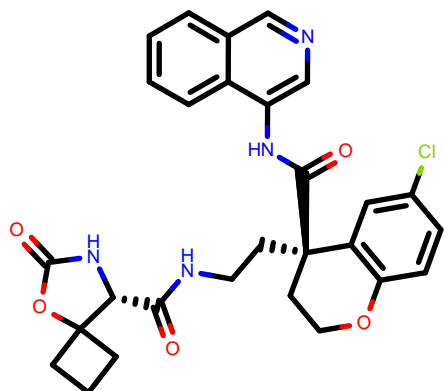
SMILES: C[C@@H]1C(=O)N(CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5)C

RUN: RUN5175

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.28

EN300-7432415_3_1_1



CID: EN300-7432415_3_1_1

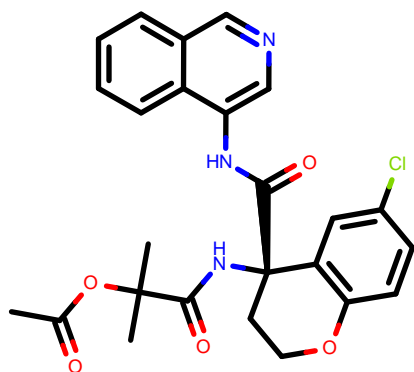
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)CCNC)C(=O)N[C@@H]5C6(CCC6)OC1=O[N5]

RUN: RUN3571

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.39

EN300-155589_1_1_1



CID: EN300-155589_1_1_1

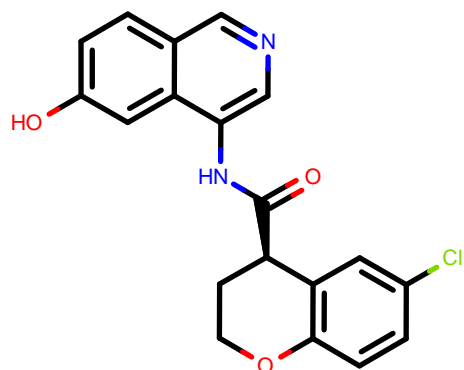
SMILES: CC(=O)OC(C)(C)C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN6175

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.26

BEN-DND-c852c98b-4_1



CID: BEN-DND-c852c98b-4_1

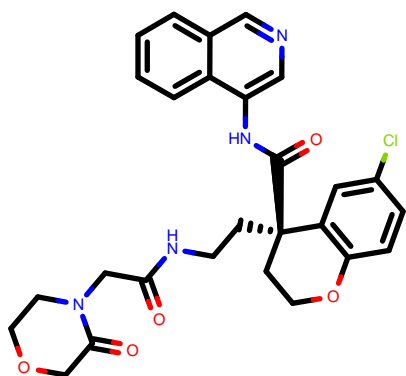
SMILES: c1cc2cnc(c2cc1O)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1097

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.04

EN300-186943_3_1_1



CID: EN300-186943_3_1_1

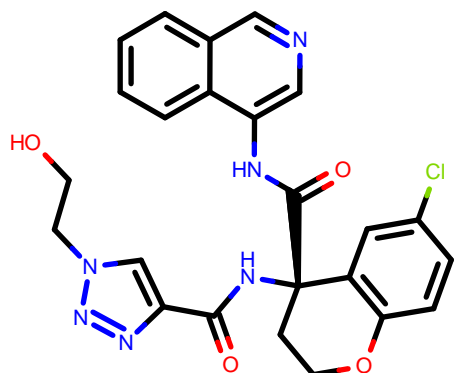
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5CCOCC5=O

RUN: RUN5349

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.32

EN300-52193_1_1_1



CID: EN300-52193_1_1_1

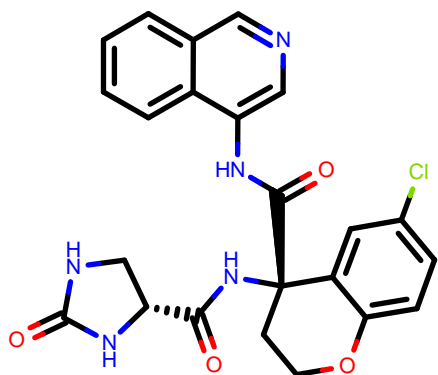
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(n5)CCO

RUN: RUN3681

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.24

EN300-222145_1_1_1



CID: EN300-222145_1_1_1

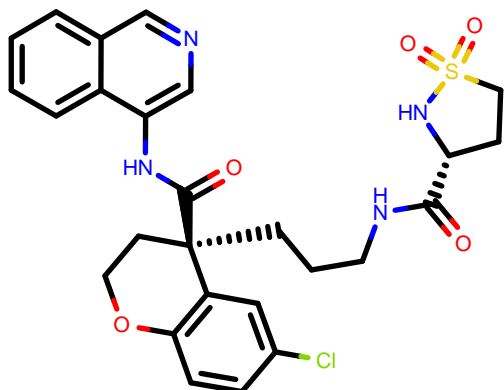
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CN(C)=O)N5

RUN: RUN3854

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.24

EN300-45049_4_2_1



CID: EN300-45049_4_2_1

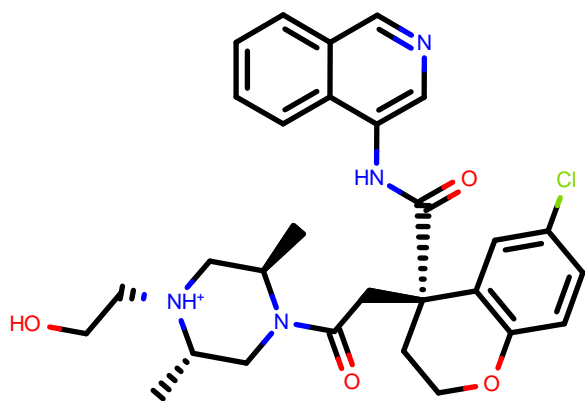
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5SCCS(=O)(=O)N5

RUN: RUN5732

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.42

EDG-MED-ba1ac7b9-26_2



CID: EDG-MED-ba1ac7b9-26_2

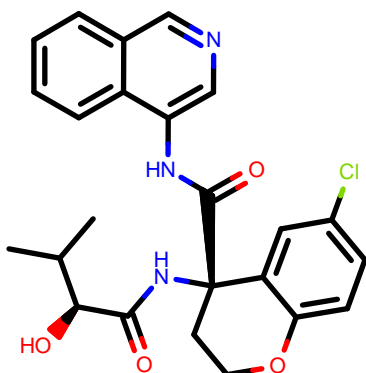
SMILES: C[C@H]1CN[BH+]](C@H)CN1C(-O)C[C@H]2(CCOc3c2cc(c3)C)C(-O)Nc4nc5c4cccc5)C(CCO

RUN: RUN2592

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.43

EN300-199359_1_1_1



CID: EN300-199359_1_1_1

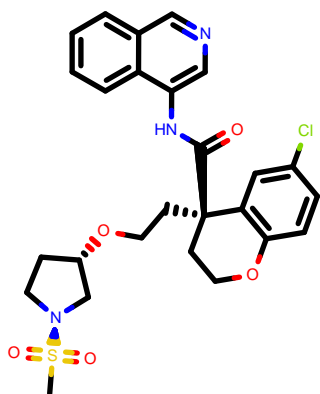
SMILES: CC(C)[C@@H](C(=O)N)C@1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4)O

RUN: RUN6139

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.24

EN300-301690_3_1_1



CID: EN300-301690_3_1_1

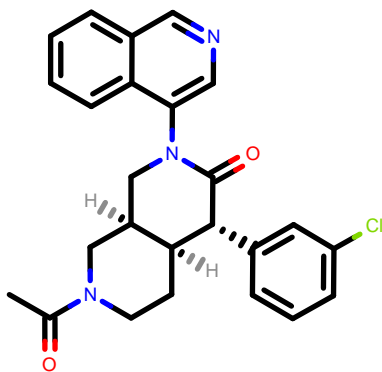
SMILES: CS(=O)(=O)[N@@]1CC[C@@H](C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN5198

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.35

MIC-UNK-9582b2c5-1_2



CID: MIC-UNK-9582b2c5-1_2

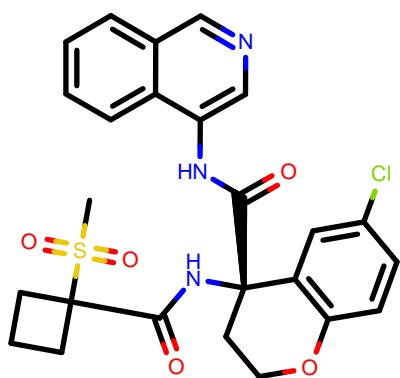
SMILES: CC(=O)N1CC[C@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4nc5c4cccc5

RUN: RUN212

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.29

EN300-191771_1_1_1



CID: EN300-191771_1_1_1

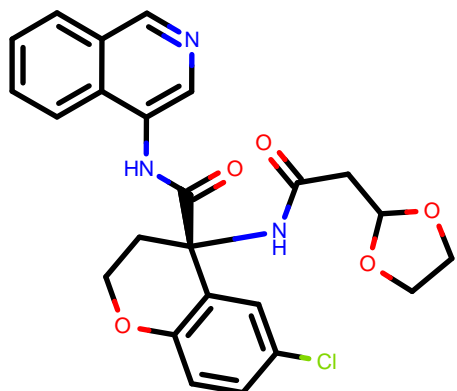
SMILES: CS(=O)(=O)C1(CCC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN5623

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.36

EN300-154944_1_1_1



CID: EN300-154944_1_1_1

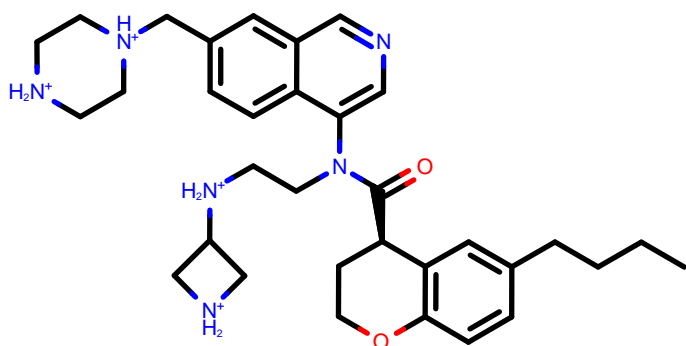
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5OCCO5

RUN: RUN5795

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.23

MAK-UNK-83e0a0b4-1_1



CID: MAK-UNK-83e0a0b4-1_1

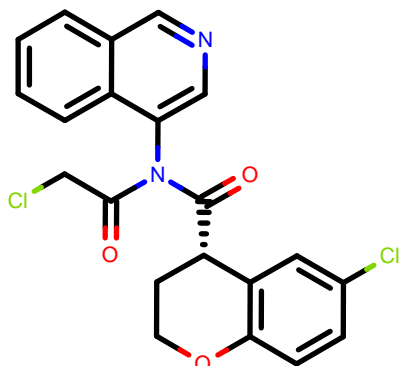
SMILES: CCCCc1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCN3C3)Nc4cnc5c4ccc(c5)CN6CCN6

RUN: RUN852

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.69

VLA-UCB-05e51b3f-9_1



CID: VLA-UCB-05e51b3f-9_1

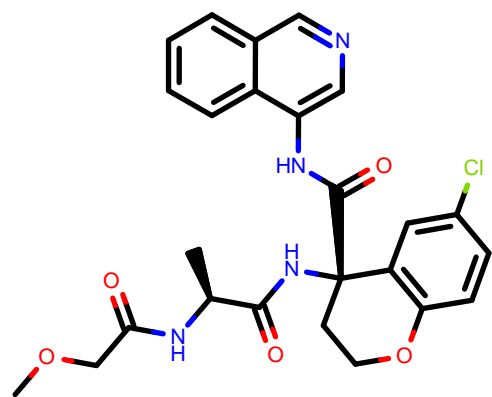
SMILES: c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN292

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.33

EN300-31183_1_1_1



CID: EN300-31183_1_1_1

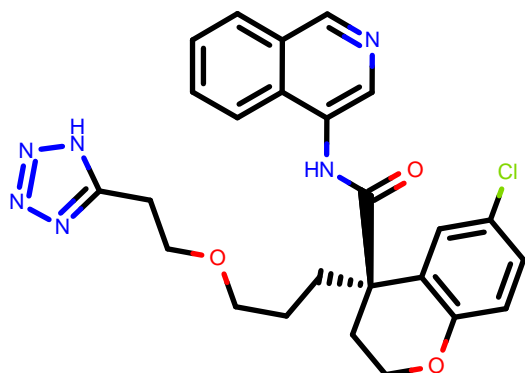
SMILES: C[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4)NC(=O)COC

RUN: RUN6812

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.27

EN300-183231_4_1_1



CID: EN300-183231_4_1_1

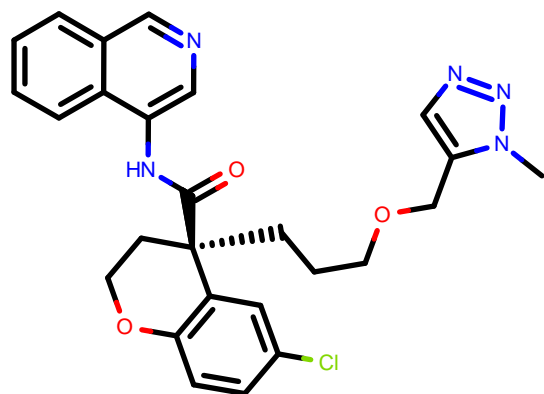
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5n[nH]n5

RUN: RUN5203

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.63

EN300-216673_4_1_1



CID: EN300-216673_4_1_1

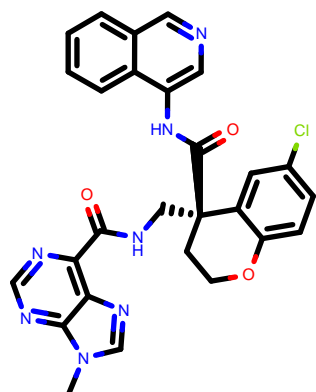
SMILES: Cn1c(cnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN5223

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.32

EN300-7434334_2_1_1



CID: EN300-7434334_2_1_1

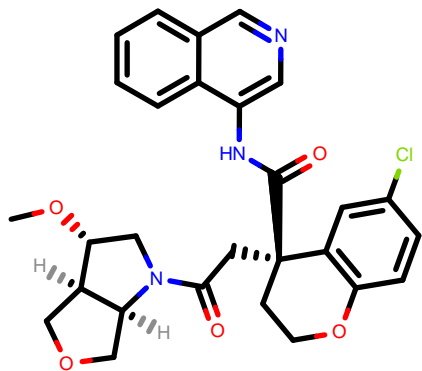
SMILES: Cn1cnc2c1ncnc2(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncnc6c5ccc6

RUN: RUN7522

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.23

EN300-6496666_1_1_1



CID: EN300-6496666_1_1_1

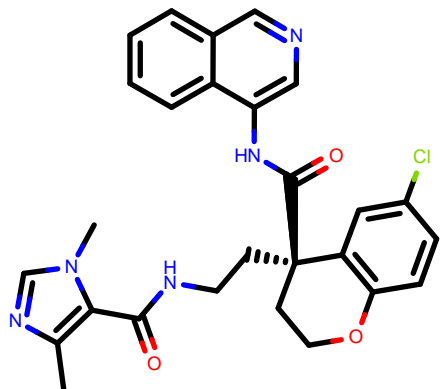
SMILES: CO[C@@H]1CN[C@@H]2[C@@H]1COC2(C)C(=O)C[C@@]3(C)COC4C3C(=O)C1(C)C(=O)Nc5ccc6c5ccc6

RUN: RUN4176

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.33

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

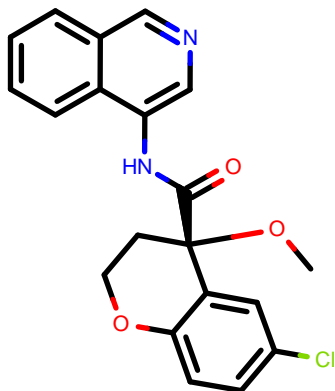
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(C)COC3C2C(=O)C(C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4476

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.30

PET-UNK-29afea89-2_1



CID: PET-UNK-29afea89-2_1

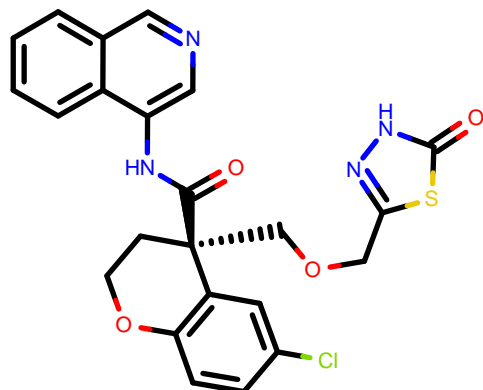
SMILES: CO[C@@]1(C)COC2C1C(=O)C(C)C(=O)Nc3ccc4c3ccc4

RUN: RUN564

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.12

EN300-171766_2_1_1



CID: EN300-171766_2_1_1

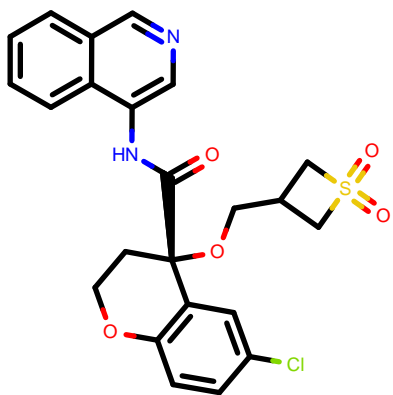
SMILES: c1ccc2c(c1)ncoc2N(C(=O)C[C@@]3(C)COC4C3C(=O)C)COC5n[nH]c(=O)s5

RUN: RUN4141

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.24

EN300-5638430_1_1_1



CID: EN300-5638430_1_1_1

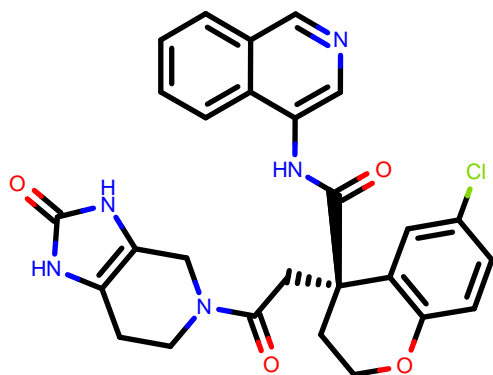
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5CS(=O)=O)CS

RUN: RUN6134

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.29

EN300-7237143_1_1_1



CID: EN300-7237143_1_1_1

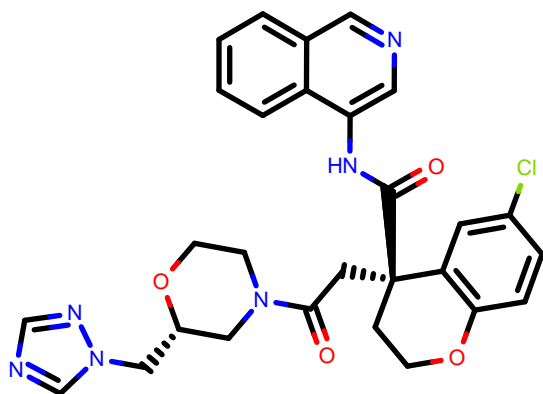
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c([nH]c(=O)[nH]6)C5

RUN: RUN7803

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.27

EN300-80241_1_2_1



CID: EN300-80241_1_2_1

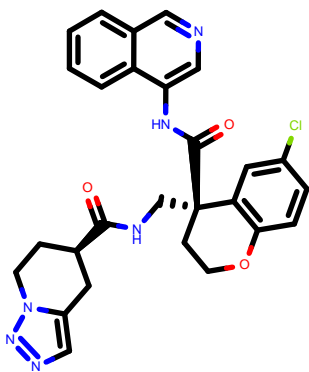
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)Cn6cn6

RUN: RUN5435

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.28

EN300-7430501_2_1_1



CID: EN300-7430501_2_1_1

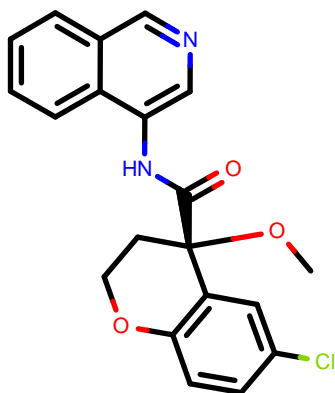
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5Cn6c(cnn6)C5

RUN: RUN6843

DDG (kcal/mol): -0.58

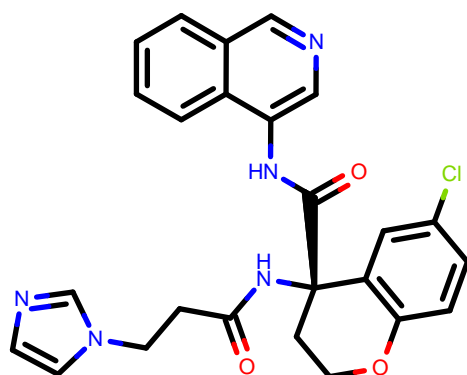
dDDG (kcal/mol): 0.29

EDG-MED-0e5afe9d-3_2



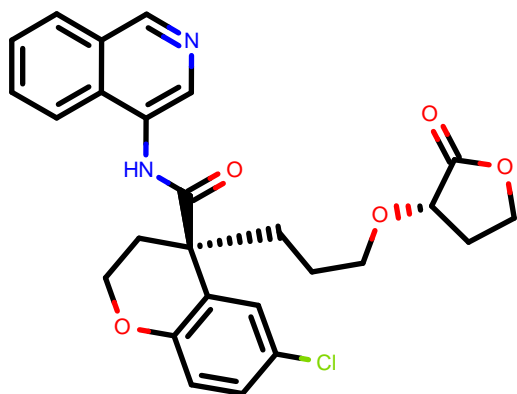
CID:	EDG-MED-0e5afe9d-3_2
SMILES:	<chem>CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN2185
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.11

EN300-75342_1_1_1



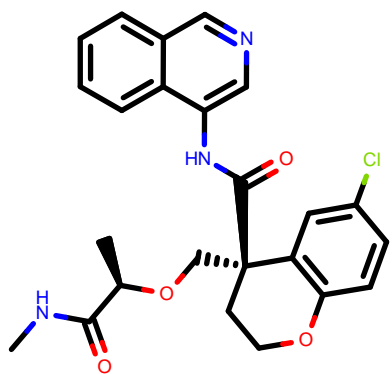
CID:	EN300-75342_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnc5</chem>
RUN:	RUN4990
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.21

EN300-20496_4_2_1



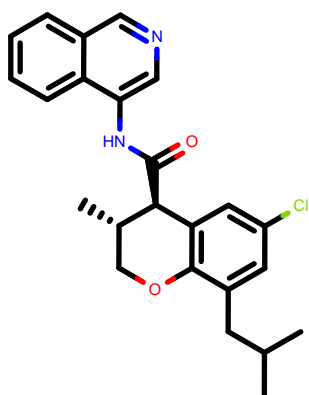
CID:	EN300-20496_4_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC@H5COCOC5=O</chem>
RUN:	RUN5110
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.33

EN300-211482_2_2_1



CID:	EN300-211482_2_2_1
SMILES:	<chem>C[C@H](C(=O)NC)OC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN5546
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.27

DAR-DIA-0d514e7d-24_1



CID: DAR-DIA-0d514e7d-24_1

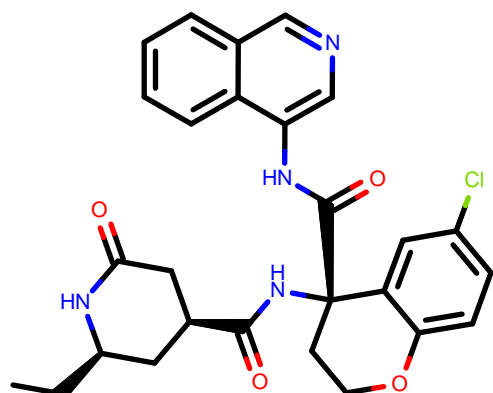
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C)CC(C)C

RUN: RUN771

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.18

EN300-7439980_1_1_1



CID: EN300-7439980_1_1_1

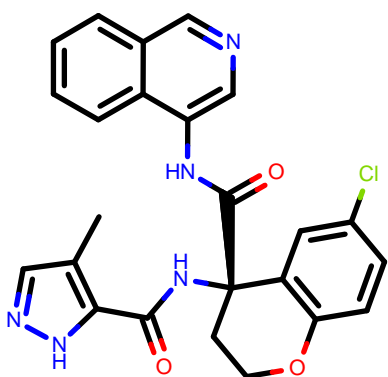
SMILES: CC[C@@H]1C[C@@H](C)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN5180

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EN300-248178_1_1_1



CID: EN300-248178_1_1_1

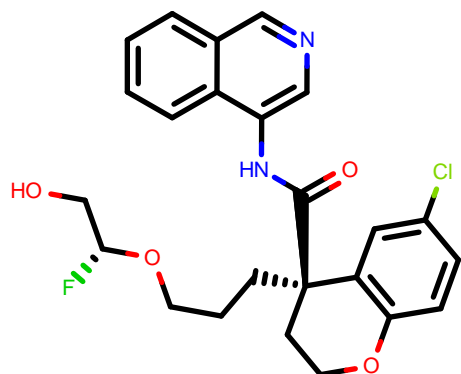
SMILES: Cc1cn[nH]c1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3697

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

EN300-861925_4_1_1



CID: EN300-861925_4_1_1

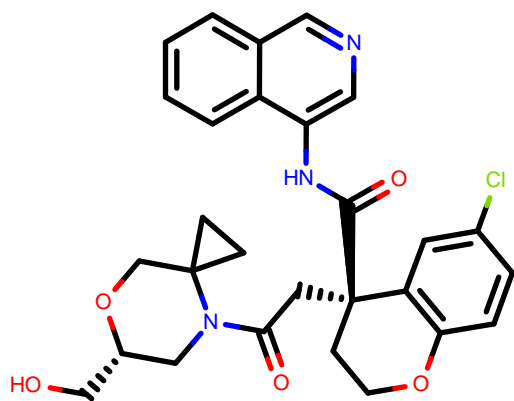
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCO[C@@H](CO)F

RUN: RUN5666

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.41

EN300-7493255_1_1_1



CID: EN300-7493255_1_1_1

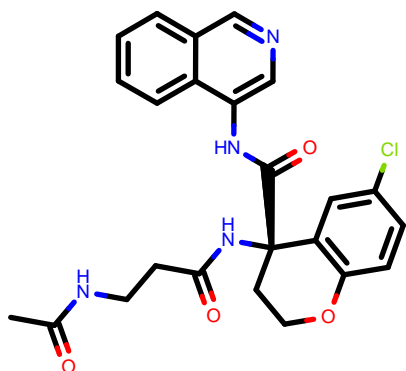
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](OCC56CC6)CO

RUN: RUN4946

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.38

EN300-04073_1_1_1



CID: EN300-04073_1_1_1

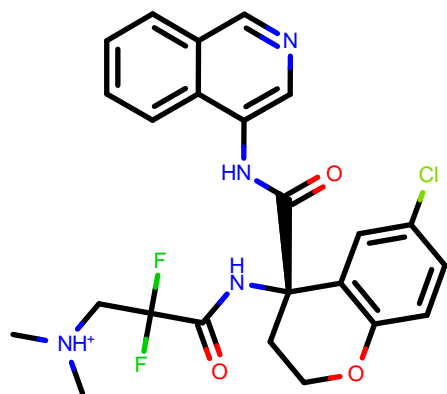
SMILES: CC(=O)NCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6694

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.28

EDG-MED-90036822-87_1



CID: EDG-MED-90036822-87_1

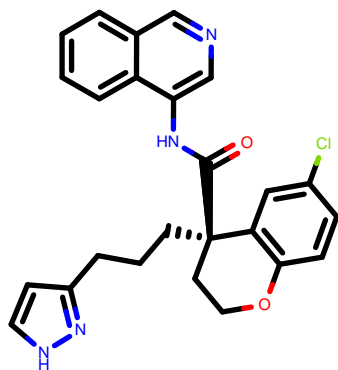
SMILES: CN(C)CC(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)(F)F

RUN: RUN1687

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.24

VLA-UCB-34f3ed0c-10_1_1



CID: VLA-UCB-34f3ed0c-10_1_1

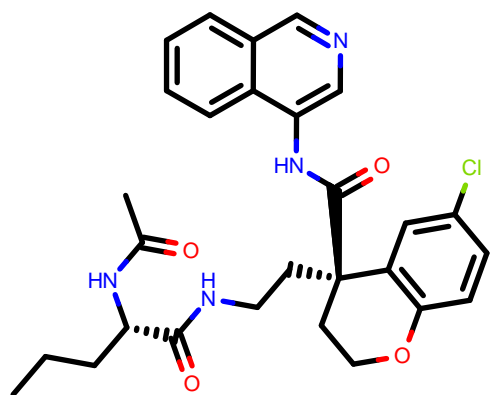
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5cc[nH]5

RUN: RUN4862

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.25

EN300-43047_3_1_1



CID: EN300-43047_3_1_1

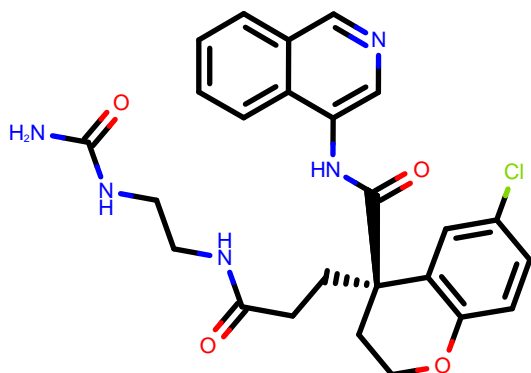
SMILES: CC(=O)N[C@@H](CC=C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7731

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.36

EN300-269419_2_1_1



CID: EN300-269419_2_1_1

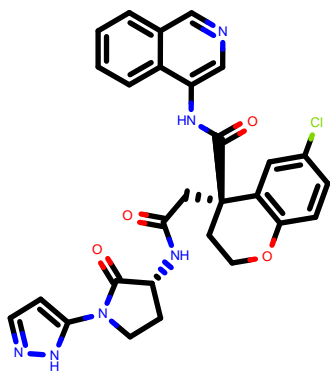
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCNC(=O)N

RUN: RUN7609

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.23

ALP-UNI-3496895b-4_1



CID: ALP-UNI-3496895b-4_1

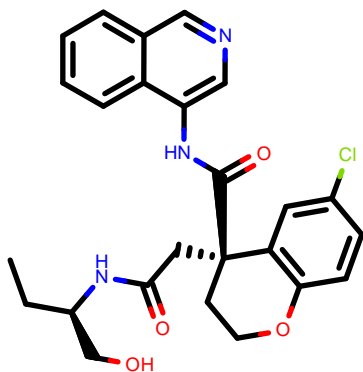
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4(C)CNC(=O)Nc5cncn4

RUN: RUN2368

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.29

EN300-125884_1_1_1



CID: EN300-125884_1_1_1

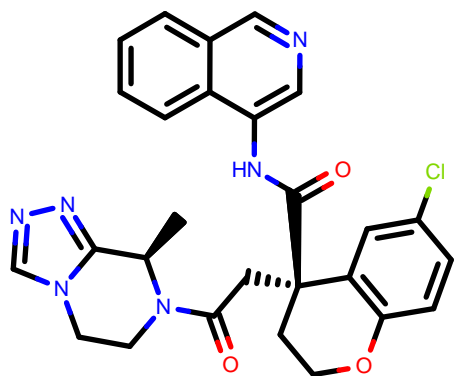
SMILES: CC[C@H](CO)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6586

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-19_3



CID: EDG-MED-ba1ac7b9-19_3

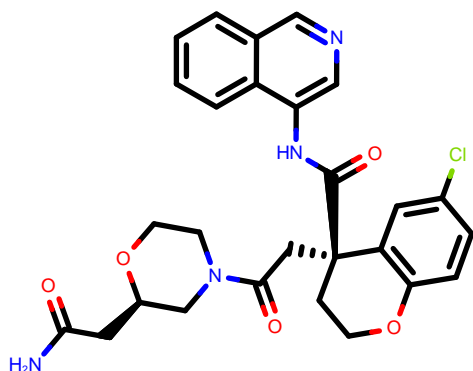
SMILES: C[C@@H]1c2nncn2CCN1C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccc6

RUN: RUN2525

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.40

EN300-321558_1_1_1



CID: EN300-321558_1_1_1

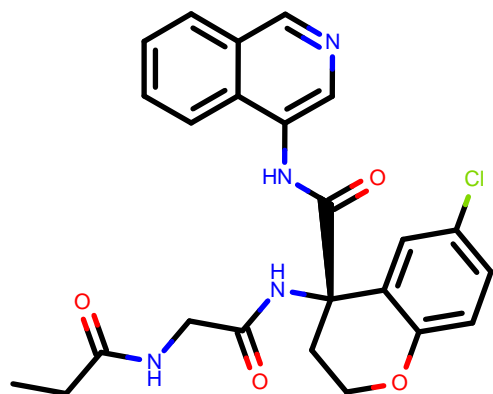
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CC(=O)N

RUN: RUN6253

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EN300-31099_1_1_1



CID: EN300-31099_1_1_1

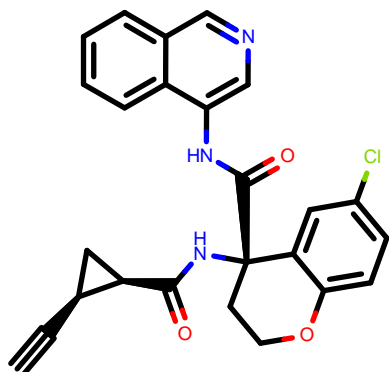
SMILES: CCC(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6018

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

EN300-254137_1_1_1



CID: EN300-254137_1_1_1

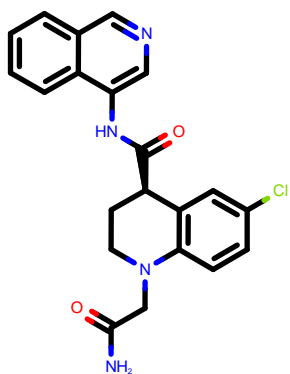
SMILES: C#C[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN3977

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.21

RAL-THA-8416115c-8_1



CID: RAL-THA-8416115c-8_1

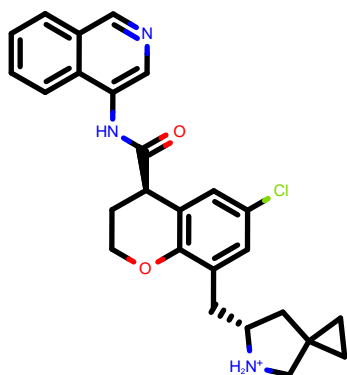
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)C)CC(=O)N

RUN: RUN1171

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.35

DAR-DIA-23e5a6a0-9_1



CID: DAR-DIA-23e5a6a0-9_1

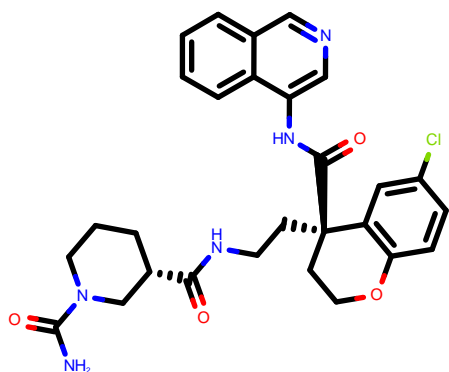
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4C3CC(C4)C[C@@H]5CC6(CC6)C(NH2+)5Cl

RUN: RUN406

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.40

EN300-14767_3_2_1



CID: EN300-14767_3_2_1

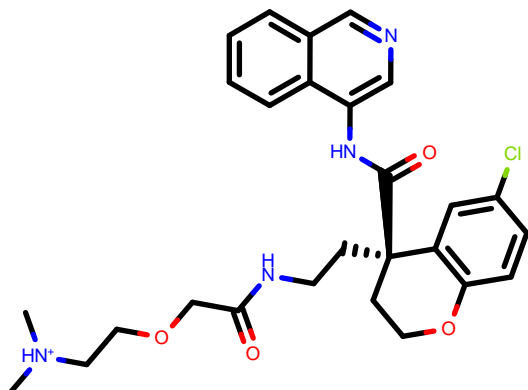
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCN(C5)C(=O)N

RUN: RUN5766

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.31

EN300-1865348_3_1_1



CID: EN300-1865348_3_1_1

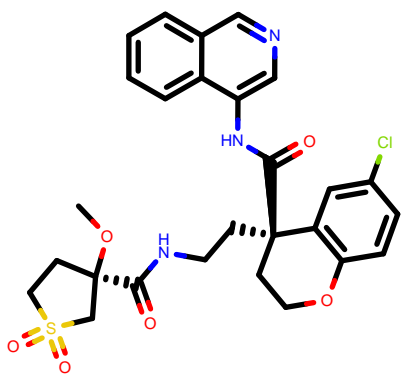
SMILES: C[NH+](C)CCOCC(=O)NCC[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4

RUN: RUN6064

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.39

EN300-385267_3_1_1



CID: EN300-385267_3_1_1

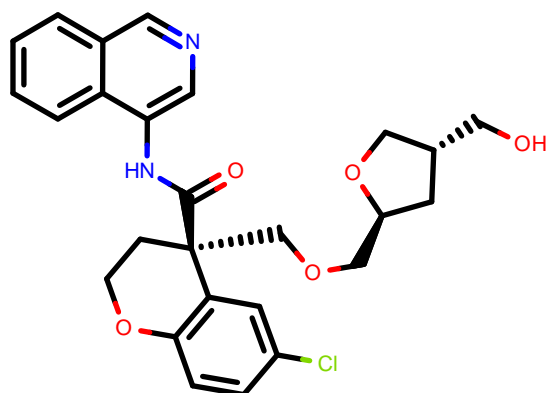
SMILES: CO[C@@]1(CCS(=O)(=O)C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5379

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.29

EN300-6494158_2_3_1



CID: EN300-6494158_2_3_1

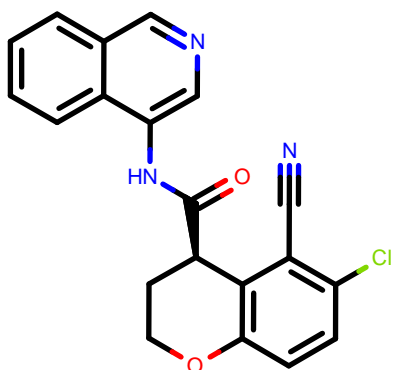
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]H5C[C@H](CO)5CO

RUN: RUN7534

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.33

RAL-THA-05e671eb-31_1



CID: RAL-THA-05e671eb-31_1

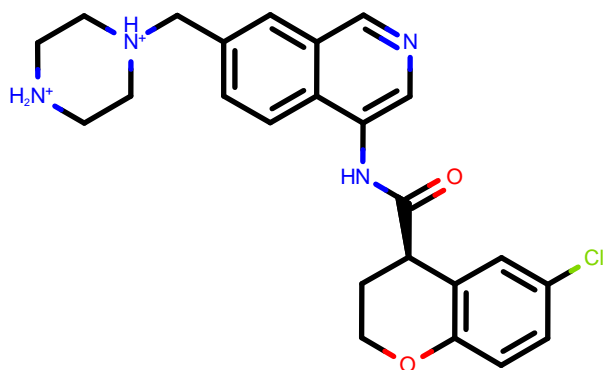
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]H3CCOCc4c3c(c(cc4)C)C#N

RUN: RUN1927

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.10

MAK-UNK-8be7dca9-1_1



CID: MAK-UNK-8be7dca9-1_1

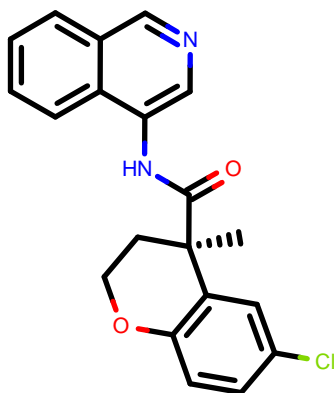
SMILES: c1cc2c(cc1CN3CC[NH2+][CC3])ncnc2NC(=O)[C@@]H4CCOCc5c4cc(cc5)Cl

RUN: RUN439

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.14

BEN-DND-a7517465-4_1



CID: BEN-DND-a7517465-4_1

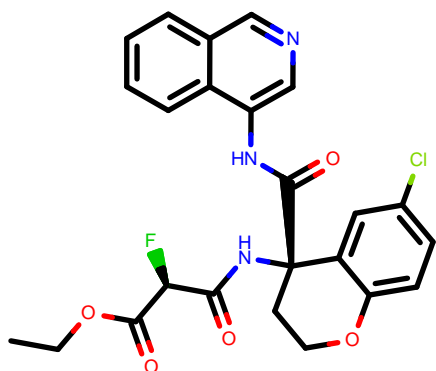
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1303

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.10

EN300-123398_1_2_1



CID: EN300-123398_1_2_1

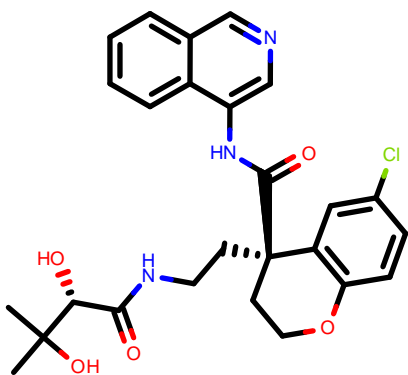
SMILES: CCOC(=O)[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3encc4c3cccc4)F

RUN: RUN5791

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.26

EN300-299532_3_1_1



CID: EN300-299532_3_1_1

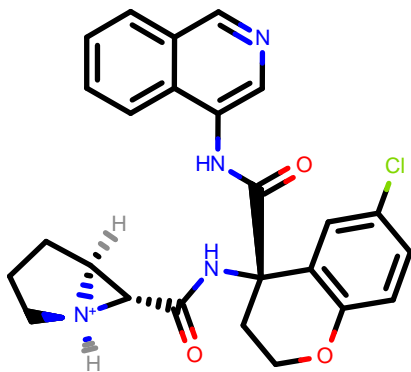
SMILES: CC(C)([C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3encc4c3cccc4)O)O

RUN: RUN5305

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.28

EDG-MED-90036822-73_4



CID: EDG-MED-90036822-73_4

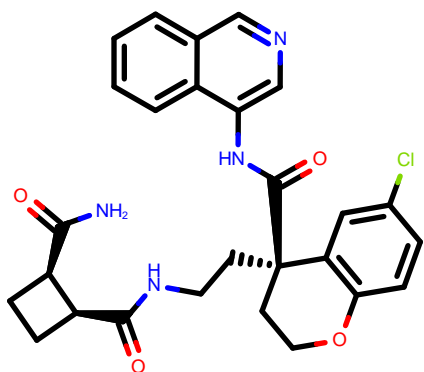
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]1(CCOc3c4cc(cc4)C)N(C=O)[C@H]2[C@@H](N)N[C@@H]1SCCOC6

RUN: RUN1595

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.35

EN300-217107_3_4_1



CID: EN300-217107_3_4_1

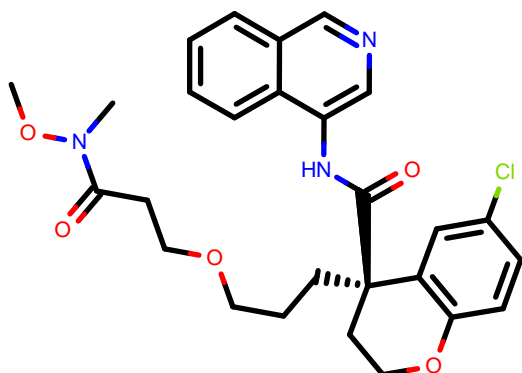
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H5CC[C@H]5C(=O)N

RUN: RUN4083

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.29

EN300-174603_4_1_1



CID: EN300-174603_4_1_1

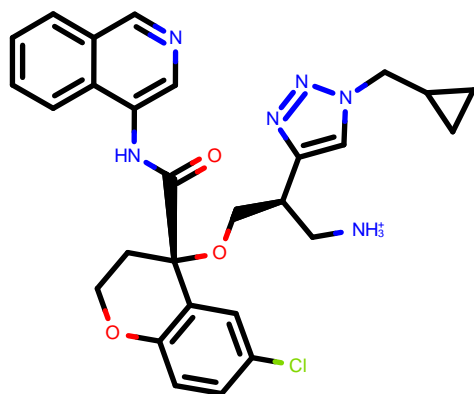
SMILES: CN(C(=O)CCOCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4)OC

RUN: RUN6029

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.40

ED_-GRI-5b13fbe2-49_2



CID: ED_-GRI-5b13fbe2-49_2

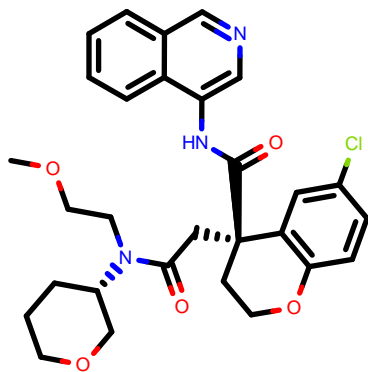
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)OC[C@H]5C(NH3+)c5cn(m5)CC6CC6

RUN: RUN1533

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.39

JAG-UCB-706446eb-5_2_1



CID: JAG-UCB-706446eb-5_2_1

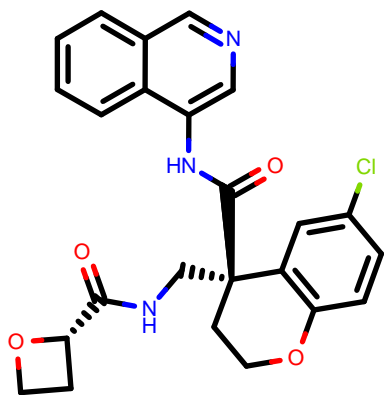
SMILES: COCCN([C@H]1CCCOC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN: RUN5511

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.45

EN300-85760_2_1_1



CID: EN300-85760_2_1_1

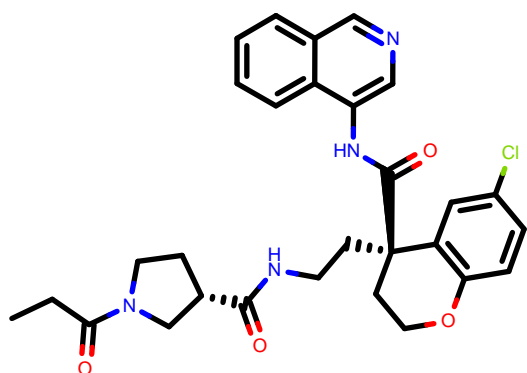
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CCO5

RUN: RUN4378

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-114133_3_1_1



CID: EN300-114133_3_1_1

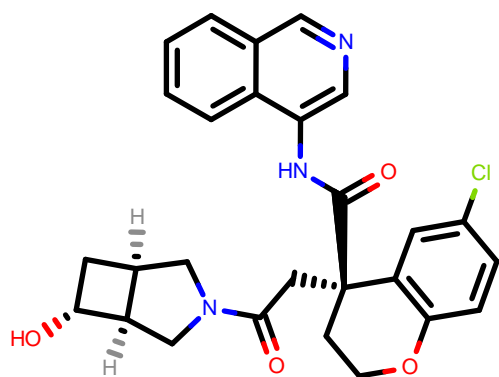
SMILES: CCC(=O)N1CC[C@@H](C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN5353

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.45

EN300-305294_1_3_1



CID: EN300-305294_1_3_1

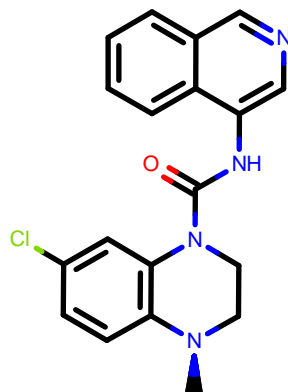
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)N[C@@]5(C)C[C@@H](C5)O

RUN: RUN7143

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.22

BEN-DND-f2e727cd-3_2



CID: BEN-DND-f2e727cd-3_2

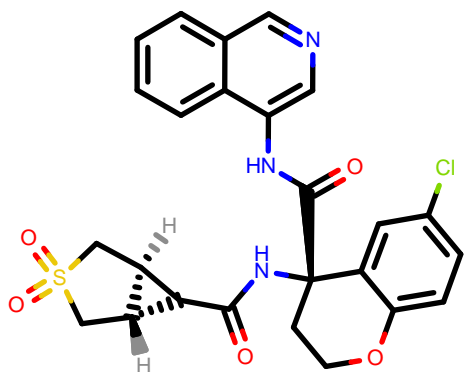
SMILES: C[N@]1CCN(c2c1ccc(c2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1059

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.31

EN300-6779469_1_3_1



CID: EN300-6779469_1_3_1

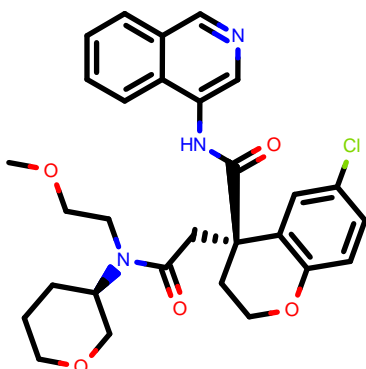
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(c4)C)N(C)C(=O)C[C@@H]5C(S(=O)(=O)C)C=C5

RUN: RUN6109

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.25

JAG-UCB-706446eb-5_1



CID: JAG-UCB-706446eb-5_1

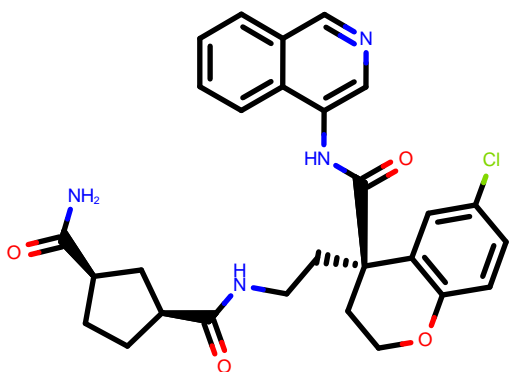
SMILES: COCCN(C[C@@H]1CCCOC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN651

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.36

EN300-370753_3_1_1



CID: EN300-370753_3_1_1

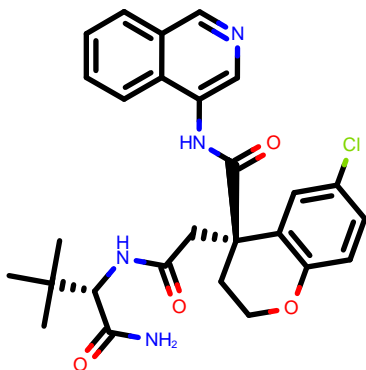
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(c4)C)N(C)C(=O)C[C@@H]5C(C)C=C5

RUN: RUN5860

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.31

EN300-96001_1_1_1



CID: EN300-96001_1_1_1

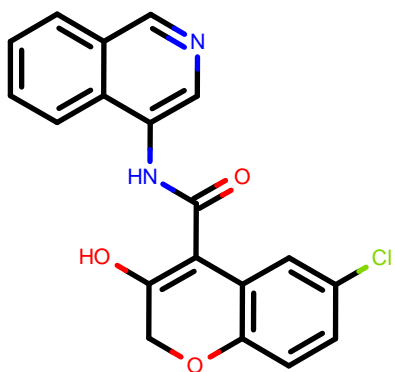
SMILES: CC(C)(C)[C@@H](C(=O)N)N(C(=O)C[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN6353

DDG (kcal/mol): -0.55

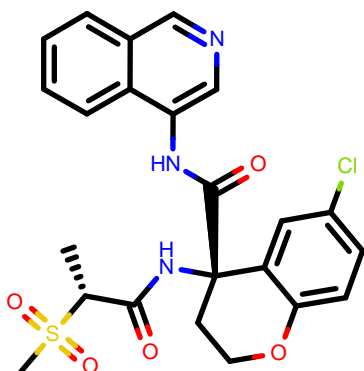
dDDG (kcal/mol): 0.27

VLA-UCB-1dbca3b4-16_1



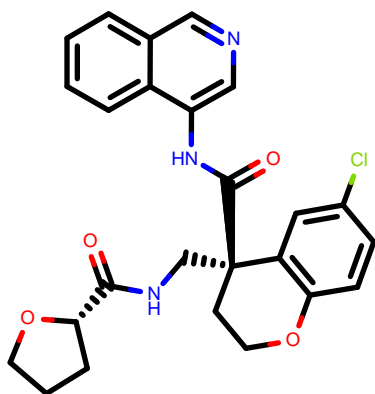
CID:	VLA-UCB-1dbca3b4-16_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)C3=C(COC4c3cc(cc4)Cl)O</chem>
RUN:	RUN121
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.27

EN300-39405_1_2_1



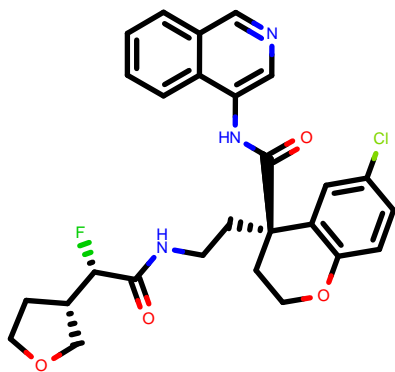
CID:	EN300-39405_1_2_1
SMILES:	<chem>C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)S(=O)(=O)C</chem>
RUN:	RUN6453
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.29

EN300-104395_2_1_1



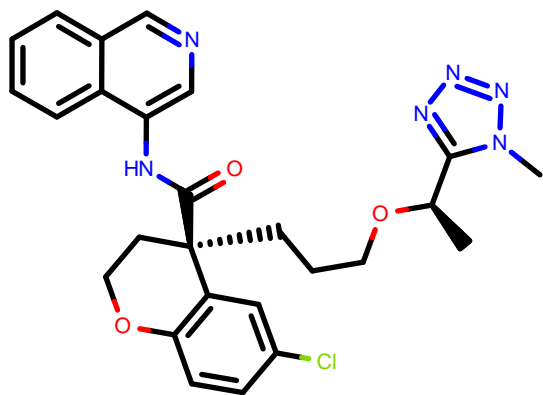
CID:	EN300-104395_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCOC5</chem>
RUN:	RUN7476
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.29

EN300-783124_3_4_1



CID:	EN300-783124_3_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]([C@@H]5CCOC5)F</chem>
RUN:	RUN3278
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.27

EN300-173006_4_2_1



CID: EN300-173006_4_2_1

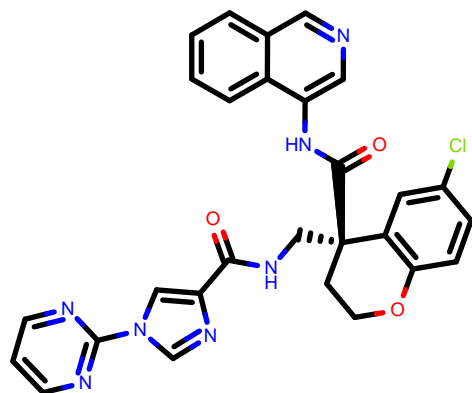
SMILES: C[C@H](c1nnc1C)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN7763

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.35

EN300-261056_2_1_1



CID: EN300-261056_2_1_1

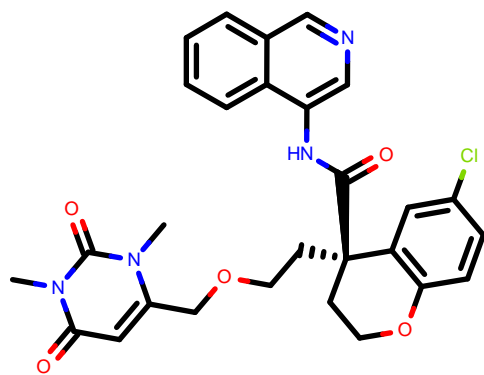
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn(cn5)c6ncoc6

RUN: RUN6462

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.30

EN300-25386_3_1_1



CID: EN300-25386_3_1_1

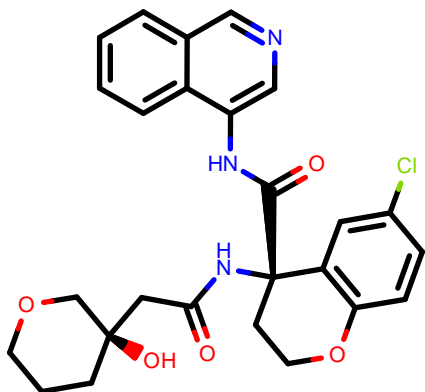
SMILES: Cn1c(cc(=O)n(c1=O)C)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5214

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.31

EN300-1071940_1_1_1



CID: EN300-1071940_1_1_1

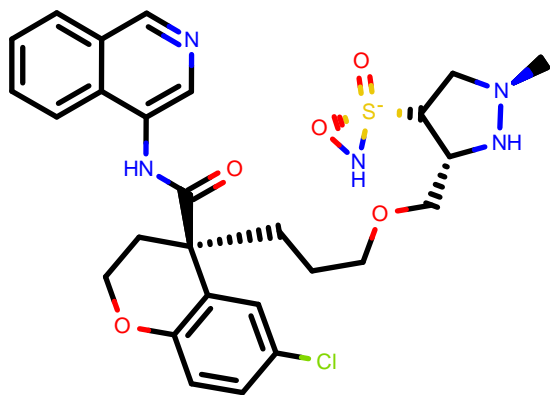
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]5(CCCOC5)O

RUN: RUN6219

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-7355737_4_1_3



CID: EN300-7355737_4_1_3

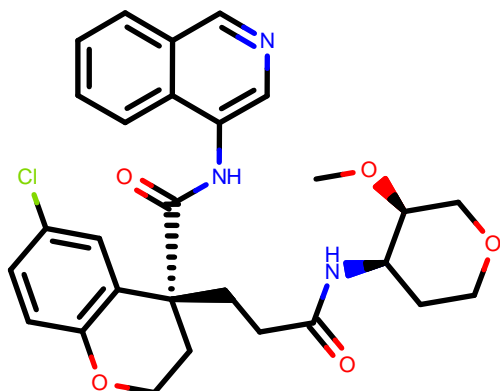
SMILES: CN1C=C([C@H](N1)C)OCCC[C@]2(C)COCc3c2cc(cc3)C(=O)Nc4ncc5c4cccc5S(=O)(=O)N

RUN: RUN6519

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.41

EN300-76451_2_4_1



CID: EN300-76451_2_4_1

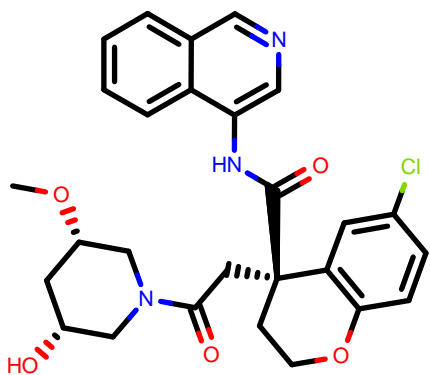
SMILES: CO[C@H]1COC[C@H](N1)C(=O)C[C@]2(C)COCc3c2cc(cc3)C(=O)Nc4ncc5c4cccc5

RUN: RUN7078

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.32

EN300-6763507_1_4_1



CID: EN300-6763507_1_4_1

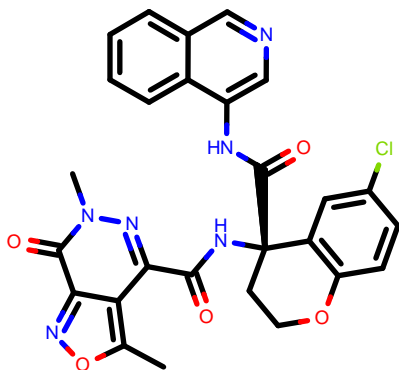
SMILES: CO[C@H]1C[C@H](CN(C1)C(=O)C)[C@]2(C)COCc3c2cc(cc3)C(=O)Nc4ncc5c4cccc5O

RUN: RUN5699

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.30

EN300-63781_1_1_1



CID: EN300-63781_1_1_1

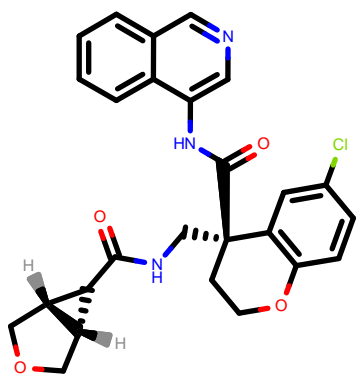
SMILES: Cc1c2c(c(=O)n(c2C(=O)N)[C@]3(C)COCc4c3cc(cc4)C(=O)Nc5ncc6c5cccc6)C)n1

RUN: RUN7676

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-257945_2_1_1



CID: EN300-257945_2_1_1

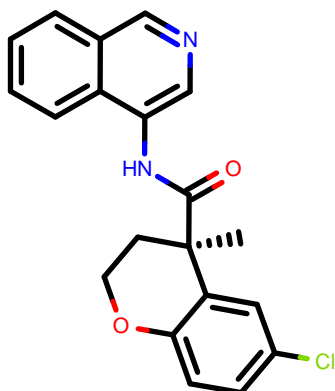
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5[C@H]6[C@@H]5COC6

RUN: RUN6364

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.28

EDJ-MED-e4b030d8-13_1_1



CID: EDJ-MED-e4b030d8-13_1_1

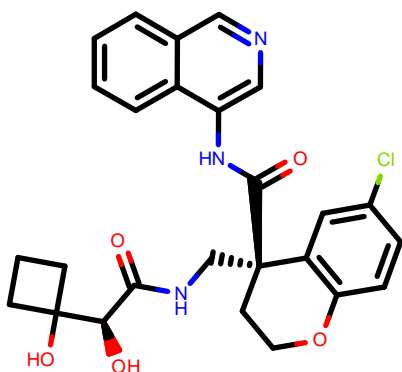
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN6122

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.10

EN300-1073320_2_2_1



CID: EN300-1073320_2_2_1

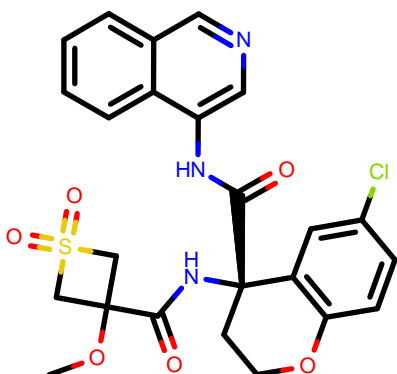
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5(CCC5)O)O

RUN: RUN6314

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-704025_1_1_1



CID: EN300-704025_1_1_1

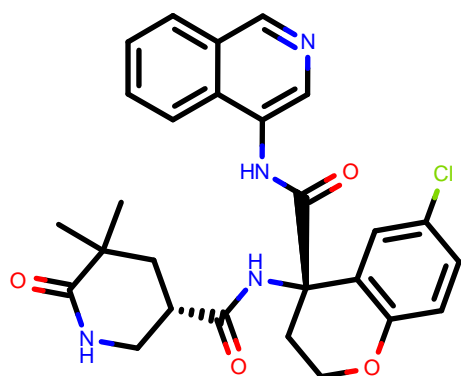
SMILES: COC1(CS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN5267

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.33

EN300-7351945_1_1_1



CID: EN300-7351945_1_1_1

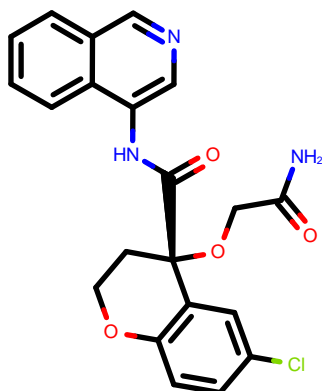
SMILES: CC1[C@@H](NC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5C

RUN: RUN2693

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.21

EN300-18249_1_1_1



CID: EN300-18249_1_1_1

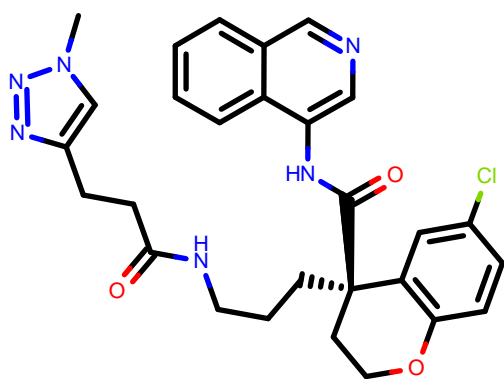
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N

RUN: RUN5798

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.19

EN300-306047_4_1_1



CID: EN300-306047_4_1_1

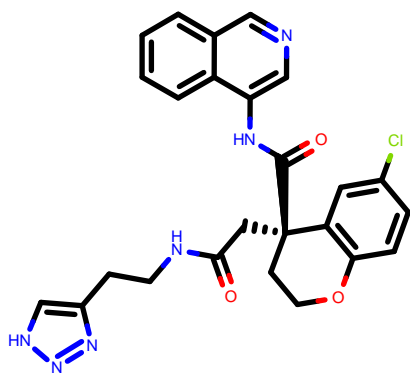
SMILES: Cn1cc(n1)CCC(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5081

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.35

EN300-1178209_1_1_1



CID: EN300-1178209_1_1_1

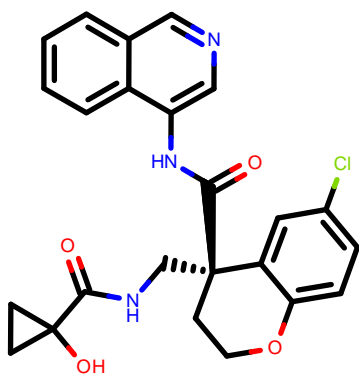
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5c5n[nH]5

RUN: RUN6413

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-25702_2_1_1



CID: EN300-25702_2_1_1

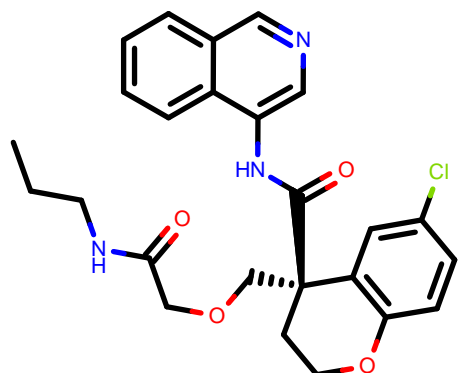
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)O

RUN: RUN4128

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-17184_2_1_1



CID: EN300-17184_2_1_1

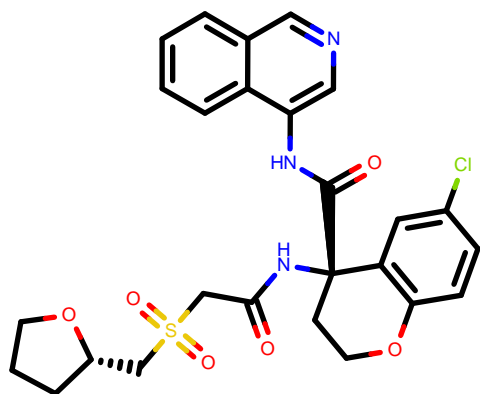
SMILES: C=CCNC(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN7314

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.23

EN300-67023_1_1_1



CID: EN300-67023_1_1_1

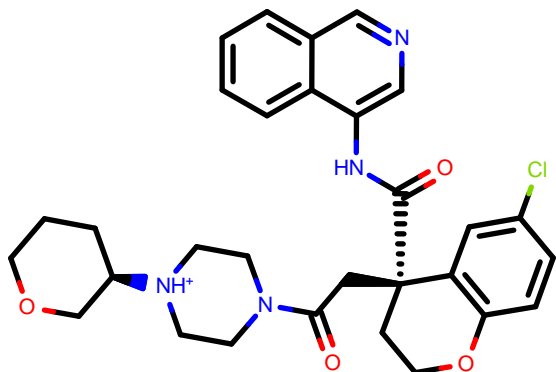
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C[C@@]5H5OCCO5

RUN: RUN6657

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.37

EDG-MED-ba1ac7b9-31_2



CID: EDG-MED-ba1ac7b9-31_2

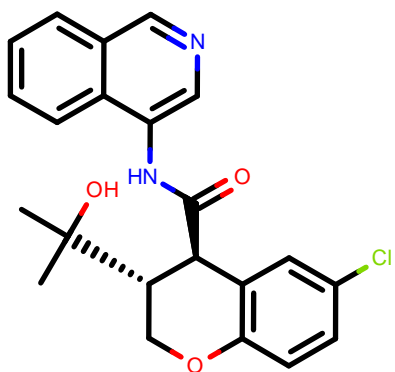
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)C(=O)N5CQ[NH+]CC5[C@@]6H6OCCO6

RUN: RUN2606

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.41

BEN-BAS-5c03e89e-1_2_1



CID: BEN-BAS-5c03e89e-1_2_1

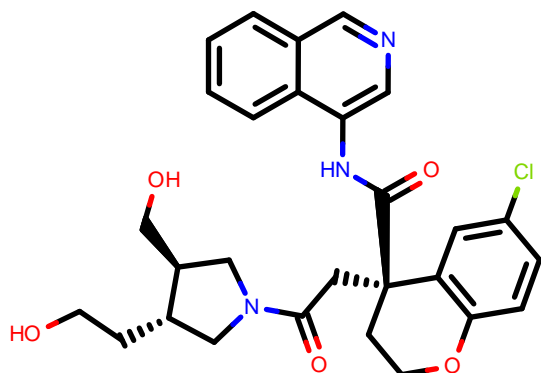
SMILES: CC(C)(C@H)1COc2ccc(cc2[C@@H]1C(=O)Nc3ccc4c3ccc4Cl)O

RUN: RUN4415

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.11

EN300-1425608_1_3_1



CID: EN300-1425608_1_3_1

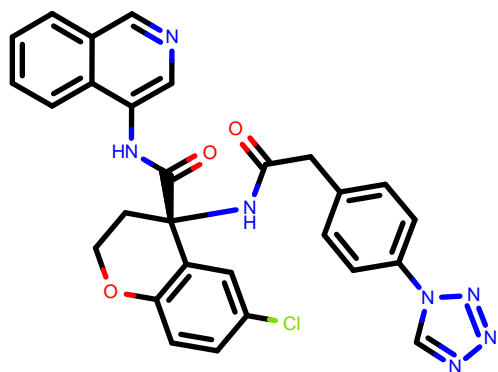
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)C(=O)N5C[C@@H](C)C5O)CO

RUN: RUN5424

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.30

ALP-UNI-dbbfd3db-1_1



CID: ALP-UNI-dbbfd3db-1_1

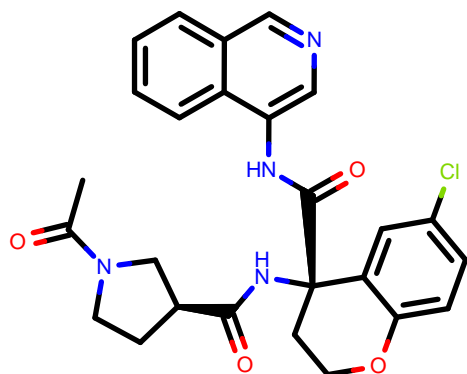
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)C(=O)N5C5ccc(c5)n6cnnn6

RUN: RUN2628

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.32

EN300-100180_1_1_1



CID: EN300-100180_1_1_1

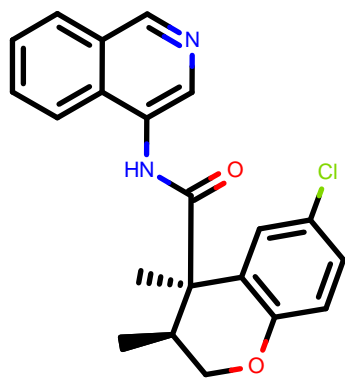
SMILES: CC(=O)N1CC[C@@H](C1)C(=O)N[C@@]2(CCOc3ccc(cc3)Cl)C(=O)N4cncnc5c4ccc5

RUN: RUN7034

DDG (kcal/mol): -0.54

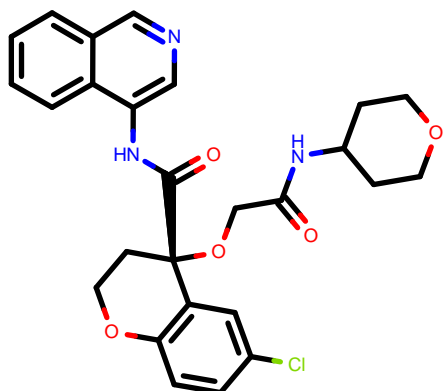
dDDG (kcal/mol): 0.45

DAR-DIA-0d514e7d-29_1



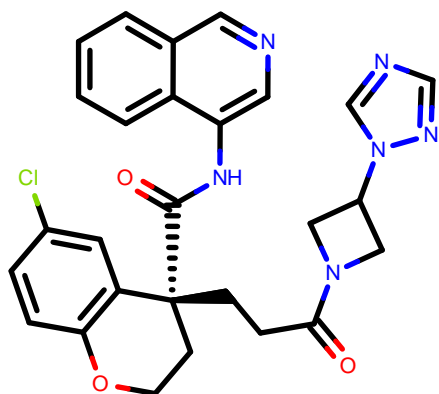
CID:	DAR-DIA-0d514e7d-29_1
SMILES:	<chem>C[C@@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN723
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.25

EN300-67573_1_1_1



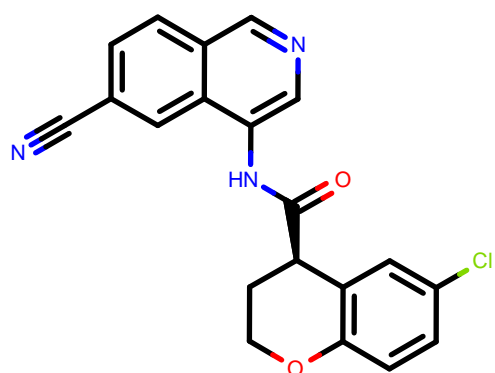
CID:	EN300-67573_1_1_1
SMILES:	<chem>c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCOCC5</chem>
RUN:	RUN5637
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.27

KAD-UNI-8a629cb0-48_1



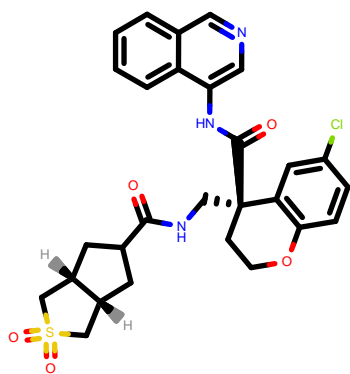
CID:	KAD-UNI-8a629cb0-48_1
SMILES:	<chem>c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)n6cncn6</chem>
RUN:	RUN2040
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.27

BEN-DND-c852c98b-1_1_1



CID:	BEN-DND-c852c98b-1_1_1
SMILES:	<chem>c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN6707
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.13

EN300-7438088_2_1_1



CID: EN300-7438088_2_1_1

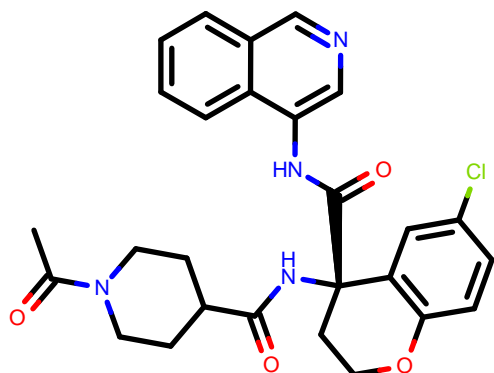
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4ccc(cc4)C)NC(=O)C3C[C@@H]5C(S(=O)(=O)O)C[C@@H]5C5

RUN: RUN7786

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.37

EN300-18557_1_1_1



CID: EN300-18557_1_1_1

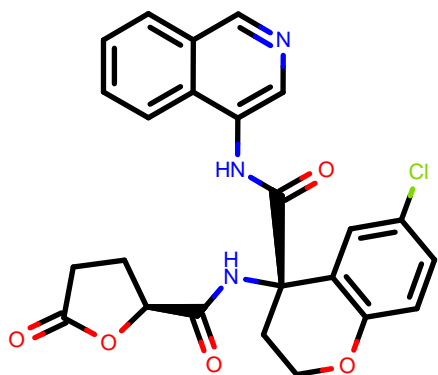
SMILES: CC(=O)N1CCC(CC1)C(=O)N[C@@2](COCc3ccc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN6814

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.32

EN300-359750_1_1_1



CID: EN300-359750_1_1_1

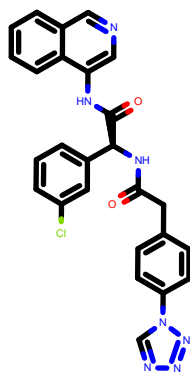
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4ccc(cc4)Cl)NC(=O)C3[C@@H]5CCCC(=O)O5

RUN: RUN6817

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.23

EDJ-MED-ee07cf00-15_2



CID: EDJ-MED-ee07cf00-15_2

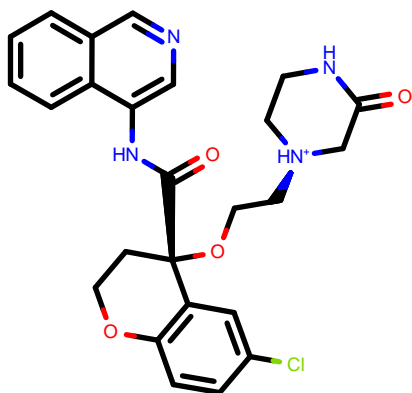
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H](c3ccccc(c3)Cl)NC(=O)C4Cccc(cc4)n5cnnn5

RUN: RUN2686

DDG (kcal/mol): -0.53

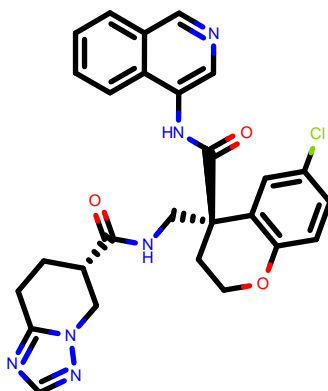
dDDG (kcal/mol): 0.37

ED_-GRI-5b13fbe2-31_2



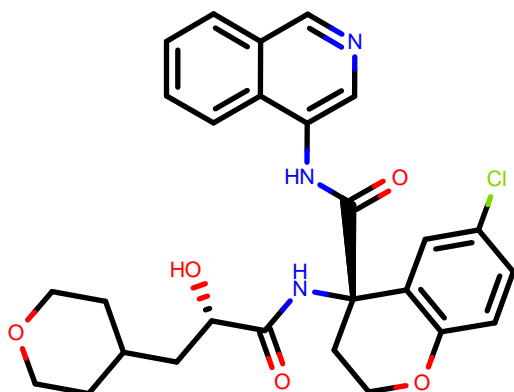
CID:	ED_-GRI-5b13fbe2-31_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@H]5CCNC(=O)C5</chem>
RUN:	RUN1416
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.34

EDJ-MED-40433386-9_1



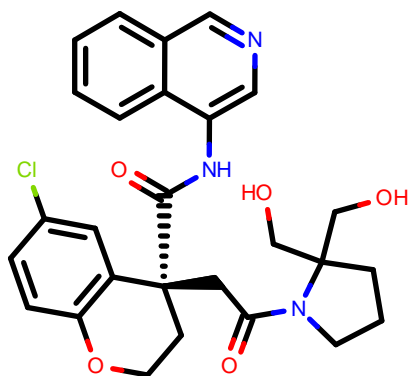
CID:	EDJ-MED-40433386-9_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC6c6nnn6C5</chem>
RUN:	RUN2365
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.28

EN300-1452069_1_2_1



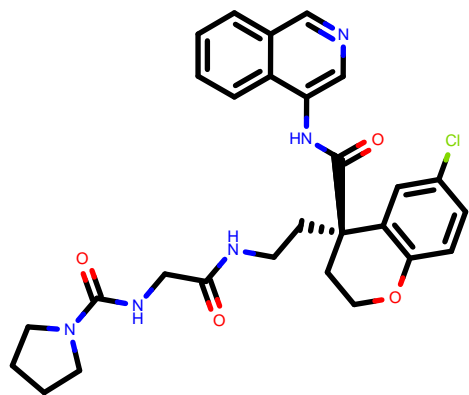
CID:	EN300-1452069_1_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C)CC5CCOCC5O</chem>
RUN:	RUN6189
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.30

EN300-1091448_1_1_1



CID:	EN300-1091448_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC5(CO)CO</chem>
RUN:	RUN3434
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.33

EN300-383906_3_1_1



CID: EN300-383906_3_1_1

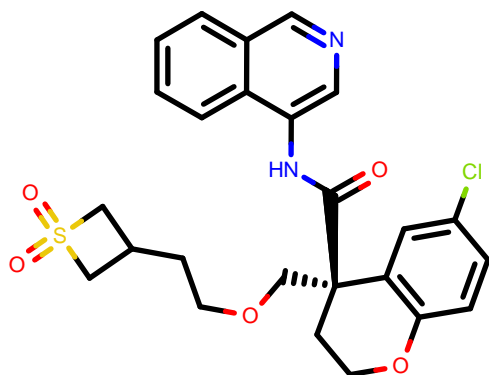
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CNC(=O)N5CCCC5

RUN: RUN6963

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.31

EN300-189563_2_1_1



CID: EN300-189563_2_1_1

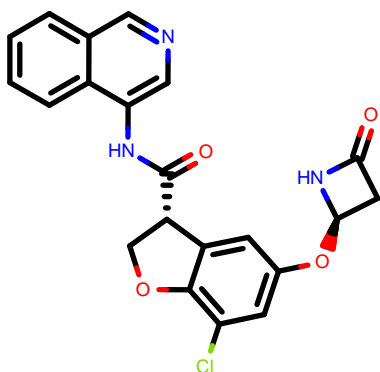
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)COCCCS(=O)(=O)C5

RUN: RUN4468

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.27

FRA-DIA-b66f7109-2_1



CID: FRA-DIA-b66f7109-2_1

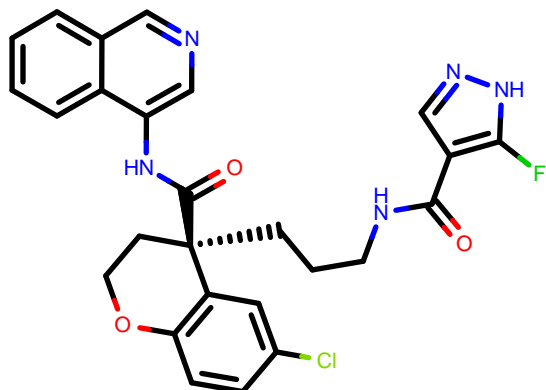
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3COc4c3cc(cc4Cl)O[C@@H]5CC(=O)N5

RUN: RUN323

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.39

EN300-7121836_4_1_1



CID: EN300-7121836_4_1_1

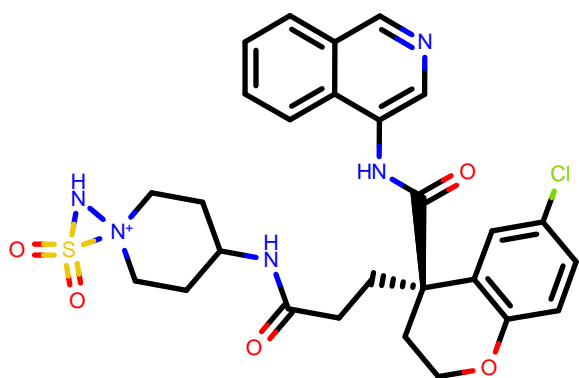
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)c5c[nH]c5F

RUN: RUN7229

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.29

EN300-310398_2_1_1



CID: EN300-310398_2_1_1

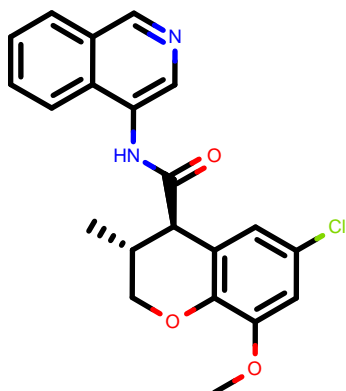
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N(C5CCN5)C(=O)NS(=O)(=O)

RUN: RUN3664

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.30

DAR-DIA-0d514e7d-1_1



CID: DAR-DIA-0d514e7d-1_1

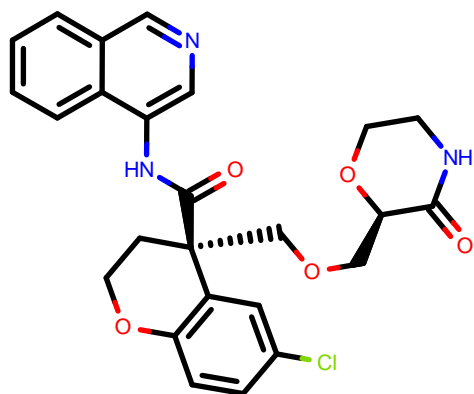
SMILES: C[C@H]1COc2c(cc2OC)C1][C@@H]1C(=O)Nc3cnc4c3cccc4

RUN: RUN728

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.11

EN300-1706036_2_1_1



CID: EN300-1706036_2_1_1

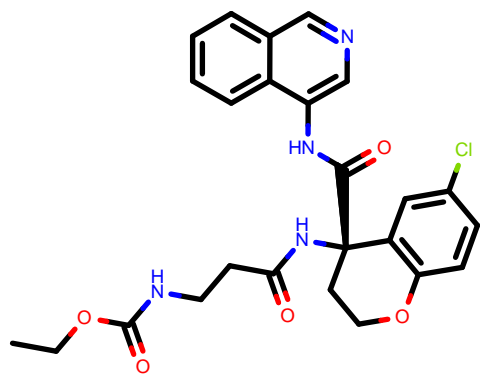
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N(C5CCN5)C(=O)N(C6CCO6)

RUN: RUN6540

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.27

EN300-36495_1_1_1



CID: EN300-36495_1_1_1

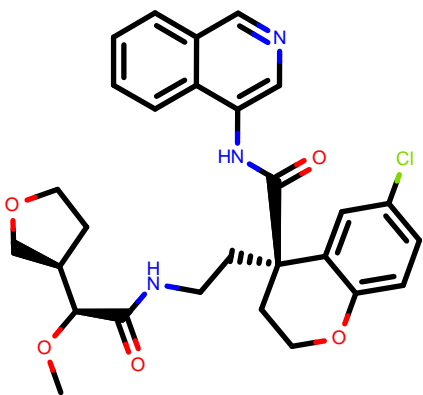
SMILES: CCOC(=O)NCCC(=O)N[C@@H]1(COCc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN6541

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.28

EN300-298552_3_1_1



CID: EN300-298552_3_1_1

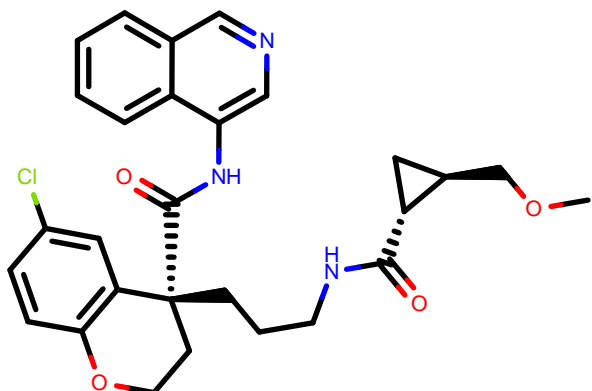
SMILES: CO[C@@H]([C@@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4782

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.23

EN300-705386_4_1_1



CID: EN300-705386_4_1_1

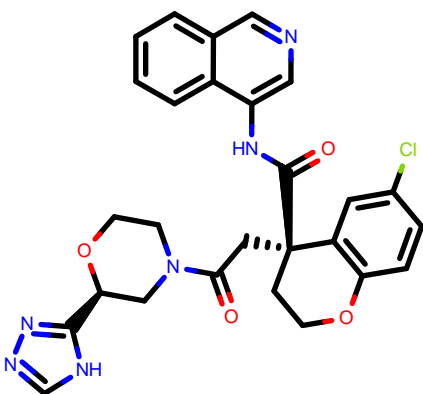
SMILES: COC[C@@H]1[C@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN7128

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.31

EN300-1709213_1_1_1



CID: EN300-1709213_1_1_1

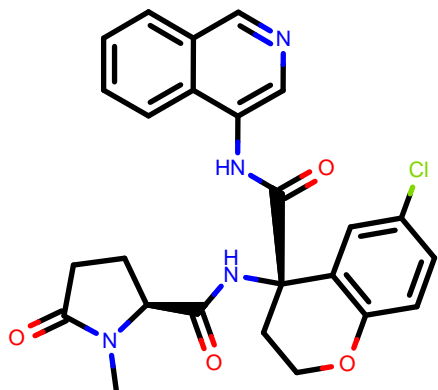
SMILES: c1cc2c(e1)ncoc2Nc1=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N6CCO[C@@H](C5)S6[H]n7c6

RUN: RUN7109

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.33

EN300-130825_1_1_1



CID: EN300-130825_1_1_1

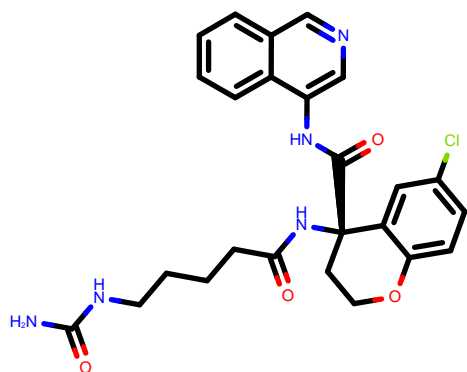
SMILES: CN1[C@@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6575

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.24

EN300-13499_1_1_1



CID: EN300-13499_1_1_1

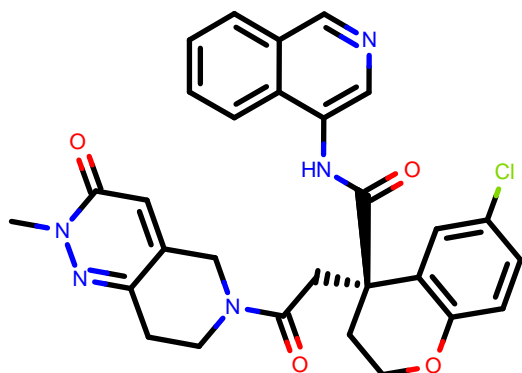
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCCNC(=O)N

RUN: RUN4014

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.28

ALP-UNI-3496895b-13_1



CID: ALP-UNI-3496895b-13_1

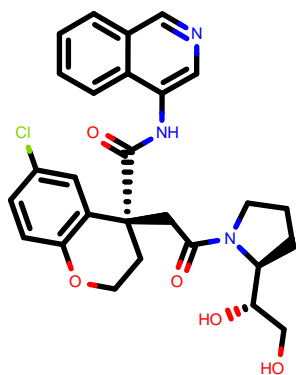
SMILES: Cn1c(=O)cc2c(n1)CCN(C2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN2364

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.28

EDJ-MED-d203f206-15_1



CID: EDJ-MED-d203f206-15_1

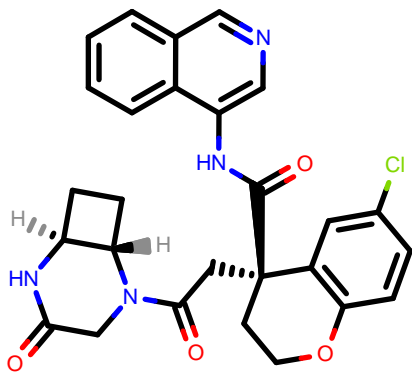
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5[C@@H](CO)O

RUN: RUN2399

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.41

EN300-6499164_1_1_1



CID: EN300-6499164_1_1_1

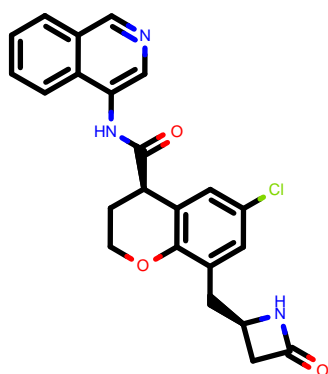
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5C[C@@H]6C[C@H]6

RUN: RUN5053

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

DAR-DIA-6a508060-5_1



CID: DAR-DIA-6a508060-5_1

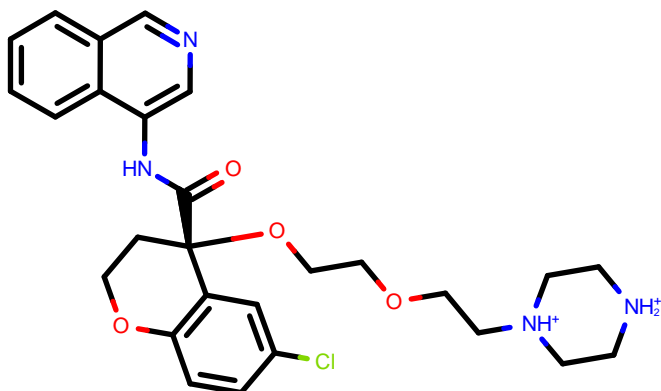
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC(=O)N5)Cl

RUN: RUN280

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.17

ED_-GRI-5b13fbe2-65_1



CID: ED_-GRI-5b13fbe2-65_1

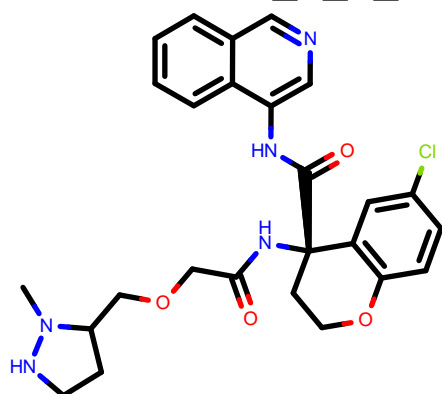
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCCOCCN5CC[NH2+]CC5

RUN: RUN1495

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.38

EN300-92472_1_1_1



CID: EN300-92472_1_1_1

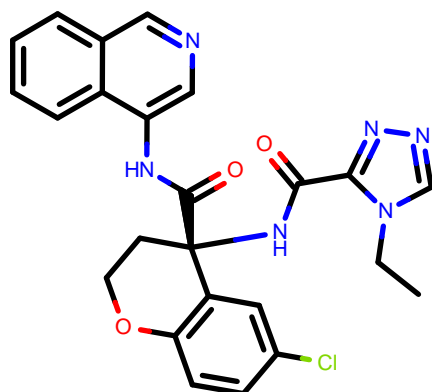
SMILES: C[n+](c1cc[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4440

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

EN300-6766760_1_1_1



CID: EN300-6766760_1_1_1

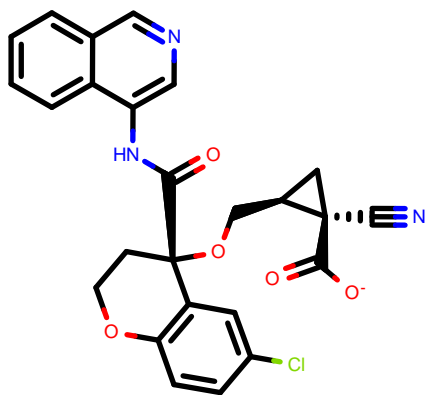
SMILES: CCn1cnnc1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6830

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.21

ED_-GRI-5b13fbe2-50_2



CID: ED_-GRI-5b13fbe2-50_2

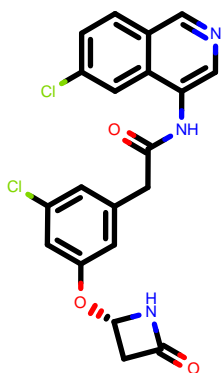
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCCOc4c3cc(cc4)C)OC[C@@H]5C[C@@]5(C#N)C(=O)[O-]

RUN: RUN1439

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

ALF-EVA-0b412456-1_2



CID: ALF-EVA-0b412456-1_2

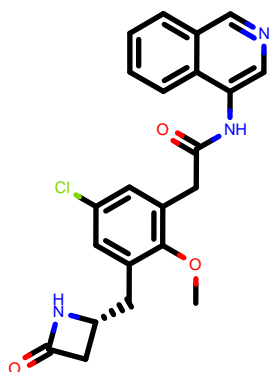
SMILES: c1cc2cnc(c2cc1Cl)NC(=O)Cc3ccc(cc3)C(O)C@H4CC(=O)N4

RUN: RUN2539

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.36

EDJ-MED-50011917-3_1



CID: EDJ-MED-50011917-3_1

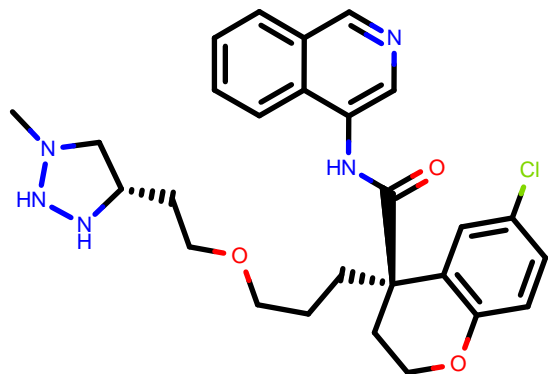
SMILES: COc1c(cc(cc1CC(=O)Nc2cnc3c2cccc3)Cl)C[C@@H]4CC(=O)N4

RUN: RUN333

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.34

EN300-1600786_4_1_1



CID: EN300-1600786_4_1_1

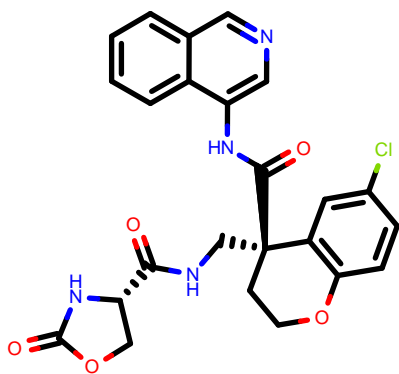
SMILES: Cn1cc(nn1)CCOCCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6877

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.39

EN300-126389_2_1_1



CID: EN300-126389_2_1_1

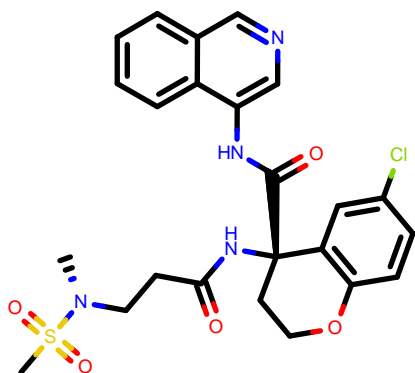
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5COC(=O)N5

RUN: RUN4749

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.23

EN300-132523_1_1_1



CID: EN300-132523_1_1_1

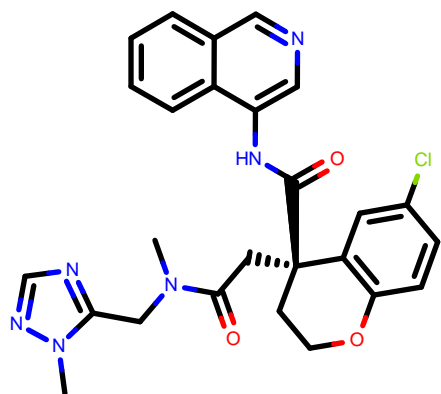
SMILES: C[N@](CCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3ccc4)S(=O)(=O)C

RUN: RUN6857

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.44

EN300-7444635_1_1_1



CID: EN300-7444635_1_1_1

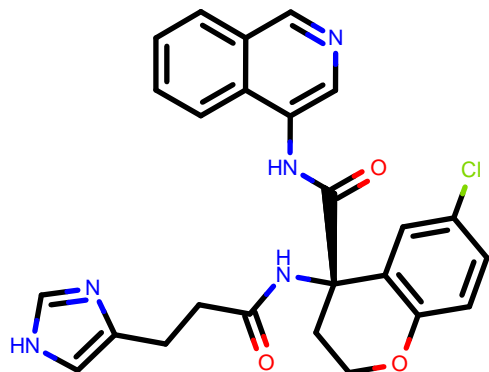
SMILES: Cn1c(nen1)CN(C)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN7742

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.33

EDG-MED-90036822-93_1



CID: EDG-MED-90036822-93_1

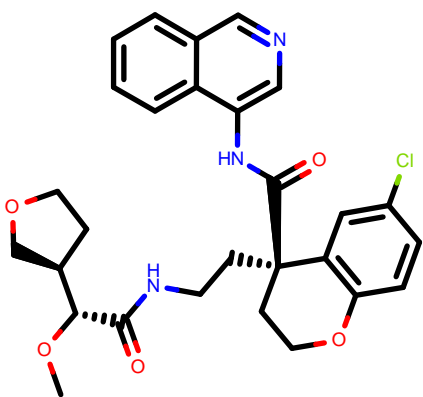
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CCc5cnc[nH]5

RUN: RUN1656

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.24

EN300-298552_3_2_1



CID: EN300-298552_3_2_1

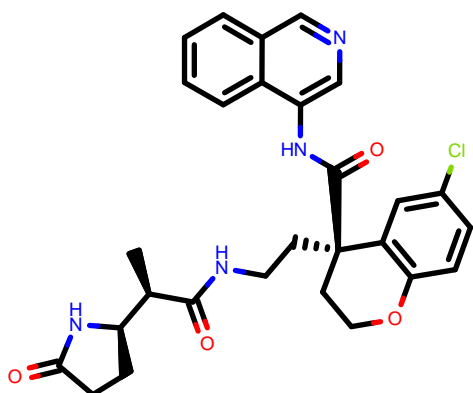
SMILES: CO[C@@H]([C@@H]1CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3809

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.24

EN300-249421_3_4_1



CID: EN300-249421_3_4_1

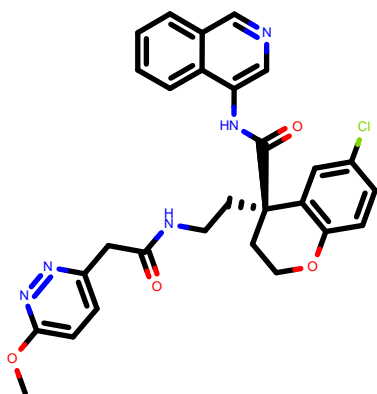
SMILES: C[C@@H]([C@@H]1CCC(=O)N1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3343

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.29

EN300-7540889_3_1_1



CID: EN300-7540889_3_1_1

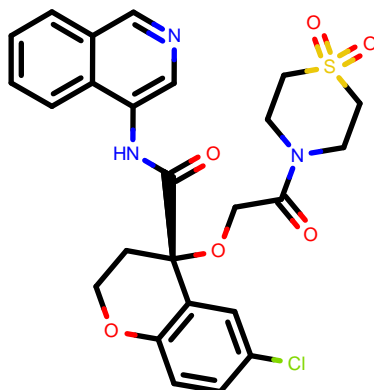
SMILES: COc1ccc(nn1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN4769

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.27

EN300-1265948_1_1_1



CID: EN300-1265948_1_1_1

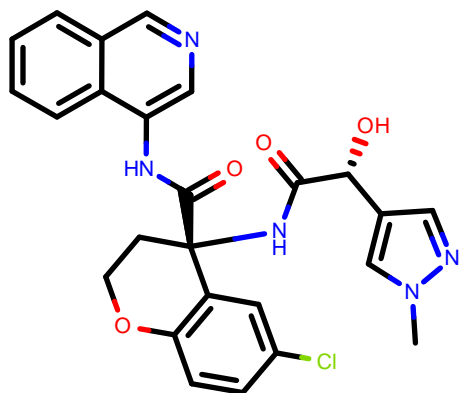
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN6065

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

EN300-198540_1_2_1



CID: EN300-198540_1_2_1

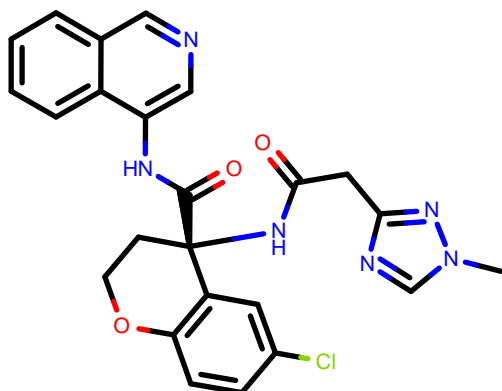
SMILES: Cn1cc(en1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN7145

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.29

EN300-7493922_1_1_1



CID: EN300-7493922_1_1_1

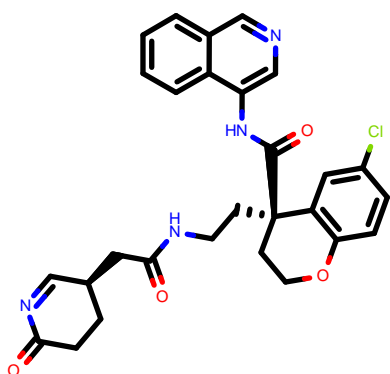
SMILES: Cn1cnc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6680

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.23

EN300-246992_3_2_1



CID: EN300-246992_3_2_1

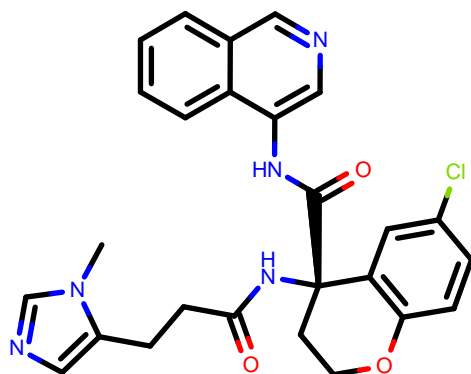
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)C[C@H]5CCC(=O)Nc5

RUN: RUN5417

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.37

EN300-174561_1_1_1



CID: EN300-174561_1_1_1

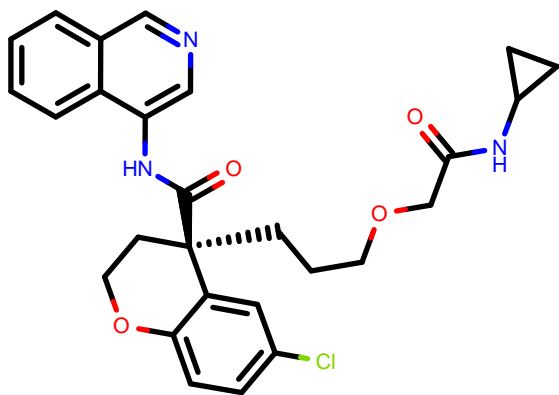
SMILES: Cn1cnc1CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6792

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.22

EN300-1253178_4_1_1



CID: EN300-1253178_4_1_1

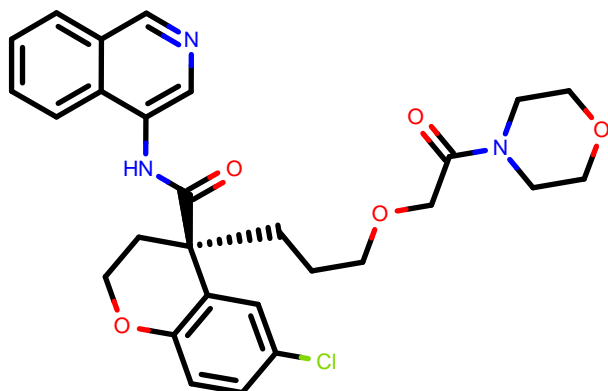
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C@H)(COC(=O)C)COC(=O)NCC3CC3

RUN: RUN7104

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.36

EN300-1241327_4_1_1



CID: EN300-1241327_4_1_1

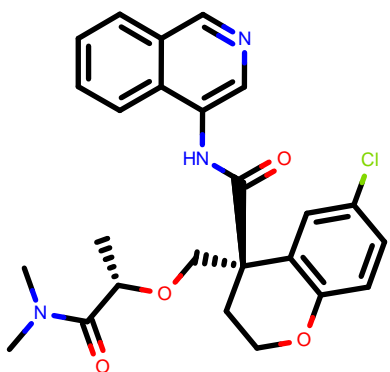
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C@H)(COC(=O)C)COC(=O)N5CCOCC5

RUN: RUN7673

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.32

EN300-14458_2_1_1



CID: EN300-14458_2_1_1

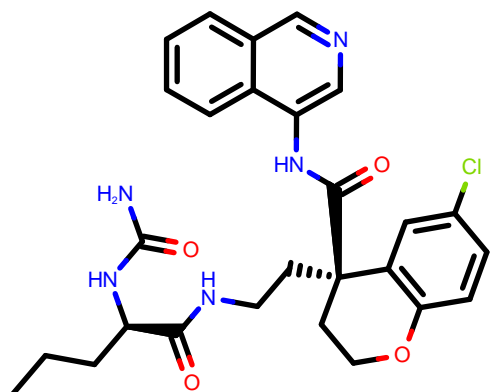
SMILES: C[C@@H](C(=O)N(C)C)OC[C@@H](COC(=O)C)C(=O)Nc3ccc(Cl)cc3

RUN: RUN6275

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.25

EN300-102901_3_1_1



CID: EN300-102901_3_1_1

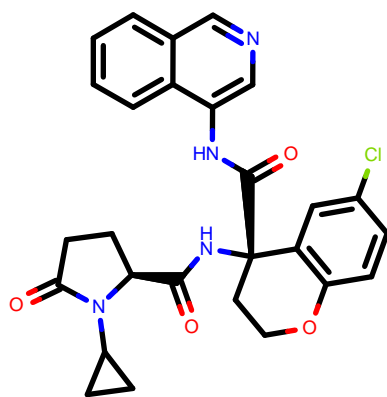
SMILES: CCC[C@@H](C(=O)NCC[C@@H](COC(=O)C)C(=O)Nc3ccc(Cl)cc3)NC(=O)N

RUN: RUN4375

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.46

EN300-3044054_1_1_1



CID: EN300-3044054_1_1_1

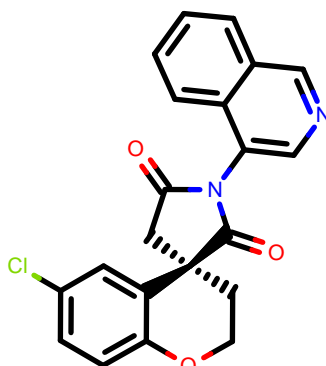
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5C5CC(=O)N5C6CC6

RUN: RUN7120

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.29

VLA-UCB-05e51b3f-5_1



CID: VLA-UCB-05e51b3f-5_1

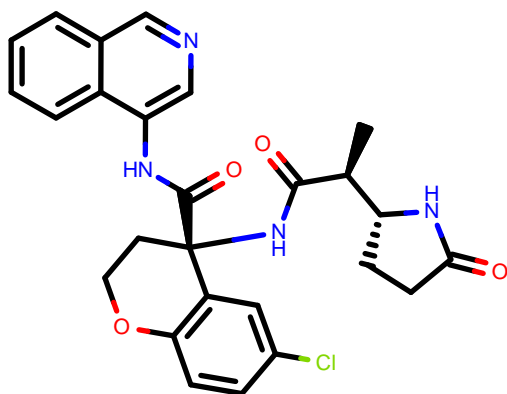
SMILES: c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CCOc5c4cc(cc5)Cl

RUN: RUN237

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.24

EN300-249421_1_3_1



CID: EN300-249421_1_3_1

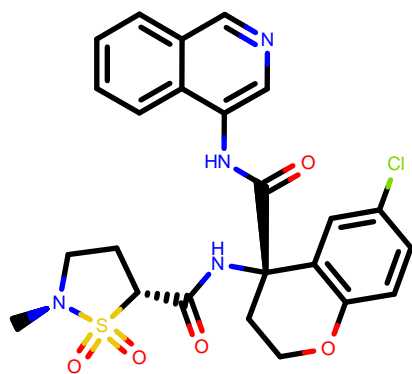
SMILES: C[C@@]1H[C@@H]1CCC(=O)N1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN6946

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.31

EN300-255496_1_1_1



CID: EN300-255496_1_1_1

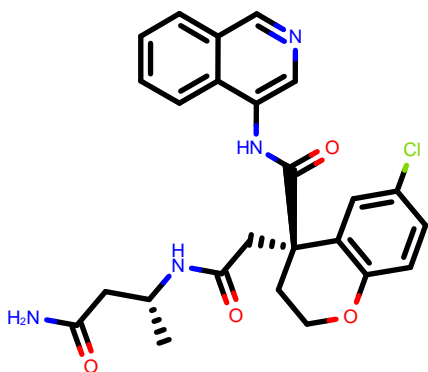
SMILES: C[N@@]1CC[C@@]1H[S1(=O)=O]C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4097

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.30

EN300-84785_1_2_1



CID: EN300-84785_1_2_1

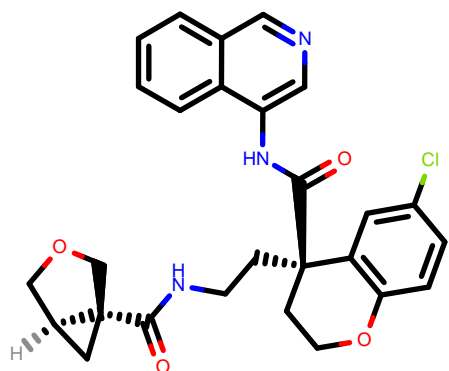
SMILES: C[C@H](CC(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3093

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.25

EN300-263669_3_1_1



CID: EN300-263669_3_1_1

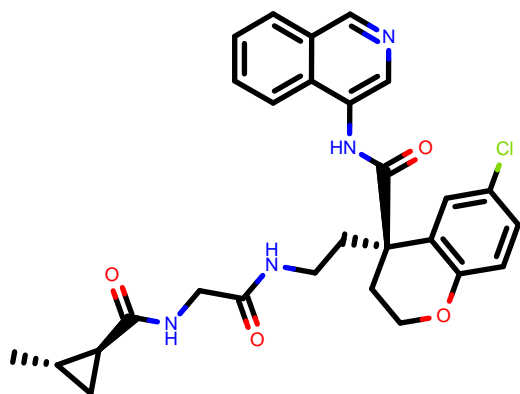
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56C[C@H]5COC6

RUN: RUN5183

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.25

EN300-30768_3_2_1



CID: EN300-30768_3_2_1

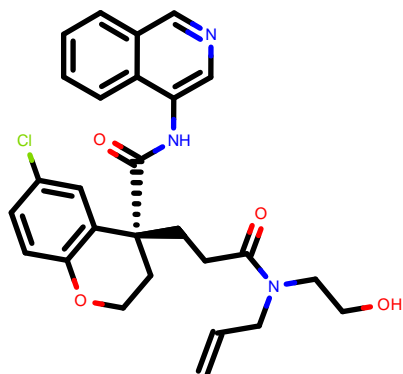
SMILES: C[C@H]1C[C@@H]1C(=O)NCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7497

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.28

EN300-79536_2_1_1



CID: EN300-79536_2_1_1

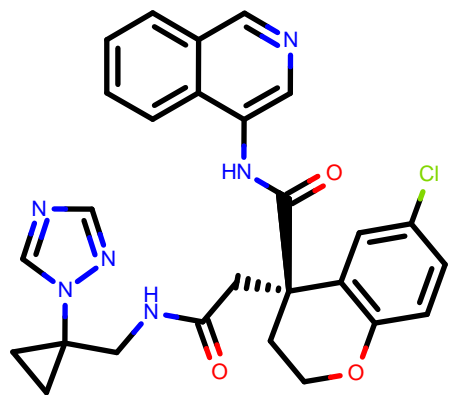
SMILES: C=CCN(CCO)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6320

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.27

EN300-6733137_1_1_1



CID: EN300-6733137_1_1_1

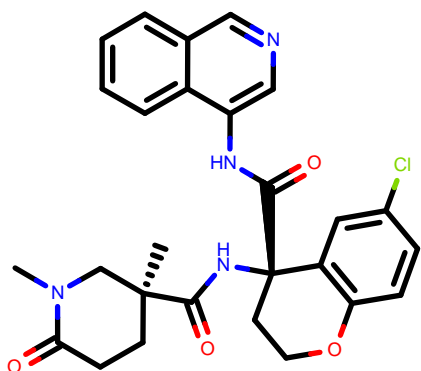
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)NCC5(CC5)n6cncn6

RUN: RUN7313

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.33

EN300-6734171_1_1_1



CID: EN300-6734171_1_1_1

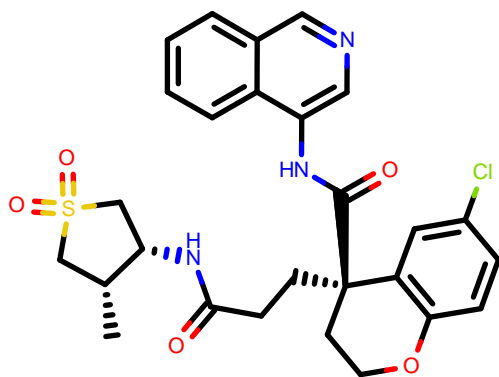
SMILES: C[C@@]1(CCC(=O)N(C1)C)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3675

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.33

EN300-371704_2_1_1



CID: EN300-371704_2_1_1

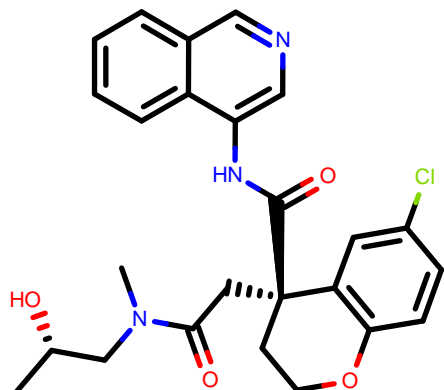
SMILES: C[C@@]1(CS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6201

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.31

EN300-210254_1_1_1



CID: EN300-210254_1_1_1

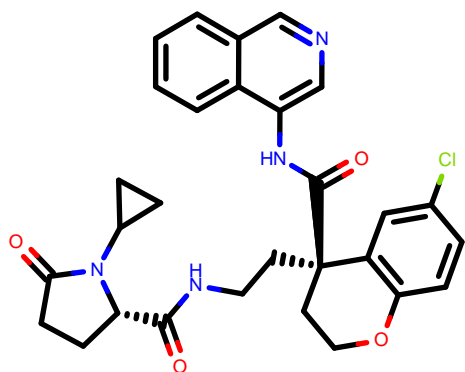
SMILES: C[C@@]1(CN(C)C(=O)C)C@1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4O

RUN: RUN4835

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.37

EN300-3044054_3_1_1



CID: EN300-3044054_3_1_1

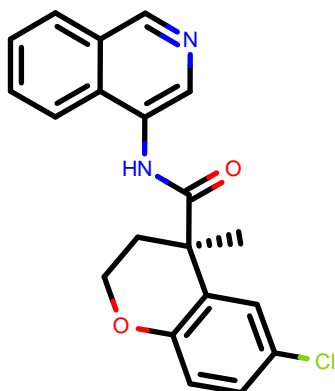
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C4=CC=CC=C4C1=CC=CC=C1O[C@@H](C)C(=O)N5CCCC5

RUN: RUN7060

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.27

DAR-DIA-6a508060-10_2



CID: DAR-DIA-6a508060-10_2

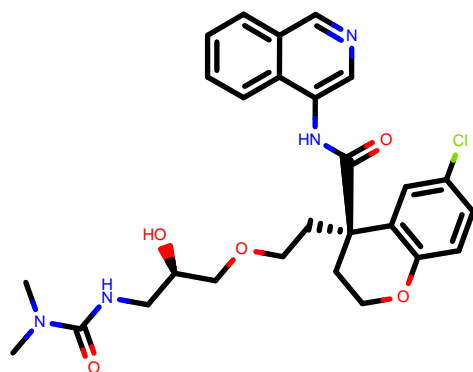
SMILES: C[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN294

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.10

EN300-6501360_3_2_1



CID: EN300-6501360_3_2_1

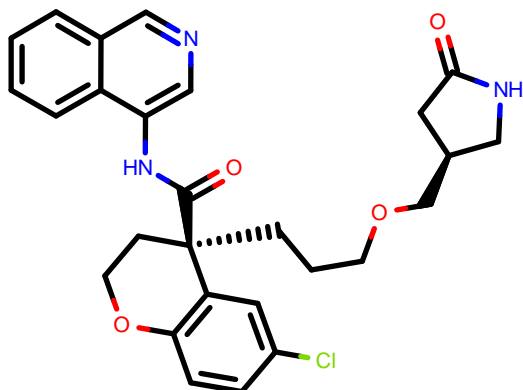
SMILES: CN(C)C(=O)N[C@@H](C)C(=O)C1=CC=CC=C1C(=O)Nc3cncc4c3cccc4O

RUN: RUN7323

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.40

EN300-246747_4_2_1



CID: EN300-246747_4_2_1

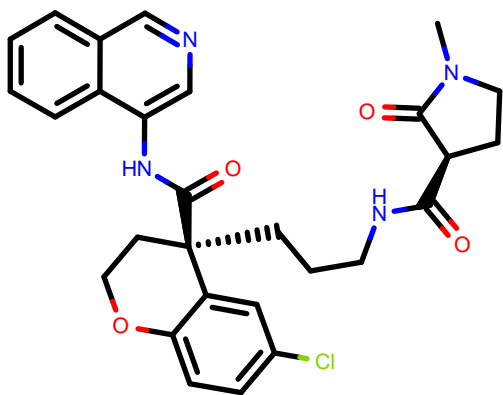
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C4=CC=CC=C4C1=CC=CC=C1O[C@@H](C)C(=O)N5CCCC5

RUN: RUN5883

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.38

EN300-141695_4_2_1



CID: EN300-141695_4_2_1

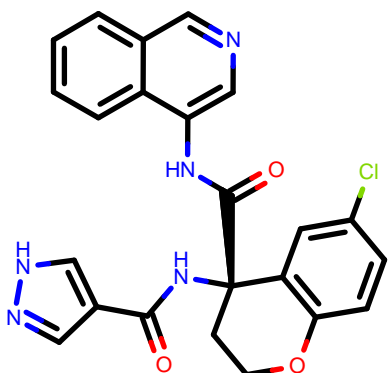
SMILES: CN1CC[C@H](C1=O)C(=O)NCCC[C@2](CCOC3C2C(C3)C)C(=O)Nc4nc5c4cccc5

RUN: RUN7096

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.35

EN300-41863_1_1_1



CID: EN300-41863_1_1_1

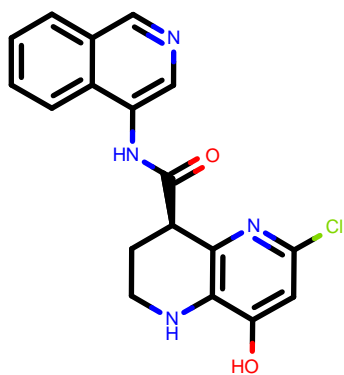
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOC4C3C(C4)C)NC(=O)c5c[nH]nc5

RUN: RUN5935

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.17

BEN-BAS-c2bc0d80-4_1



CID: BEN-BAS-c2bc0d80-4_1

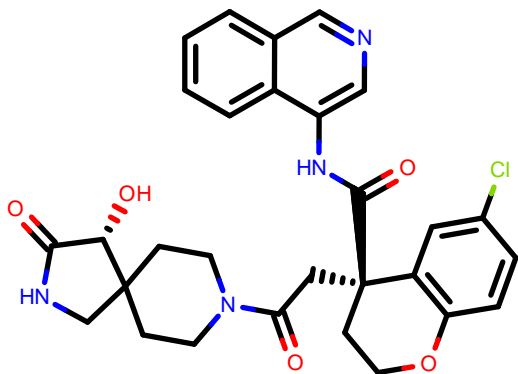
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC=Nc4c3[nH]c(cc4=O)Cl

RUN: RUN1012

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.31

EN300-6478434_1_1_1



CID: EN300-6478434_1_1_1

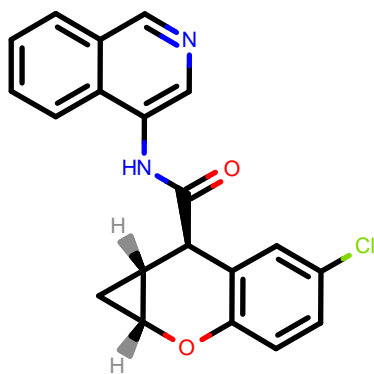
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3](CCOC4C3C(C4)C)C(=O)N5CCCC(C5)CNC1=O[C@@H]5O

RUN: RUN6249

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.48

DAR-DIA-0d514e7d-33_2



CID: DAR-DIA-0d514e7d-33_2

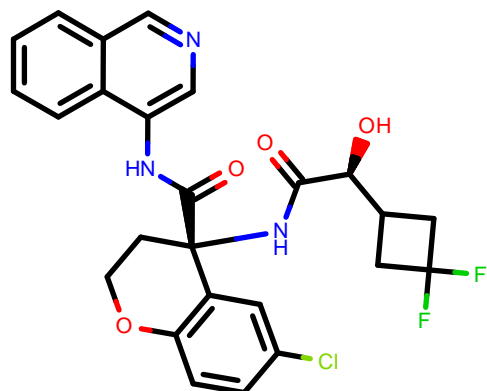
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@H]3c4cc(ccc4O[C@H]5[C@@H]3C5)Cl

RUN: RUN783

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.26

EDG-MED-90036822-101_2



CID: EDG-MED-90036822-101_2

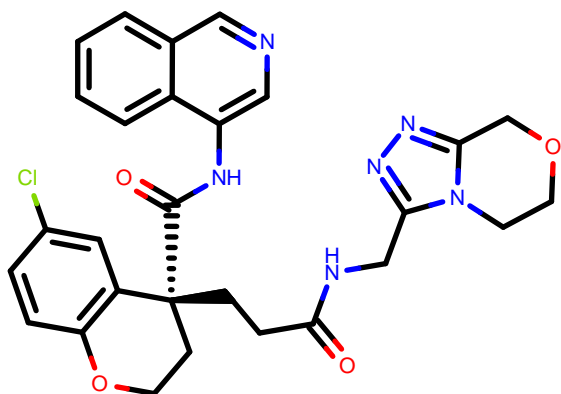
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](C5CC(C5)(F)F)O

RUN: RUN1712

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.24

EN300-155447_2_1_1



CID: EN300-155447_2_1_1

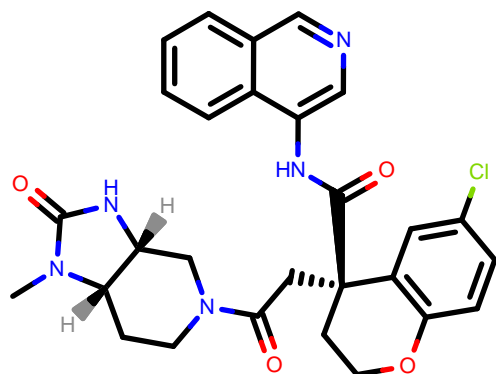
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC5nnc6n5CCOC6

RUN: RUN6213

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.23

EN300-216968_1_1_1



CID: EN300-216968_1_1_1

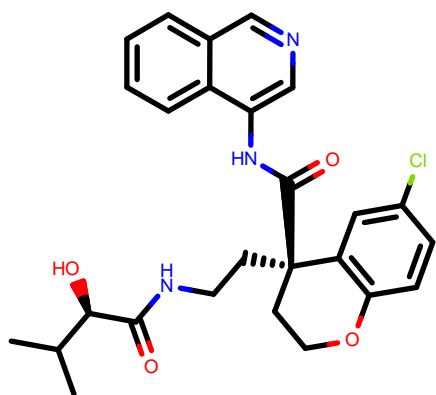
SMILES: CN1[C@H]2CN(C)[C@H]2NC1=O[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5cnc6c5ccccc6

RUN: RUN6852

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.32

EN300-115017_3_1_1



CID: EN300-115017_3_1_1

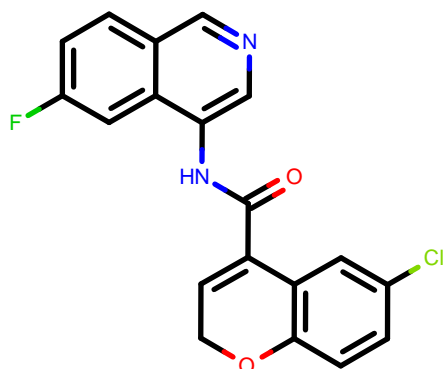
SMILES: CC(C)[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5824

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

ALP-POS-ce760d3f-5_1



CID: ALP-POS-ce760d3f-5_1

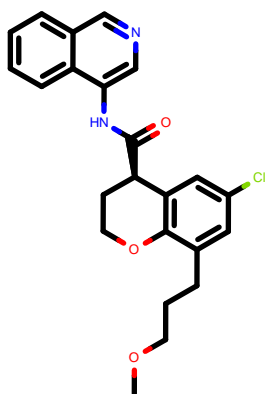
SMILES: c1cc2cncc(c2cc1F)NC(=O)C3=CCOc4c3cc(cc4)Cl

RUN: RUN1279

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

LAU-MED-88a3970a-13_1



CID: LAU-MED-88a3970a-13_1

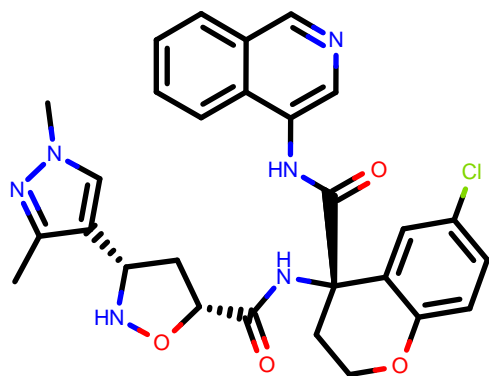
SMILES: COCCc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3ccoc4)Cl

RUN: RUN1360

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.18

EN300-92684_1_2_1



CID: EN300-92684_1_2_1

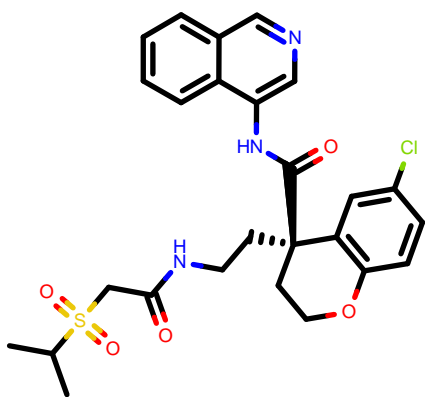
SMILES: Cc1c([n+])[nH]1)C(C@@H)2C(C@@H)3ON2C1=O)N1C@]3(CCOc4c3cc(cc4)Cl)C1=O)Nc5ncoc6c5ccoc6

RUN: RUN3021

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.34

EN300-51028_3_1_1



CID: EN300-51028_3_1_1

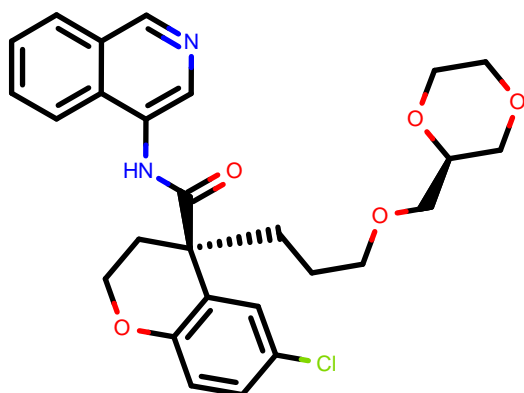
SMILES: CC(C)S(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7278

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.34

EN300-139167_4_1_1



CID: EN300-139167_4_1_1

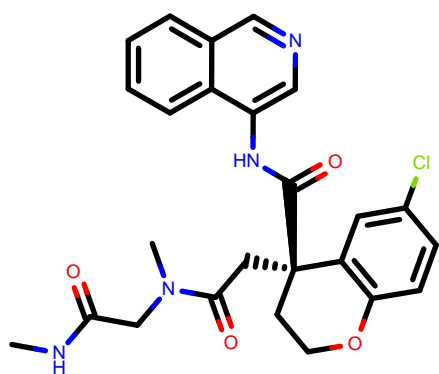
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCOC[C@]5H5COCOC5

RUN: RUN4895

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

EN300-34491_1_1_1



CID: EN300-34491_1_1_1

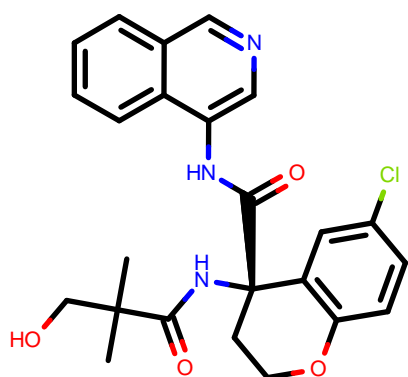
SMILES: CNC(=O)CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5515

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

EN300-65050_1_1_1



CID: EN300-65050_1_1_1

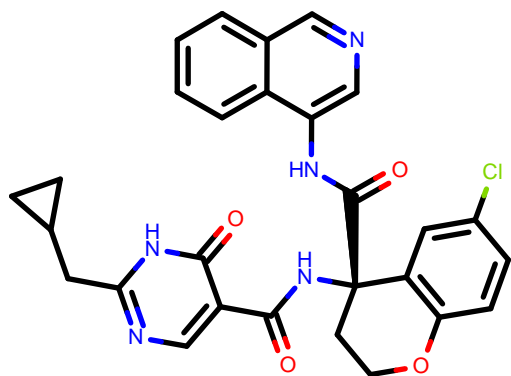
SMILES: CC(C)(CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5003

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.32

EN300-363154_1_1_1



CID: EN300-363154_1_1_1

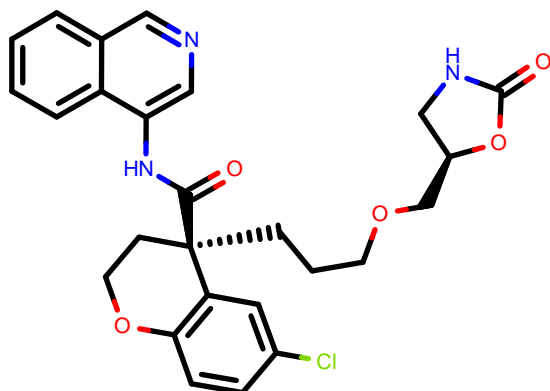
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncn([nH]c5=O)CC6CC6

RUN: RUN6007

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.42

EN300-203293_4_2_1



CID: EN300-203293_4_2_1

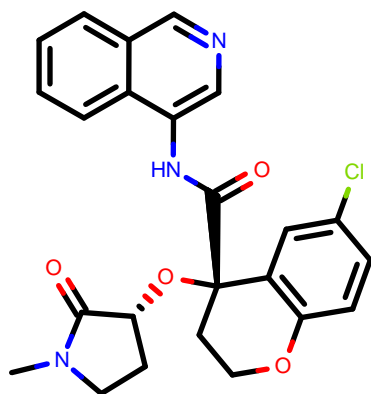
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CNC(=O)O5

RUN: RUN5406

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

EN300-98648_1_2_1



CID: EN300-98648_1_2_1

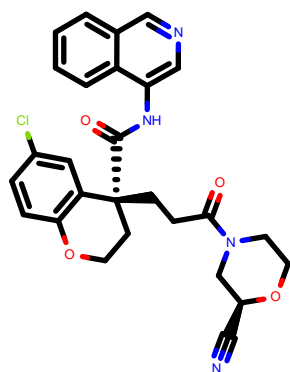
SMILES: CN1CC[C@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN5387

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.19

EN300-70489_2_2_1



CID: EN300-70489_2_2_1

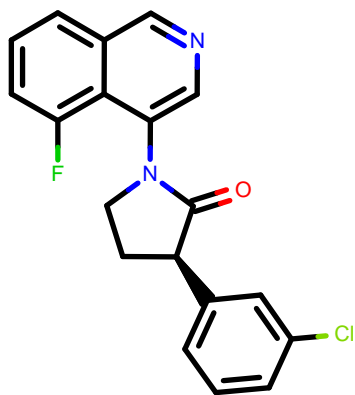
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCO[C@H](C5)C#N

RUN: RUN4993

DDG (kcal/mol): -0.49

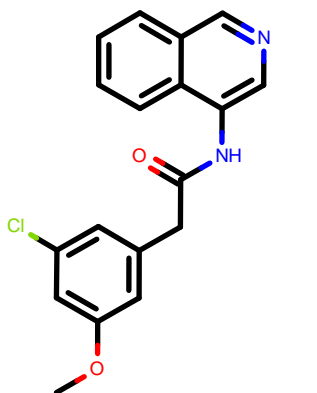
dDDG (kcal/mol): 0.31

MIC-UNK-50cce87d-5_2



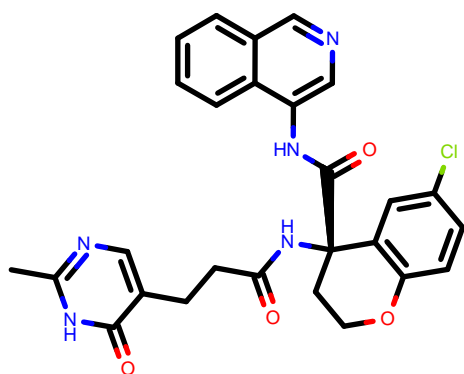
CID:	MIC-UNK-50cce87d-5_2
SMILES:	<chem>c1cc(cc(c1)Cl)[C@H]2CCN(C2=O)c3cncc4c3c(ccc4)F</chem>
RUN:	RUN538
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.23

ALP-POS-3b848b35-1_1



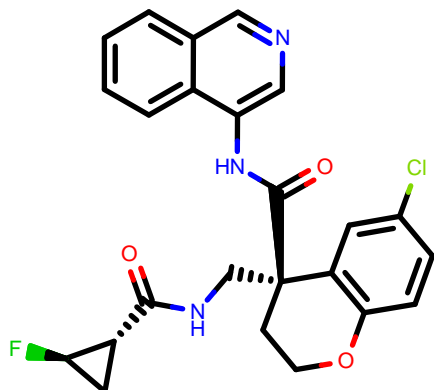
CID:	ALP-POS-3b848b35-1_1
SMILES:	<chem>COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN11
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.28

EN300-6734334_1_1_1



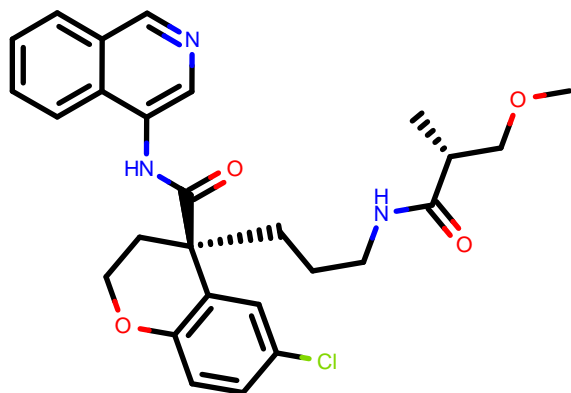
CID:	EN300-6734334_1_1_1
SMILES:	<chem>Cc1[nH]c(=O)c(en1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN7379
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.23

EN300-97300_2_3_1



CID:	EN300-97300_2_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5C[C@H]5F</chem>
RUN:	RUN5268
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.15

EN300-69162_4_2_1



CID: EN300-69162_4_2_1

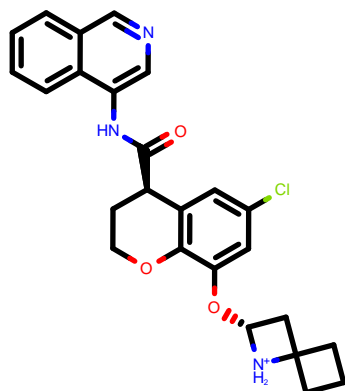
SMILES: C[C@H](COC)C(=O)NCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnoc4c3ccc4

RUN: RUN6622

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.31

DAR-DIA-23e5a6a0-2_1



CID: DAR-DIA-23e5a6a0-2_1

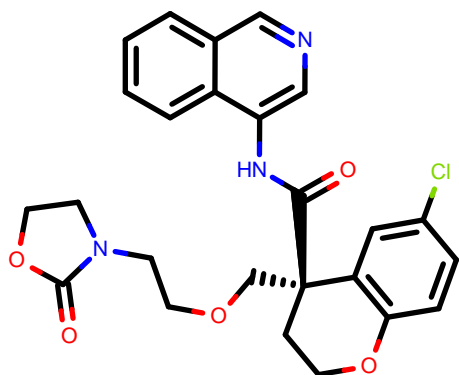
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@@H]5CC6([NH2+][5])CC6)Cl

RUN: RUN388

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.40

EN300-370967_2_1_1



CID: EN300-370967_2_1_1

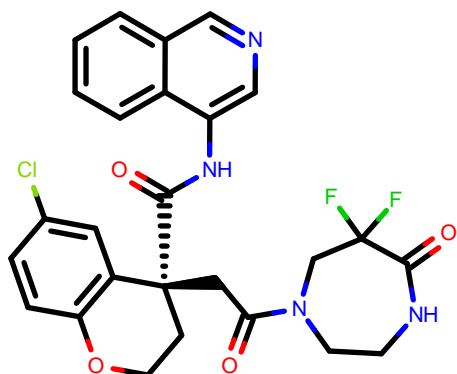
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCNC5CCOC5=O

RUN: RUN4616

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.28

EN300-1083988_1_1_1



CID: EN300-1083988_1_1_1

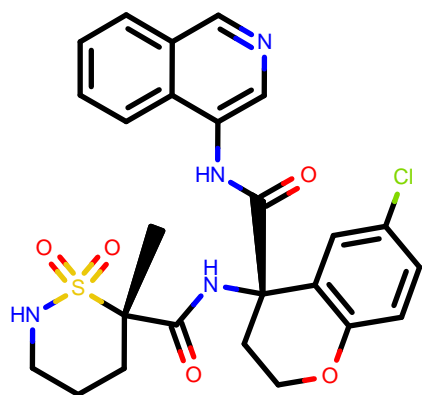
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)C(C5)(F)F

RUN: RUN7436

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.30

EN300-1709315_1_2_1



CID: EN300-1709315_1_2_1

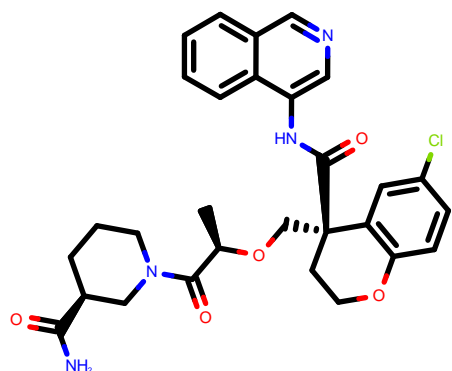
SMILES: C[C@]1(CCCNS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccccc5

RUN: RUN7217

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.34

EN300-28177_2_2_1



CID: EN300-28177_2_2_1

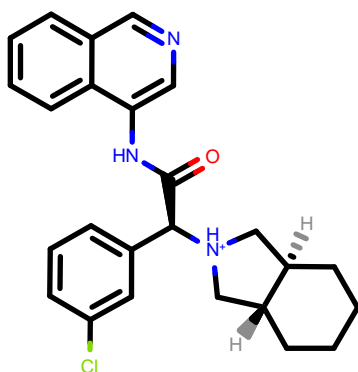
SMILES: C[C@H](C(=O)NCC[C@]([H])(C1)C(=O)NOC1C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccccc5

RUN: RUN7011

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.33

MIC-UNK-5a93dd5f-2_4



CID: MIC-UNK-5a93dd5f-2_4

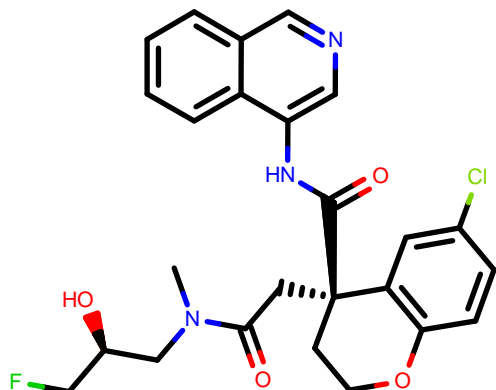
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccccc(c3)Cl)N[H+]JC[C@H]5CCCC[C@]([H])5C4

RUN: RUN614

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.37

EN300-1651623_1_1_1



CID: EN300-1651623_1_1_1

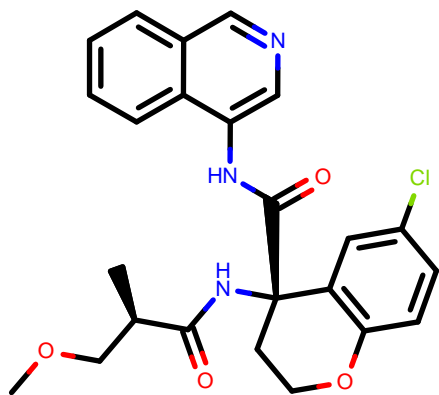
SMILES: CN(C[C@]([H])(CF)O)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccccc4

RUN: RUN7258

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

EN300-69162_1_2_1



CID: EN300-69162_1_2_1

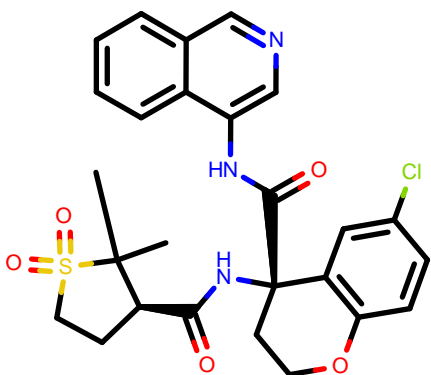
SMILES: C[C@H](COC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6508

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.22

EN300-2007564_1_2_1



CID: EN300-2007564_1_2_1

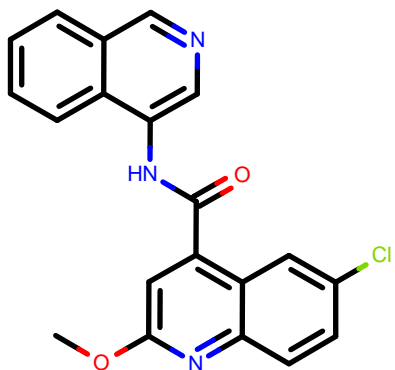
SMILES: CC1([C@H](CCS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN3757

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.37

MAT-POS-89e65850-3_1



CID: MAT-POS-89e65850-3_1

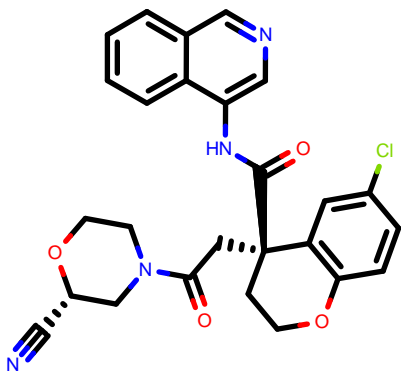
SMILES: COC1cc(c2cc(ccc2n1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1994

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.30

EN300-70489_1_2_1



CID: EN300-70489_1_2_1

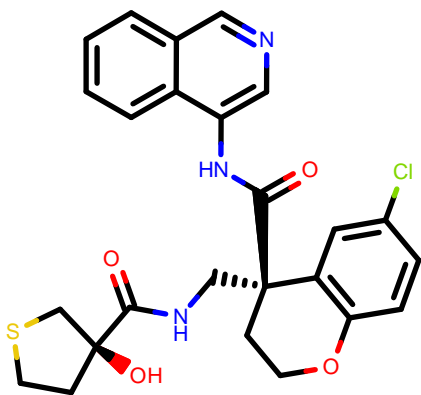
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)C#N

RUN: RUN6699

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.29

EN300-122656_2_1_1



CID: EN300-122656_2_1_1

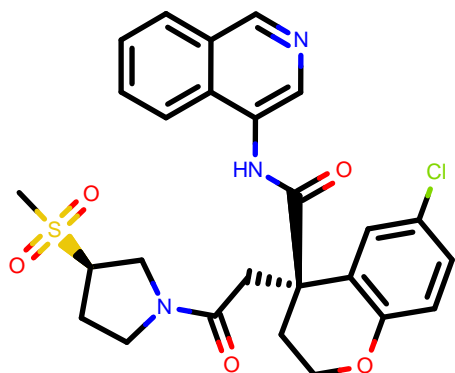
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCSC5)O

RUN: RUN3635

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.40

EN300-200609_1_1_1



CID: EN300-200609_1_1_1

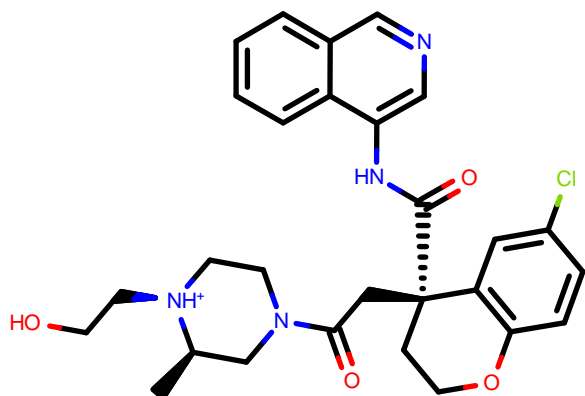
SMILES: CS(=O)(=O)[C@@H]1CCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5

RUN: RUN5910

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.42

EDG-MED-ba1ac7b9-25_1



CID: EDG-MED-ba1ac7b9-25_1

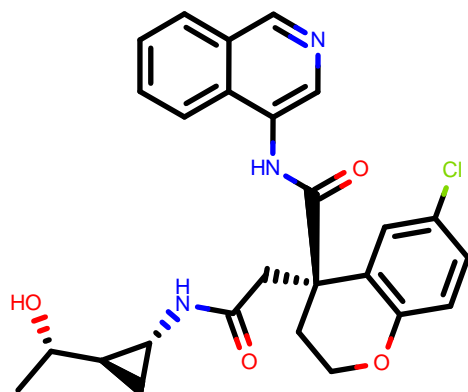
SMILES: C[C@@H]1CNCCN1[C@@H]2CCO[C@@H]3C[C@@]4(CCOc5c3cc(cc5)C)C(=O)Nc6cncc5c6ccc5

RUN: RUN2564

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.77

EN300-7463275_1_1_1



CID: EN300-7463275_1_1_1

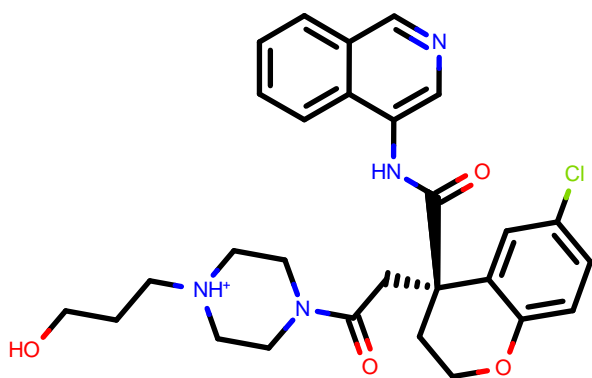
SMILES: C[C@@H]1[C@@H]2C[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5)O

RUN: RUN6406

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.25

ALP-UNI-3496895b-8_1



CID: ALP-UNI-3496895b-8_1

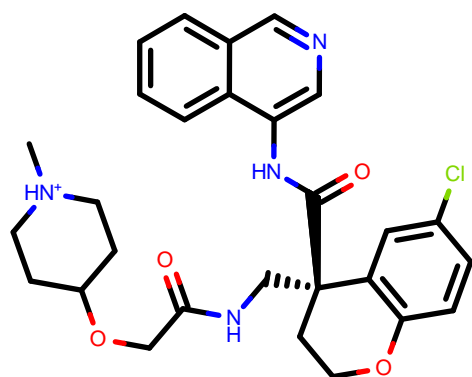
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)CCCCO

RUN: RUN2348

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.31

ALP-UNI-0676e700-30_1



CID: ALP-UNI-0676e700-30_1

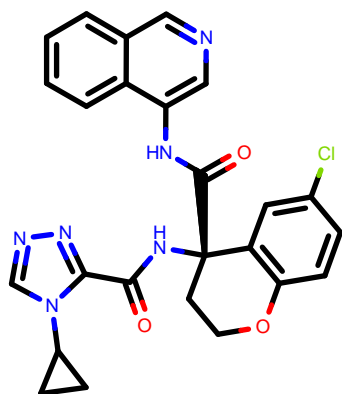
SMILES: C[NH+]1CCC(CC1)OCC(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccnc5c4ccc5

RUN: RUN2381

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.45

EN300-6745581_1_1_1



CID: EN300-6745581_1_1_1

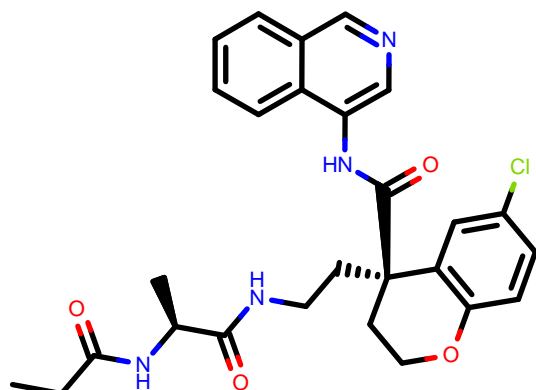
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nncnc5C6CC6

RUN: RUN5841

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.26

EN300-31148_3_1_1



CID: EN300-31148_3_1_1

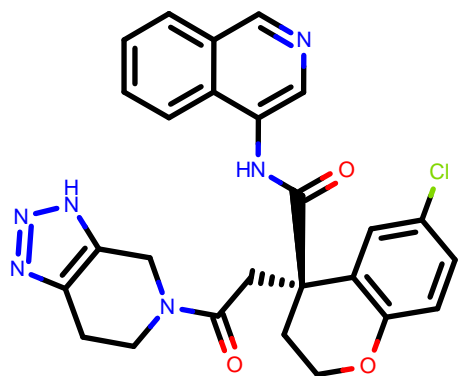
SMILES: CCC(=O)N[C@@H](C)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4

RUN: RUN5455

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.34

EN300-90293_1_1_1



CID: EN300-90293_1_1_1

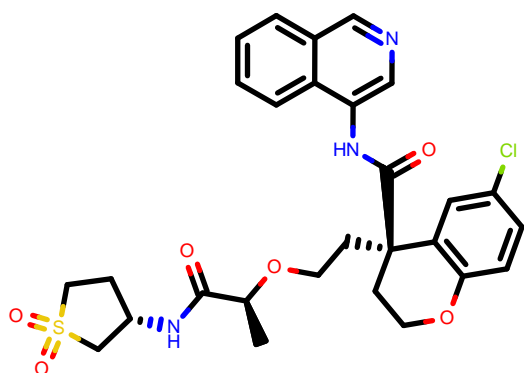
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)N5CCc6c(n[nH]6)C5

RUN: RUN4634

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-23318_3_3_1



CID: EN300-23318_3_3_1

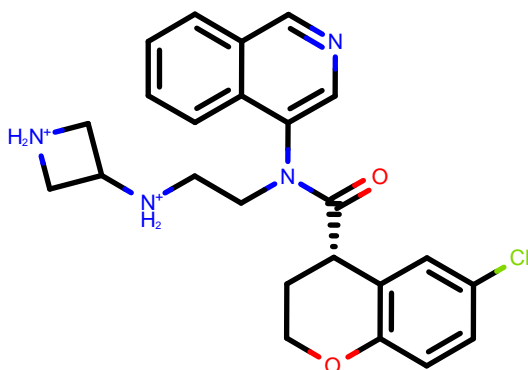
SMILES: C[C@@H](Cl)O[N]C(=O)[C@@H](CCS(=O)(=O)O)C(=O)C[C@@]3(CCOc4c3cc(c4)Cl)C[C@@]4Nc5ccsc54

RUN: RUN4433

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.39

MAK-UNK-83e0a0b4-3_2



CID: MAK-UNK-83e0a0b4-3_2

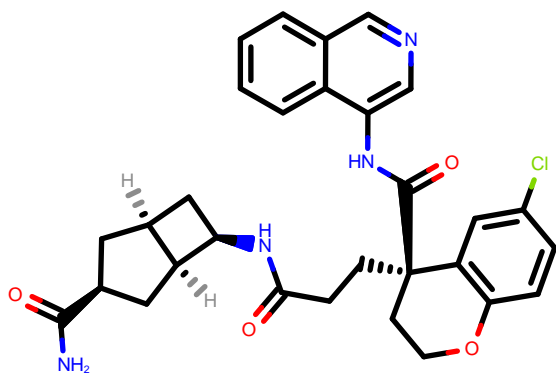
SMILES: c1ccc2c(c1)cncc2N(CCN(C3CC[NH2+]C3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN689

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.49

EN300-1268016_2_11_1



CID: EN300-1268016_2_11_1

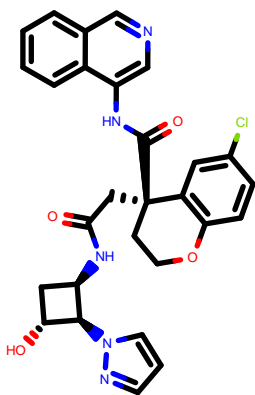
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)N[C@@]5(C)C[C@@H]6[C@@]5(C)C[C@@H]6Cl

RUN: RUN7190

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.35

EN300-260696_1_3_1



CID: EN300-260696_1_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N[C@@H]5C[C@@H]3[C@@H]5c6ccc(O)

RUN:

RUN4119

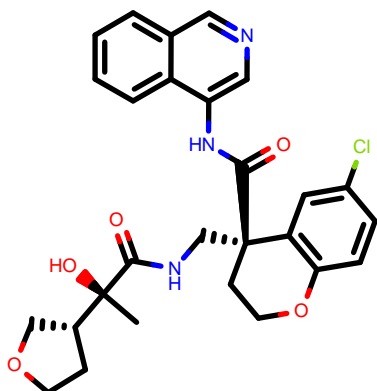
DDG (kcal/mol):

-0.47

dDDG (kcal/mol):

0.32

EN300-217494_2_2_1



CID: EN300-217494_2_2_1

SMILES:

C[C@@]([C@@H]1CCOC1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN:

RUN3919

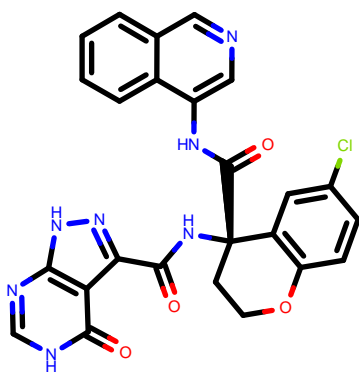
DDG (kcal/mol):

-0.47

dDDG (kcal/mol):

0.33

EN300-1266218_1_1_1



CID: EN300-1266218_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N[C@@]5(C(=O)c5c6c(=O)[nH]cnc6[nH]5)

RUN:

RUN6544

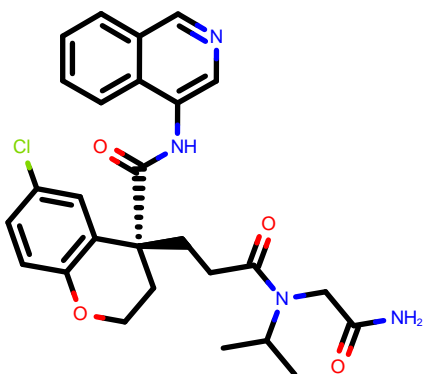
DDG (kcal/mol):

-0.47

dDDG (kcal/mol):

0.25

EN300-35450_2_1_1



CID: EN300-35450_2_1_1

SMILES:

CC(C)N(CC(=O)N)C(=O)CC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN:

RUN5579

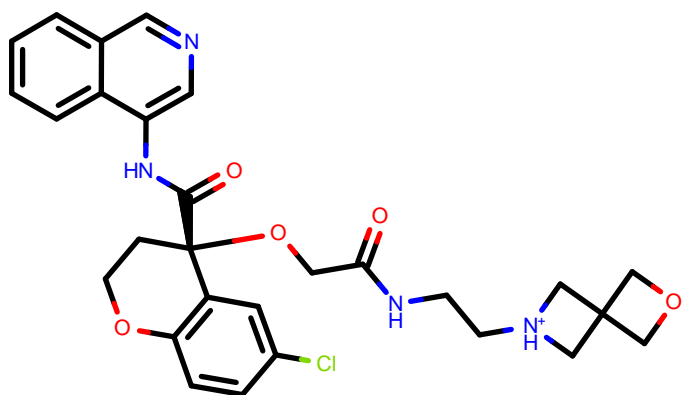
DDG (kcal/mol):

-0.47

dDDG (kcal/mol):

0.26

EDG-MED-4c68219f-5_1



CID: EDG-MED-4c68219f-5_1

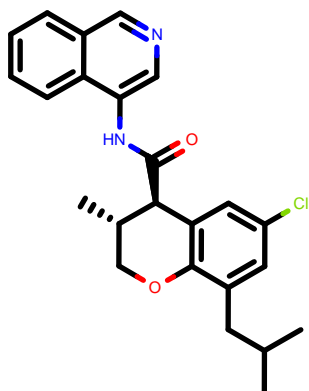
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)NCC[NH+]5CC6(C5)COC6

RUN: RUN1562

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-24_1_1



CID: DAR-DIA-0d514e7d-24_1_1

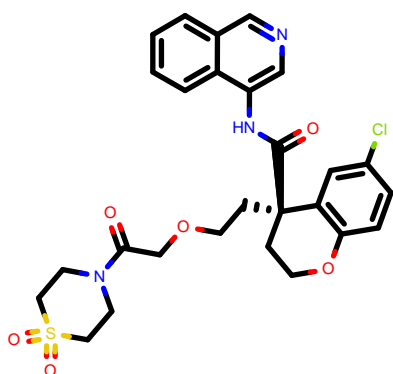
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3ncnc4c3cccc4)C)CC(C)C

RUN: RUN7219

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.17

EN300-1265948_3_1_1



CID: EN300-1265948_3_1_1

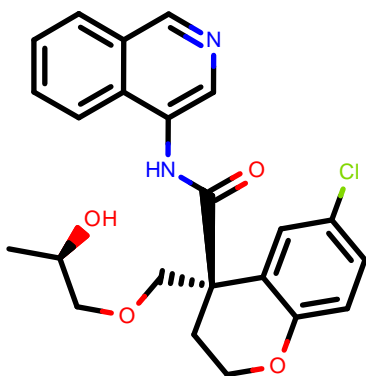
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN3783

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.37

EN300-185378_2_2_1



CID: EN300-185378_2_2_1

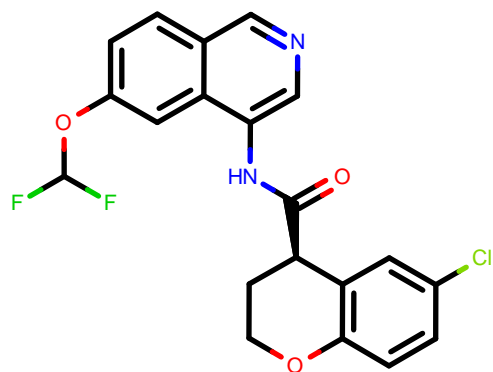
SMILES: C[C@H](COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncnc4c3cccc4)O

RUN: RUN4995

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.24

BEN-DND-c852c98b-6_1_1



CID: BEN-DND-c852c98b-6_1_1

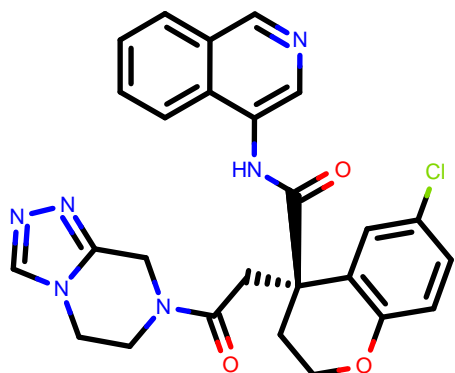
SMILES: c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN7570

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.06

EN300-71125_1_1_1



CID: EN300-71125_1_1_1

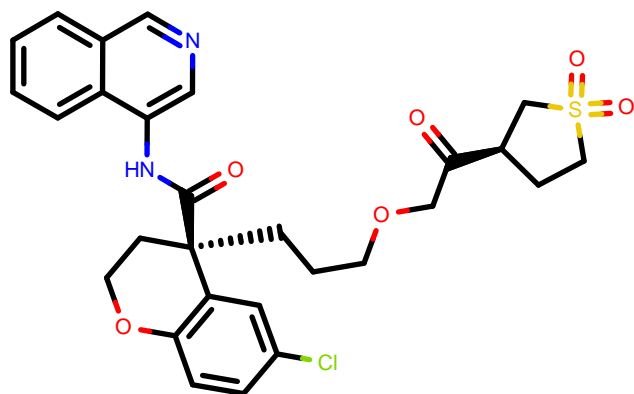
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CN6cnn6C5

RUN: RUN7023

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.31

EN300-226314_4_1_1



CID: EN300-226314_4_1_1

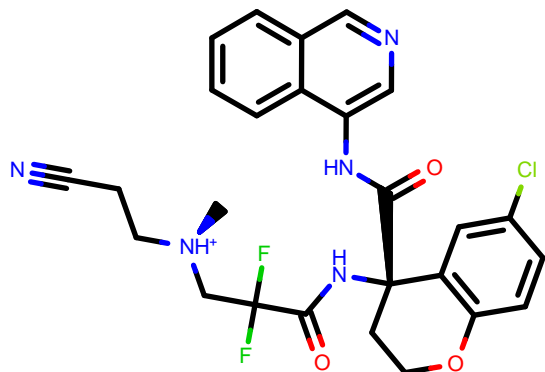
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@@H]5CCS(=O)(=O)C5

RUN: RUN6269

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.39

EDG-MED-90036822-92_2



CID: EDG-MED-90036822-92_2

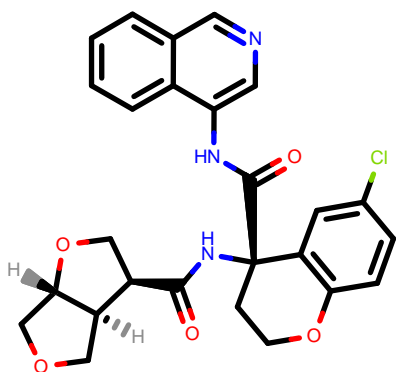
SMILES: C[N+](CCC#N)CC(C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)F)F

RUN: RUN1688

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.30

EN300-6482296_1_1_1



CID: EN300-6482296_1_1_1

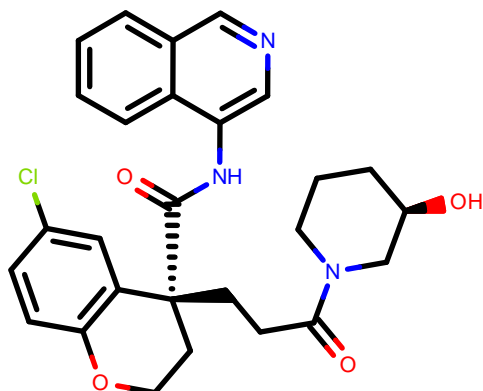
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@H](Cl)C(CO)C(=O)Nc3ccc4c3ccc4

RUN: RUN7669

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.26

EN300-266117_2_1_1



CID: EN300-266117_2_1_1

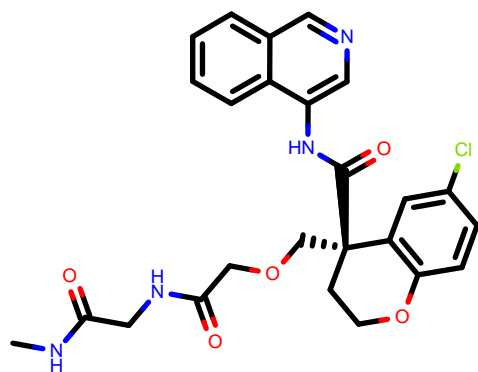
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@H](Cl)C(CO)C(=O)N5CCCC5

RUN: RUN5090

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.34

EN300-23223_2_1_1



CID: EN300-23223_2_1_1

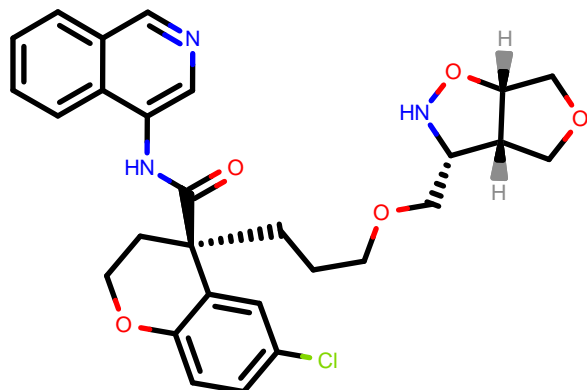
SMILES: CNC(=O)CNC(=O)COC[C@@H](Cl)C(CO)C(=O)Nc3ccc4c3ccc4

RUN: RUN4327

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-7436306_4_1_2



CID: EN300-7436306_4_1_2

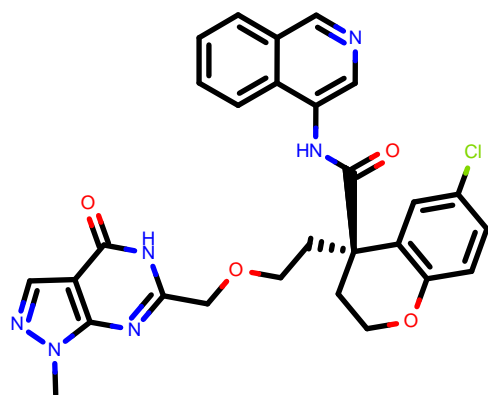
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@H](Cl)C(CO)C(=O)Nc3ccc4c3ccc4

RUN: RUN5462

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.37

EN300-44149_3_1_1



CID: EN300-44149_3_1_1

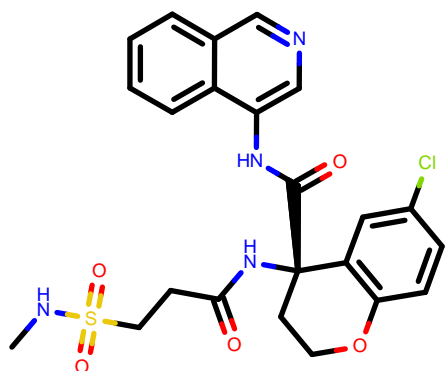
SMILES: Cn1c2c(en1)c(=O)[nH]c(n2)C(=O)CC[C@@]3(C(=O)O4C3CC(=O)C4)C(=O)Nc5ncc6c5ccc6

RUN: RUN4772

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.34

EN300-123205_1_1_1



CID: EN300-123205_1_1_1

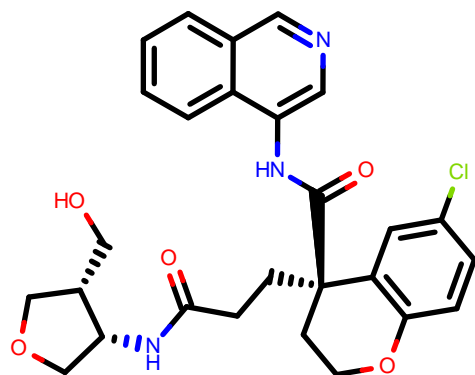
SMILES: CNS(=O)(=O)CCC(=O)N[C@@]1(C(=O)O2C1CC(=O)C2)C(=O)Nc3ncc4c3ccc4

RUN: RUN5835

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.30

EN300-1663228_2_1_1



CID: EN300-1663228_2_1_1

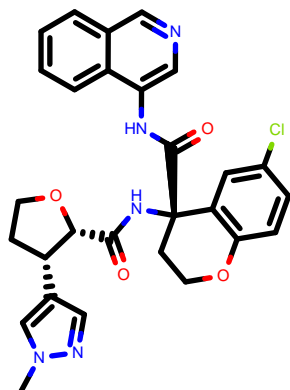
SMILES: c1ccc2c(c1)ncnc2N[C@@]3(C(=O)O4C3CC(=O)C4)C(=O)N[C@@]5C(=O)C5

RUN: RUN7264

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

EN300-305454_1_1_1



CID: EN300-305454_1_1_1

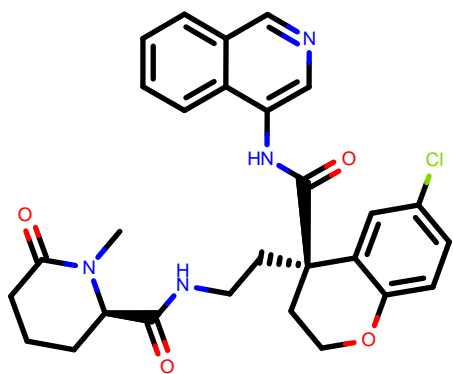
SMILES: Cn1cc(en1)[C@@]2(C(=O)O3C2CC(=O)C3)C(=O)N[C@@]4(C(=O)O5C4CC(=O)C5)C(=O)Nc6ncc7c6ccc7

RUN: RUN3882

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

EN300-325738_3_2_1



CID: EN300-325738_3_2_1

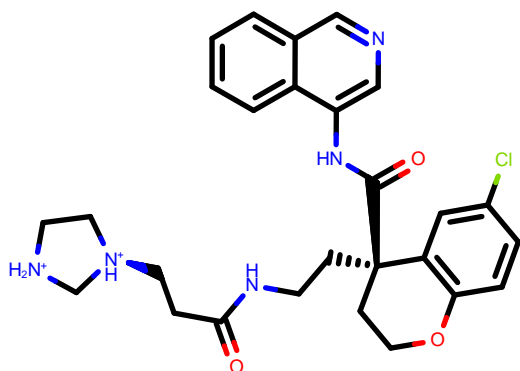
SMILES: CN1C@H](CCCC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN4708

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

EN300-75342_3_1_1



CID: EN300-75342_3_1_1

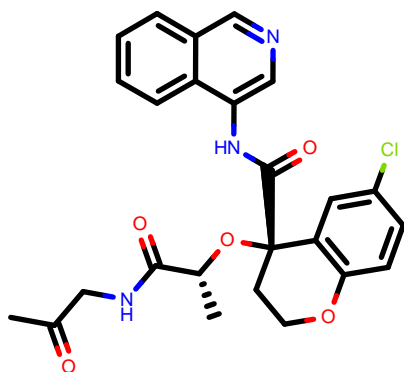
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5ccnc5

RUN: RUN3504

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.28

EN300-131093_1_2_1



CID: EN300-131093_1_2_1

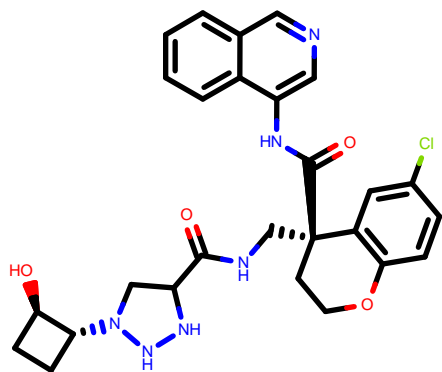
SMILES: C[C@@H](C(=O)NCC(=O)O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4

RUN: RUN5340

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

EN300-316196_2_1_1



CID: EN300-316196_2_1_1

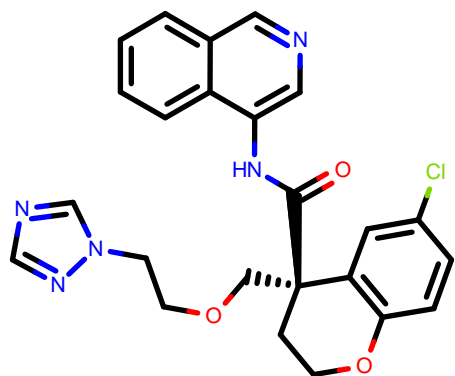
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(m5)[C@@H]6CC[C@@H]6O

RUN: RUN7221

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.35

EN300-6255179_2_1_1



CID: EN300-6255179_2_1_1

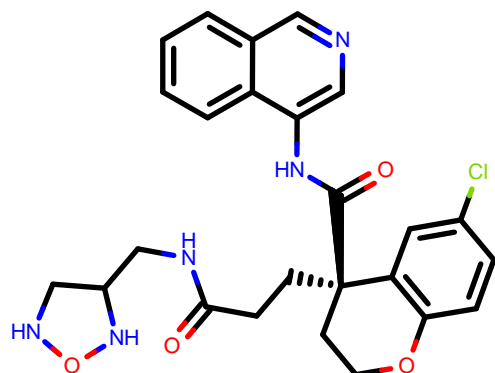
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5ncn5

RUN: RUN6440

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.24

EN300-1068239_2_1_1



CID: EN300-1068239_2_1_1

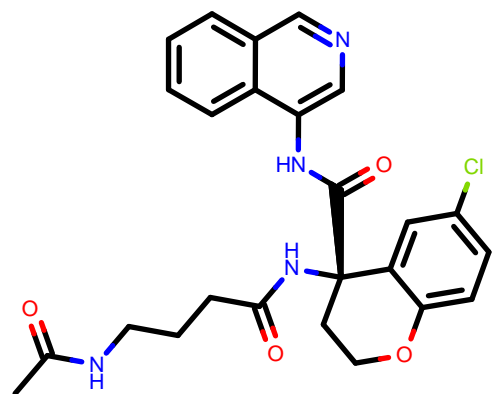
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5=NON5

RUN: RUN7020

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.26

EN300-18564_1_1_1



CID: EN300-18564_1_1_1

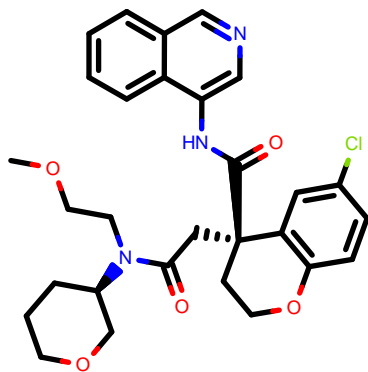
SMILES: CC(=O)NCCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4

RUN: RUN4469

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.25

JAG-UCB-706446eb-5_1_1



CID: JAG-UCB-706446eb-5_1_1

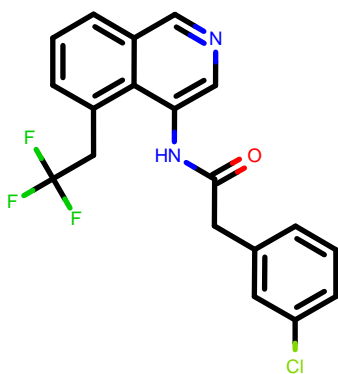
SMILES: COCCN([C@@H]1CCCOC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4cccc5

RUN: RUN3981

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.48

JOH-UNI-ee5ed7c8-3_1



CID: JOH-UNI-ee5ed7c8-3_1

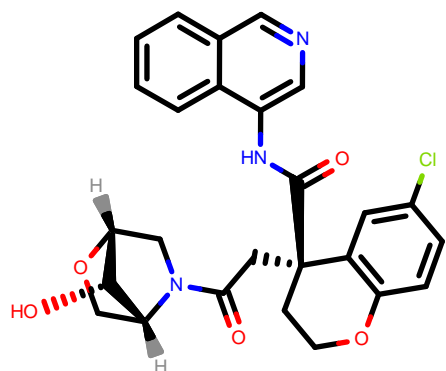
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)CC(F)(F)F

RUN: RUN1727

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.25

EN300-6504714_1_1_1



CID: EN300-6504714_1_1_1

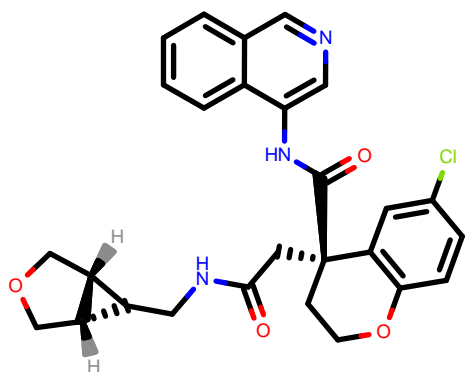
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOC4c3cc(cc4)C1CC(=O)N5C[C@@H]6[C@@H]7C[C@@H]5CO6

RUN: RUN5358

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.24

EN300-210089_1_1_1



CID: EN300-210089_1_1_1

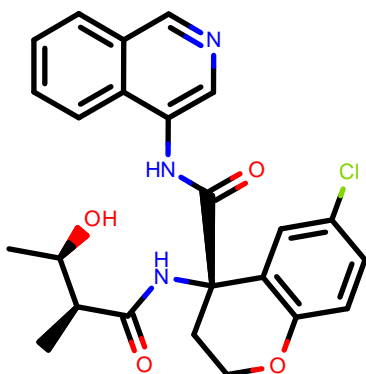
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOC4c3cc(cc4)C1CC(=O)NCC5[C@@H]6[C@@H]5CO6

RUN: RUN7367

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-7089802_1_1_1



CID: EN300-7089802_1_1_1

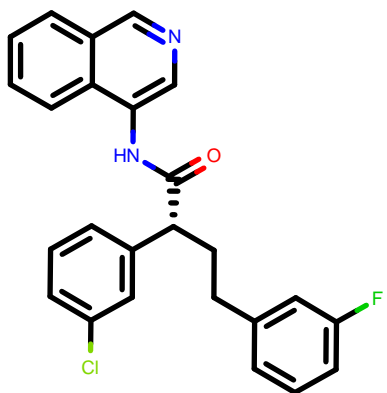
SMILES: C[C@@H]3[C@@H]4[C@@H](C)O[C@@H]3C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN5097

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.28

MIC-UNK-c66144cb-1_2



CID: MIC-UNK-c66144cb-1_2

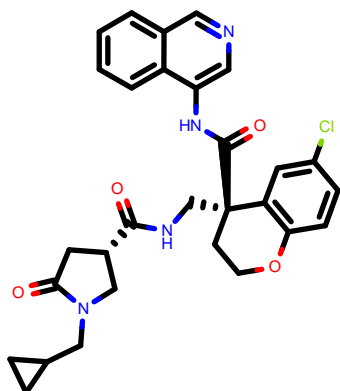
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(c3)F)c4cccc(c4)Cl

RUN: RUN122

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.31

EN300-31969_2_2_1



CID: EN300-31969_2_2_1

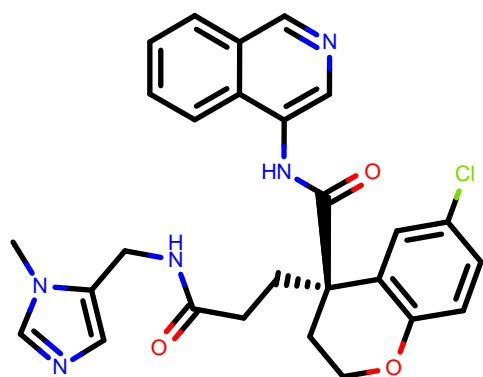
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C3COCc4cc3cc4)C1CN(C=O)N(C5)COC6C6

RUN: RUN7192

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.31

EN300-216594_2_1_1



CID: EN300-216594_2_1_1

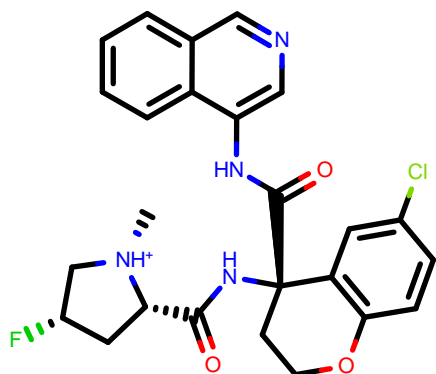
SMILES: Cn1cnc1CNC(=O)CC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6648

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EDG-MED-90036822-74_8



CID: EDG-MED-90036822-74_8

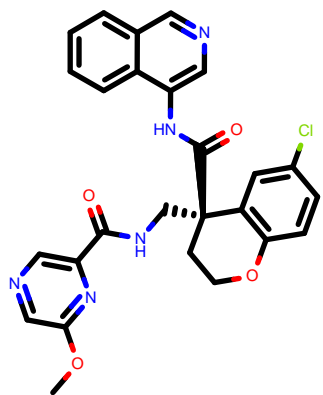
SMILES: C[N@H]1C[C@H](C[C@H]1C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)F

RUN: RUN1629

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-172870_2_1_1



CID: EN300-172870_2_1_1

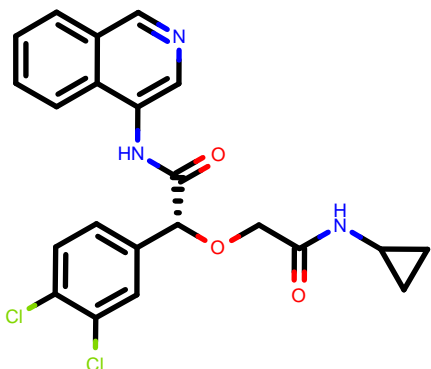
SMILES: COc1cncc(n1)C(=O)NC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5329

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

MAT-POS-de59a476-6_1



CID: MAT-POS-de59a476-6_1

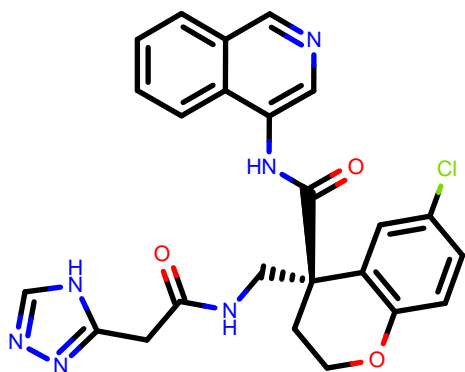
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccc(c(c3)Cl)Cl)OCC(=O)NC4CC4

RUN: RUN2093

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.44

EN300-96159_2_1_1



CID: EN300-96159_2_1_1

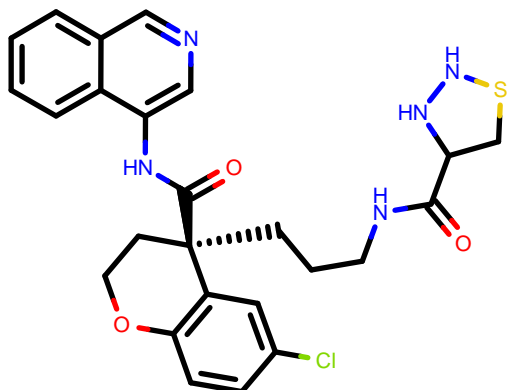
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5[nH]n5

RUN: RUN7660

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-24297_4_1_1



CID: EN300-24297_4_1_1

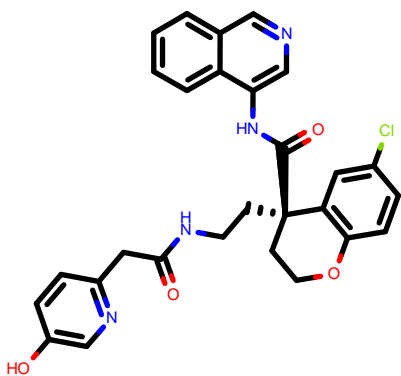
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5csn5

RUN: RUN3680

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.37

EN300-188341_3_1_1



CID: EN300-188341_3_1_1

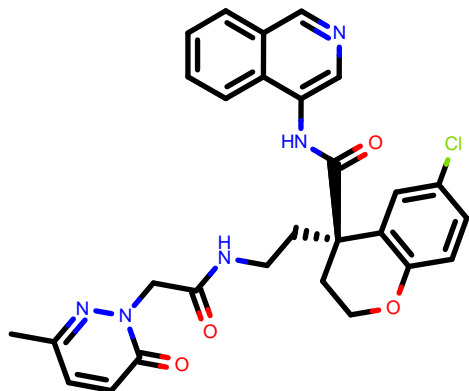
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccocn5O

RUN: RUN4127

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.29

EN300-69556_3_1_1



CID: EN300-69556_3_1_1

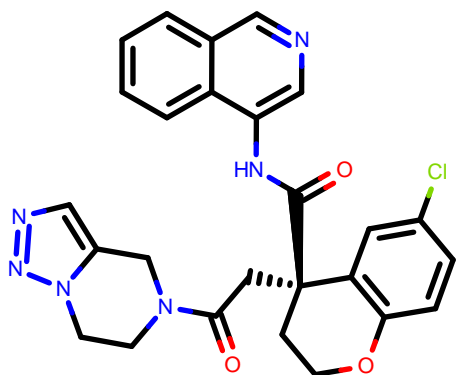
SMILES: Cc1ccc(=O)n(n1)CC(=O)NCC[C@@]2(CCOc4c3cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5138

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.38

EN300-29228_1_1_1



CID: EN300-29228_1_1_1

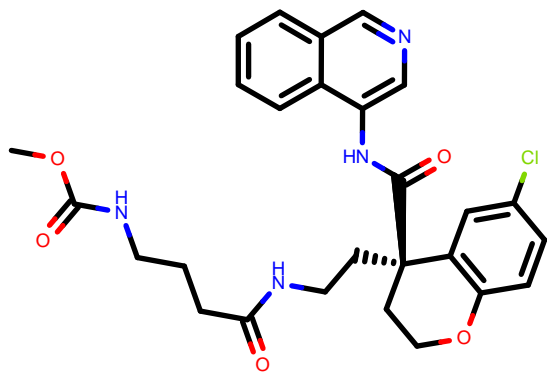
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N5Ccn6c4cn6)C5

RUN: RUN6205

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.29

EN300-71560_3_1_1



CID: EN300-71560_3_1_1

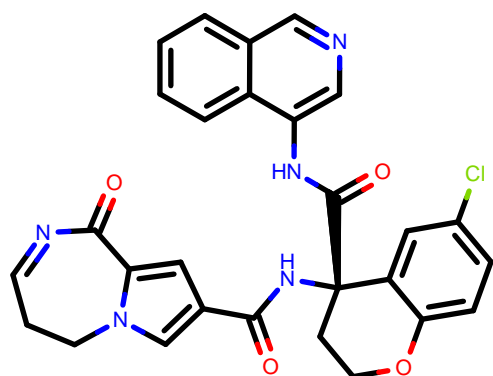
SMILES: COC(=O)NCCCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5496

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.37

EN300-7431365_1_1_1



CID: EN300-7431365_1_1_1

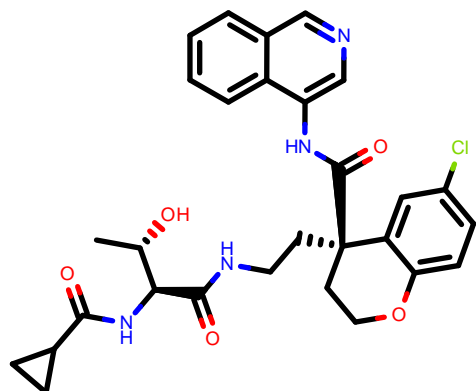
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6n(c5)CCNC6=O

RUN: RUN6480

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.26

EN300-96362_3_1_1



CID: EN300-96362_3_1_1

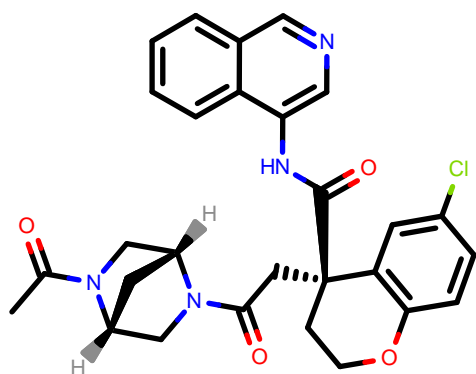
SMILES: C[C@@H](C[C@@H](C1=O)NC[C@@H]1)(CCO)c1ccc(cc1)C[C@@H]3(CCOc4c3ccccc4)NC(=O)C5CC5=O

RUN: RUN7059

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.58

ALP-UNI-76695c4f-6_1



CID: ALP-UNI-76695c4f-6_1

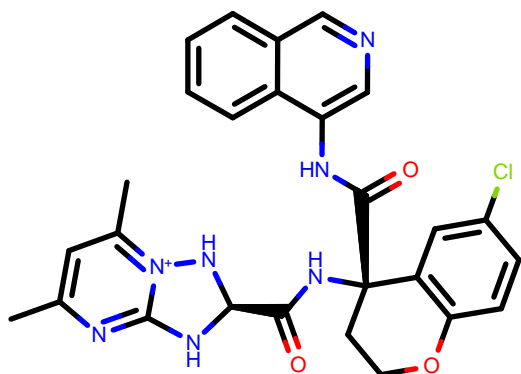
SMILES: CC(=O)N1[C@@H]2[C@@H]3[C@@H]1CN2C(=O)C[C@@H]3(CCOc4c3cc(cc4)C)C(=O)Nc5nc6c65ccccc6

RUN: RUN2061

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.25

EN300-00904_1_1_1



CID: EN300-00904_1_1_1

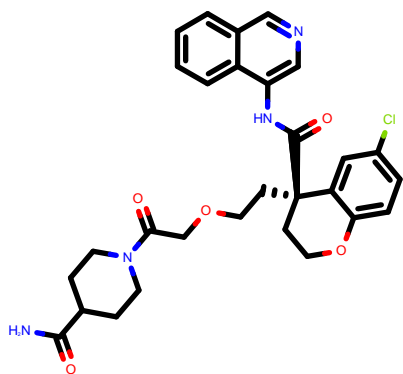
SMILES: Cc1ccc([n+]2c(n1)N[C@@H](N2)C(=O)N[C@@H]3(CCOc4c3cc(cc4)C)C(=O)Nc5nc6c65ccccc6)C

RUN: RUN3380

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.31

EN300-08063_3_1_1



CID: EN300-08063_3_1_1

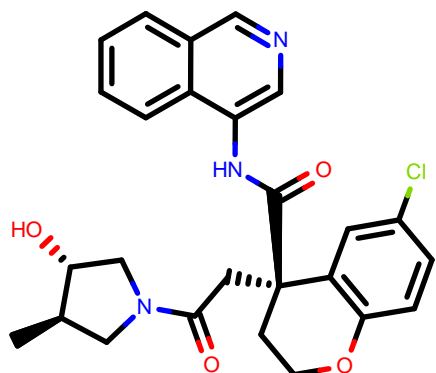
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCCC(C5)C(=O)N

RUN: RUN6290

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.37

EN300-6497226_1_1_1



CID: EN300-6497226_1_1_1

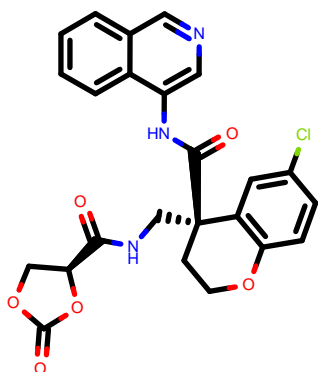
SMILES: C[C@@H]1CN(C[C@H]1O)C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7026

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.20

EN300-5253939_2_1_1



CID: EN300-5253939_2_1_1

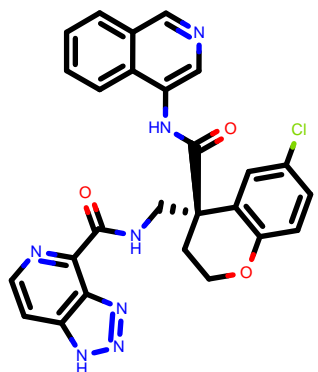
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COCC(=O)O5

RUN: RUN4222

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.26

EN300-7426383_2_1_1



CID: EN300-7426383_2_1_1

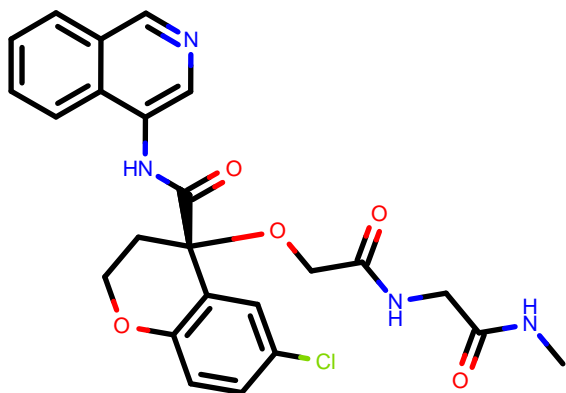
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c6c(ccn5)n[nH]6

RUN: RUN6587

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-23223_1_1_1



CID: EN300-23223_1_1_1

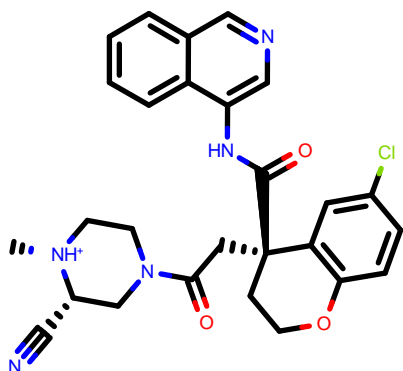
SMILES: CNC(=O)CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4

RUN: RUN5079

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.25

EDG-MED-ba1ac7b9-14_5



CID: EDG-MED-ba1ac7b9-14_5

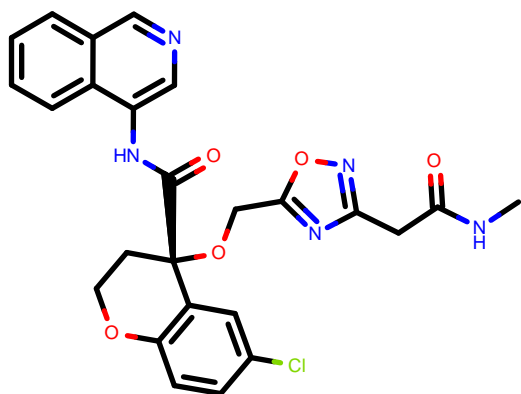
SMILES: C[N+]1CCN(C[C@@H]1C#N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN2506

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-99983_1_1_1



CID: EN300-99983_1_1_1

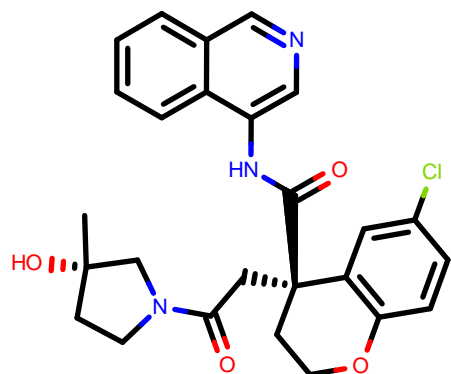
SMILES: CNC(=O)Cc1nc(on1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN3644

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-99161_1_1_1



CID: EN300-99161_1_1_1

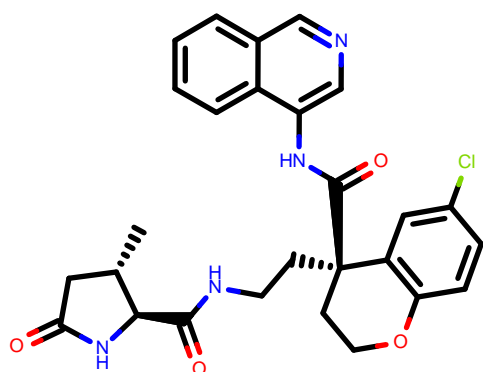
SMILES: C[C@]1(CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5)O

RUN: RUN4108

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.32

EN300-155362_3_2_1



CID: EN300-155362_3_2_1

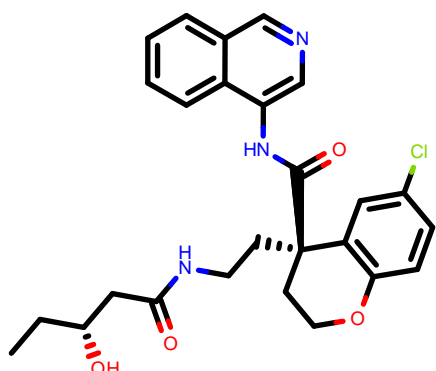
SMILES: C[C@H]1CC(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN7769

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.30

EN300-224741_3_2_1



CID: EN300-224741_3_2_1

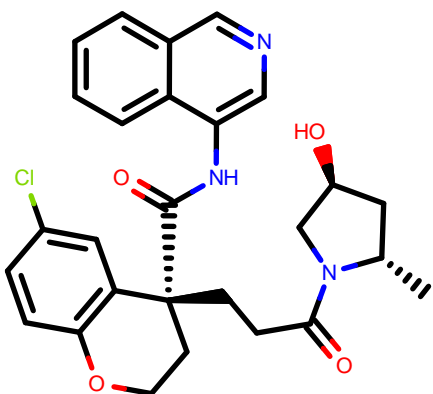
SMILES: CC[C@H](CC(=O)NOC[C@]1(CCOc2c1cc(cc2)Cl)Cl)C(=O)Nc3ncnc4c3cccc4O

RUN: RUN6596

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.32

EN300-173562_2_2_1



CID: EN300-173562_2_2_1

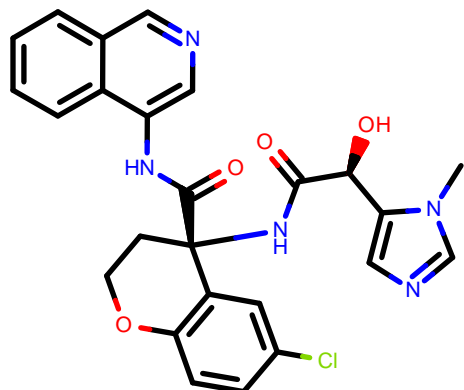
SMILES: C[C@H]1C[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)O

RUN: RUN7312

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.26

EN300-190283_1_1_1



CID: EN300-190283_1_1_1

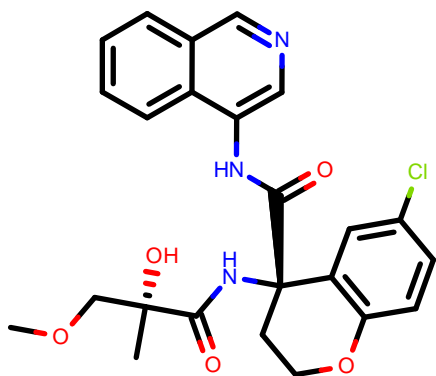
SMILES: Cn1cnc1[C@@H](C(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)O

RUN: RUN7787

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.39

EN300-76841_1_1_1



CID: EN300-76841_1_1_1

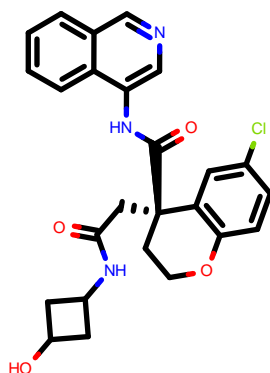
SMILES: C[C@@](COC)(C=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4O

RUN: RUN4164

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.31

EN300-100583_1_1_1



CID: EN300-100583_1_1_1

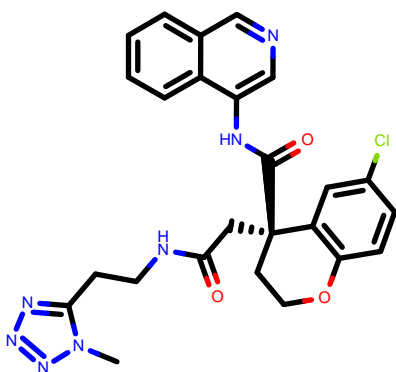
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CC(=O)NC5CC(C5)O

RUN: RUN4885

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.23

EN300-124904_1_1_1



CID: EN300-124904_1_1_1

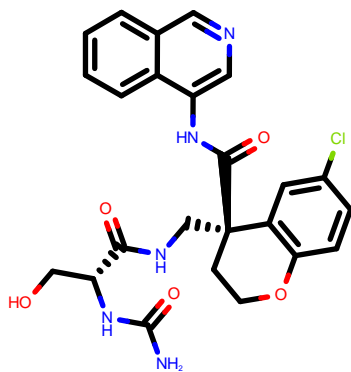
SMILES: Cn1c(nnn1)CCNC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncoc5c4ccoc5

RUN: RUN6637

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-10170_2_1_1



CID: EN300-10170_2_1_1

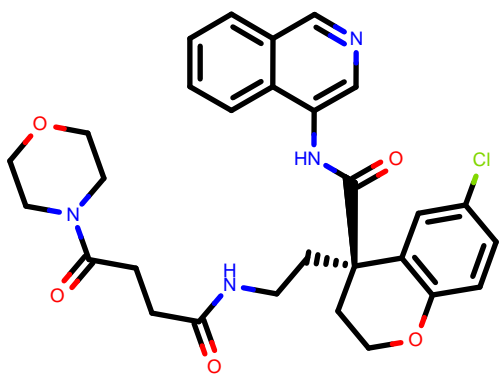
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CNC(=O)[C@@]5(CO)NC(=O)N

RUN: RUN7667

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.39

EN300-05277_3_1_1



CID: EN300-05277_3_1_1

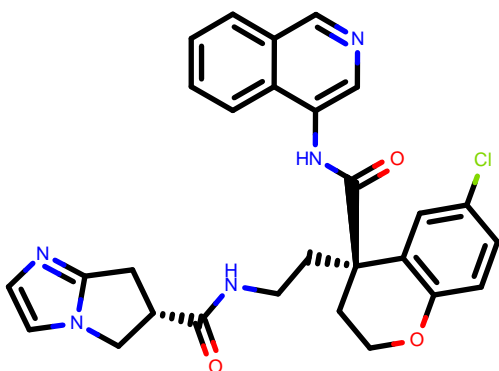
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCC(=O)N5CCOCC5

RUN: RUN5856

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

KAD-UNI-8a629cb0-12_1



CID: KAD-UNI-8a629cb0-12_1

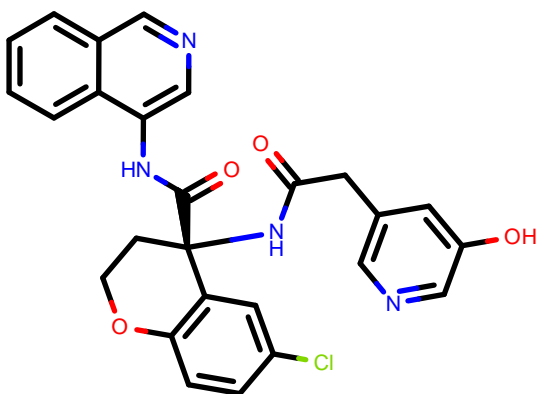
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5Cn6[nH+]cn6C5

RUN: RUN1996

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.38

EN300-222620_1_1_1



CID: EN300-222620_1_1_1

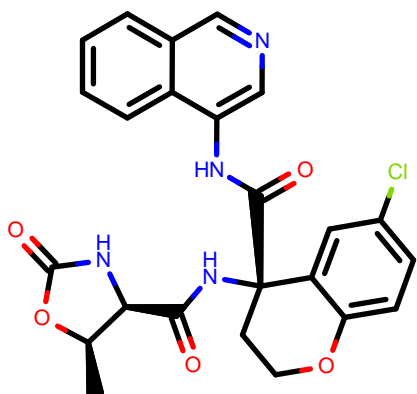
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccncc5O

RUN: RUN3814

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.27

EN300-172640_1_1_1



CID: EN300-172640_1_1_1

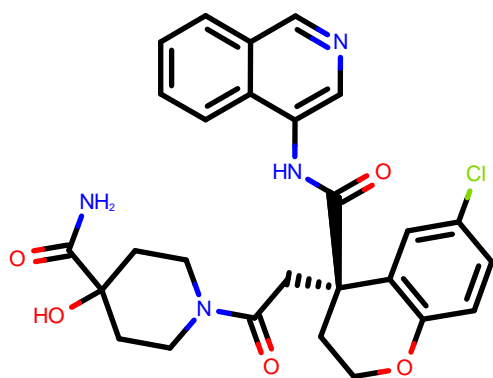
SMILES: C[C@@H]1[C@@H](NC(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN4373

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EN300-203306_1_1_1



CID: EN300-203306_1_1_1

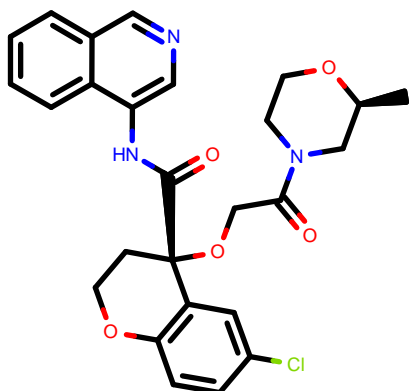
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC(CC5)(C(=O)N)O

RUN: RUN4039

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.40

EN300-25572_1_2_1



CID: EN300-25572_1_2_1

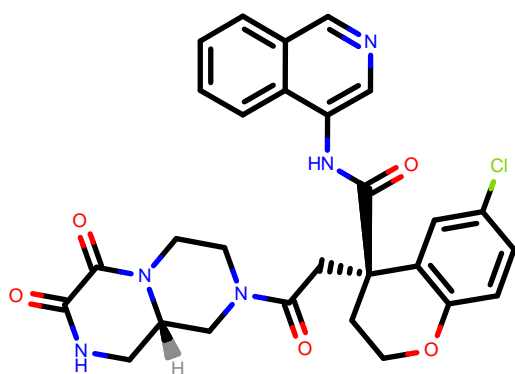
SMILES: C[C@H]1CN(CCO1)C(=O)CO[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6441

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EN300-100768_1_2_1



CID: EN300-100768_1_2_1

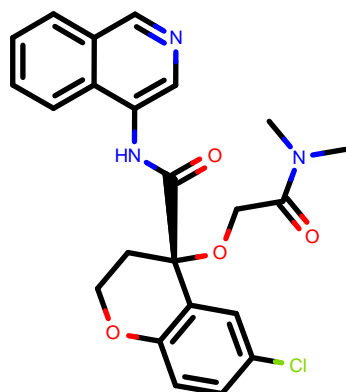
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN(C@H)C5)CNCl=O)O)O

RUN: RUN6751

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.27

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

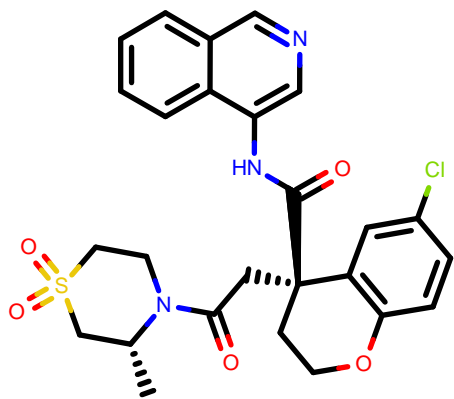
SMILES: CN(C)C(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5519

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.22

EN300-171215_1_1_1



CID: EN300-171215_1_1_1

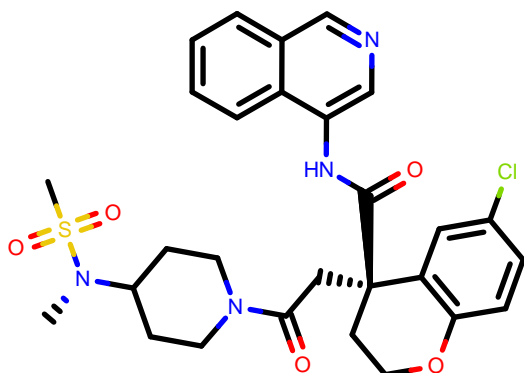
SMILES: C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5445

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.26

KAD-UNI-8a629cb0-17_1



CID: KAD-UNI-8a629cb0-17_1

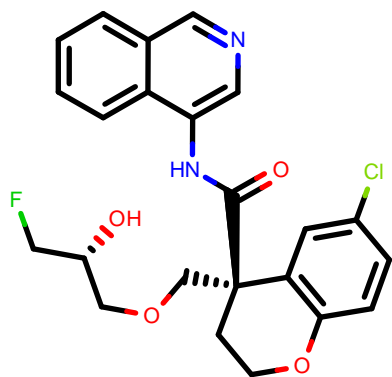
SMILES: CN@@]1C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5S(=O)(=O)C

RUN: RUN2017

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.33

EN300-1968342_2_2_1



CID: EN300-1968342_2_2_1

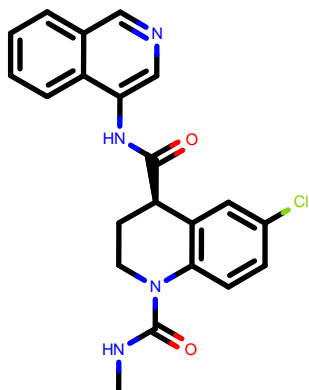
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN4289

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.28

RAL-THA-4aa06b95-3_2



CID: RAL-THA-4aa06b95-3_2

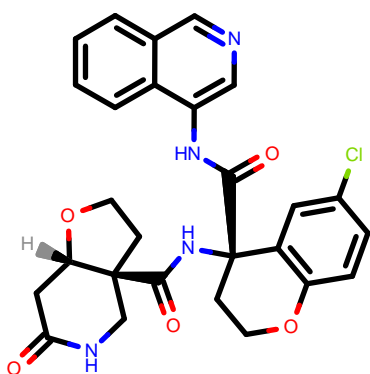
SMILES: CNC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1123

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.28

EN300-6731226_1_1_1



CID: EN300-6731226_1_1_1

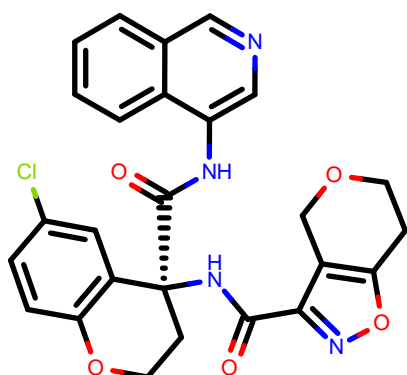
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@56CC(C@H)5CC(=O)N6

RUN: RUN4194

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.41

EN300-88819_1_1_1



CID: EN300-88819_1_1_1

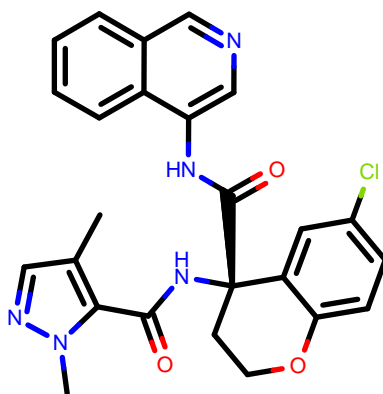
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6c(on5)CCOC6

RUN: RUN4358

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.25

EN300-233079_1_1_1



CID: EN300-233079_1_1_1

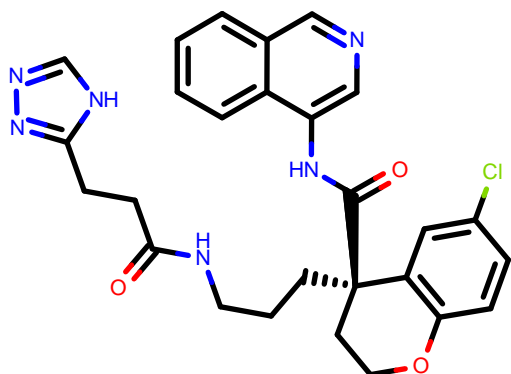
SMILES: Cc1cnn(c1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5)C

RUN: RUN5977

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.23

EN300-101197_4_1_1



CID: EN300-101197_4_1_1

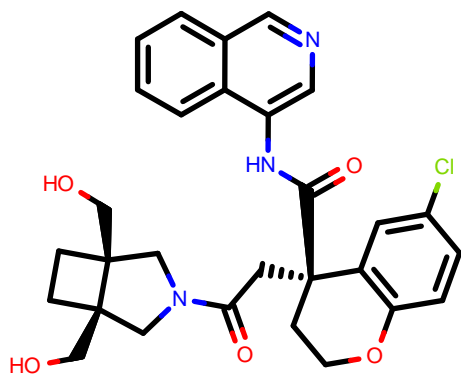
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCc5[nH]n5

RUN: RUN7411

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.35

EN300-1272865_1_1_1



CID: EN300-1272865_1_1_1

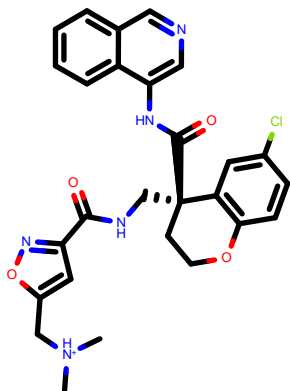
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(C)COC(=O)N5C[C@@]3(C)C[C@@]4(C)C5

RUN: RUN4607

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.34

EN300-124457_2_1_1



CID: EN300-124457_2_1_1

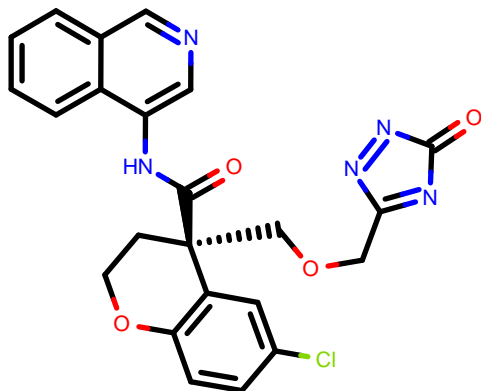
SMILES: C[NH+](C)Cc1cc(nc1)C(=O)NC[C@@]2(C)COC(=O)Nc3ccccc3

RUN: RUN6886

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-10_1



CID: EDJ-MED-fcba3f31-10_1

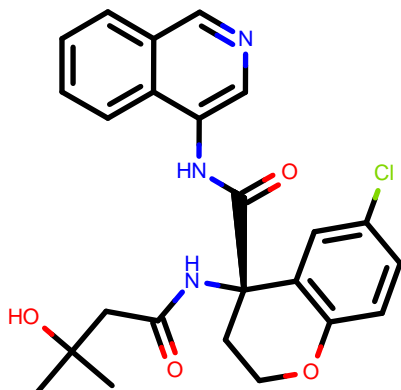
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(C)COC(=O)N5C[C@@]3(C)C[C@@]4(C)C5

RUN: RUN2350

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.22

EN300-117931_1_1_1



CID: EN300-117931_1_1_1

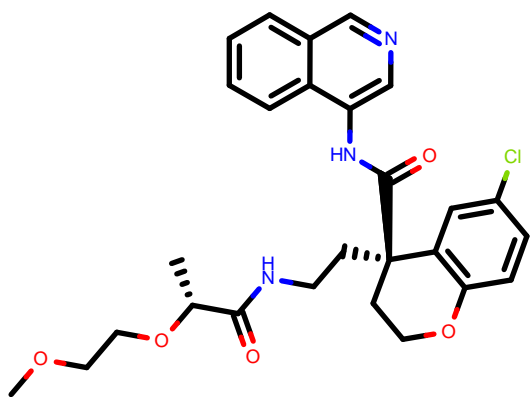
SMILES: CC(C)(CC(=O)N[C@@]1(C)COC(=O)Nc2ccccc2)C(=O)Nc3ccccc3

RUN: RUN5137

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.24

EN300-77359_3_2_1



CID: EN300-77359_3_2_1

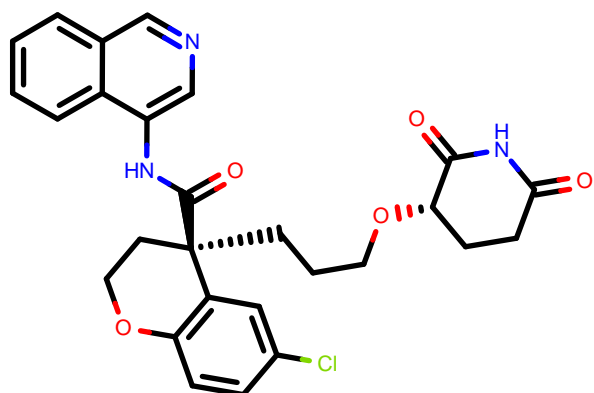
SMILES: C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)OCCOC

RUN: RUN3800

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.27

EN300-120920_4_2_1



CID: EN300-120920_4_2_1

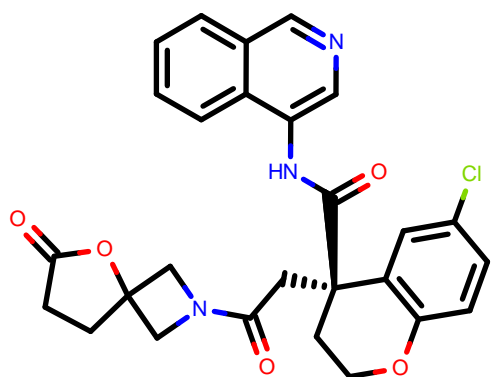
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@H]5CCCC(=O)NC5=O

RUN: RUN6674

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.31

EN300-7534935_1_1_1



CID: EN300-7534935_1_1_1

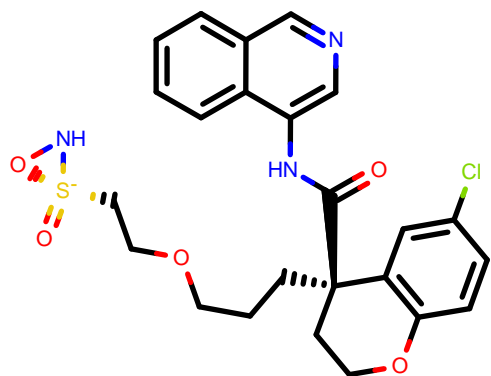
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CCC(=O)O6

RUN: RUN6021

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.25

EN300-270710_4_1_1



CID: EN300-270710_4_1_1

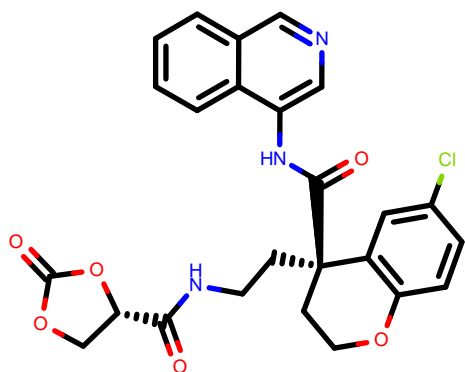
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)N

RUN: RUN5645

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.35

EN300-5253939_3_1_1



CID: EN300-5253939_3_1_1

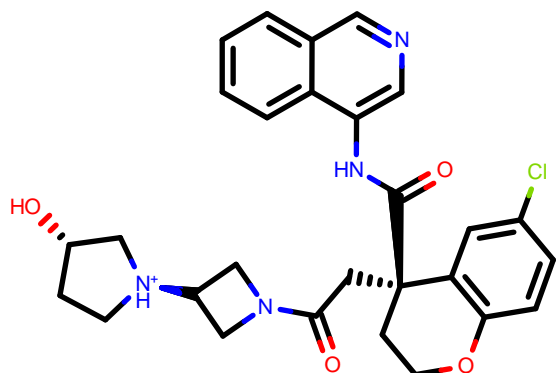
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5[C@@H]5COC(=O)O5

RUN: RUN3835

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-4_3



CID: EDG-MED-ba1ac7b9-4_3

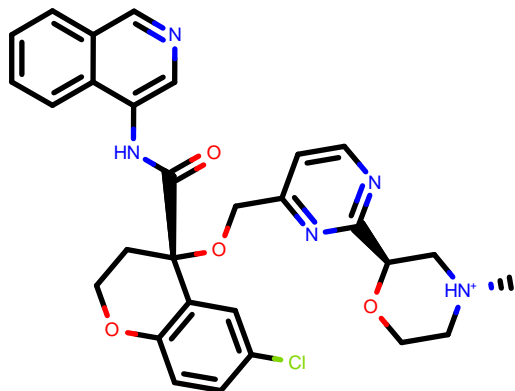
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)C(=O)N5CC(C5)[N+](H)C[C@@]6[C@@H]6CO

RUN: RUN2479

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.39

ED_-GRI-5b13fbe2-74_3



CID: ED_-GRI-5b13fbe2-74_3

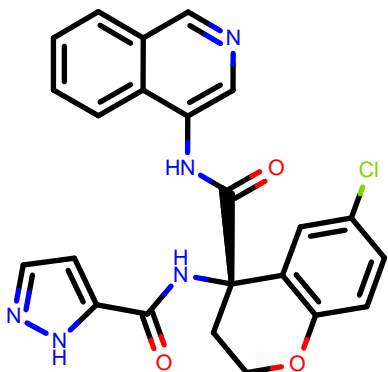
SMILES: C[N+](H)1CC[C@@H](C1)C2=CC=NC(=O)C2[C@@]3[C@@](CCOc4c3cc(cc4)C)C(=O)N5C6CC65CCCC6

RUN: RUN1546

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.35

EN300-37077_1_1_1



CID: EN300-37077_1_1_1

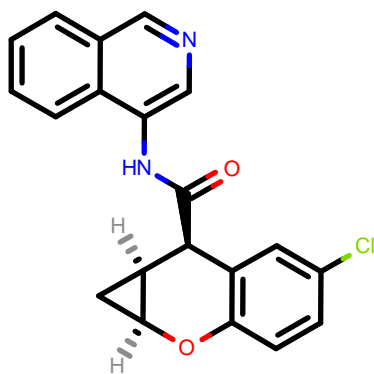
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)c5c[nH]5

RUN: RUN6229

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.20

DAR-DIA-0d514e7d-33_3



CID: DAR-DIA-0d514e7d-33_3

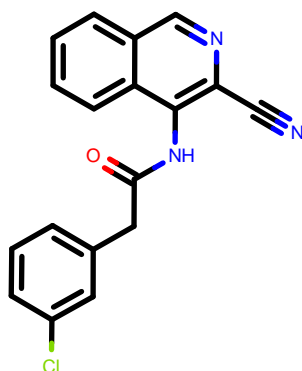
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@H]3c4cc(ccc4O)[C@@H]5[C@H]3C5)Cl

RUN: RUN809

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.22

JOH-UNI-ee5ed7c8-8_1



CID: JOH-UNI-ee5ed7c8-8_1

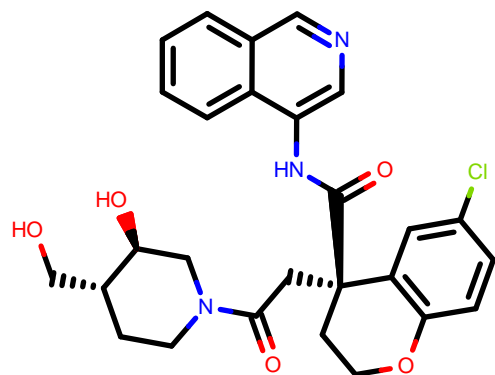
SMILES: c1ccc2c(c1)cnc(c2NC(=O)Cc3ccccc(c3)Cl)C#N

RUN: RUN1713

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.26

EN300-95639_1_3_1



CID: EN300-95639_1_3_1

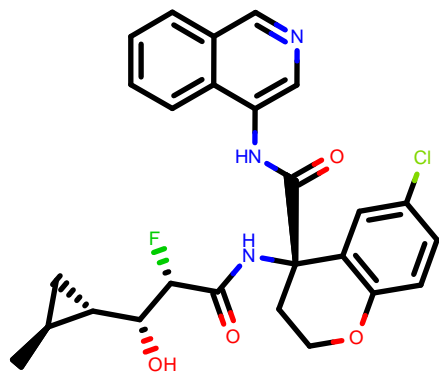
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H]4[C@H](O)[C@@H](O)[C@H]3C(=O)N5C[C@H]4[C@H]5)Cl

RUN: RUN6108

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.39

EDG-MED-90036822-94_6



CID: EDG-MED-90036822-94_6

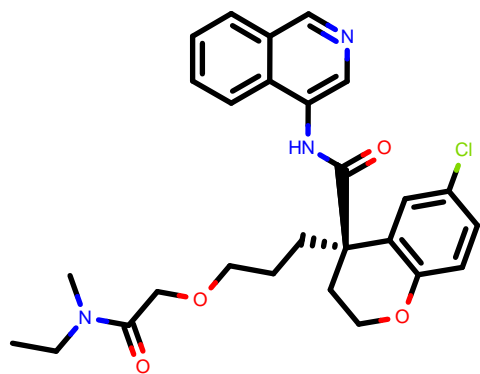
SMILES: C[C@H]1[C@@H]2[C@H]3[C@@H]4[C@H](O)[C@@H](F)C(=O)N[C@@H]3[C@@H]2[C@H]1)C(=O)N5C[C@H]4[C@H]5)Cl

RUN: RUN1674

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.28

EN300-1253122_4_1_1



CID: EN300-1253122_4_1_1

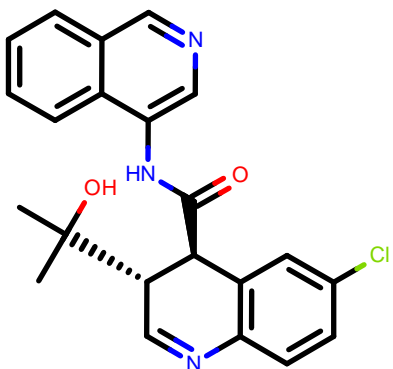
SMILES: CCN(C)C(=O)COC[C@]1(C)COCc2c1cc(cc2)C(=O)Nc3ncc4c3cccc4

RUN: RUN7450

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

BEN-BAS-5c03e89e-2_2



CID: BEN-BAS-5c03e89e-2_2

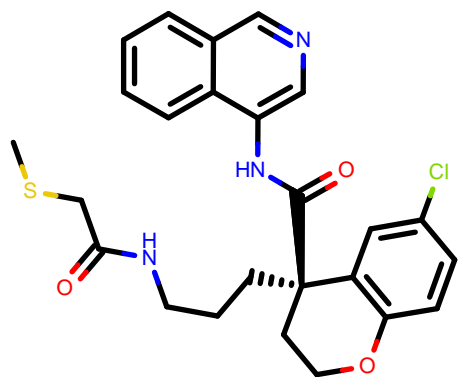
SMILES: CC(C)([C@H]1C=Nc2ccc(cc2)[C@@H]1C(=O)Nc3ncc4c3cccc4)ClO

RUN: RUN1061

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.23

EN300-07879_4_1_1



CID: EN300-07879_4_1_1

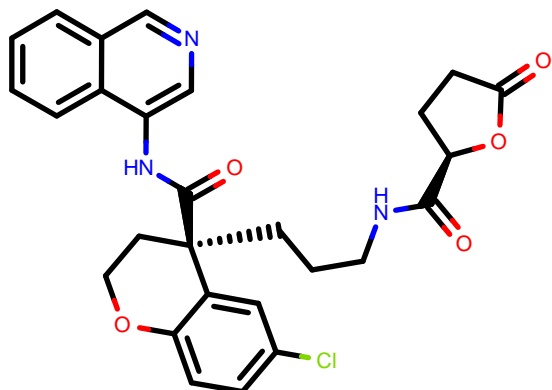
SMILES: CSCC(=O)NCCC[C@]1(C)COCc2c1cc(cc2)C(=O)Nc3ncc4c3cccc4

RUN: RUN6332

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

EN300-332606_4_1_1



CID: EN300-332606_4_1_1

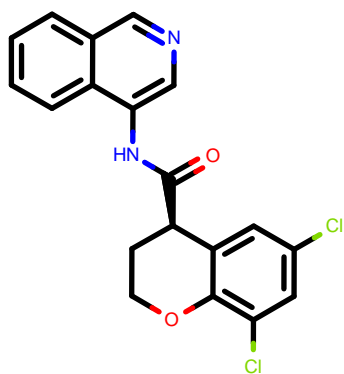
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C(=O)Nc5cnc6c5cccc6

RUN: RUN6368

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.34

RAL-THA-05e671eb-16_1



CID: RAL-THA-05e671eb-16_1

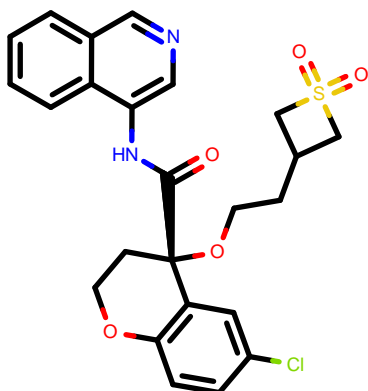
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4Cl)Cl

RUN: RUN1894

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.08

EN300-189563_1_1_1



CID: EN300-189563_1_1_1

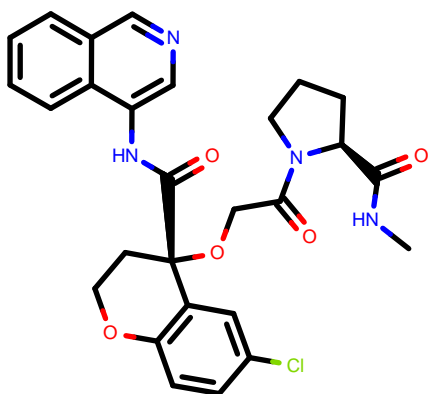
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)Cl)OCCCS(=O)(=O)CS

RUN: RUN4736

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.31

EN300-48902_1_1_1



CID: EN300-48902_1_1_1

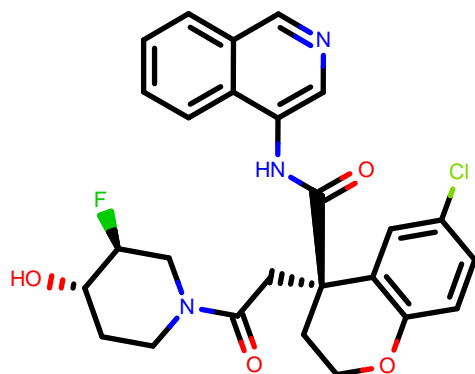
SMILES: CNC(=O)[C@@H]3(CCN1C(=O)CO[C@@H]2(CCOc3c2cc(cc3Cl)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN5568

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.34

EN300-741926_1_3_1



CID: EN300-741926_1_3_1

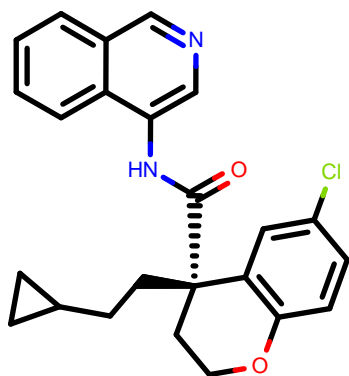
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)Cl)CC(=O)N5CC[C@@H]([C@@H](C5)F)O

RUN: RUN5225

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.28

ALP-POS-477dc5b7-3_2_1



CID: ALP-POS-477dc5b7-3_2_1

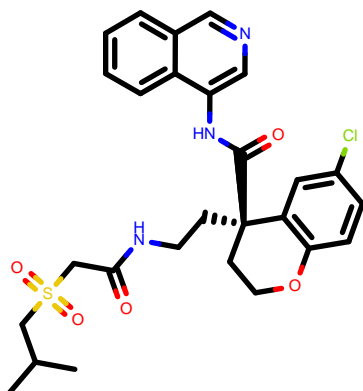
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCC5CC5

RUN: RUN6547

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.32

EN300-42243_3_1_1



CID: EN300-42243_3_1_1

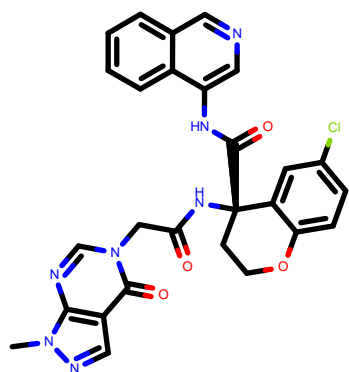
SMILES: CC(C)S(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5356

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.43

EN300-25865_1_1_1



CID: EN300-25865_1_1_1

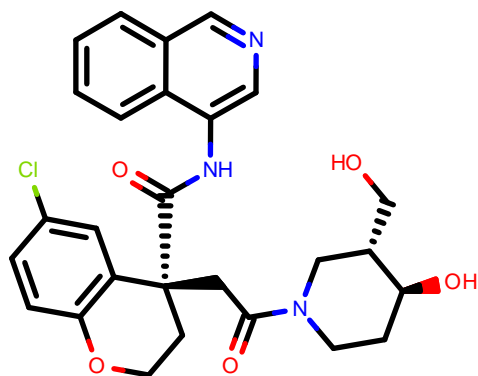
SMILES: Cn1c2c(cn1)c(=O)n(cn2)CC(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4480

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.31

EN300-233678_1_3_1



CID: EN300-233678_1_3_1

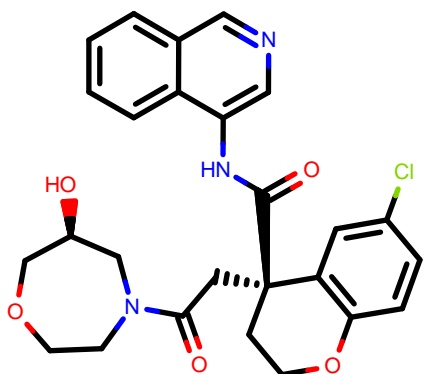
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]3[C@H](C5)CO

RUN: RUN5454

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

EN300-233951_1_2_1



CID: EN300-233951_1_2_1

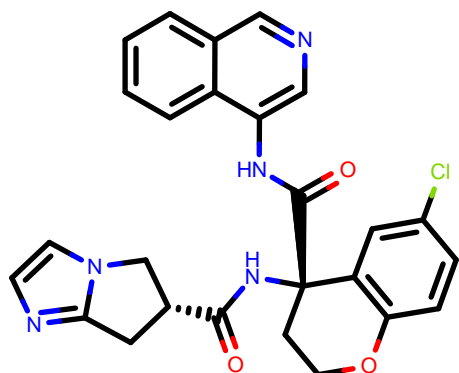
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)O

RUN: RUN4109

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EN300-7385329_1_1_1



CID: EN300-7385329_1_1_1

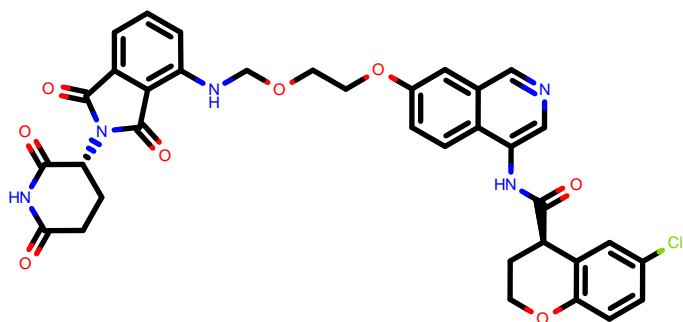
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNC6[C@H]C[C@H]6C5

RUN: RUN3802

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.23

DAR-DIA-9e4459de-13_3



CID: DAR-DIA-9e4459de-13_3

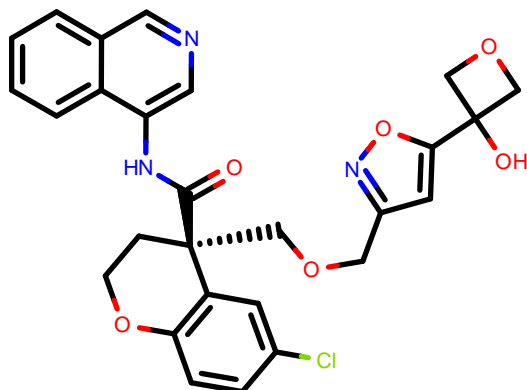
SMILES: c1cc2c(c1)NC(=O)C3CC4C(C3)C(=O)N(C4)C(=O)N5C(=O)C6C(=O)N(C5)C6

RUN: RUN1340

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.36

EN300-7457159_2_1_1



CID: EN300-7457159_2_1_1

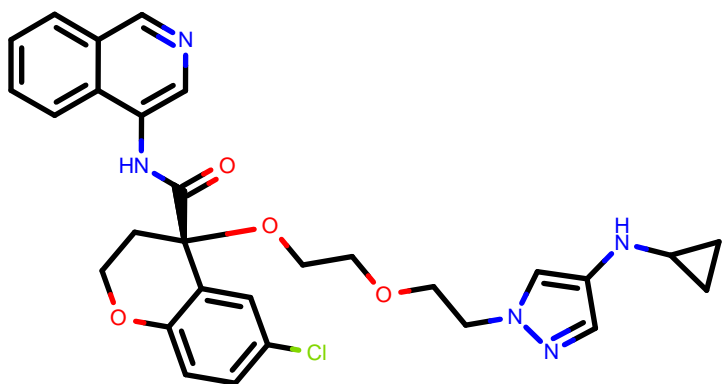
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC5Cz(on5)C6(COC6)O

RUN: RUN6266

DDG (kcal/mol): -0.41

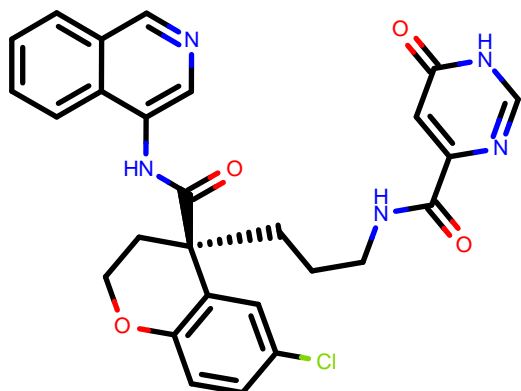
dDDG (kcal/mol): 0.33

ED_-GRI-5b13fbe2-75_1



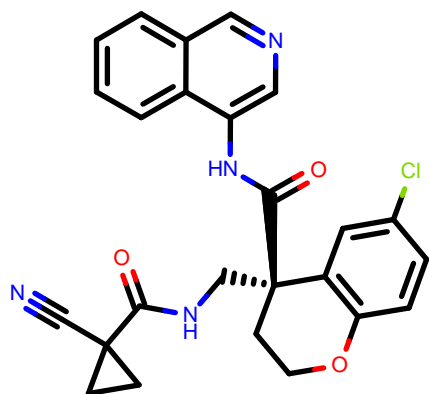
CID:	ED_-GRI-5b13fbe2-75_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCOCc5cc(cn5)NC6CC6</chem>
RUN:	RUN1529
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.31

EN300-817811_4_1_1



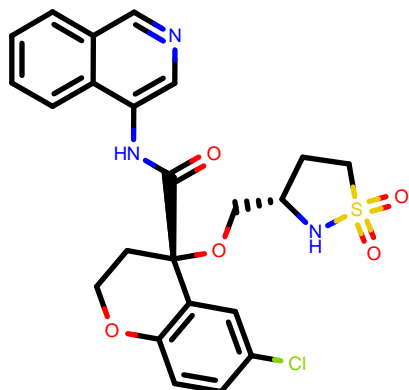
CID:	EN300-817811_4_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cc(=O)[nH]cn5</chem>
RUN:	RUN7293
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.26

EN300-114082_2_1_1



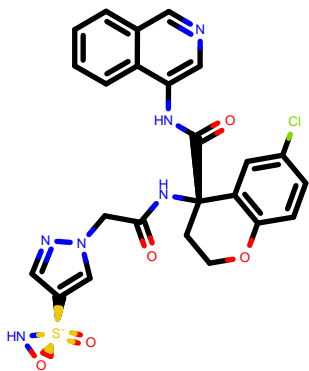
CID:	EN300-114082_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(C)C#N</chem>
RUN:	RUN3404
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.19

EN300-1699871_1_1_1



CID:	EN300-1699871_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5SCCS(=O)(=O)N5</chem>
RUN:	RUN6582
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.26

EN300-60514_1_1_1



CID: EN300-60514_1_1_1

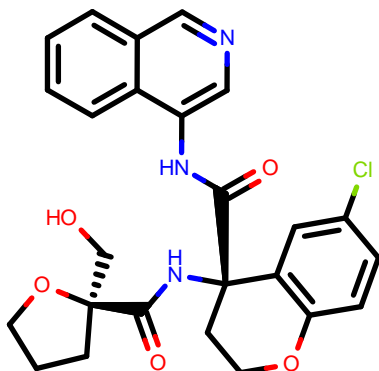
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ccn(s5)S(=O)(=O)N

RUN: RUN6964

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.38

EN300-1425677_1_2_1



CID: EN300-1425677_1_2_1

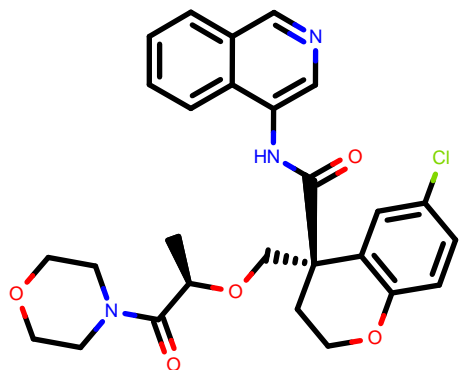
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCO5)CO

RUN: RUN5695

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.31

EN300-05754_2_2_1



CID: EN300-05754_2_2_1

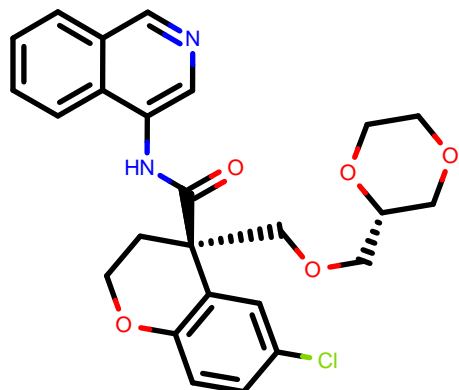
SMILES: C[C@@H](C(=O)N1CCOCC1)OC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5S

RUN: RUN6984

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.28

EN300-139167_2_2_1



CID: EN300-139167_2_2_1

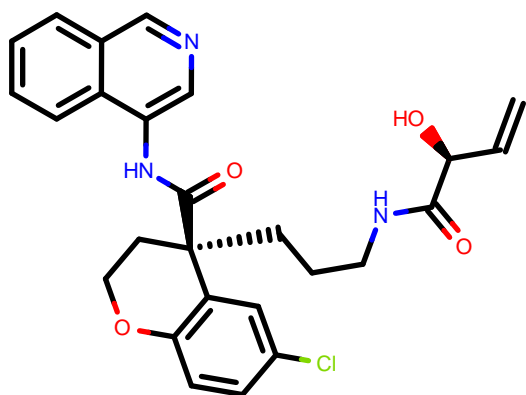
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]5COC5

RUN: RUN4396

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

EN300-181492_4_1_1



CID: EN300-181492_4_1_1

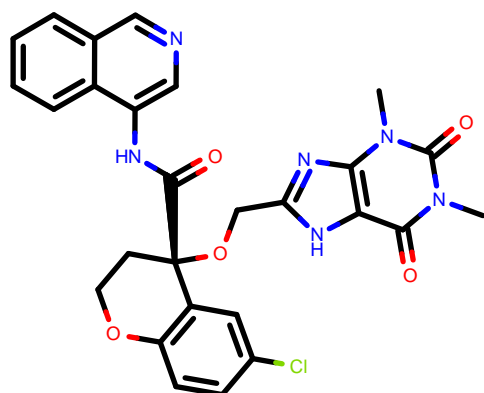
SMILES: C=C[C@@H](Cl)(C(=O)NCCC[C@@]1(CCOc2c1cc(oc2)Cl)C(=O)Nc3ncc4c3cccc4O

RUN: RUN5949

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.39

EN300-31037_1_1_1



CID: EN300-31037_1_1_1

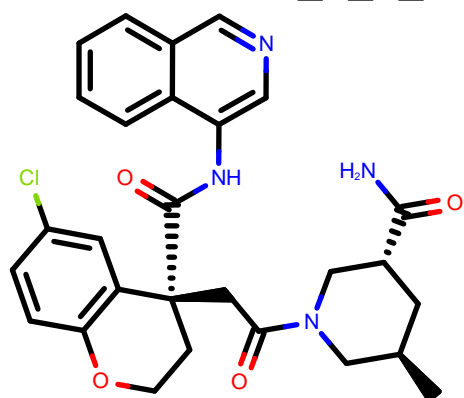
SMILES: Cn1c2c(c(=O)n(c1=O)C)[nH]c(n2)CO[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN6632

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.29

EN300-1724086_1_3_1



CID: EN300-1724086_1_3_1

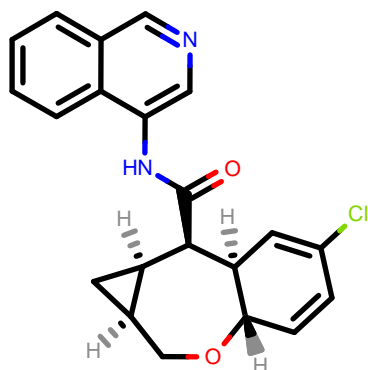
SMILES: C[C@@]1(C)[C@@H](CN(C1)Cl)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5Cl=ON

RUN: RUN2917

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-32_1



CID: DAR-DIA-0d514e7d-32_1

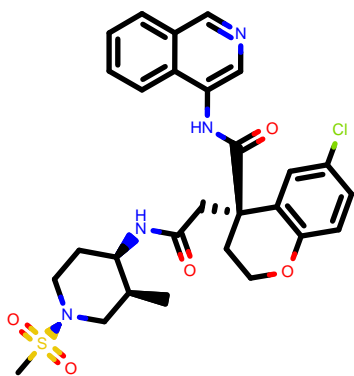
SMILES: c1ccc2c(c1)cnc2N(C(=O)[C@@]1(C)C[C@@H]3C[C@@H]4C[C@@H]5C[C@@H]3C[C@@H]5[C@@H]4C=C)Cl

RUN: RUN764

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.21

ALP-POS-2da19ca7-7_6



CID: ALP-POS-2da19ca7-7_6

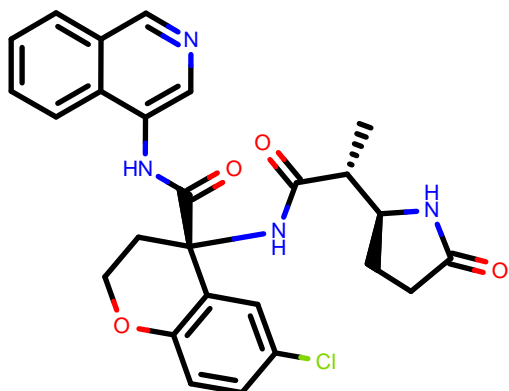
SMILES: C[C@H]1C[N@@](C)C[C@@H]1NC(=O)C(C)C(=O)C2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5S(=O)(=O)C

RUN: RUN2275

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.33

EN300-249421_1_2_1



CID: EN300-249421_1_2_1

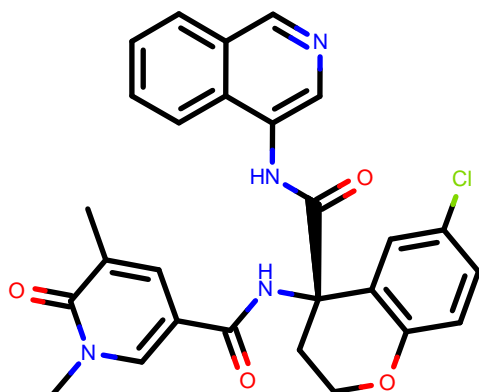
SMILES: C[C@H]1[C@@H](C)CCC(=O)N1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5S

RUN: RUN5851

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.23

EN300-1703340_1_1_1



CID: EN300-1703340_1_1_1

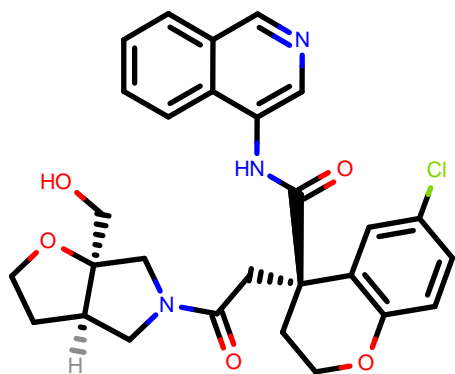
SMILES: Cc1cc(en1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5S

RUN: RUN5653

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.32

EN300-7466671_1_1_1



CID: EN300-7466671_1_1_1

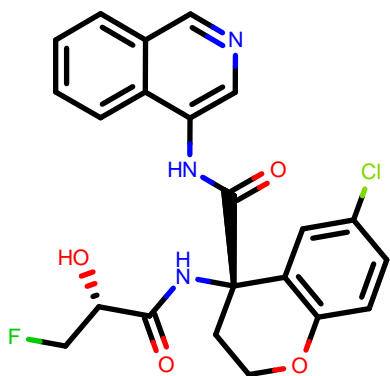
SMILES: c1ccc2c(c1)encc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5C[C@@H]6CCO[C@@]6(C)C5CO

RUN: RUN7486

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.35

EDG-MED-90036822-17_2



CID: EDG-MED-90036822-17_2

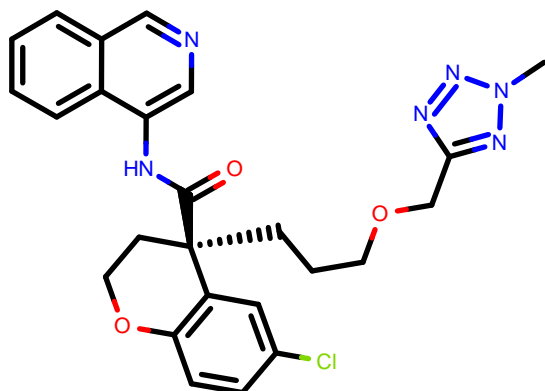
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](CF)O

RUN: RUN1521

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.29

EN300-90225_4_1_1



CID: EN300-90225_4_1_1

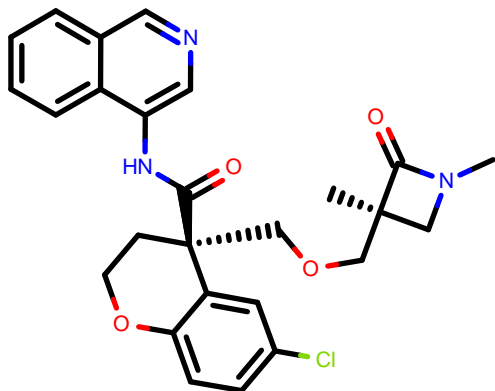
SMILES: Cn1nc(nn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3629

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.30

EN300-1273362_2_2_1



CID: EN300-1273362_2_2_1

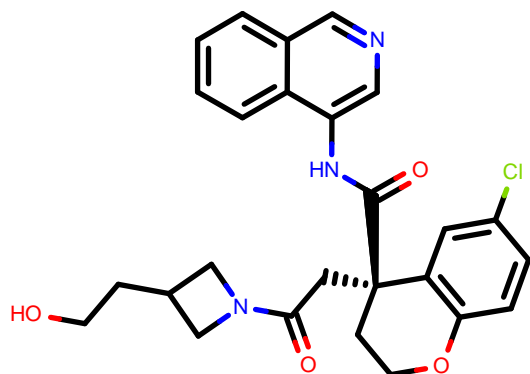
SMILES: C[C@]1(CN(C1=O)C)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3617

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.29

EN300-7413100_1_1_1



CID: EN300-7413100_1_1_1

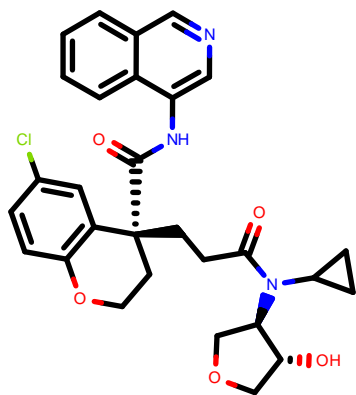
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CCO

RUN: RUN5199

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.26

EN300-1214616_2_1_1



CID: EN300-1214616_2_1_1

SMILES:

c1ccc2c(c1)cnc2N[C@@H](C)C(=O)Nc3ccc(Cl)cc3[C@@H](C)C(=O)N[C@@H](C)C(=O)Nc4ccc(Cl)cc4

RUN:

RUN6190

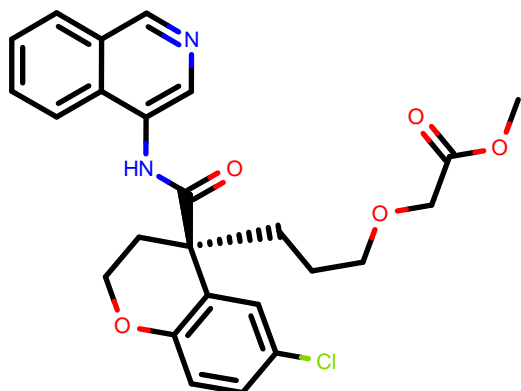
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.23

EN300-19700_4_1_1



CID: EN300-19700_4_1_1

SMILES:

COC(=O)COCC[C@H](C)C(=O)Nc3ccc(Cl)cc3[C@@H](C)C(=O)Nc4ccc(Cl)cc4

RUN:

RUN4379

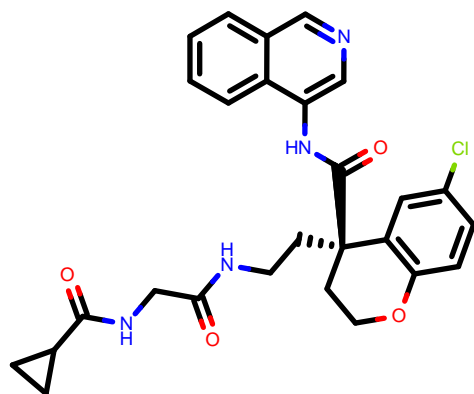
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.35

EN300-36522_3_1_1



CID: EN300-36522_3_1_1

SMILES:

c1ccc2c(c1)cnc2N[C@@H](C)C(=O)Nc3ccc(Cl)cc3[C@@H](C)C(=O)Nc4ccc(Cl)cc4

RUN:

RUN4595

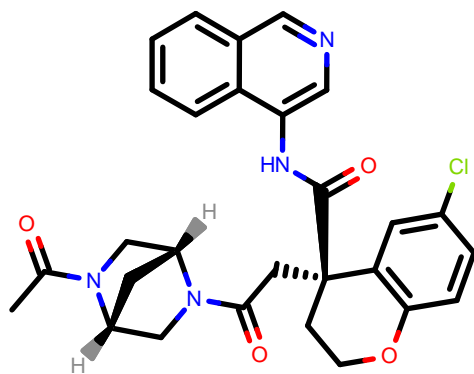
DDG (kcal/mol):

-0.39

dDDG (kcal/mol):

0.29

ALP-UNI-3496895b-3_1



CID: ALP-UNI-3496895b-3_1

SMILES:

CC(=O)N1C[C@H]2C[C@@H](C)C(=O)Nc3ccc(Cl)cc3[C@@H](C)C(=O)Nc4ccc(Cl)cc4

RUN:

RUN2334

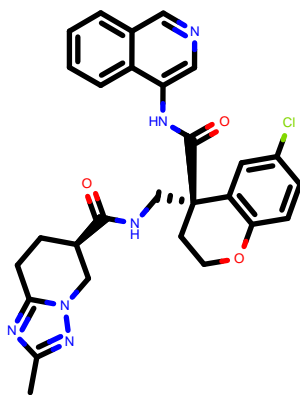
DDG (kcal/mol):

-0.39

dDDG (kcal/mol):

0.28

EN300-746187_2_1_1



CID: EN300-746187_2_1_1

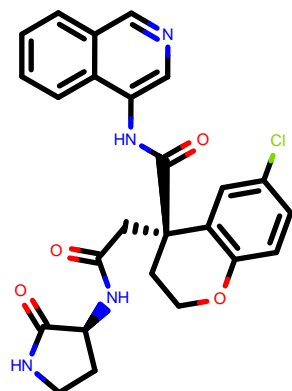
SMILES: Cc1nc2n(n1)C[C@@H](CC2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccc6

RUN: RUN7664

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

EN300-307333_1_1_1



CID: EN300-307333_1_1_1

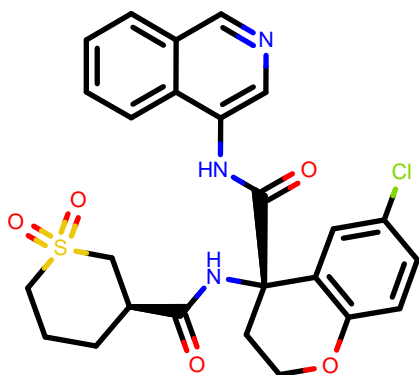
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCNC5=O

RUN: RUN7818

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-77778_1_2_1



CID: EN300-77778_1_2_1

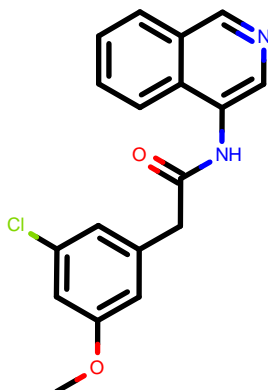
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCS(=O)(=O)C5

RUN: RUN3249

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.25

RAL-THA-2d450e86-18_1



CID: RAL-THA-2d450e86-18_1

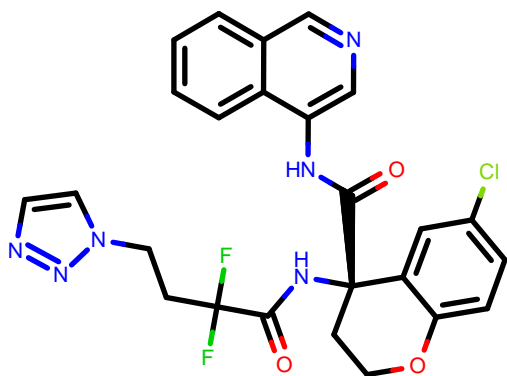
SMILES: COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3

RUN: RUN1825

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

EN300-6474220_1_1_1



CID: EN300-6474220_1_1_1

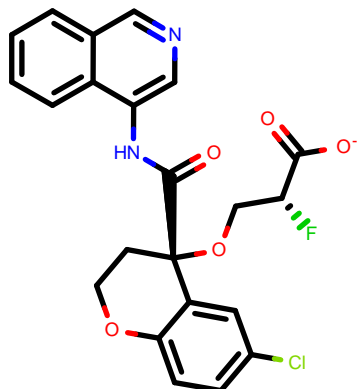
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(Cn5cnn5)F

RUN: RUN4059

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-47_2



CID: ED_-GRI-5b13fbe2-47_2

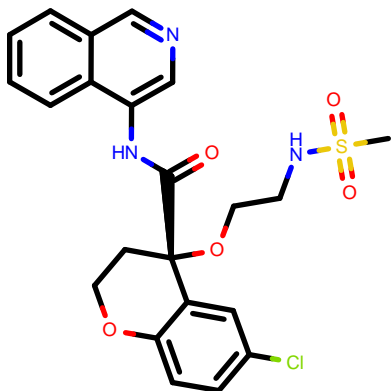
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](C(=O)O)F

RUN: RUN1420

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-1238839_1_1_1



CID: EN300-1238839_1_1_1

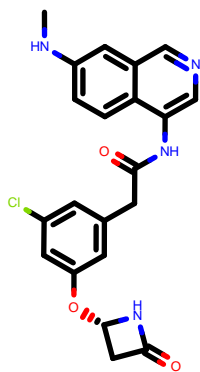
SMILES: CS(=O)(=O)NCCO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7588

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

ALF-EVA-0b412456-6_2



CID: ALF-EVA-0b412456-6_2

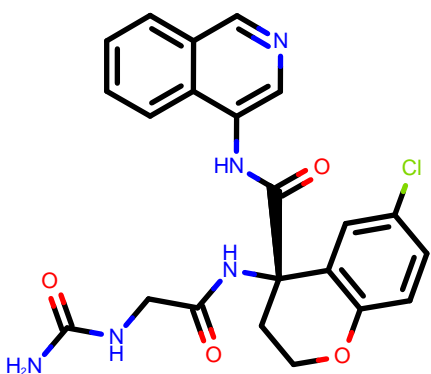
SMILES: CNc1ccc2c(c1)ncnc2NC(=O)Cc3ccc(cc3)ClO[C@H]4CC(=O)N4

RUN: RUN2572

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.38

EN300-10397_1_1_1



CID: EN300-10397_1_1_1

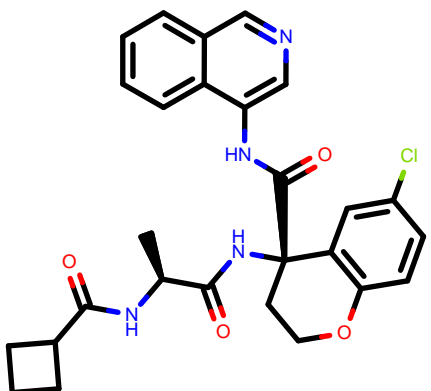
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N

RUN: RUN6565

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.21

ALP-UNI-dbbfd3db-15_1



CID: ALP-UNI-dbbfd3db-15_1

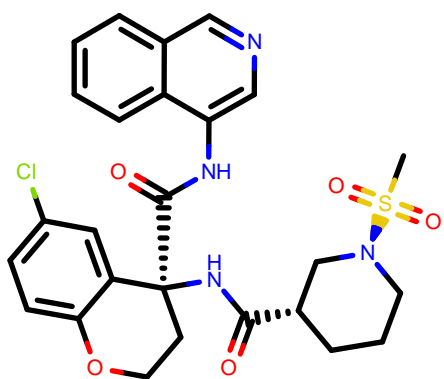
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)NC(=O)C5CC5

RUN: RUN2627

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.32

EN300-27341_1_1_1



CID: EN300-27341_1_1_1

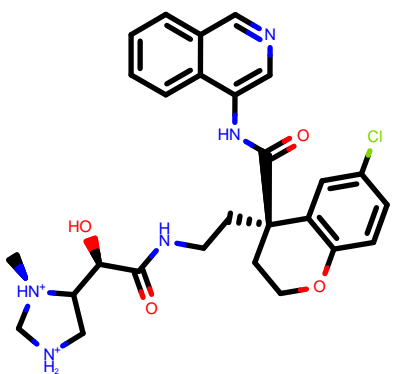
SMILES: CS(=O)(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)NC(=O)N5CCCC5

RUN: RUN3036

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

EN300-190283_3_2_1



CID: EN300-190283_3_2_1

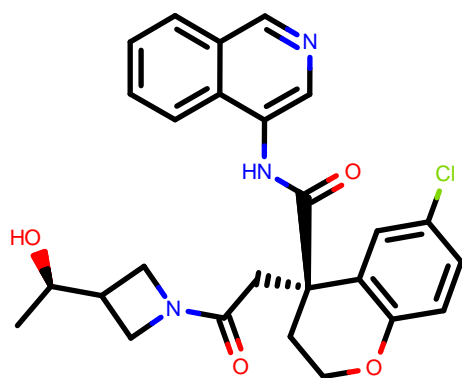
SMILES: C[n+][c-]nHcc1[C@@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O

RUN: RUN5399

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.46

EN300-301721_1_2_1



CID: EN300-301721_1_2_1

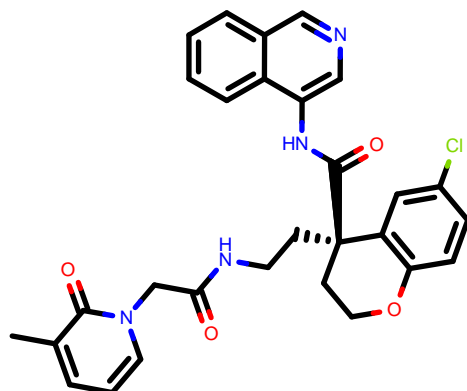
SMILES: C[C@H](C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN6576

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

EN300-126104_3_1_1



CID: EN300-126104_3_1_1

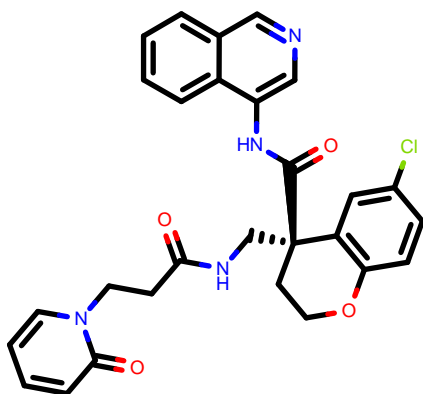
SMILES: Cc1cccn(c1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5086

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

EN300-36622_2_1_1



CID: EN300-36622_2_1_1

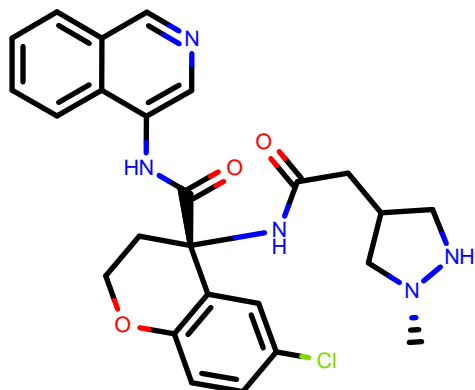
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5ccccc5=O

RUN: RUN7777

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.27

EN300-63872_1_1_1



CID: EN300-63872_1_1_1

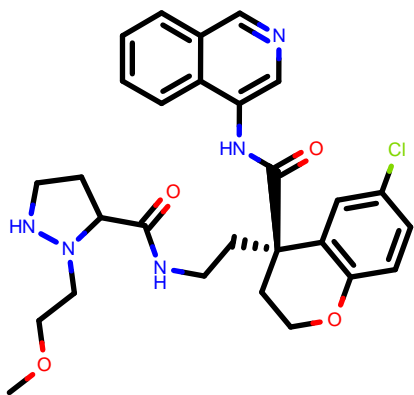
SMILES: Cn1cc(en1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4878

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.27

EN300-92664_3_1_1



CID: EN300-92664_3_1_1

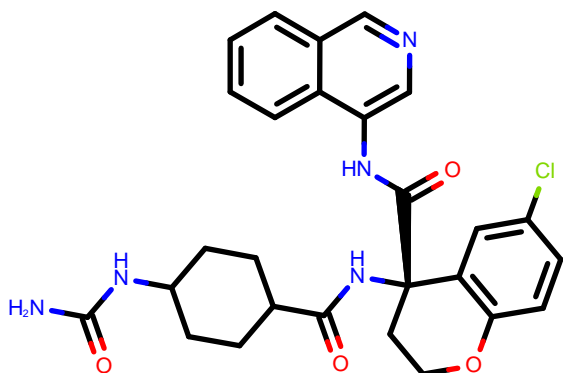
SMILES: COCc1c(ccn1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5710

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

EN300-53591_1_1_1



CID: EN300-53591_1_1_1

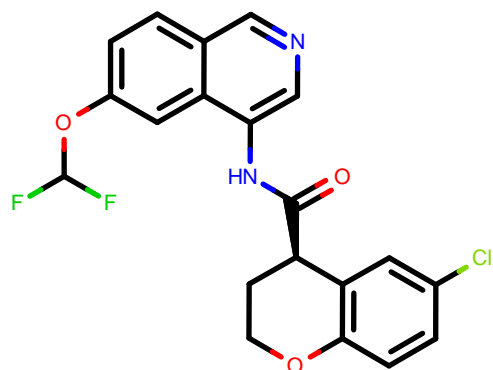
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CCC(C5)NC(=O)N

RUN: RUN3397

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.28

BEN-DND-c852c98b-6_1



CID: BEN-DND-c852c98b-6_1

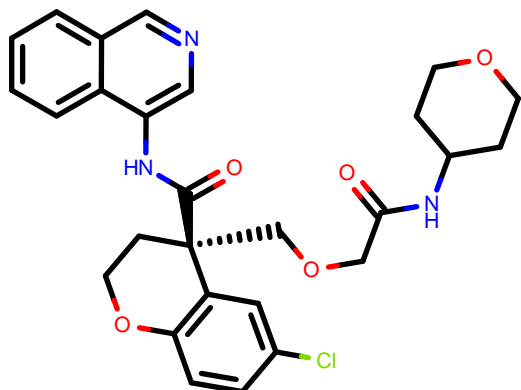
SMILES: c1cc2cnc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN1135

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.06

EN300-67573_2_1_1



CID: EN300-67573_2_1_1

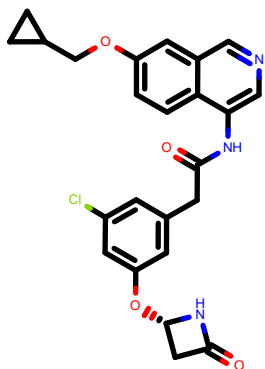
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)N5CCOC5

RUN: RUN6333

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

ALF-EVA-0b412456-7_2



CID: ALF-EVA-0b412456-7_2

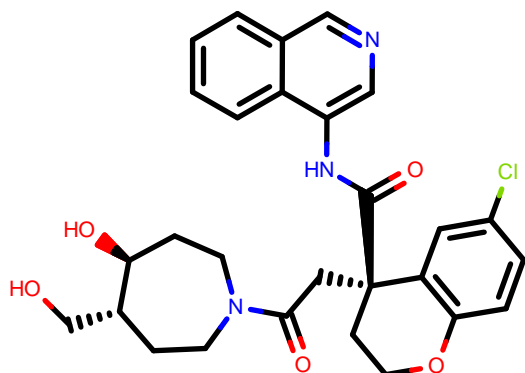
SMILES: c1cc2c(cc1OCC3CC3)ncnc2NC(=O)Cc4cc(cc(c4)Cl)O[C@H]5CC(=O)N5

RUN: RUN2559

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.38

EN300-7353672_1_3_1



CID: EN300-7353672_1_3_1

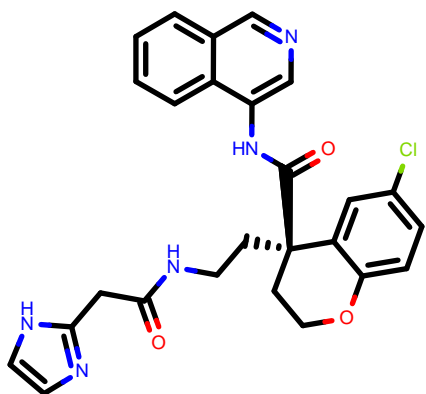
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C1=O)N5CC[C@@H]([C@@H]5)O)CO

RUN: RUN4505

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.32

EN300-220527_3_1_1



CID: EN300-220527_3_1_1

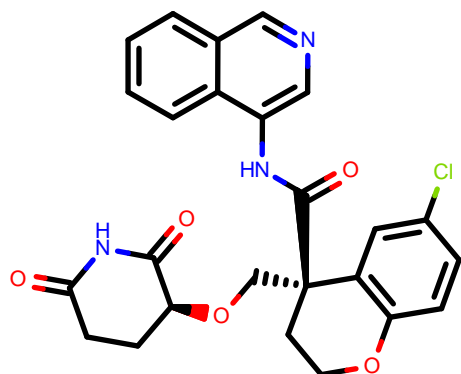
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5[nH]cn5

RUN: RUN5212

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.30

EN300-120920_2_2_1



CID: EN300-120920_2_2_1

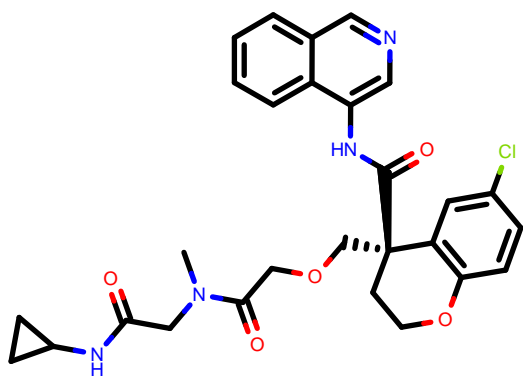
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCCC(=O)NC5=O

RUN: RUN7230

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.23

EN300-13668_2_1_1



CID: EN300-13668_2_1_1

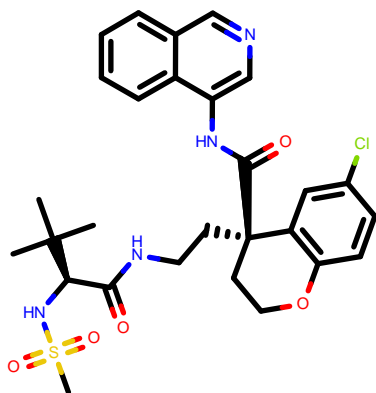
SMILES: CN(CC(=O)NC1CC1)C(=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5296

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

EN300-112872_3_1_1



CID: EN300-112872_3_1_1

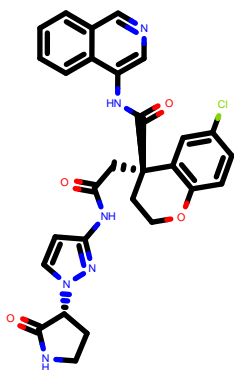
SMILES: CC(C)C(C@H)(Cl)O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4NS(=O)(=O)C

RUN: RUN7574

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.44

ALP-UNI-3496895b-12_1



CID: ALP-UNI-3496895b-12_1

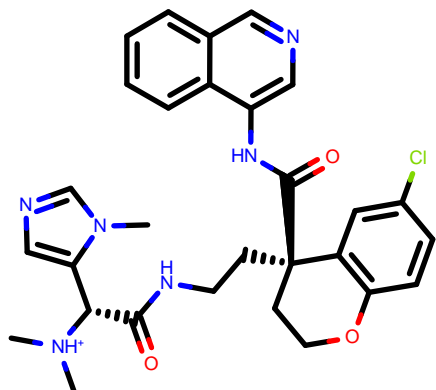
SMILES: c1ccc2c(c1)ncoc2N(C)C(=O)C[C@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5ncoc6c5cnc6=O

RUN: RUN2344

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.31

EN300-192809_3_2_1



CID: EN300-192809_3_2_1

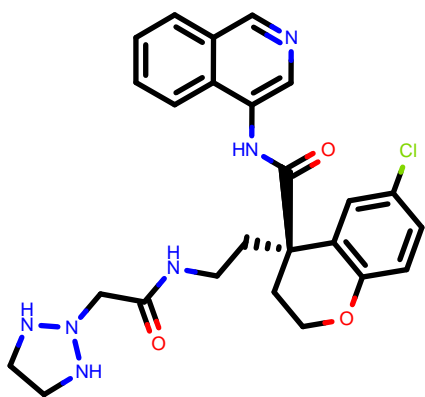
SMILES: Cn1cnc1[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5)[NH+](C)C

RUN: RUN7658

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.55

EN300-100916_3_1_1



CID: EN300-100916_3_1_1

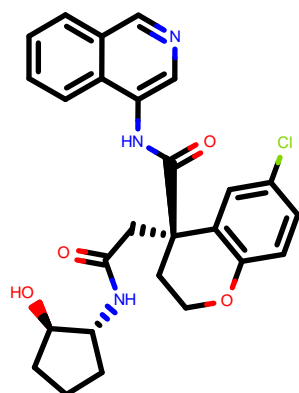
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[N@@]5NCC=N5

RUN: RUN4935

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.30

EN300-60314_1_1_1



CID: EN300-60314_1_1_1

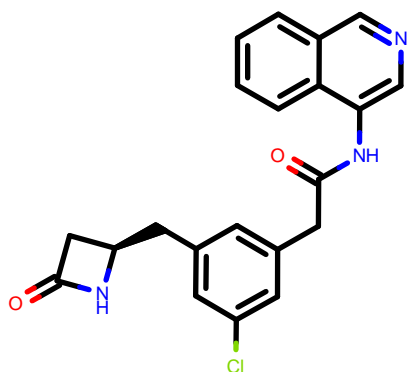
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5H5CCC[C@@]5O

RUN: RUN4549

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

EDJ-MED-50011917-1_1



CID: EDJ-MED-50011917-1_1

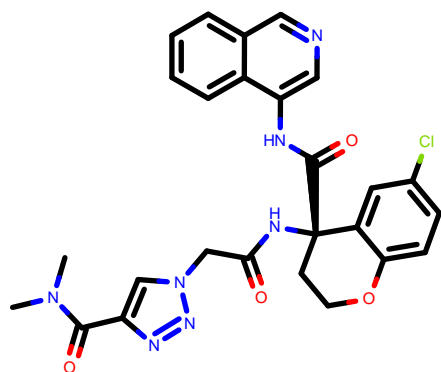
SMILES: c1ccc2c(c1)ncnc2NC(=O)Cc3cc(cc(c3)C)C[C@@]4H4CC(=O)N4

RUN: RUN305

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.39

EN300-2853791_1_1_1



CID: EN300-2853791_1_1_1

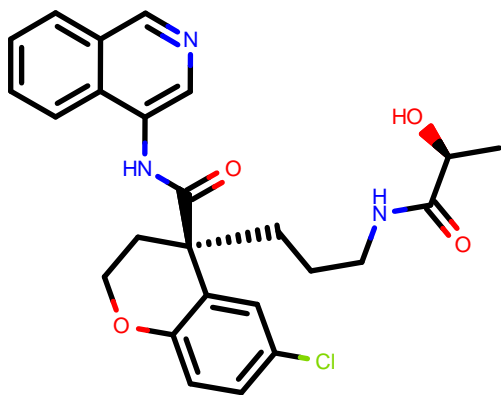
SMILES: CN(C)C(=O)c1cn(nn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN7252

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

EN300-91905_4_1_1



CID: EN300-91905_4_1_1

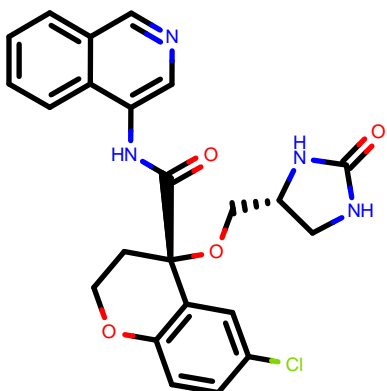
SMILES: C[C@@H](C(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN6128

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.38

ED_-GRI-5b13fbe2-39_1



CID: ED_-GRI-5b13fbe2-39_1

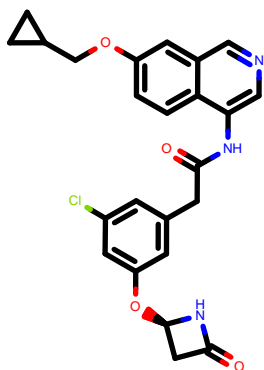
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CNC(=O)N5

RUN: RUN1415

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.25

ALF-EVA-0b412456-7_1



CID: ALF-EVA-0b412456-7_1

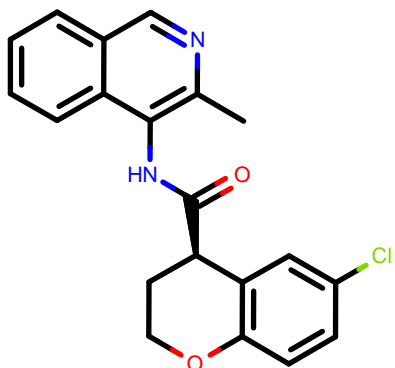
SMILES: c1cc2c(cc1OCC3CC3)ncoc2NC(=O)Cc4cc(cc(c4)Cl)O[C@@H]5CC(=O)N5

RUN: RUN2597

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.35

ADA-UCB-dc2b944c-10_1



CID: ADA-UCB-dc2b944c-10_1

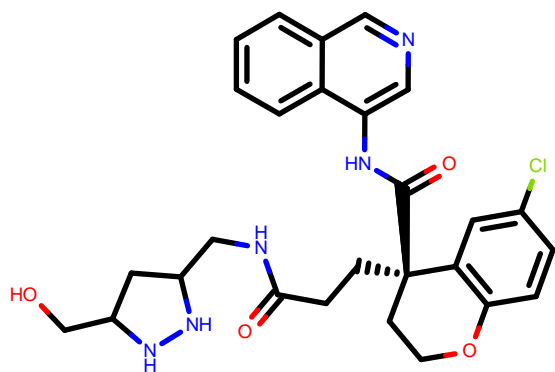
SMILES: Cc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN497

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.09

EN300-7439043_2_1_1



CID: EN300-7439043_2_1_1

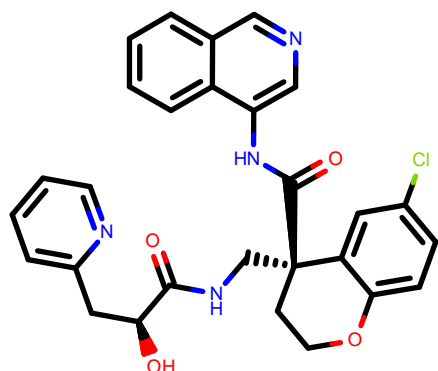
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cc[nH]n5CO

RUN: RUN5428

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.25

EN300-6762327_2_2_1



CID: EN300-6762327_2_2_1

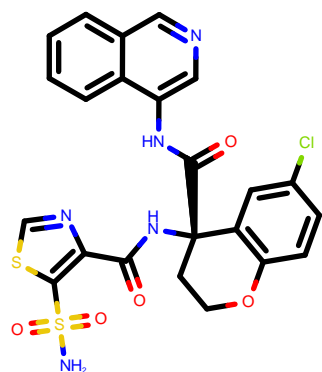
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](Cc5ccccc5)O

RUN: RUN6084

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.31

EN300-132613_1_1_1



CID: EN300-132613_1_1_1

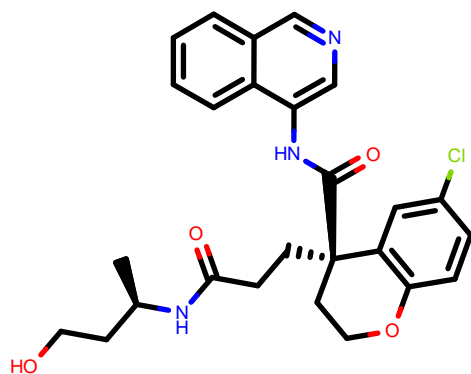
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[sn5]S(=O)(=O)N

RUN: RUN4582

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.25

EN300-117685_2_1_1



CID: EN300-117685_2_1_1

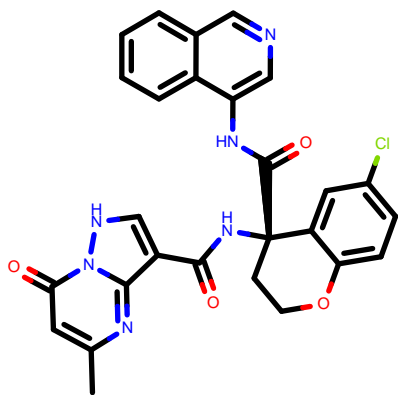
SMILES: C[C@H](CCO)NC(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4533

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

EN300-181178_1_1_1



CID: EN300-181178_1_1_1

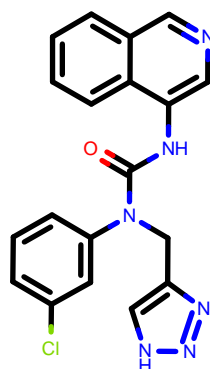
SMILES: Cc1cc(=O)n2c(n1)c(c[nH]2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN6146

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

MIC-UNK-bcd487e9-7_1



CID: MIC-UNK-bcd487e9-7_1

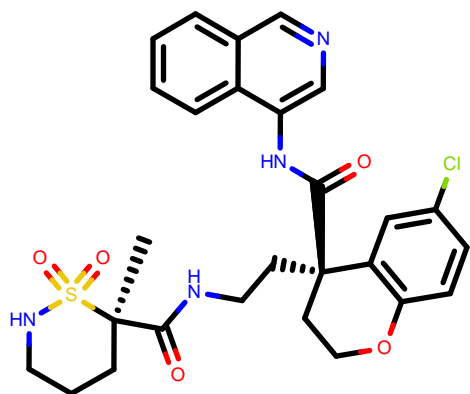
SMILES: c1ccc2c(c1)cnc2NC(=O)N(Cc3cn[nH]n3)c4cccc(c4)Cl

RUN: RUN499

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.38

EN300-1709315_3_1_1



CID: EN300-1709315_3_1_1

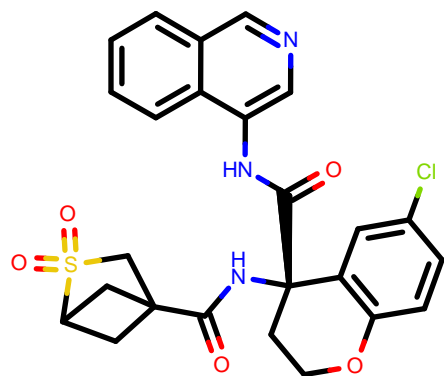
SMILES: C[C@@]1(CCCNS1(=O)=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN6460

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.34

EN300-7354033_1_1_1



CID: EN300-7354033_1_1_1

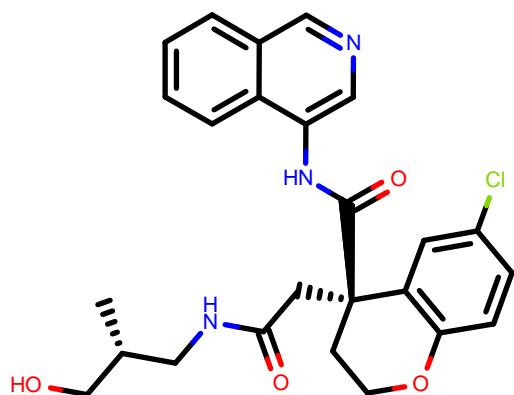
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(C5)S(=O)(=O)C6

RUN: RUN4174

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.24

EN300-53656_1_2_1



CID: EN300-53656_1_2_1

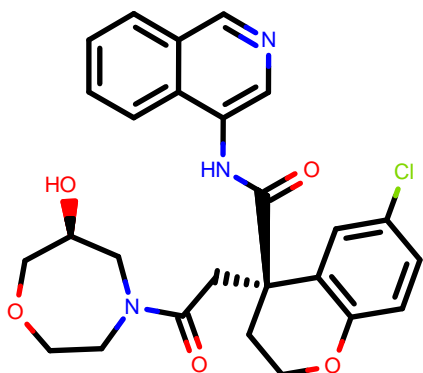
SMILES: C[C@H](CNC(=O)C[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)CO

RUN: RUN6718

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-233951_1_2_1



CID: EN300-233951_1_2_1

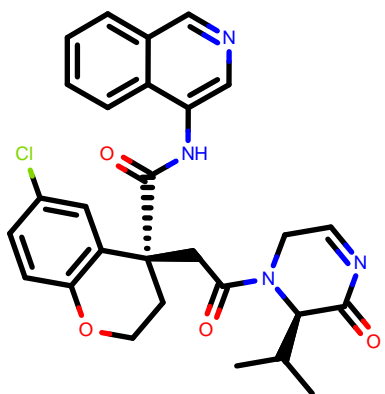
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)O

RUN: RUN6895

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.28

EN300-67791_1_1_1



CID: EN300-67791_1_1_1

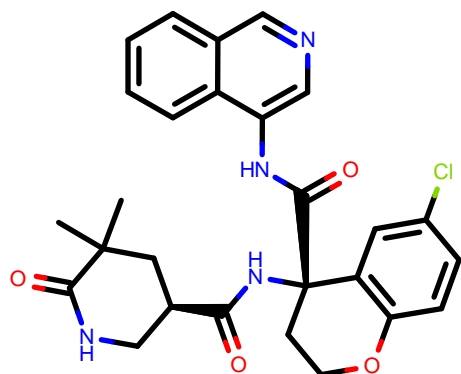
SMILES: CC(C)[C@@]1[C@H](C(=O)NCCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4cccc5

RUN: RUN6602

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.38

EN300-7351945_1_2_1



CID: EN300-7351945_1_2_1

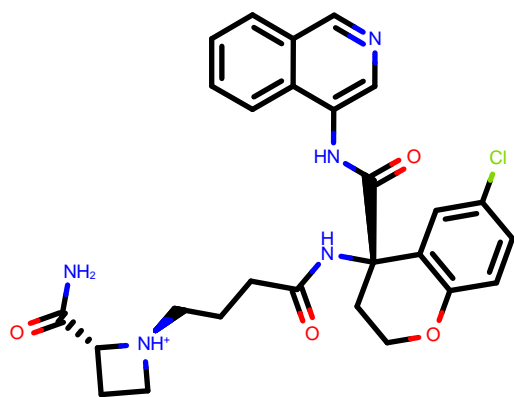
SMILES: CC1(C[C@H](CNC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4cccc5)C

RUN: RUN6312

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.23

EDG-MED-90036822-12_2



CID: EDG-MED-90036822-12_2

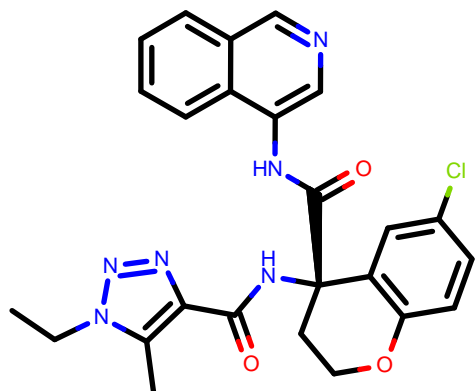
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C3c4cc5cc(O)C=C(C)N4H5CC[C@@H]6C[C@@H]6

RUN: RUN1570

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.32

EN300-151411_1_1_1



CID: EN300-151411_1_1_1

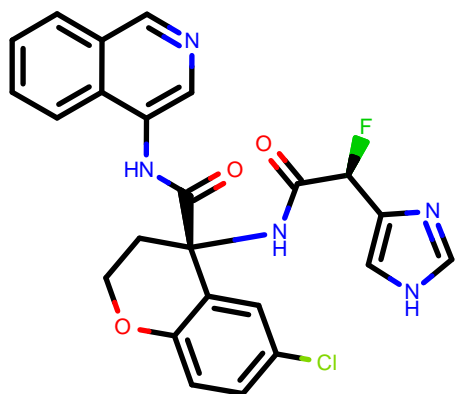
SMILES: CCn1c(c(nn1)C(=O)N[C@@]2(C)C(CO)C2c3cc(O)C=C(C)N4C5C6C7C8C9C5)C

RUN: RUN7053

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.29

EDG-MED-90036822-20_2



CID: EDG-MED-90036822-20_2

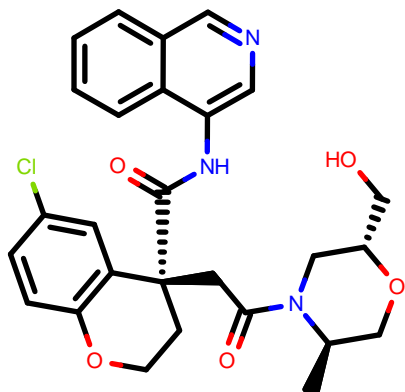
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C3c4cc5cc(O)C=C(C)N4H5C6C7C8C9C5)F

RUN: RUN1560

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.23

EN300-109920_1_3_1



CID: EN300-109920_1_3_1

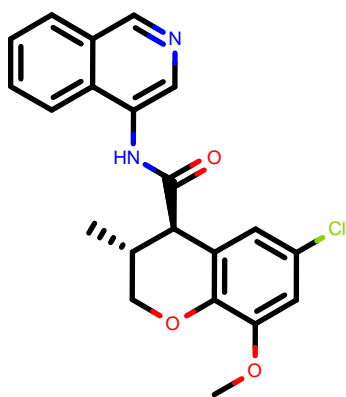
SMILES: C[C@@H]1CO[C@@H](CN1C(=O)C[C@@]2(C)C(CO)C2c3cc(O)C=C(C)N4C5C6C7C8C9C5)CO

RUN: RUN5691

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.57

DAR-DIA-0d514e7d-1_1_1



CID: DAR-DIA-0d514e7d-1_1_1

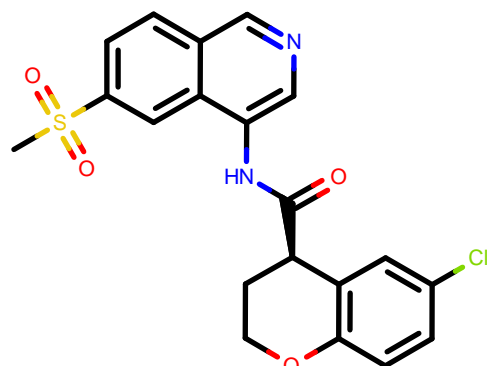
SMILES: C[C@H]1COc2c(cc2OC)C1[C@@H]1C(=O)Nc3ccc4c3cccc4

RUN: RUN6515

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.12

BEN-DND-c852c98b-5_1



CID: BEN-DND-c852c98b-5_1

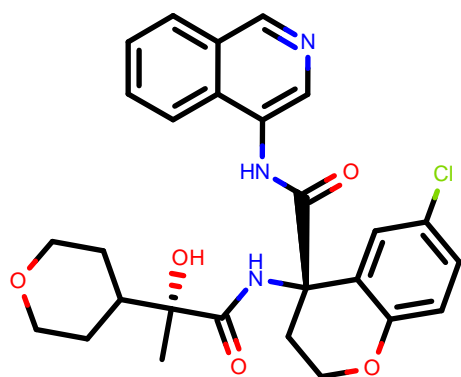
SMILES: CS(=O)(=O)c1ccc2nccc(c2c1)NC(=O)[C@@H]3CCOCc4c3cc(c4)Cl

RUN: RUN1104

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.08

EN300-217499_1_1_1



CID: EN300-217499_1_1_1

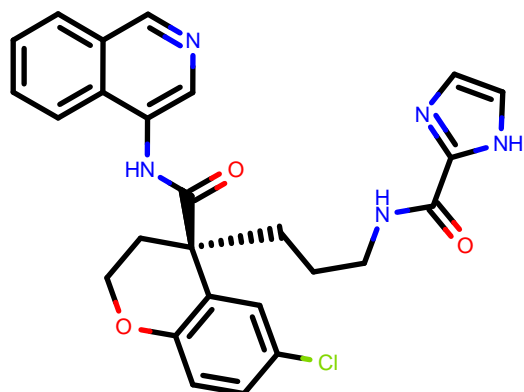
SMILES: C[C@@H](C1CCOCC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5O

RUN: RUN7647

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.22

EN300-315836_4_1_1



CID: EN300-315836_4_1_1

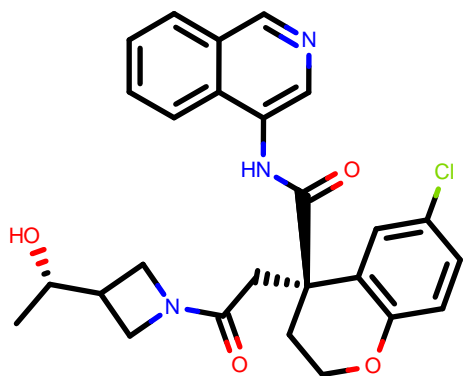
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5[nH]cnc5

RUN: RUN6304

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.31

EN300-365650_1_1_1



CID: EN300-365650_1_1_1

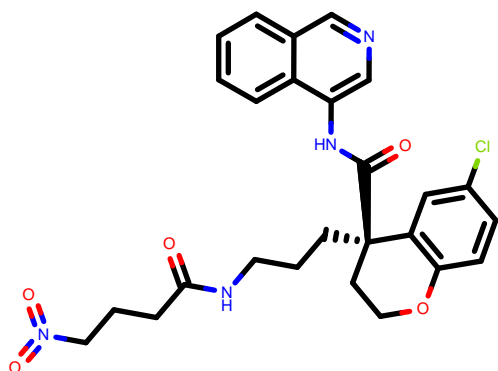
SMILES: C[C@@H](C1CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7639

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-143449_4_1_1



CID: EN300-143449_4_1_1

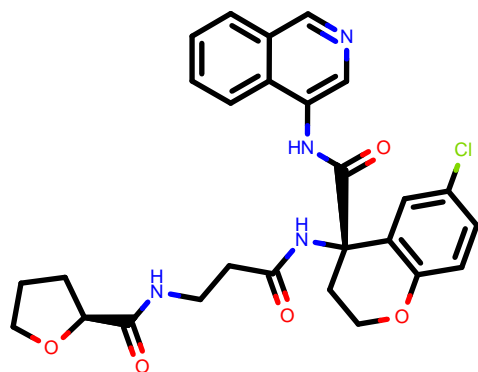
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCN(=O)=O

RUN: RUN5467

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.31

EN300-86732_1_1_1



CID: EN300-86732_1_1_1

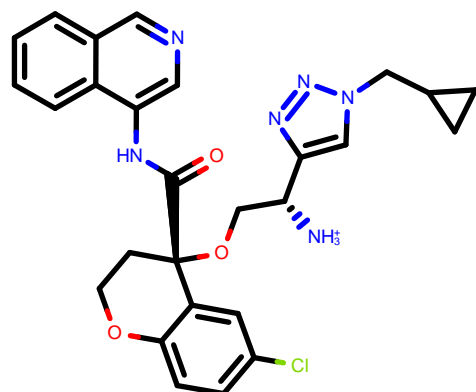
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)[C@@]5H5CCCCO5

RUN: RUN5488

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-17_1



CID: ED_-GRI-5b13fbe2-17_1

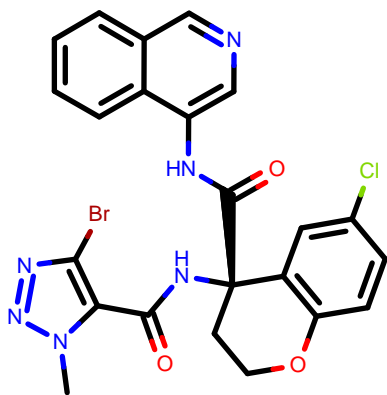
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5cn(m5)CC6CC6)[NH3+]

RUN: RUN1429

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.38

EN300-218288_1_1_1



CID: EN300-218288_1_1_1

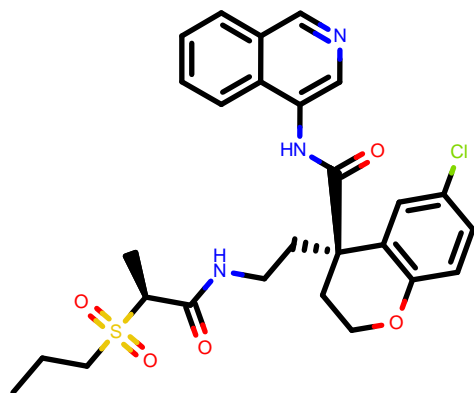
SMILES: Cn1c(c(nn1)Br)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5363

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.21

EN300-52768_3_1_1



CID: EN300-52768_3_1_1

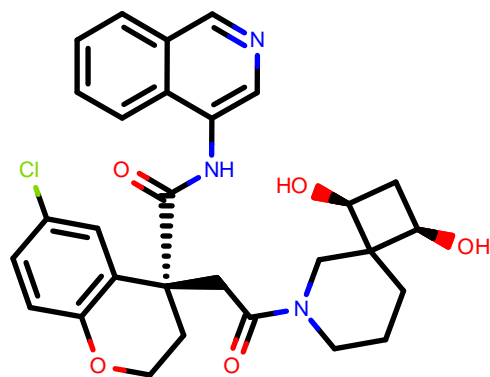
SMILES: CCCS(=O)(=O)[C@@H](C)C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6141

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.44

EDJ-MED-d203f206-10_1



CID: EDJ-MED-d203f206-10_1

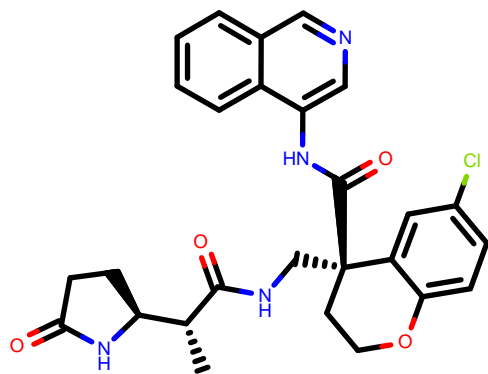
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)Cl)C(=O)N5CCCC6(C5)[C@@H](C)[C@@H]6O

RUN: RUN2425

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.39

EN300-249421_2_2_1



CID: EN300-249421_2_2_1

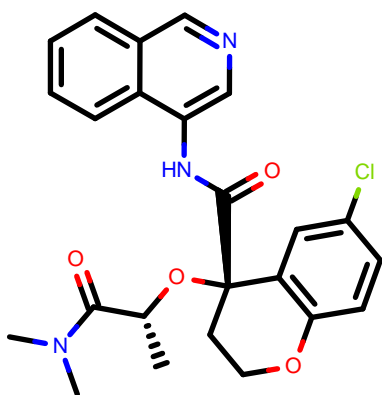
SMILES: C[C@@H]([C@@H]1CC(=O)N1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6755

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.34

EN300-14458_1_2_1



CID: EN300-14458_1_2_1

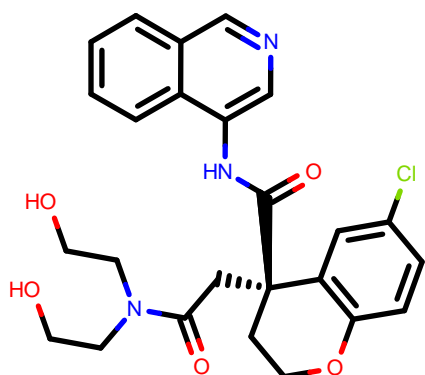
SMILES: C[C@H](C(=O)N(C)C)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7173

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.21

EN300-19762_1_1_1



CID: EN300-19762_1_1_1

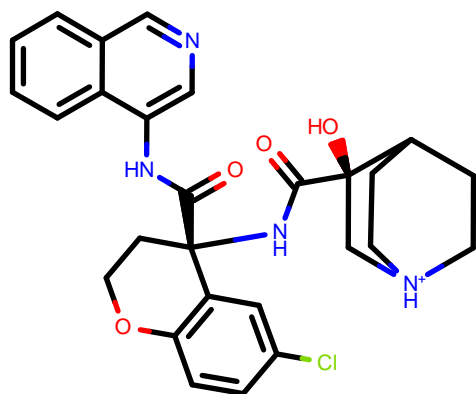
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)CCO

RUN: RUN3000

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.39

EN300-7442191_1_2_1



CID: EN300-7442191_1_2_1

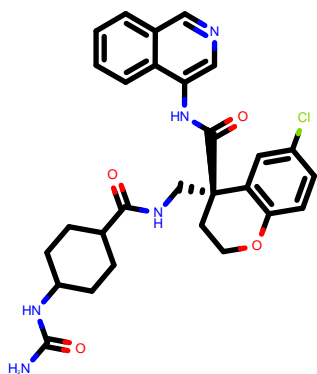
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(C)N+J6CCC5OC6O

RUN: RUN7083

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.40

EN300-53591_2_1_1



CID: EN300-53591_2_1_1

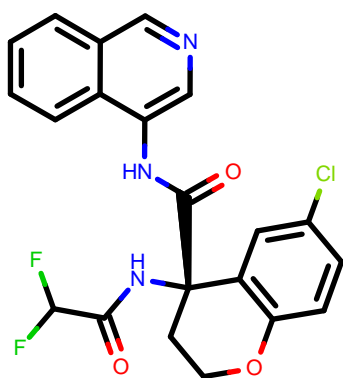
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CCCC(C5)NC(=O)N

RUN: RUN7449

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.29

EDG-MED-90036822-63_1



CID: EDG-MED-90036822-63_1

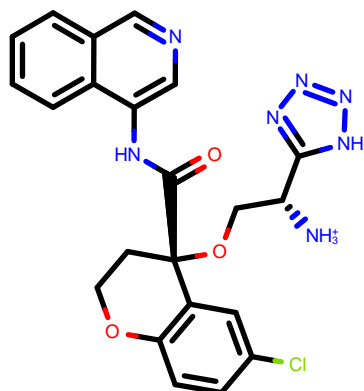
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(F)F

RUN: RUN1586

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.15

ED_-GRI-5b13fbe2-4_1



CID: ED_-GRI-5b13fbe2-4_1

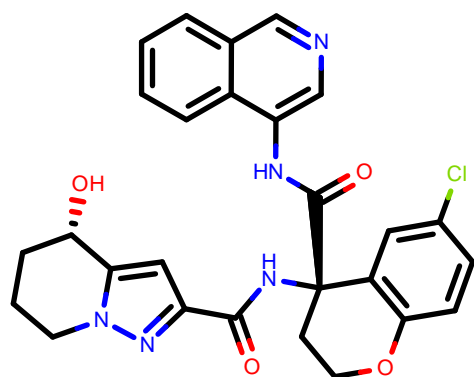
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5[n-]nn5)[NH3+]

RUN: RUN1386

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.30

EN300-399606_1_1_1



CID: EN300-399606_1_1_1

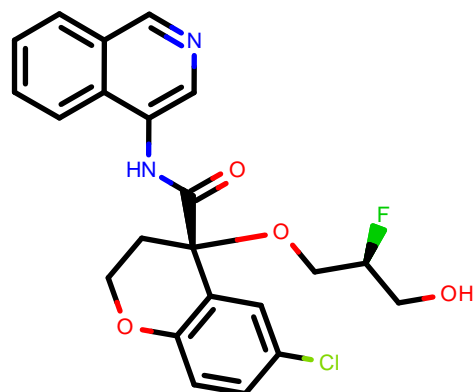
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CC[C@]3@@H6O

RUN: RUN3538

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.24

EN300-1600517_1_2_1



CID: EN300-1600517_1_2_1

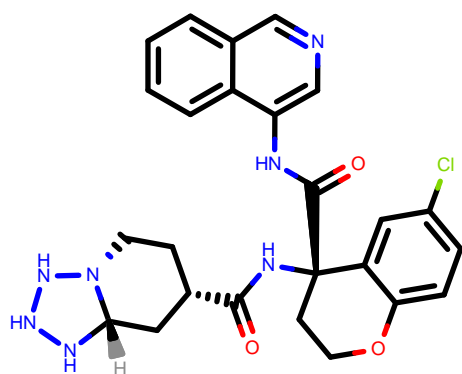
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CO)F

RUN: RUN7795

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-1653482_1_2_2



CID: EN300-1653482_1_2_2

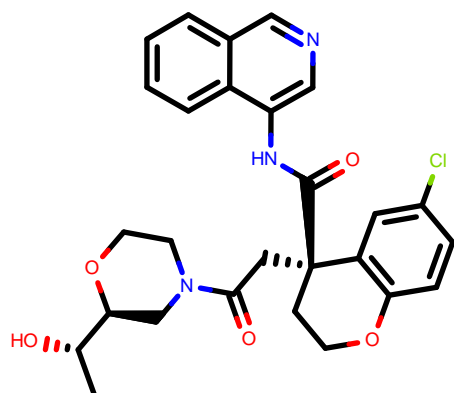
SMILES: c1ccc2c(c1)cnc2NC(=O)C(C)C3(C)COC4C3C(=O)C(NC1=O)C1C@H5CCN@H5C@H(C5)N(H)2+3N(H)2+9

RUN: RUN3251

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.44

EN300-254840_1_1_1



CID: EN300-254840_1_1_1

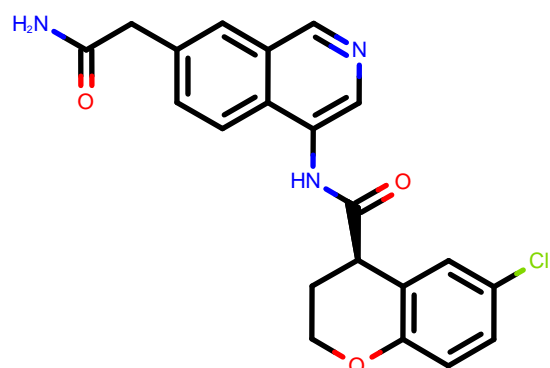
SMILES: C[C@@H]1[C@@H]1CN(CCO1)C(=O)C(C)C2(C)COC3C2C(=O)C(C)C(=O)N4cnc5c4ccc5O

RUN: RUN4357

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.40

MAK-UNK-8be7dca9-2_1



CID: MAK-UNK-8be7dca9-2_1

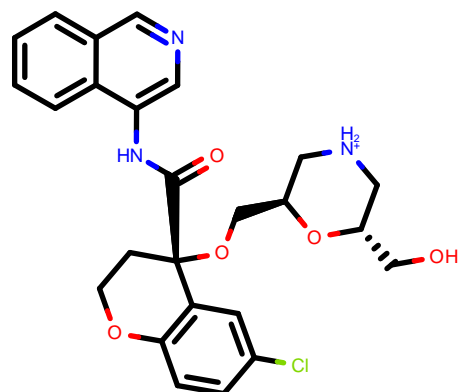
SMILES: c1cc2c(cc1CC(=O)N)cnc2NC(=O)C(C)C@H3CCOC4C3C(=O)C4Cl

RUN: RUN429

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.07

ED_-GRI-5b13fbe2-20_1



CID: ED_-GRI-5b13fbe2-20_1

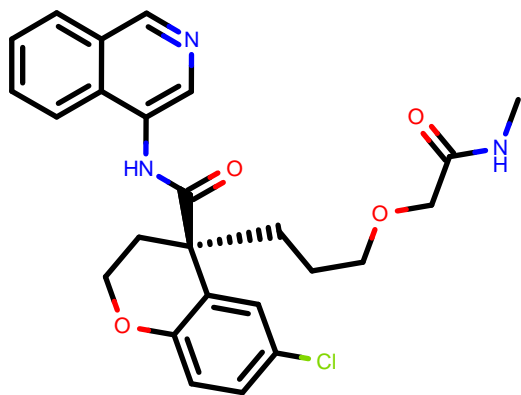
SMILES: c1ccc2c(c1)cnc2NC(=O)C(C)C3(C)COC4C3C(=O)C(NC1=O)C1C@H5C[NH2+]C(C)C@H(O5)CO

RUN: RUN1431

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.41

EN300-2977549_4_1_1



CID: EN300-2977549_4_1_1

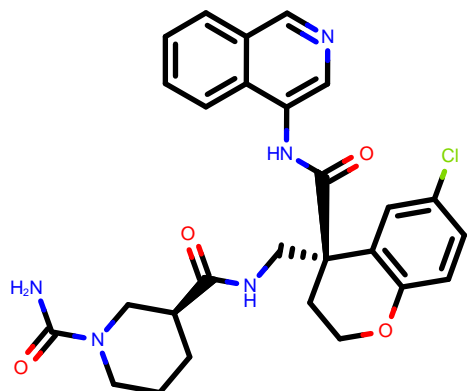
SMILES: CNC(=O)COCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN4392

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.30

EN300-14767_2_2_1



CID: EN300-14767_2_2_1

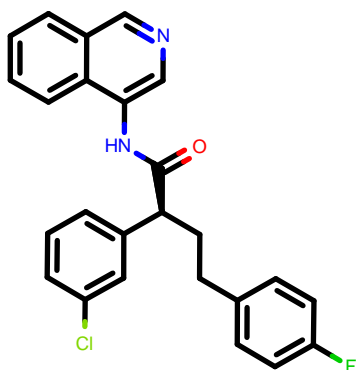
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCN(C5)C(=O)N

RUN: RUN5298

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.27

MIC-UNK-c66144cb-2_1



CID: MIC-UNK-c66144cb-2_1

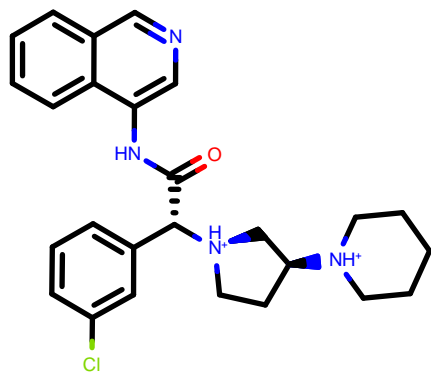
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc3)F)c4cccc(c4)Cl

RUN: RUN143

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.34

MIC-UNK-5a93dd5f-12_3



CID: MIC-UNK-5a93dd5f-12_3

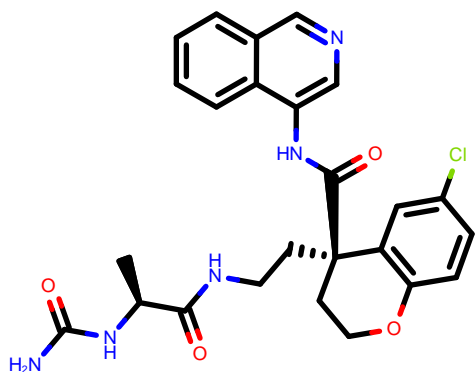
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc3)Cl)N@]4CC[C@]3(C4)N[+]5CCCCC5

RUN: RUN701

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.37

EN300-152705_3_1_1



CID: EN300-152705_3_1_1

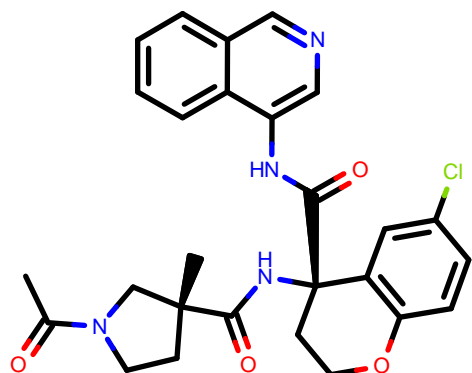
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)NC(=O)N

RUN: RUN4240

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.28

EN300-98018_1_1_1



CID: EN300-98018_1_1_1

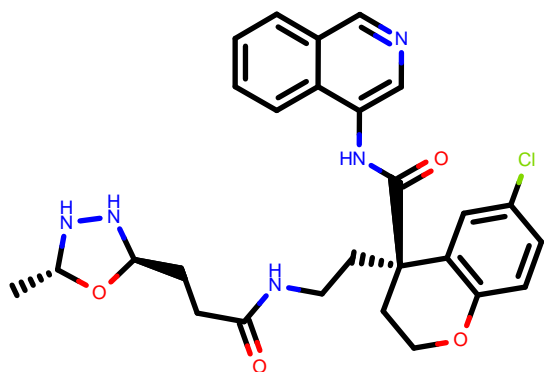
SMILES: CC(=O)N1CC[C@@](C1)(C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3666

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.36

EN300-304662_3_1_3



CID: EN300-304662_3_1_3

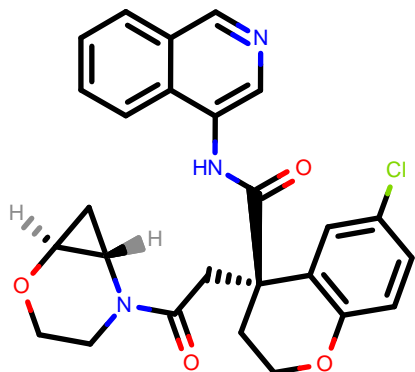
SMILES: C[C@@H]1NN[C@H](O1)CCCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7001

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.33

EN300-91609_1_1_1



CID: EN300-91609_1_1_1

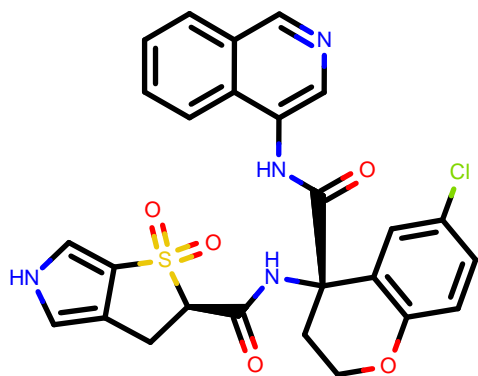
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H]6[C@@H]5C6

RUN: RUN6411

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.27

EN300-7445396_1_2_1



CID: EN300-7445396_1_2_1

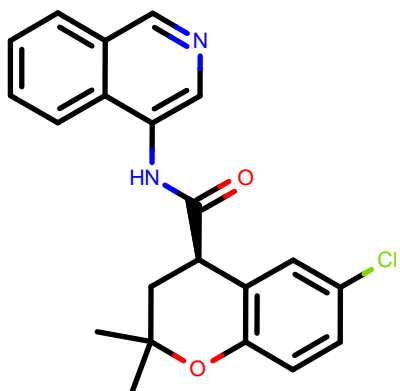
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@[3](CCOc4ccc(cc4)Cl)NC(=O)C@H]5Cc6c[nH]sc6S5(=O)=O

RUN: RUN2951

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.45

ADA-UCB-dc2b944c-16_1_1



CID: ADA-UCB-dc2b944c-16_1_1

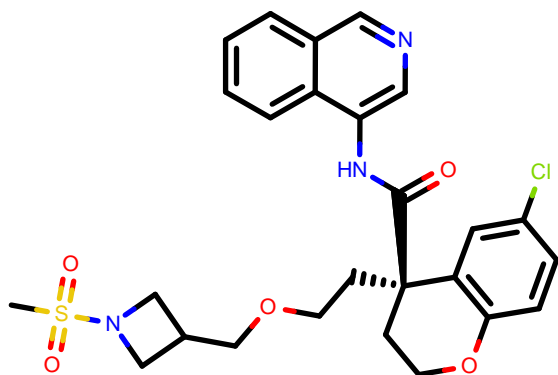
SMILES: CC1(C)[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3ccc4)C

RUN: RUN5395

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.10

EN300-302290_3_1_1



CID: EN300-302290_3_1_1

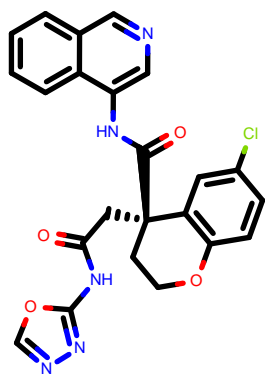
SMILES: CS(=O)(=O)N1CC(C1)COC[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN5772

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.33

EDJ-MED-d203f206-1_1



CID: EDJ-MED-d203f206-1_1

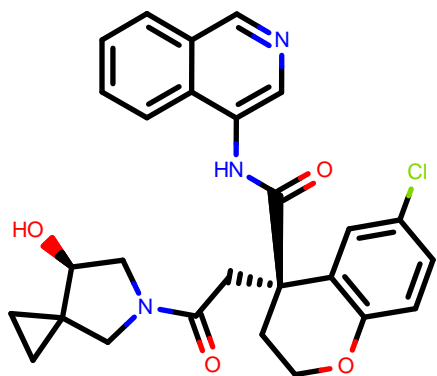
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@[3](CCOc4ccc(cc4)Cl)CC(=O)Nc5nnc5

RUN: RUN2380

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.22

EN300-142333_1_1_1



CID: EN300-142333_1_1_1

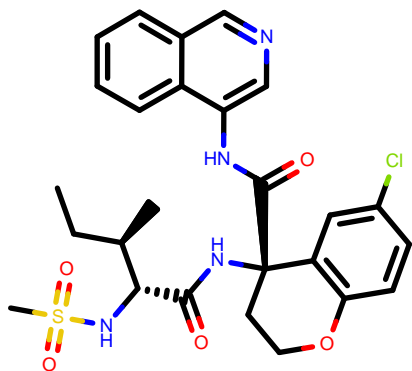
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H](C6(C5)CC6)O

RUN: RUN5376

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.27

EN300-76541_1_3_1



CID: EN300-76541_1_3_1

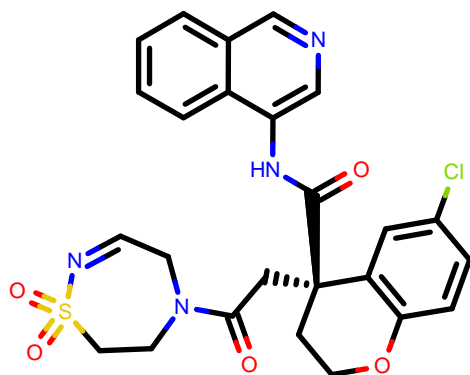
SMILES: CC[C@@H](C)[C@@H](C)N(C)C(=O)N1(CCOc2c1ccccc2)C(=O)Nc3ccc4c3ccc4NS(=O)(=O)C

RUN: RUN2743

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.47

EN300-6489145_1_1_1



CID: EN300-6489145_1_1_1

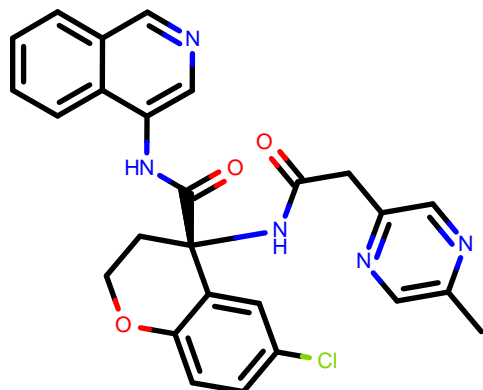
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNS(=O)(=O)CC5

RUN: RUN6467

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.33

EN300-1709295_1_1_1



CID: EN300-1709295_1_1_1

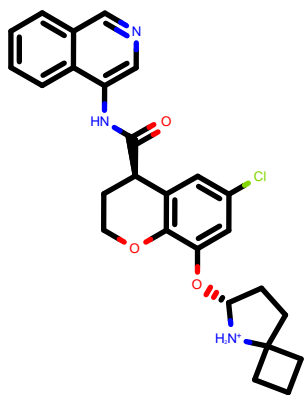
SMILES: Cc1nc(cn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN5449

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.27

DAR-DIA-23e5a6a0-1_1_1



CID: DAR-DIA-23e5a6a0-1_1_1

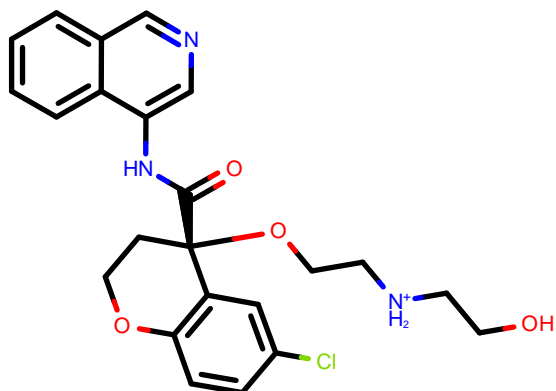
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4O)[C@@H]5CCCC6([NH2+][5])CC6)Cl

RUN: RUN6217

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.36

ED_-GRI-5b13fbe2-30_1



CID: ED_-GRI-5b13fbe2-30_1

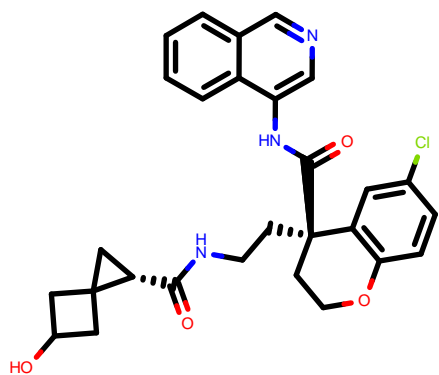
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+][CCO]

RUN: RUN1410

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.58

EN300-1717166_3_2_1



CID: EN300-1717166_3_2_1

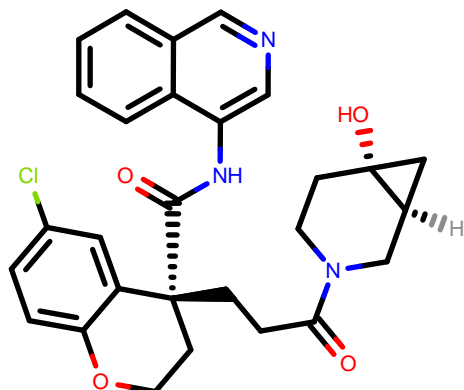
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC56C(C)C6)O

RUN: RUN4831

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.31

EN300-303908_2_1_1



CID: EN300-303908_2_1_1

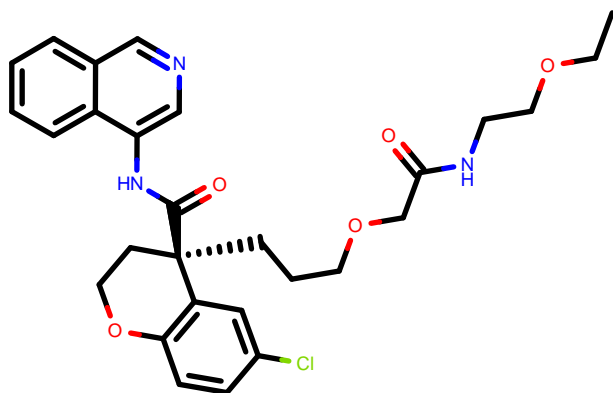
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@]6(C)[C@H]6C5)O

RUN: RUN5811

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.26

EN300-103187_4_1_1



CID: EN300-103187_4_1_1

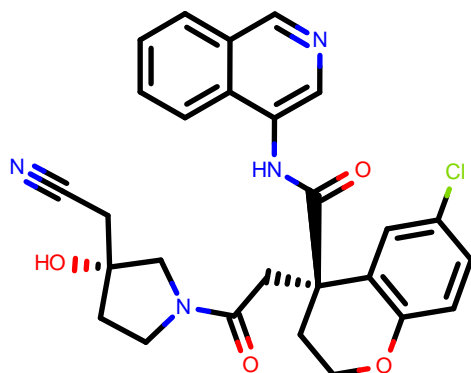
SMILES: CCOCCNC(=O)COC[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6823

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.35

EN300-257405_1_2_1



CID: EN300-257405_1_2_1

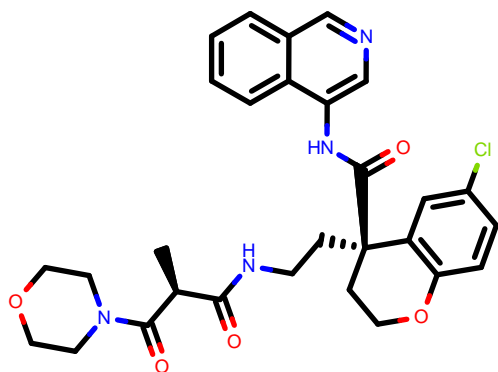
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)Cl)CC(=O)N5CC[C@]1(C5)CC#N1O

RUN: RUN5005

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.33

EN300-2855057_3_1_1



CID: EN300-2855057_3_1_1

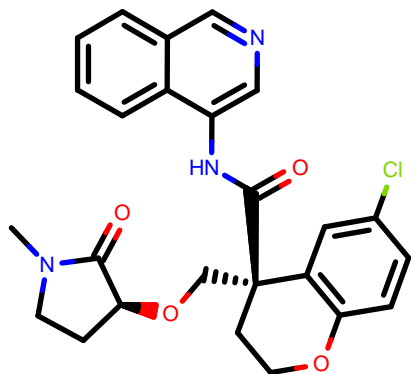
SMILES: C[C@@H](Cl)C(=O)NCC[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)C(=O)N5CCOCC5

RUN: RUN7775

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.45

EN300-98648_2_1_1



CID: EN300-98648_2_1_1

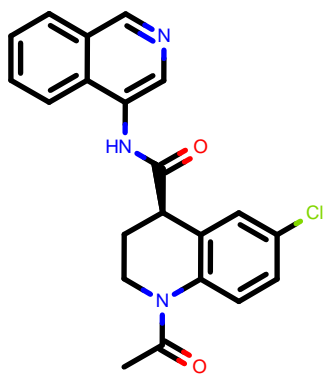
SMILES: CN1CC[C@@H](Cl)C(=O)OC[C@]2(C)COCc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3997

DDG (kcal/mol): -0.35

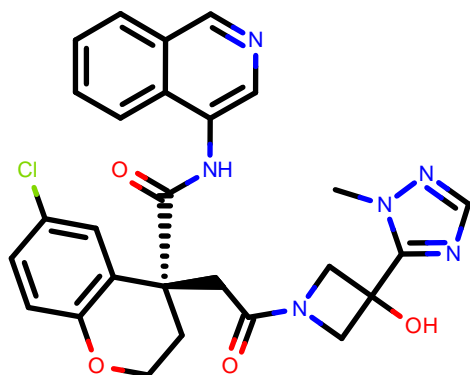
dDDG (kcal/mol): 0.24

RAL-THA-c11c1343-1_2



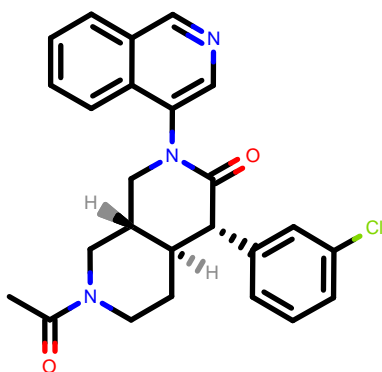
CID:	RAL-THA-c11c1343-1_2
SMILES:	<chem>CC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN1121
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.24

EN300-381149_1_1_1



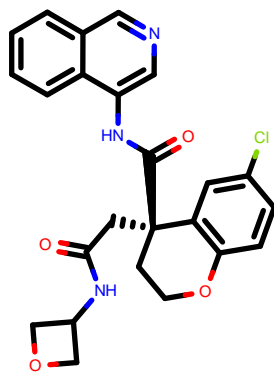
CID:	EN300-381149_1_1_1
SMILES:	<chem>Cn1c(ncn1)C2(CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6)O</chem>
RUN:	RUN5963
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.32

MIC-UNK-9582b2c5-1_4



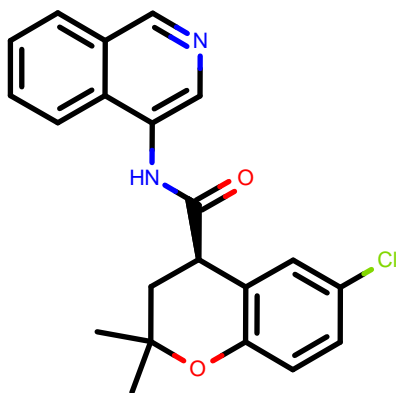
CID:	MIC-UNK-9582b2c5-1_4
SMILES:	<chem>CC(=O)N1CC[C@H]2[C@@H](C1)CN(C(=O)C)[C@@H]2c3cccc(c3)Cl)c4ncc5c4cccc5</chem>
RUN:	RUN199
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.28

EN300-49064_1_1_1



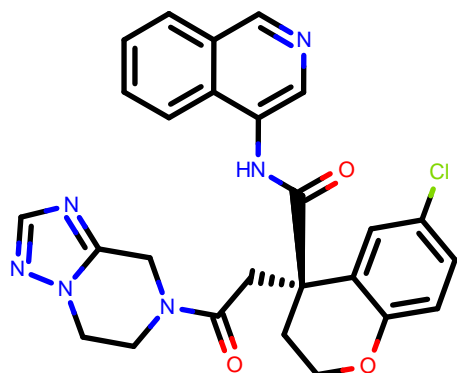
CID:	EN300-49064_1_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5COC5</chem>
RUN:	RUN7265
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.24

ADA-UCB-dc2b944c-16_1



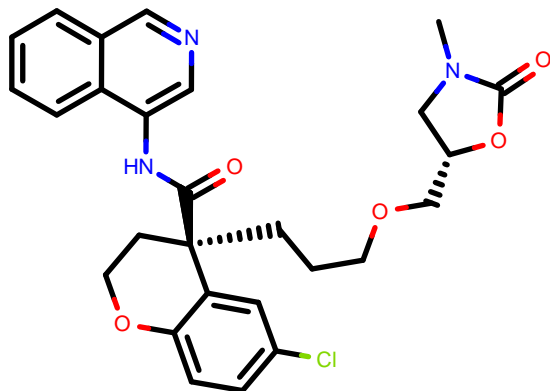
CID:	ADA-UCB-dc2b944c-16_1
SMILES:	<chem>CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C</chem>
RUN:	RUN557
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.09

EN300-141224_1_1_1



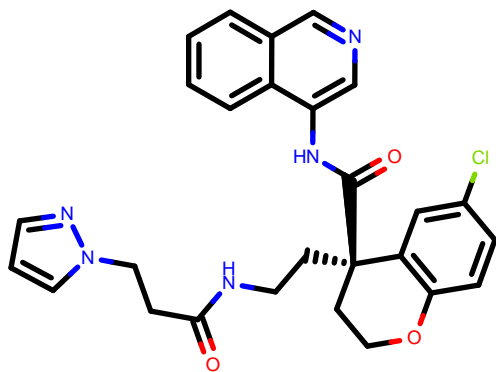
CID:	EN300-141224_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cn6c6n6c5</chem>
RUN:	RUN5407
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.28

EN300-222969_4_2_1



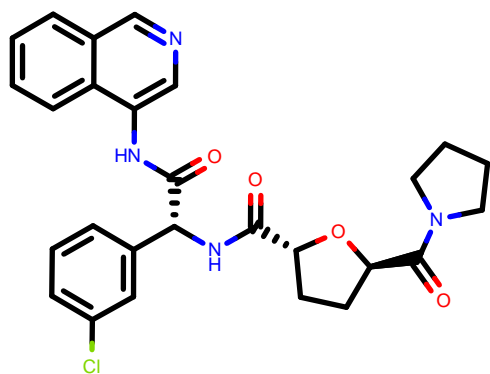
CID:	EN300-222969_4_2_1
SMILES:	<chem>CN1C[C@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5</chem>
RUN:	RUN7513
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.45

EN300-25986_3_1_1



CID:	EN300-25986_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn5</chem>
RUN:	RUN3710
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.29

EDJ-MED-ee07cf00-11_3



CID: EDJ-MED-ee07cf00-11_3

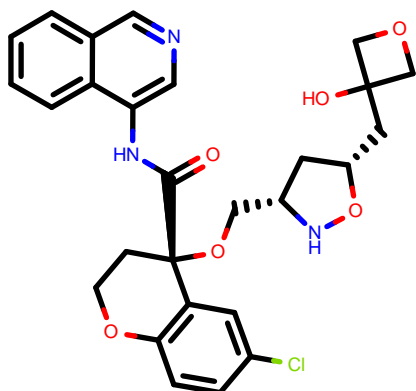
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)ccc3c3)C]NC(=O)[C@@H](Cl)CC[C@@H](O4)C1=O)N6CCCC5

RUN: RUN2682

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.40

EN300-7457160_1_2_1



CID: EN300-7457160_1_2_1

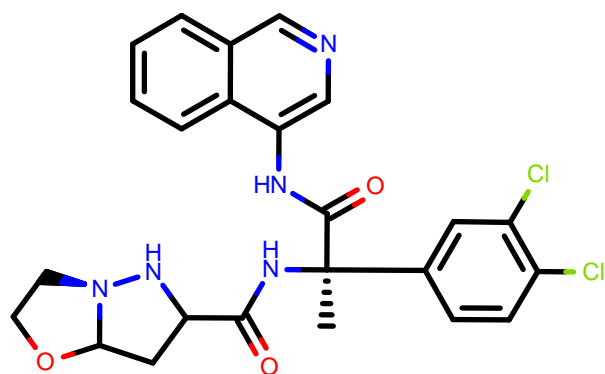
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)ccc3c3)C]NC(=O)[C@@H](Cl)CC[C@@H](O4)C1=O)N6CCCC5

RUN: RUN5703

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.32

MAT-POS-e9e99895-5_1



CID: MAT-POS-e9e99895-5_1

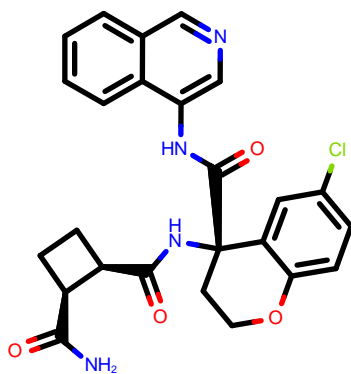
SMILES: C[C@@H](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2nc3c2ccc3)NC(=O)c4cc5n(n4)CCO5

RUN: RUN2074

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.33

EN300-217107_1_1_1



CID: EN300-217107_1_1_1

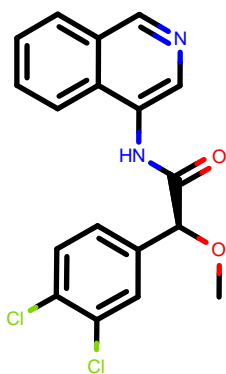
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)ccc3c3)C]NC(=O)[C@@H](Cl)CC[C@@H](O4)C1=O)N6CCCC5

RUN: RUN3317

DDG (kcal/mol): -0.34

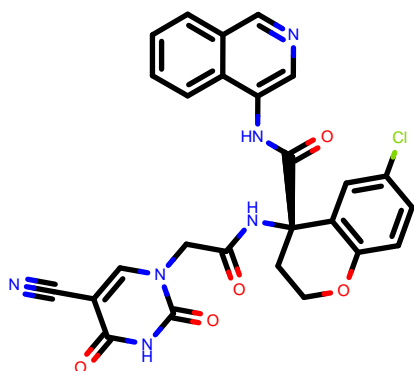
dDDG (kcal/mol): 0.27

MAT-POS-de59a476-2_1



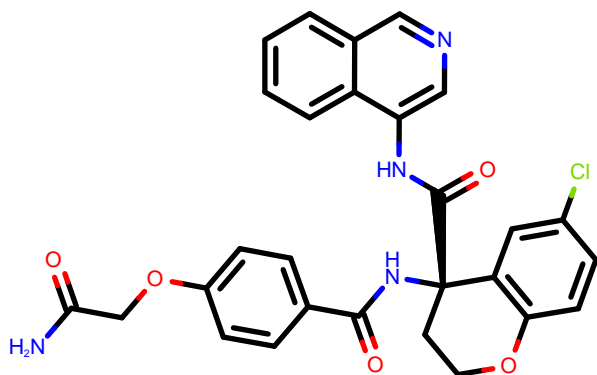
CID:	MAT-POS-de59a476-2_1
SMILES:	<chem>CO[C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN2038
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.29

ALP-UNI-dbbfd3db-11_1



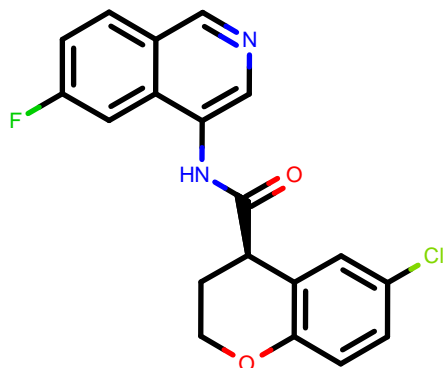
CID:	ALP-UNI-dbbfd3db-11_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(c(=O)[nH]c5=O)C#N</chem>
RUN:	RUN2615
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.35

EN300-14949_1_1_1



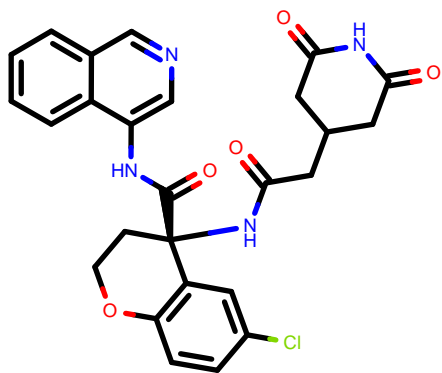
CID:	EN300-14949_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)OCC(=O)N</chem>
RUN:	RUN6182
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.31

EDG-MED-5d232de5-1_1



CID:	EDG-MED-5d232de5-1_1
SMILES:	<chem>c1cc2cncc(c2cc1F)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)</chem>
RUN:	RUN2191
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.04

EN300-225165_1_1_1



CID: EN300-225165_1_1_1

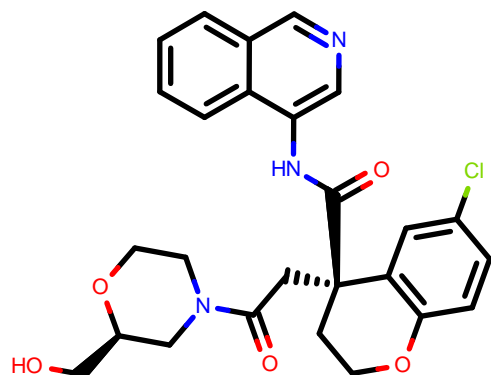
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)CC5CC(=O)NC(=O)C5

RUN: RUN4940

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.26

EN300-175487_1_1_1



CID: EN300-175487_1_1_1

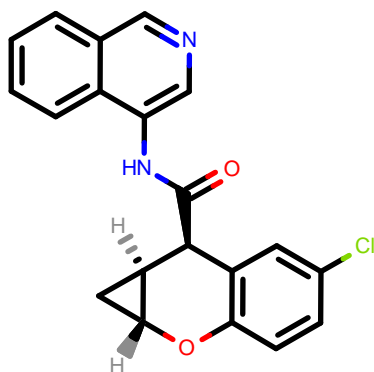
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CCO[C@@H](C5)CO

RUN: RUN4256

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.40

DAR-DIA-0d514e7d-33_4



CID: DAR-DIA-0d514e7d-33_4

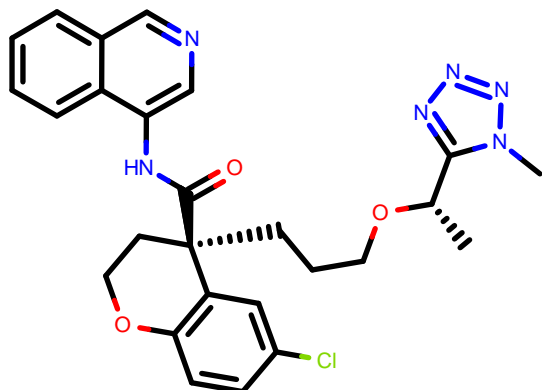
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3c4cc(cc4O[C@@H]5[C@@H]3C5)Cl

RUN: RUN779

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.24

EN300-173006_4_1_1



CID: EN300-173006_4_1_1

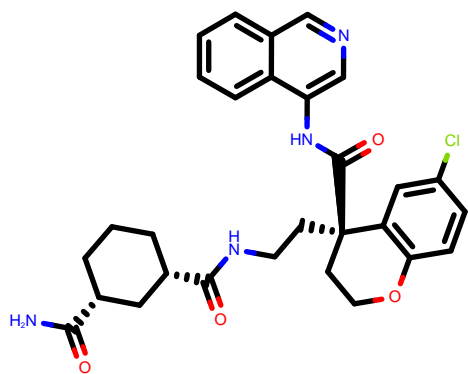
SMILES: C[C@@H](c1nncn1)OCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncnc5c4ccoc5

RUN: RUN6306

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.36

EN300-90142_3_4_1



CID: EN300-90142_3_4_1

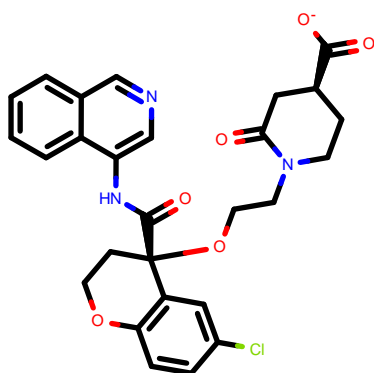
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCN(C=O)[C@@H]5CC[C@H](C5)Cl=O

RUN: RUN4037

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.31

ED_-GRI-5b13fbe2-46_1



CID: ED_-GRI-5b13fbe2-46_1

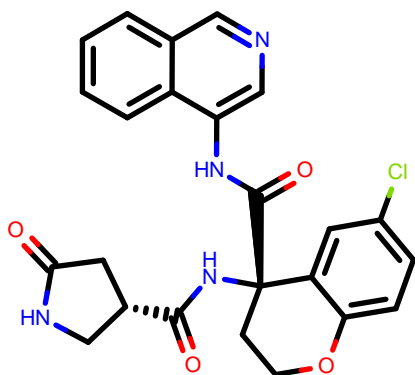
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)OCCN5CC[C@@H](CC5=O)C(=O)[O-]

RUN: RUN1461

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.53

EN300-59487_1_2_1



CID: EN300-59487_1_2_1

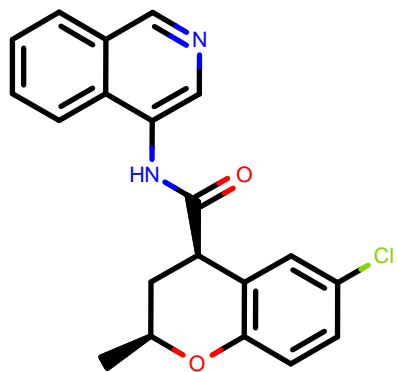
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)NC(=O)[C@@H]5CC(=O)N5

RUN: RUN5796

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.26

EDJ-MED-e4b030d8-3_1



CID: EDJ-MED-e4b030d8-3_1

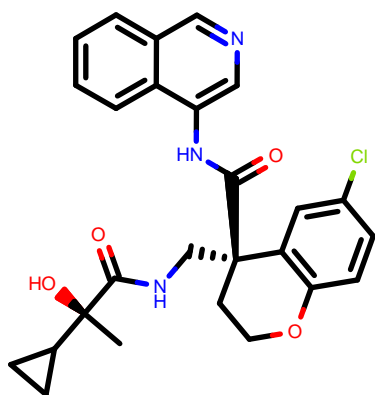
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN241

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.09

EN300-118760_2_2_1



CID: EN300-118760_2_2_1

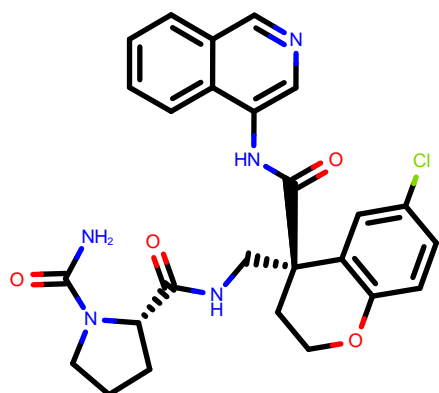
SMILES: C[C@]1(CC1)(C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7071

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.35

EN300-87536_2_1_1



CID: EN300-87536_2_1_1

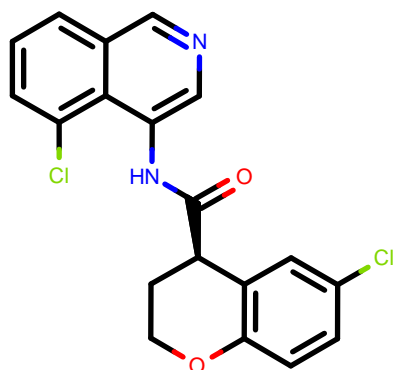
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]@H5CCCN5C(=O)N

RUN: RUN3450

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.34

BEN-DND-a7517465-3_1



CID: BEN-DND-a7517465-3_1

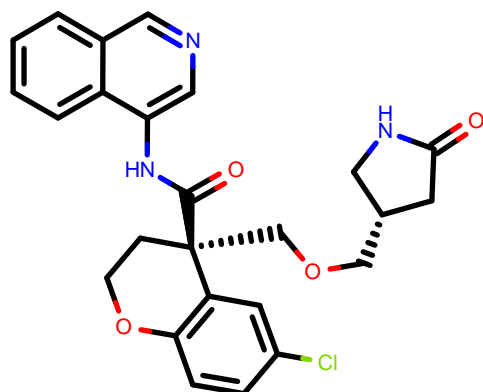
SMILES: c1cc2cncc(c2c(c1)Cl)NC(=O)[C@@]@H3CCOc4c3cc(cc4)Cl

RUN: RUN1287

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.22

EN300-246747_2_2_1



CID: EN300-246747_2_2_1

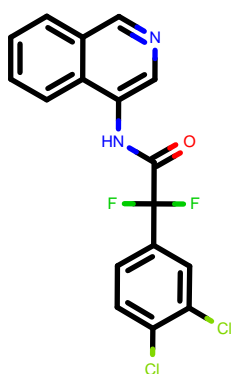
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]H5CC(=O)NCS

RUN: RUN5062

DDG (kcal/mol): -0.33

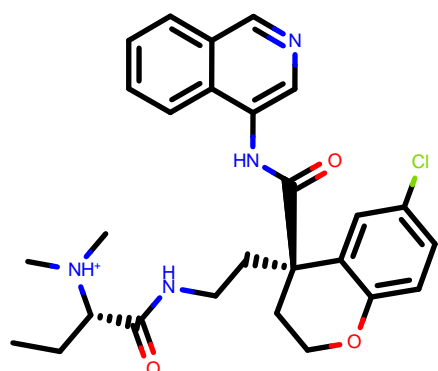
dDDG (kcal/mol): 0.24

MAT-POS-fce787c2-6_1



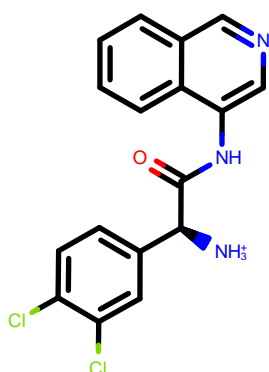
CID:	MAT-POS-fce787c2-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)C(c3ccc(c(c3)Cl)Cl)(F)F</chem>
RUN:	RUN1941
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.27

EN300-223964_3_1_1



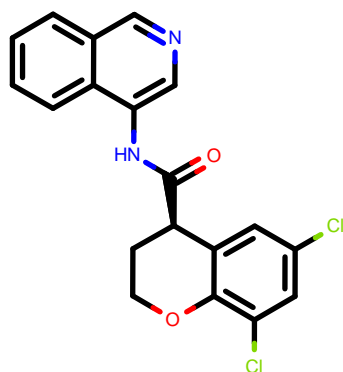
CID:	EN300-223964_3_1_1
SMILES:	<chem>CC[C@@H](C(=O)NCC[C@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)[NH+](C)C</chem>
RUN:	RUN5958
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.35

MAT-POS-1f3f1a6f-1_2



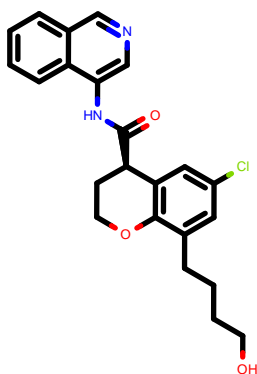
CID:	MAT-POS-1f3f1a6f-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)[NH3+]</chem>
RUN:	RUN2091
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.36

ALP-UNI-3735e77e-2_1



CID:	ALP-UNI-3735e77e-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4Cl)Cl</chem>
RUN:	RUN1781
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.08

LAU-MED-88a3970a-7_1



CID: LAU-MED-88a3970a-7_1

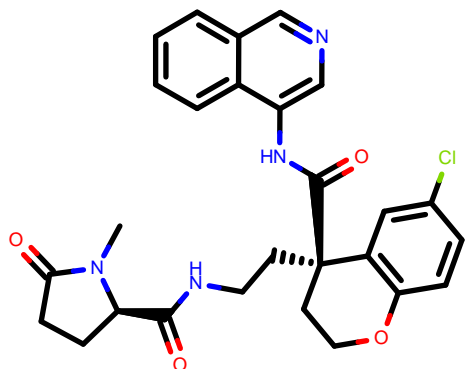
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4CCCCO)Cl

RUN: RUN1351

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.18

EN300-132963_3_2_1



CID: EN300-132963_3_2_1

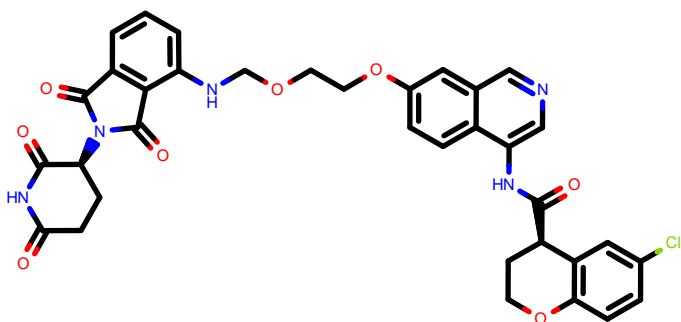
SMILES: CN1[C@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5920

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.30

DAR-DIA-9e4459de-13_7



CID: DAR-DIA-9e4459de-13_7

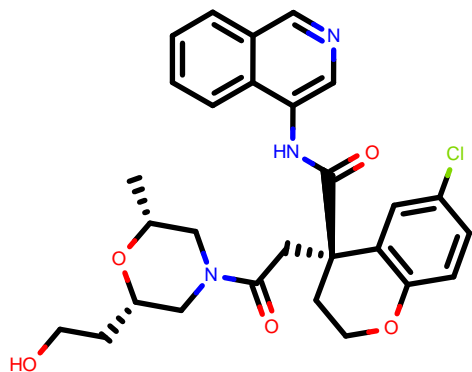
SMILES: c1cc2c(c1)NCOCCO3ccc4c(c3)cncc4NC(=O)[C@]5(C@H)SCOCc6c5cc(cc6)Cl)c1c(c2O)[C@H]7CCCl7=O

RUN: RUN1325

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.33

EN300-212814_1_1_1



CID: EN300-212814_1_1_1

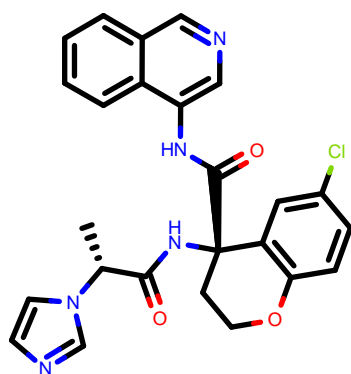
SMILES: C[C@]5(H)CN(C[C@]5[H](O1)COC1C(=O)C[C@]2(COC3c32cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6068

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.32

EDG-MED-90036822-60_2



CID: EDG-MED-90036822-60_2

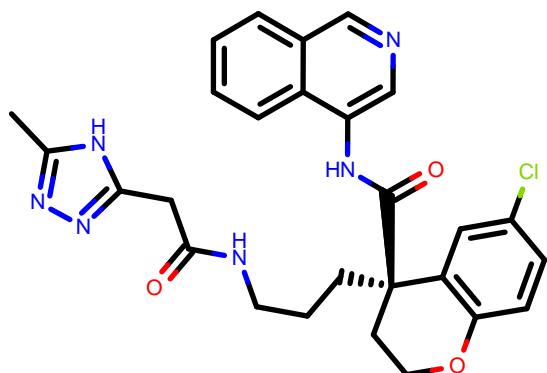
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)n5ccnc5

RUN: RUN1608

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.24

EN300-119126_4_1_1



CID: EN300-119126_4_1_1

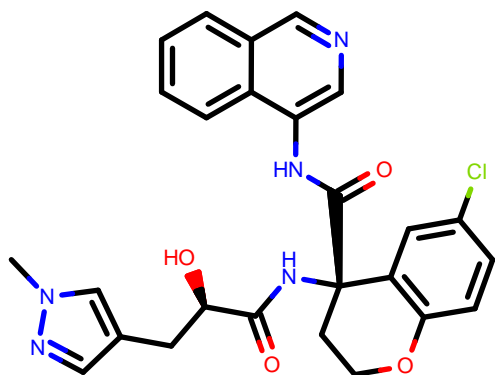
SMILES: Cc1[nH]nc(n1)CC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6479

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.38

EN300-172020_1_2_1



CID: EN300-172020_1_2_1

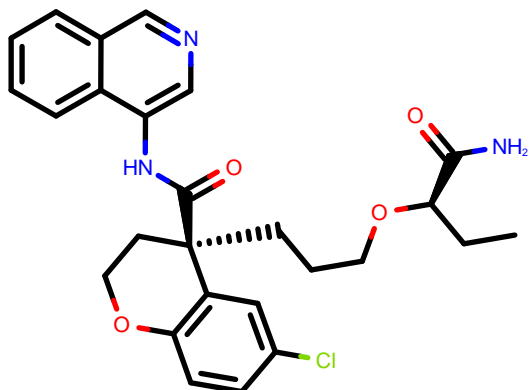
SMILES: Cn1cc(en1)C[C@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN6385

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.29

EN300-65839_4_2_1



CID: EN300-65839_4_2_1

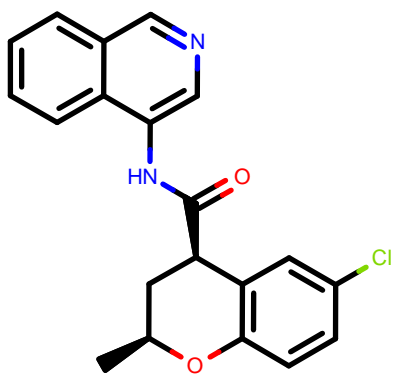
SMILES: CC[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4669

DDG (kcal/mol): -0.33

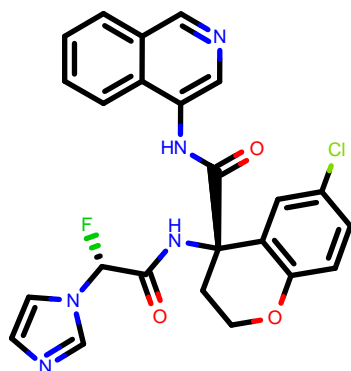
dDDG (kcal/mol): 0.40

ALP-POS-d3acb8cc-1_1



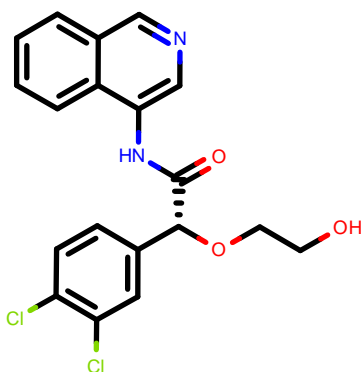
CID:	ALP-POS-d3acb8cc-1_1
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1008
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.09

EDG-MED-90036822-36_2



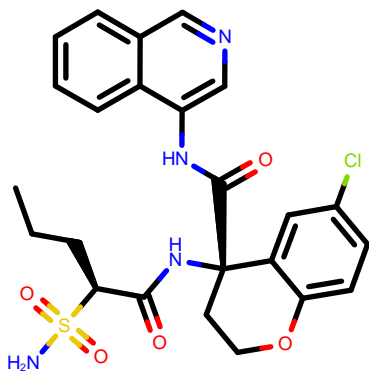
CID:	EDG-MED-90036822-36_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](n5cncc5)F</chem>
RUN:	RUN1564
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.23

MAT-POS-de59a476-5_1



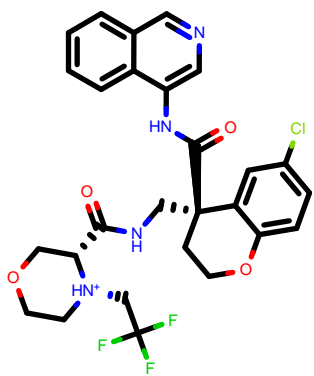
CID:	MAT-POS-de59a476-5_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO</chem>
RUN:	RUN2073
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.35

EN300-206592_1_1_1



CID:	EN300-206592_1_1_1
SMILES:	<chem>CCC[C@@]3(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N</chem>
RUN:	RUN7065
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.23

EN300-201551_2_2_1



CID: EN300-201551_2_2_1

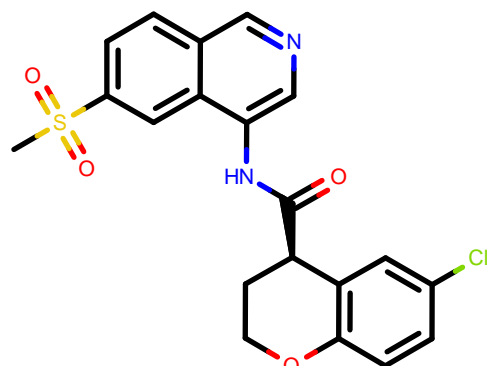
SMILES: c1ccc2c(e1)ncnc2NC(=O)C(C(F)(F)F)C1CCN(C1)C(=O)C1=CC=C(C=C1)Cl

RUN: RUN6105

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.34

BEN-DND-c852c98b-5_1_1



CID: BEN-DND-c852c98b-5_1_1

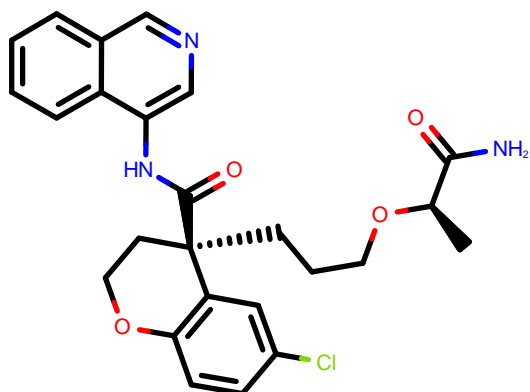
SMILES: CS(=O)(=O)c1ccc2ncnc(c2c1)NC(=O)C1=CC=C(C=C1)Cl

RUN: RUN7628

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.09

EN300-17381_4_2_1



CID: EN300-17381_4_2_1

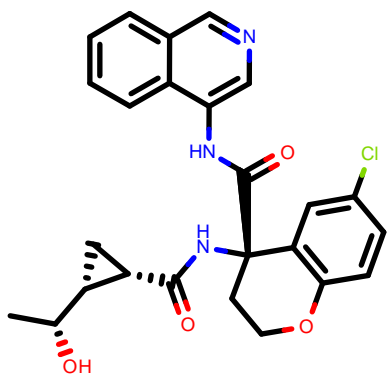
SMILES: C[C@H](C(=O)N)OCC[C@]1(C)CCOc2c1cc(cc2)C1C(=O)Nc3ncnc4c3cccc4

RUN: RUN4003

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.31

EN300-6729572_1_2_1



CID: EN300-6729572_1_2_1

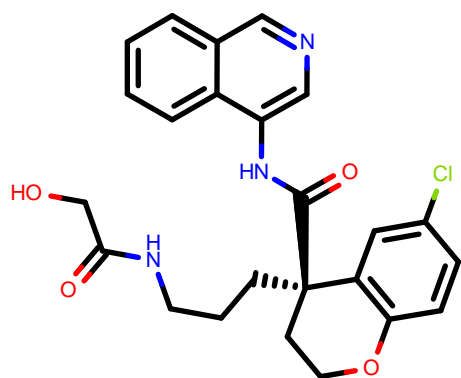
SMILES: C[C@H](C1=CC=C(C=C1)C1=CC=C(C=C1)C(=O)N)C1=CC=C(C=C1)C1=CC=C(C=C1)C(=O)Nc2ncnc3c2cccc3O

RUN: RUN4528

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.22

EN300-19242_4_1_1



CID: EN300-19242_4_1_1

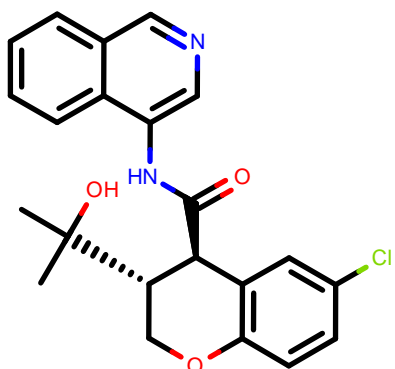
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CO

RUN: RUN4041

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.32

BEN-BAS-5c03e89e-1_2



CID: BEN-BAS-5c03e89e-1_2

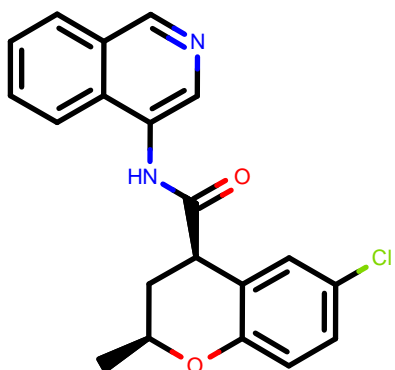
SMILES: CC(C)(C)[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cnc4c3ccc4)Cl)O

RUN: RUN1073

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.11

EDJ-MED-e4b030d8-3_1_1



CID: EDJ-MED-e4b030d8-3_1_1

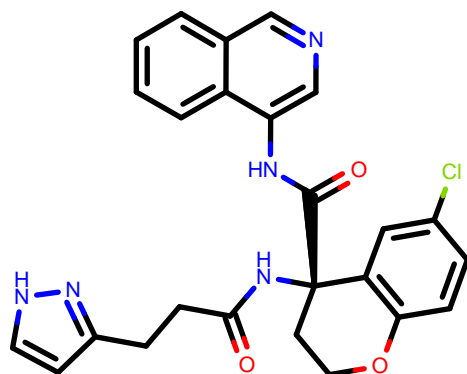
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3ccc4

RUN: RUN5751

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.09

EN300-1664603_1_1_1



CID: EN300-1664603_1_1_1

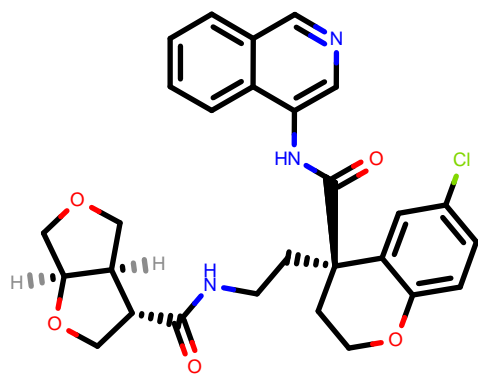
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5cnc[nH]5

RUN: RUN4540

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.21

EN300-6482296_3_5_1



CID: EN300-6482296_3_5_1

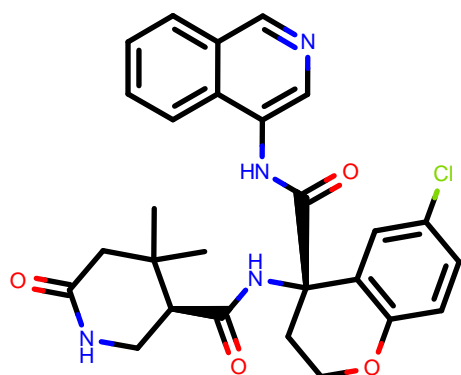
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(C)CNC(=O)[C@@H]5C[C@@H]5COC6

RUN: RUN6050

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.31

EN300-1212475_1_1_1



CID: EN300-1212475_1_1_1

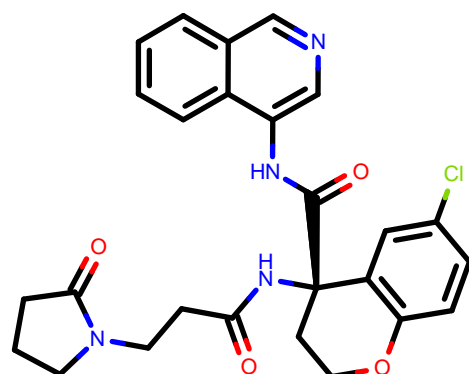
SMILES: CC1(CC(=O)NC[C@@H]1C(=O)N[C@@]2(COCc3cc2cc3)C)C(=O)Nc4cnc5c4cccc5)C

RUN: RUN5911

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.24

EN300-67191_1_1_1



CID: EN300-67191_1_1_1

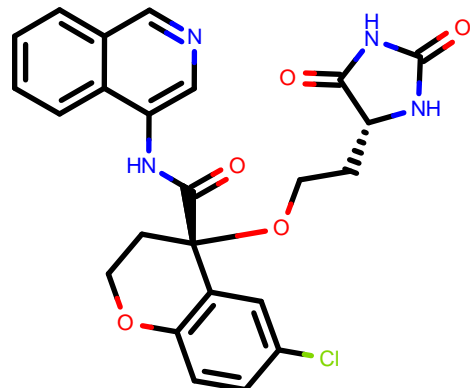
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C)N(C(=O)CN5CCCC5=O

RUN: RUN7721

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.27

EN300-6498856_1_1_1



CID: EN300-6498856_1_1_1

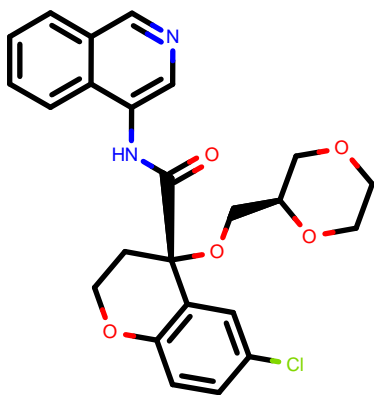
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C)OCC[C@@H]5C(=O)NC(=O)N5

RUN: RUN6316

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.24

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5COCOC5

RUN:

RUN4574

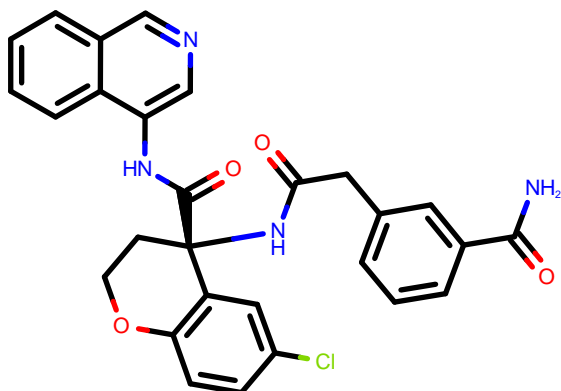
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.23

EN300-1179673_1_1_1



CID: EN300-1179673_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(N)cc5C(=O)N

RUN:

RUN5752

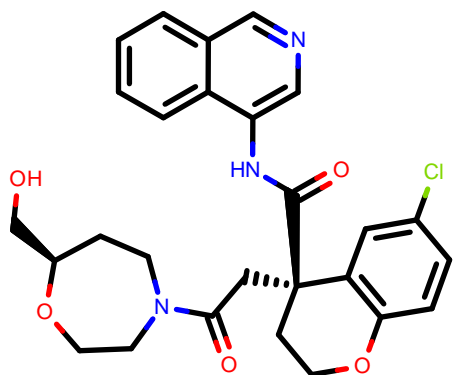
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.29

EN300-2007620_1_1_1



CID: EN300-2007620_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](OCC5)CO

RUN:

RUN6142

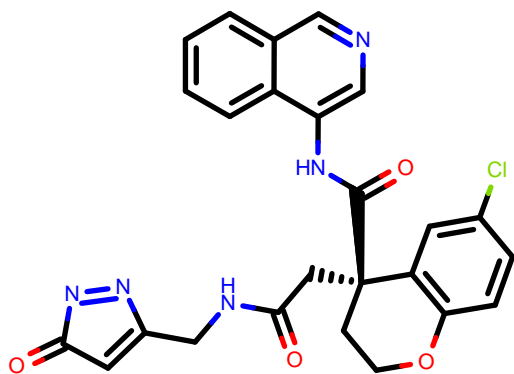
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.29

EN300-260760_1_1_1



CID: EN300-260760_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5cnc(=O)[nH]5

RUN:

RUN7049

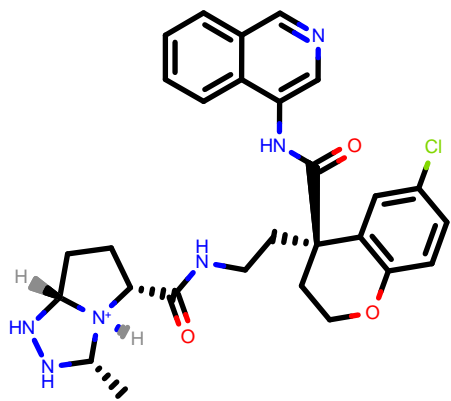
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.28

EN300-6489289_3_2_3



CID: EN300-6489289_3_2_3

SMILES:

C[C@@H]1NN[C@@H]2N[BH+]1[C@@H](CC2)C(=O)NC[C@@]3(C)CCO=C3C(=O)C(C)C(=O)N5CCCC5

RUN:

RUN4661

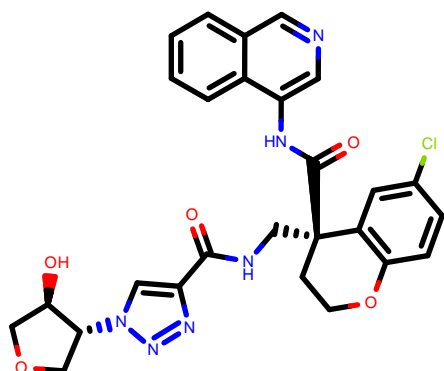
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.42

EN300-637424_2_1_1



CID: EN300-637424_2_1_1

SMILES:

C1CC(O)C1N2C=NC=C2N[C@@H](C)C(=O)NC[C@@]3(C)CCO=C3C(=O)C(C)C(=O)N5CCCC5

RUN:

RUN6612

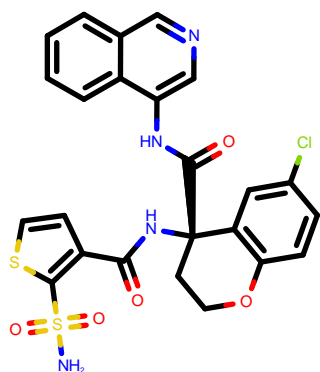
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.37

EN300-294602_1_1_1



CID: EN300-294602_1_1_1

SMILES:

C1CC(O)C1N2C=NC=C2N[C@@H](C)C(=O)NC[C@@]3(C)CCO=C3C(=O)C(C)C(=O)N5CCCC5

RUN:

RUN3264

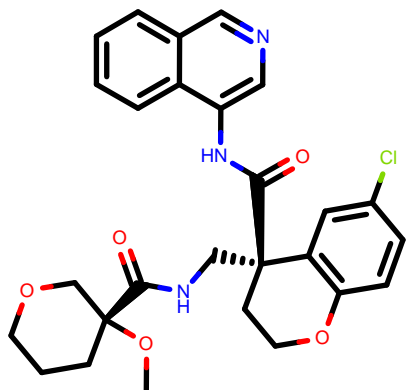
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.26

EN300-1072199_2_1_1



CID: EN300-1072199_2_1_1

SMILES:

COC1CCOC1N[C@@H](C)C(=O)NC[C@@]2(C)CCO=C2C(=O)C(C)C(=O)N3CCCC3

RUN:

RUN7461

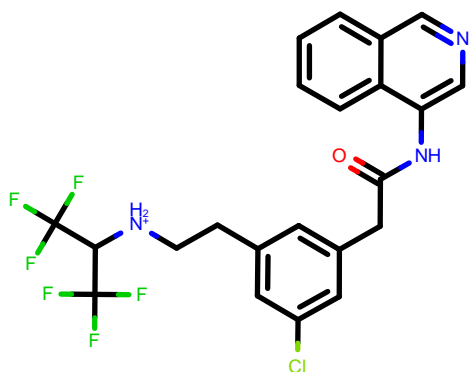
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.32

MIC-UNK-644c43c7-2_1



CID: MIC-UNK-644c43c7-2_1

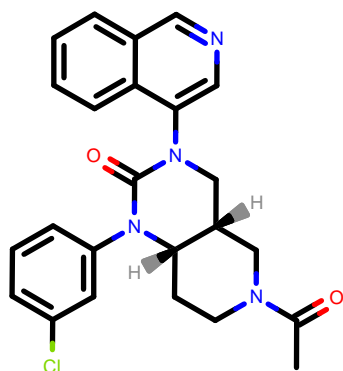
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CCNC(C(F)F)F(C(F)F)F

RUN: RUN420

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.52

MIC-UNK-9582b2c5-3_2



CID: MIC-UNK-9582b2c5-3_2

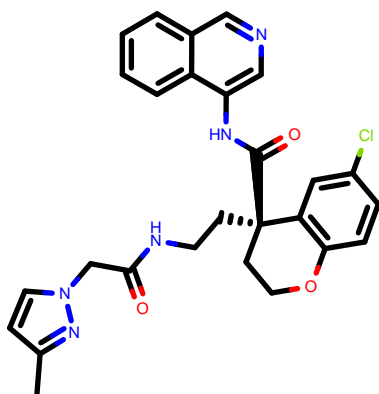
SMILES: CC(=O)N1CC[C@H]2[C@@H](C1)CN(C(=O)N2c3ccc(c3)Cl)c4cncc5c4cccc5

RUN: RUN192

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.37

EN300-226964_3_1_1



CID: EN300-226964_3_1_1

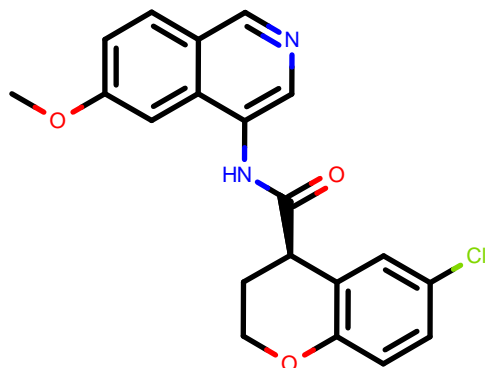
SMILES: Cc1ccn(n1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4209

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.26

MAT-POS-f9802937-7_1



CID: MAT-POS-f9802937-7_1

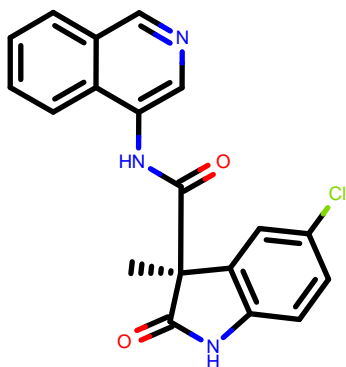
SMILES: COc1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2231

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.06

EDJ-MED-9e38fd34-1_1



CID: EDJ-MED-9e38fd34-1_1

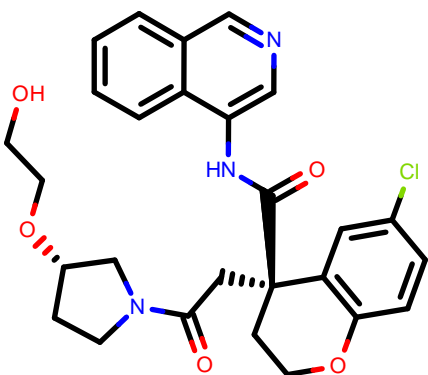
SMILES: C[C@@]1(c2cc(ccc2NC(=O)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2179

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

EN300-6764893_1_1_1



CID: EN300-6764893_1_1_1

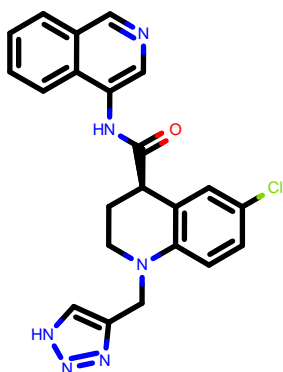
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)OCCO

RUN: RUN7288

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.32

RAL-THA-8416115c-14_3



CID: RAL-THA-8416115c-14_3

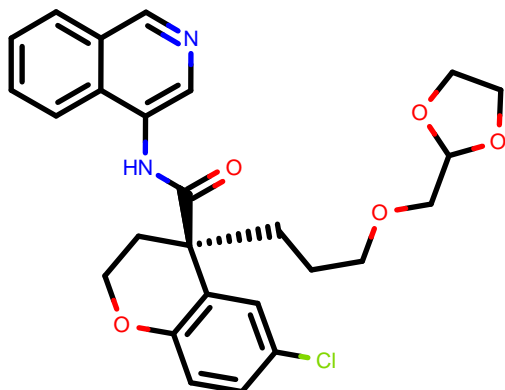
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3CCCN(c4c3cc(cc4)Cl)Cc5cn[nH]5

RUN: RUN1201

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.29

EN300-77092_4_1_1



CID: EN300-77092_4_1_1

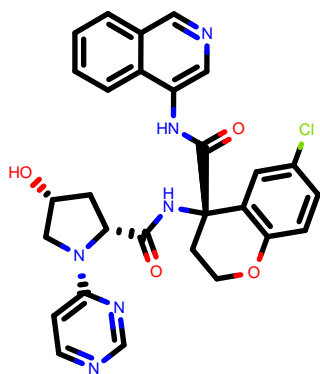
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5OCCO5

RUN: RUN6019

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.36

EN300-310022_1_4_1



CID: EN300-310022_1_4_1

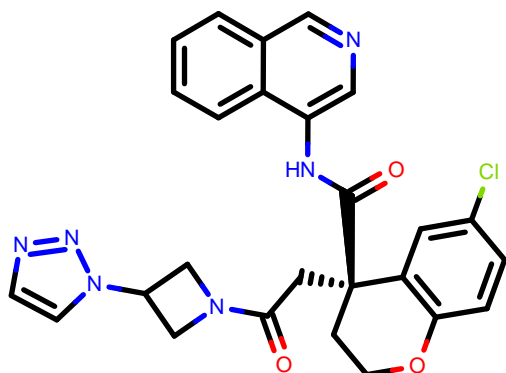
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)C@H)C(C@H)CN5c6ccccc6O

RUN: RUN4463

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.30

EN300-367405_1_1_1



CID: EN300-367405_1_1_1

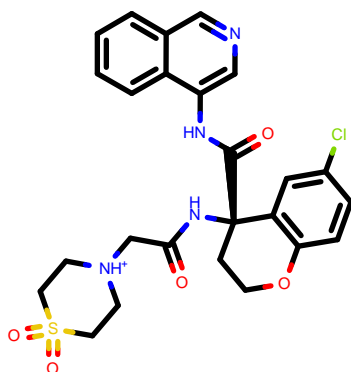
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6ccccc6

RUN: RUN7247

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

EN300-39305_1_1_1



CID: EN300-39305_1_1_1

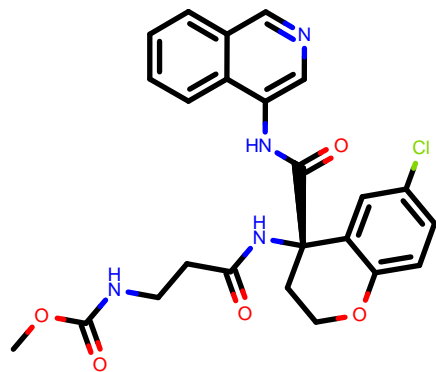
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)CN5CCS(=O)(=O)C5

RUN: RUN6636

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.30

EN300-71558_1_1_1



CID: EN300-71558_1_1_1

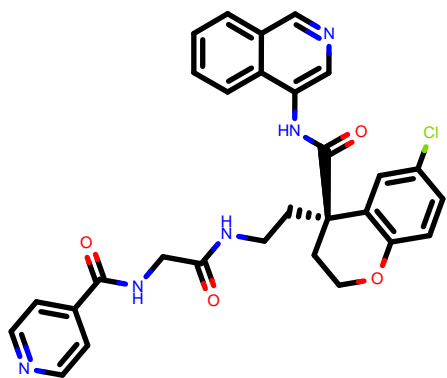
SMILES: COC(=O)NCCC(=O)N[C@@]1(C)CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN5520

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.23

EN300-36089_3_1_1



CID: EN300-36089_3_1_1

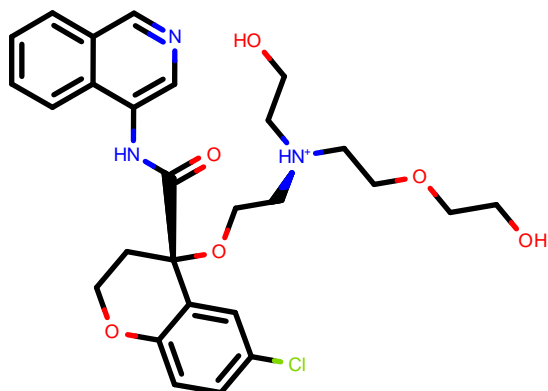
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CNC(=O)c5ccncc5

RUN: RUN4988

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.39

ED_-GRI-5b13fbe2-12_1



CID: ED_-GRI-5b13fbe2-12_1

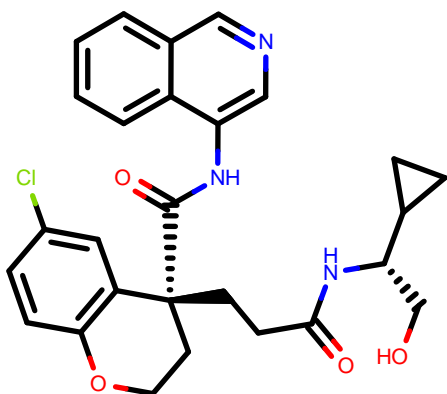
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC[N@@H](CO)CCOCCO

RUN: RUN1445

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.88

EN300-77885_2_1_1



CID: EN300-77885_2_1_1

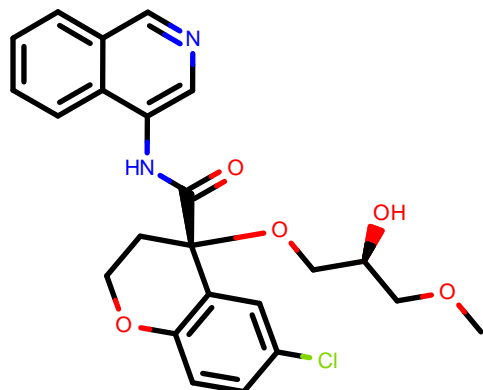
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H](CO)C5CC5

RUN: RUN5334

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.28

EN300-1915260_1_1_1



CID: EN300-1915260_1_1_1

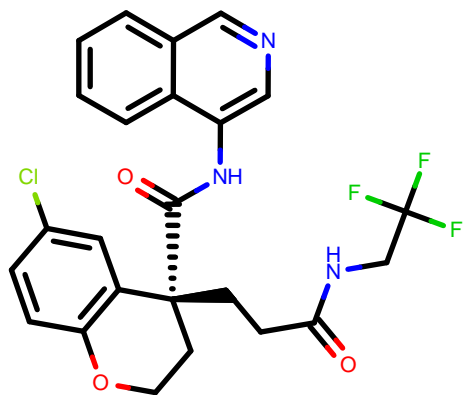
SMILES: COC[C@@H](CO)[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4O

RUN: RUN5641

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.39

JAG-UCB-706446eb-1_1_1



CID: JAG-UCB-706446eb-1_1_1

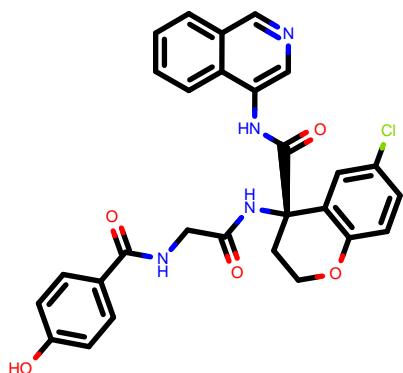
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCC(F)(F)F

RUN: RUN7061

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.22

EN300-66800_1_1_1



CID: EN300-66800_1_1_1

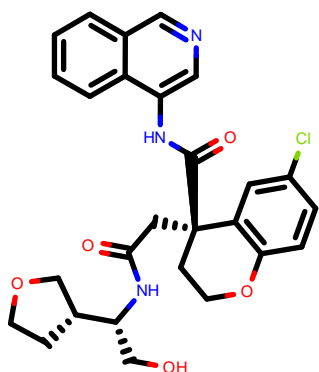
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)c5ccc(O)cc5

RUN: RUN7382

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.33

EN300-104493_1_2_1



CID: EN300-104493_1_2_1

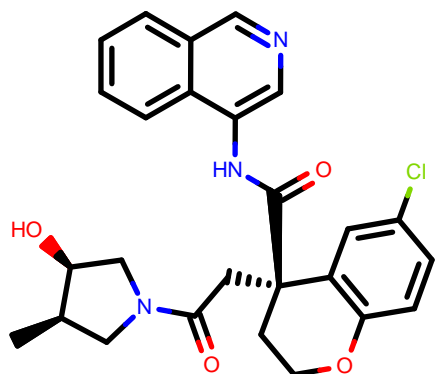
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@H](CO)[C@@]5H5COC5

RUN: RUN6177

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.35

EN300-124052_1_1_1



CID: EN300-124052_1_1_1

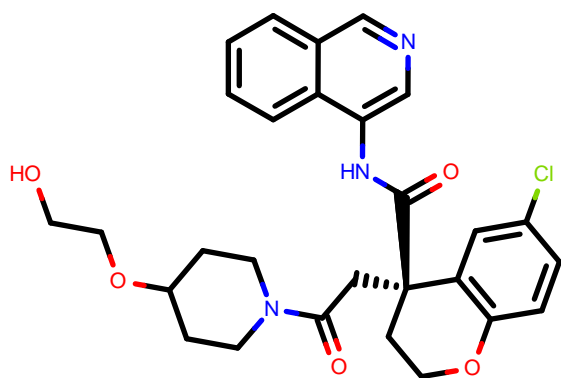
SMILES: C[C@@]1CN(C[C@@]1O)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7103

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.33

EN300-104088_1_1_1



CID: EN300-104088_1_1_1

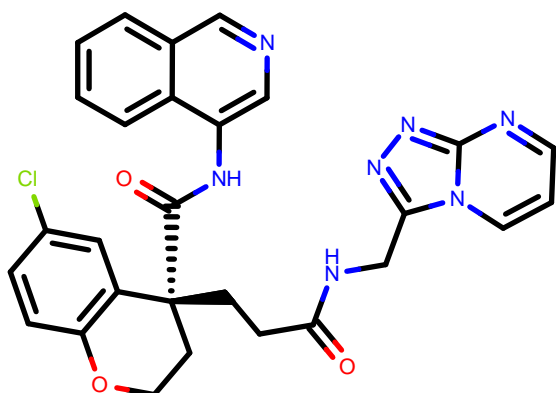
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C)CC5)OCCO

RUN: RUN6447

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.30

EN300-61021_2_1_1



CID: EN300-61021_2_1_1

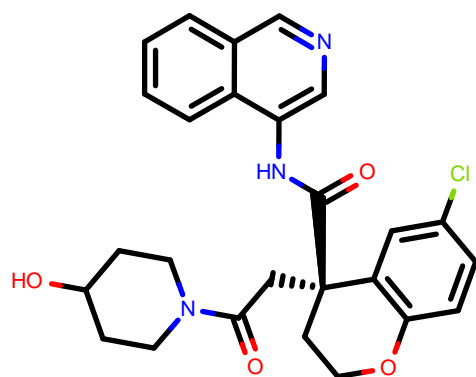
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC5nn6n5cccn6

RUN: RUN6236

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.27

EN300-379533_1_1_1



CID: EN300-379533_1_1_1

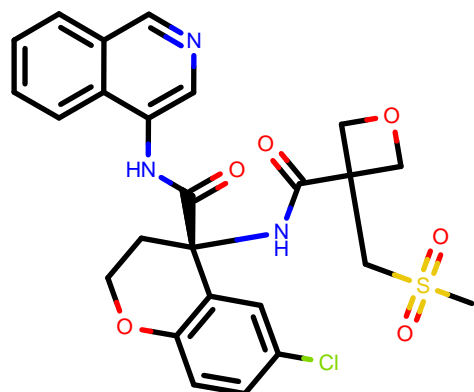
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C)CC5)O

RUN: RUN6248

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-262204_1_1_1



CID: EN300-262204_1_1_1

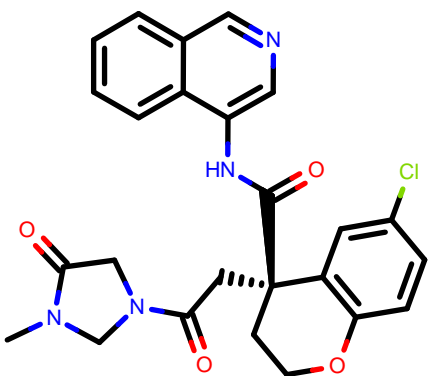
SMILES: CS(=O)(=O)CC1(COC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN7819

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.34

EN300-126548_1_1_1



CID: EN300-126548_1_1_1

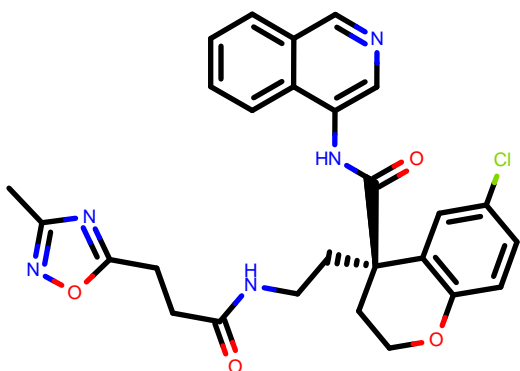
SMILES: CN1CN(CC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN7341

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

EN300-27268_3_1_1



CID: EN300-27268_3_1_1

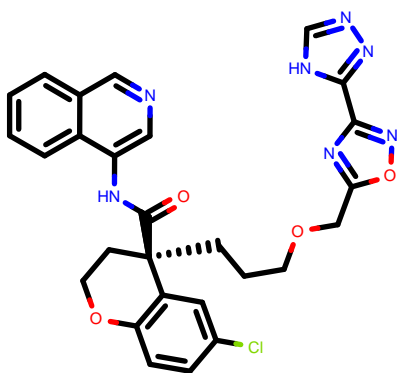
SMILES: Cc1nc(on1)CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6322

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.29

EN300-92031_4_1_1



CID: EN300-92031_4_1_1

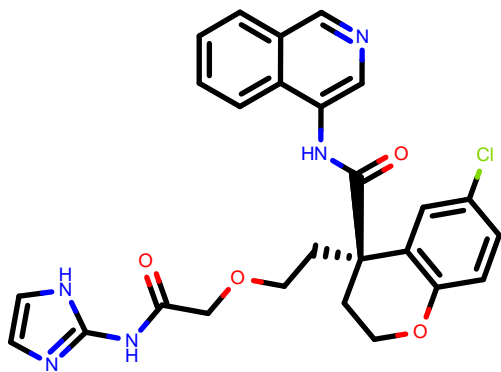
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5ncc6[nH]ncn6

RUN: RUN7263

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-331993_3_1_1



CID: EN300-331993_3_1_1

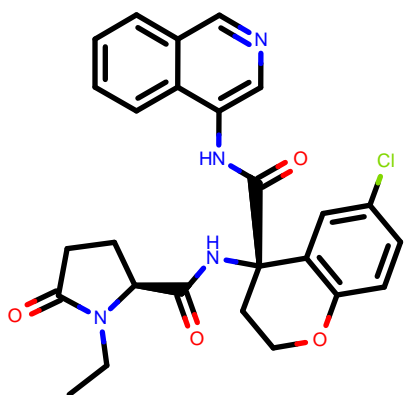
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5[nH]ncn5

RUN: RUN4036

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.24

EN300-718785_1_1_1



CID: EN300-718785_1_1_1

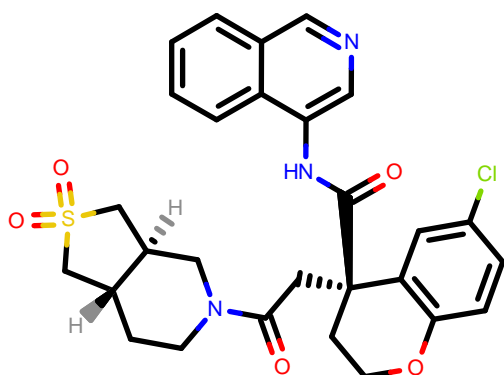
SMILES: CCN1[C@@H](CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN4484

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.26

KAD-UNI-80f122c8-3_5



CID: KAD-UNI-80f122c8-3_5

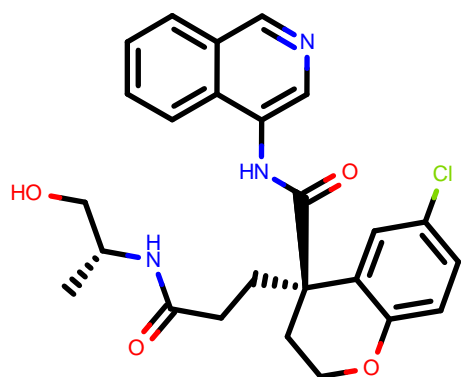
SMILES: c1ccc2c(c1)ncnc2N[C@@]3(C)C(=O)C(=O)N[C@@]4(C)C(=O)Nc5cnc6c4ccccc65

RUN: RUN2215

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.26

EN300-29387_2_2_1



CID: EN300-29387_2_2_1

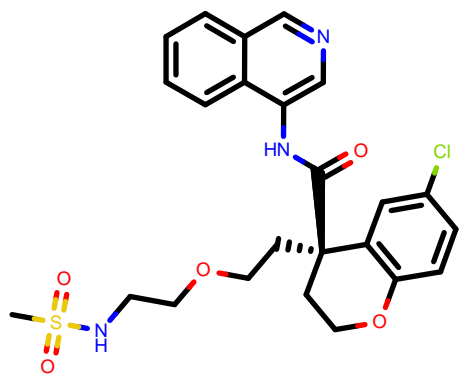
SMILES: C[C@@H](CO)NC(=O)CC[C@@]1(C)C(=O)C(=O)Nc2cnc3c1ccccc32

RUN: RUN7340

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.29

EN300-1238839_3_1_1



CID: EN300-1238839_3_1_1

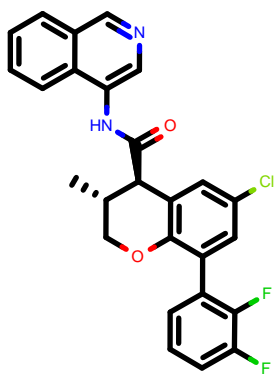
SMILES: CS(=O)(=O)NCCOCC[C@@]1(C)C(=O)C(=O)Nc2cnc3c1ccccc32

RUN: RUN5422

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.33

DAR-DIA-0d514e7d-14_1



CID: DAR-DIA-0d514e7d-14_1

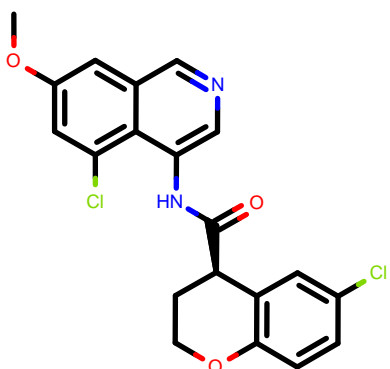
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3ncc4c3ccc4)Cl)c5ccc(c5F)F

RUN: RUN776

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.25

ALF-EVA-ced740bd-2_1



CID: ALF-EVA-ced740bd-2_1

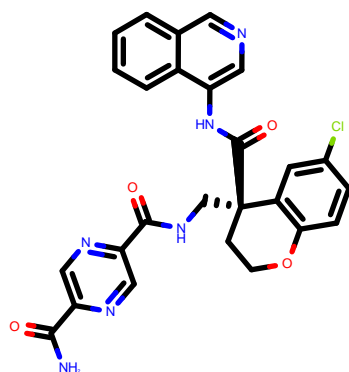
SMILES: COc1cc2cnccc(c2c(c1)Cl)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2611

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.21

EN300-1273172_2_1_1



CID: EN300-1273172_2_1_1

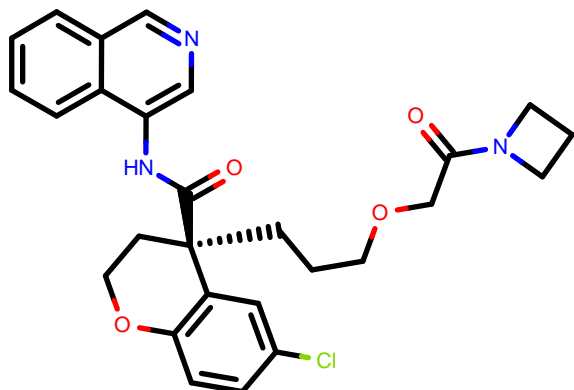
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ncnc5C(=O)N

RUN: RUN7668

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-11195_4_1_1



CID: EN300-11195_4_1_1

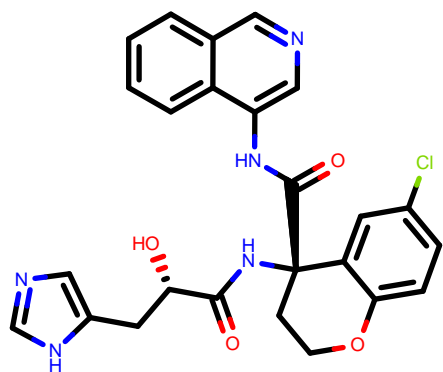
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCCS

RUN: RUN6315

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.28

EN300-6503811_1_1_1



CID: EN300-6503811_1_1_1

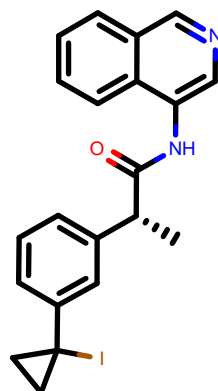
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](Cc5cn[nH]5)O

RUN: RUN5884

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.22

DAR-DIA-0cde14eb-58_2



CID: DAR-DIA-0cde14eb-58_2

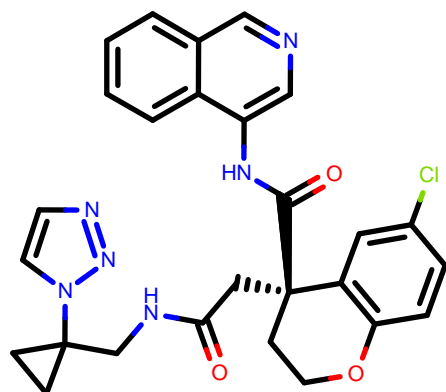
SMILES: C[C@H](c1cccc(c1)C2(CC2)I)C(=O)Nc3cncc4c3cccc4

RUN: RUN27

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.38

EN300-1721883_1_1_1



CID: EN300-1721883_1_1_1

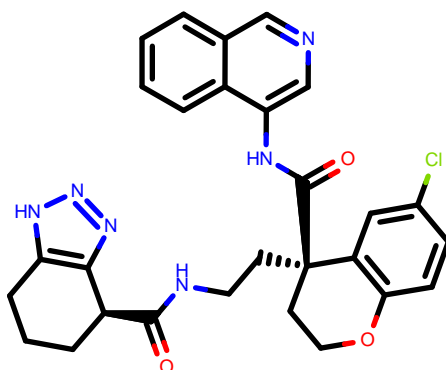
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC5(CC5)n6cn[nH]6

RUN: RUN6348

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.31

EN300-208236_3_2_1



CID: EN300-208236_3_2_1

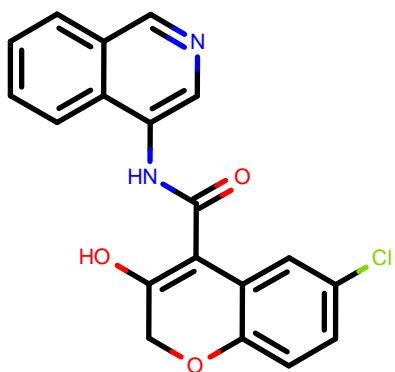
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H](H)5CCc6c5n[nH]6

RUN: RUN3048

DDG (kcal/mol): -0.29

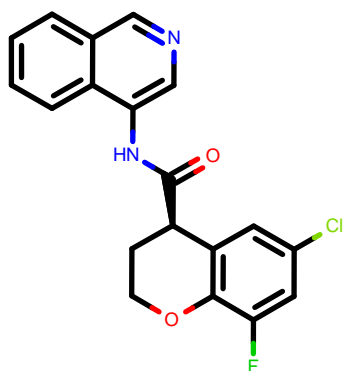
dDDG (kcal/mol): 0.39

VLA-UCB-1dbca3b4-16_2



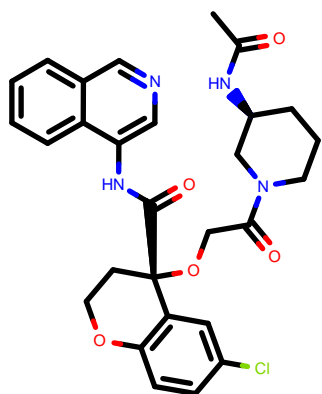
CID:	VLA-UCB-1dbca3b4-16_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)C3=C(COC4c3cc(cc4)Cl)O</chem>
RUN:	RUN112
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.28

RAL-THA-05e671eb-17_1



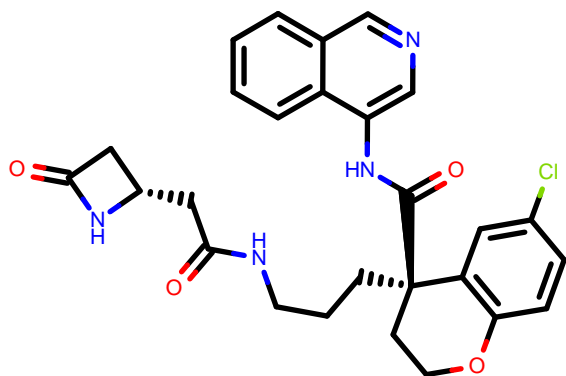
CID:	RAL-THA-05e671eb-17_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4F)Cl</chem>
RUN:	RUN1910
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.05

EN300-48886_1_2_1



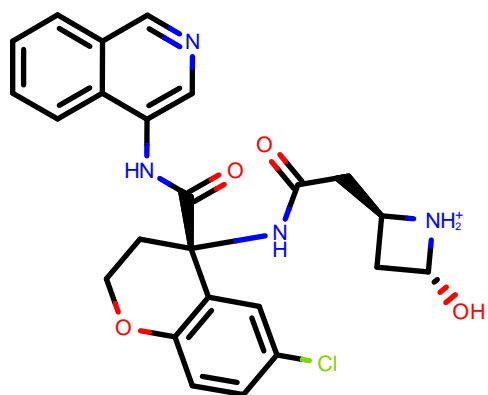
CID:	EN300-48886_1_2_1
SMILES:	<chem>CC(=O)N[C@@H]1CCCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5</chem>
RUN:	RUN6898
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.26

EN300-250593_4_2_1



CID:	EN300-250593_4_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CC(=O)N5</chem>
RUN:	RUN6102
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.26

EN300-250593_1_1_1



CID: EN300-250593_1_1_1

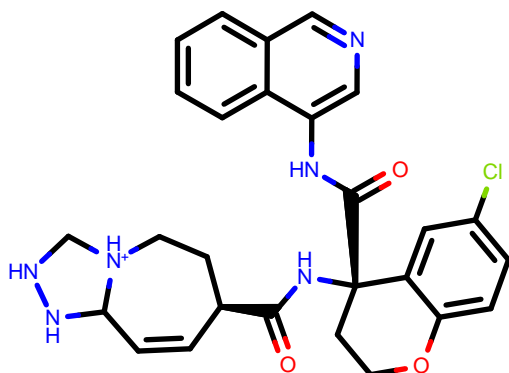
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(=O)N5

RUN: RUN6247

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-366687_1_2_1



CID: EN300-366687_1_2_1

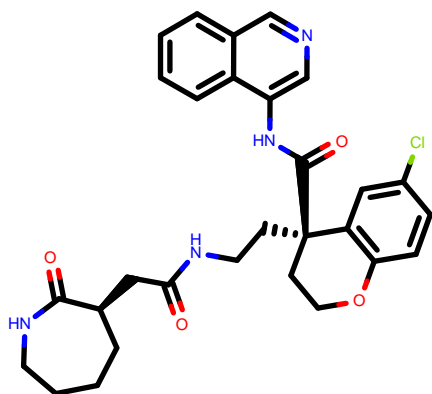
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCc6nnc6CC5

RUN: RUN4335

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.27

EN300-198633_3_2_1



CID: EN300-198633_3_2_1

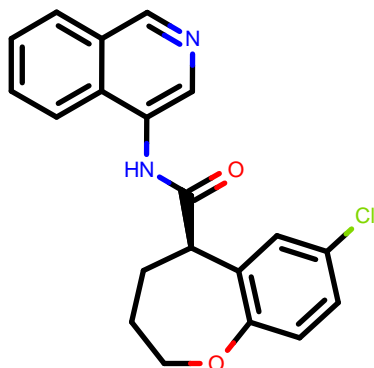
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CCCCC5=O

RUN: RUN6633

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.32

ALF-EVA-5b152d2f-1_1



CID: ALF-EVA-5b152d2f-1_1

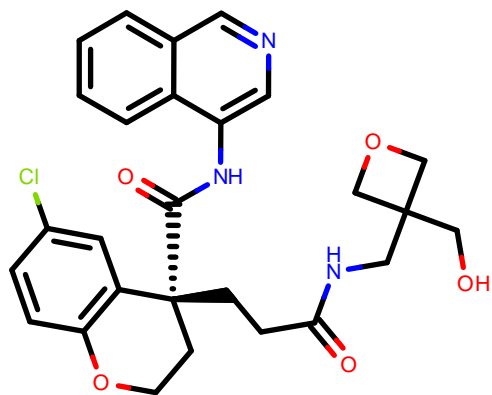
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCCCc4c3cc(cc4)Cl

RUN: RUN2167

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.19

EN300-105482_2_1_1



CID: EN300-105482_2_1_1

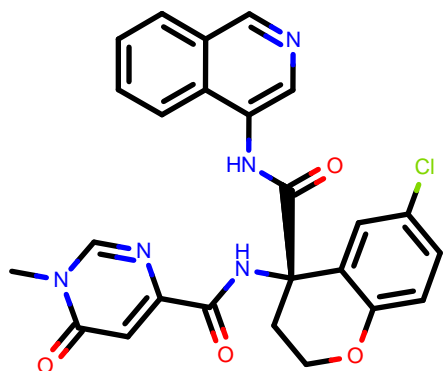
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCC(=O)NCC5(COC5)CO

RUN: RUN6832

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.24

EN300-299248_1_1_1



CID: EN300-299248_1_1_1

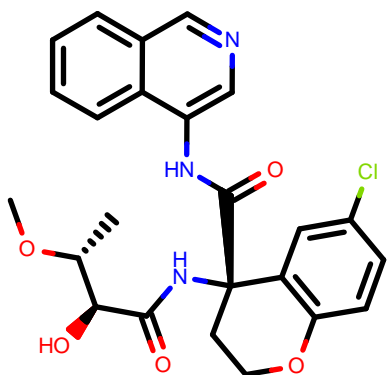
SMILES: Cn1cnc(cc1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6955

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.22

EN300-220194_1_2_1



CID: EN300-220194_1_2_1

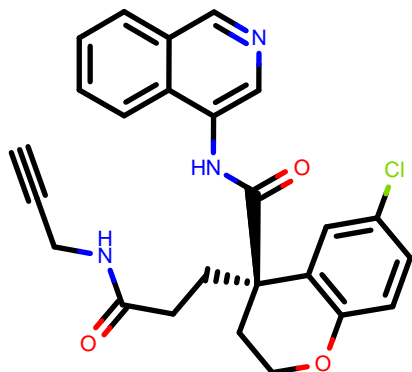
SMILES: C[C@@H]([C@@H](C=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O

RUN: RUN6773

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.24

EN300-21409_2_1_1



CID: EN300-21409_2_1_1

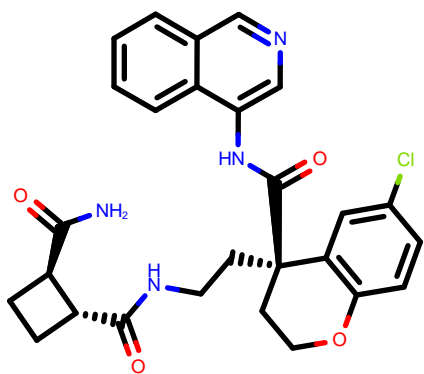
SMILES: C#CCNC(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5460

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.21

EN300-217107_3_3_1



CID: EN300-217107_3_3_1

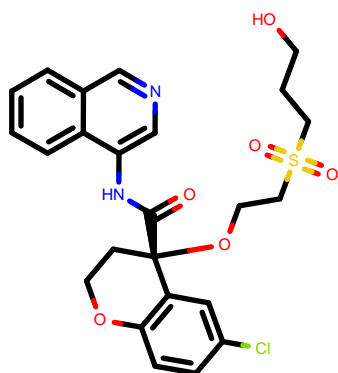
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc(Cl)cc4)CNC1=O[C@@H]5CC[C@@H]5C1=O

RUN: RUN4575

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.29

EN300-7456499_1_1_1



CID: EN300-7456499_1_1_1

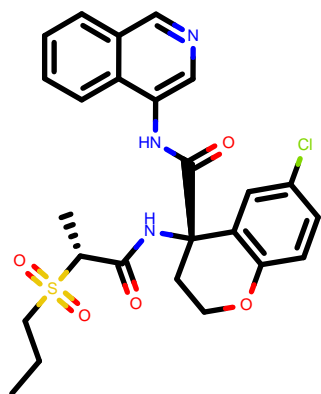
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc(Cl)cc4)CNC(=O)CCCS

RUN: RUN5241

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.33

EN300-52768_1_2_1



CID: EN300-52768_1_2_1

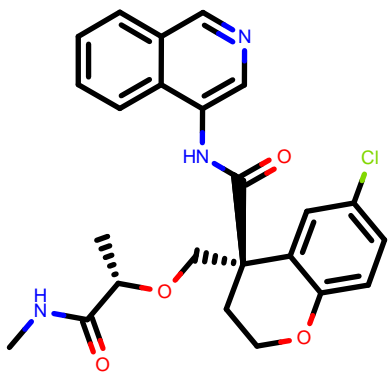
SMILES: CCCS(=O)(=O)[C@H](C)C(=O)N[C@@H]1(C)COCc2c(Cl)cc(Cl)cc2C1=O

RUN: RUN6392

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.35

EN300-211482_2_1_1



CID: EN300-211482_2_1_1

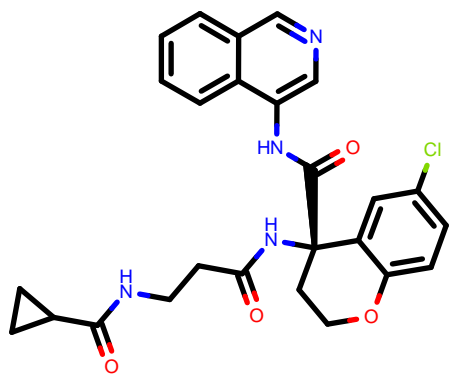
SMILES: C[C@@H](C(=O)NC)OC[C@@H]1(C)COCc2c(Cl)cc(Cl)cc2C1=O

RUN: RUN6880

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.22

EN300-31147_1_1_1



CID: EN300-31147_1_1_1

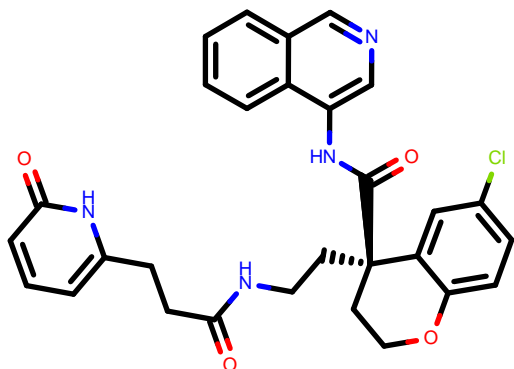
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5CC5

RUN: RUN7113

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.27

EN300-6491697_3_1_1



CID: EN300-6491697_3_1_1

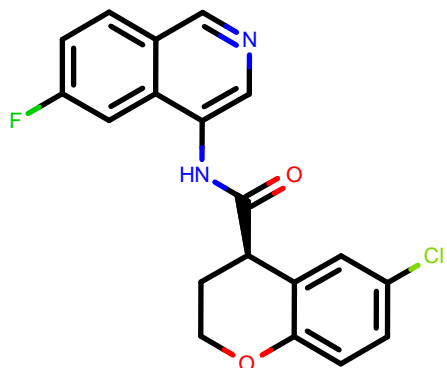
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5cccc(=O)[nH]5

RUN: RUN6529

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.24

ALP-POS-696356e4-1_1



CID: ALP-POS-696356e4-1_1

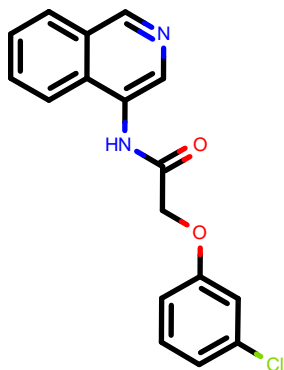
SMILES: c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1198

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.04

ALP-POS-f13221e1-2_1



CID: ALP-POS-f13221e1-2_1

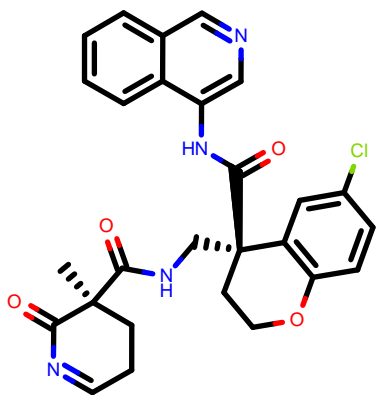
SMILES: c1ccc2c(c1)cncc2NC(=O)COc3cccc(c3)Cl

RUN: RUN147

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.31

EN300-178876_2_1_1



CID: EN300-178876_2_1_1

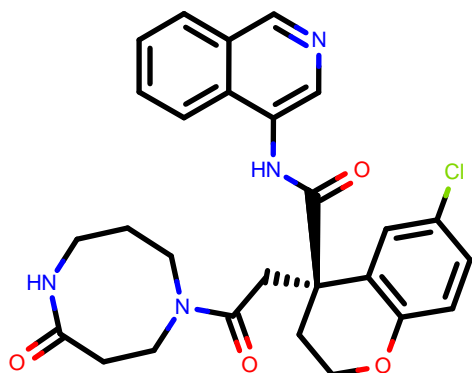
SMILES: C[C@@]1(CCCNC1=O)C(=O)NC[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6786

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.41

EN300-1072874_1_1_1



CID: EN300-1072874_1_1_1

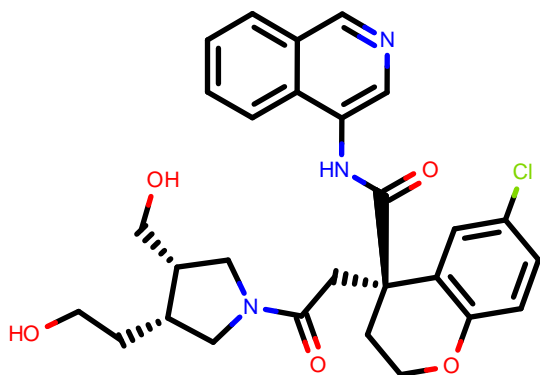
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)CC(=O)N5CCCCNC(=O)CC5

RUN: RUN4694

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.40

EN300-1425608_1_1_1



CID: EN300-1425608_1_1_1

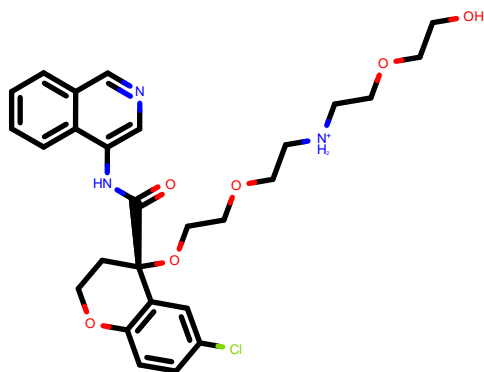
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)CC(=O)N5C[C@@H](C)C[C@H](O)CO5

RUN: RUN6429

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.33

ED_-GRI-5b13fbe2-19_1



CID: ED_-GRI-5b13fbe2-19_1

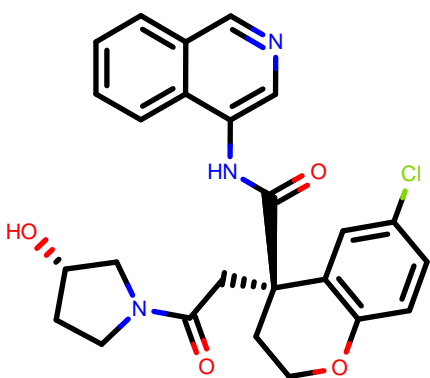
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)OCCOCC[NH2+][C]OCCO

RUN: RUN1467

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.90

EN300-69312_1_1_1



CID: EN300-69312_1_1_1

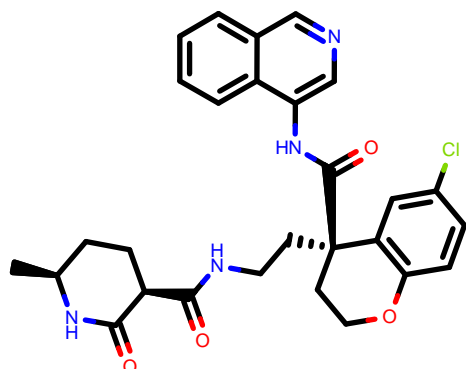
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H](C5)O

RUN: RUN7405

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.25

EN300-6505003_3_4_1



CID: EN300-6505003_3_4_1

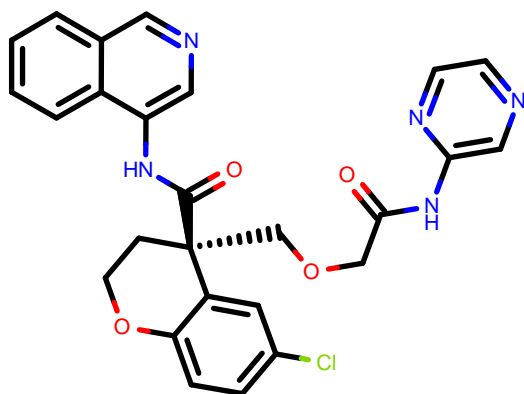
SMILES: C[C@@H]1CC[C@H](C(=O)N1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccc5ccc5

RUN: RUN4649

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.35

EN300-105267_2_1_1



CID: EN300-105267_2_1_1

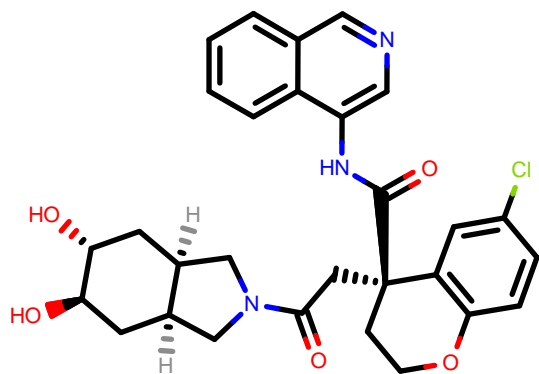
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)Nc5nccn5

RUN: RUN4803

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.27

EN300-7355477_1_3_1



CID: EN300-7355477_1_3_1

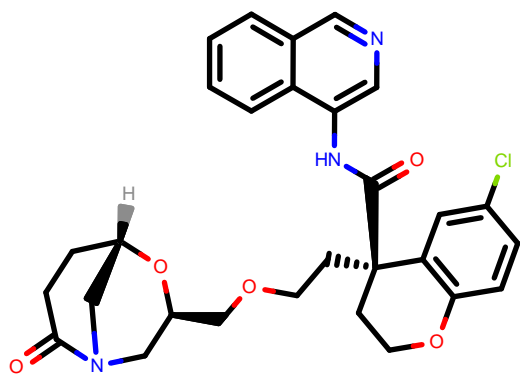
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H]6C[C@@H](C5)O

RUN: RUN6757

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.30

EN300-2008102_3_2_1



CID: EN300-2008102_3_2_1

SMILES:

c1ccc2c(c1)ncnc2N(C(=O)C[C@@H]3C[C@@H](O)CCO3)C

RUN:

RUN6280

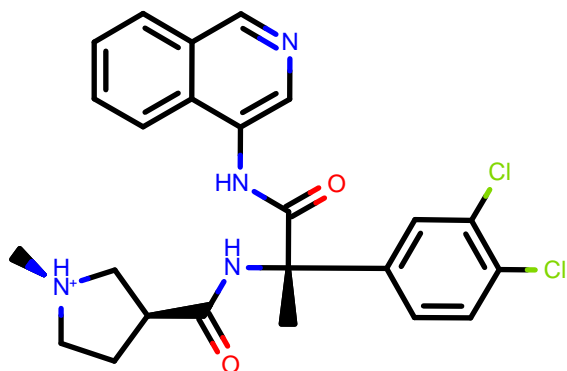
DDG (kcal/mol):

-0.27

dDDG (kcal/mol):

0.44

MAT-POS-e9e99895-13_8



CID: MAT-POS-e9e99895-13_8

SMILES:

C[C@H](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2ccc3c2ccc3NC(=O)[C@H]4CC[N@H]4)C

RUN:

RUN2114

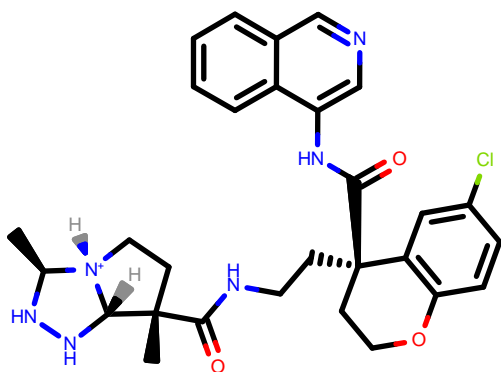
DDG (kcal/mol):

-0.27

dDDG (kcal/mol):

0.40

EN300-7431629_3_2_1



CID: EN300-7431629_3_2_1

SMILES:

C[C@H]1N[C@@H]2[N@H]1CC[C@@H]2[C@@]3(C)C(=O)NCC[C@@]3(C)COC4C3CC(=O)C(C)C(=O)Nc5ccc6c5ccc6

RUN:

RUN3205

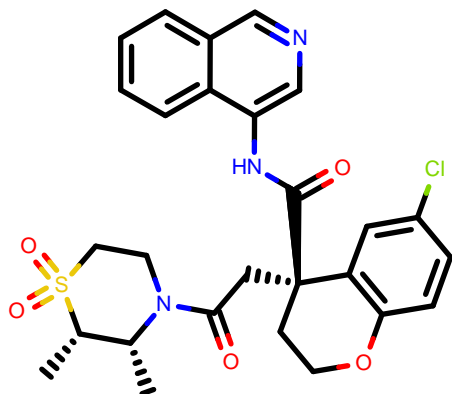
DDG (kcal/mol):

-0.27

dDDG (kcal/mol):

0.69

EN300-80940_1_1_1



CID: EN300-80940_1_1_1

SMILES:

C[C@@H]1[C@@H](C[C@@H]2[C@@H](O)C(=O)N1C(=O)C[C@@]2(C)COC3C2CC(=O)C(C)C(=O)Nc4ccc5c4ccc5

RUN:

RUN3490

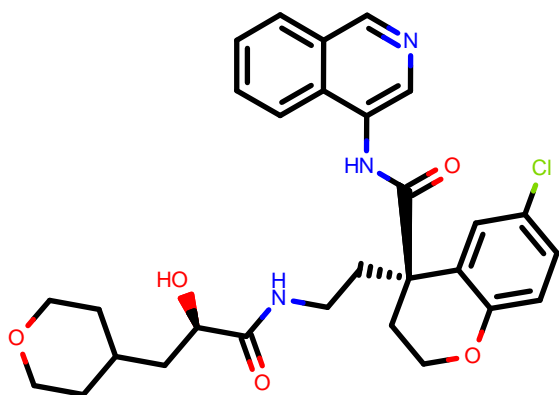
DDG (kcal/mol):

-0.27

dDDG (kcal/mol):

0.31

EN300-1452069_3_1_1



CID: EN300-1452069_3_1_1

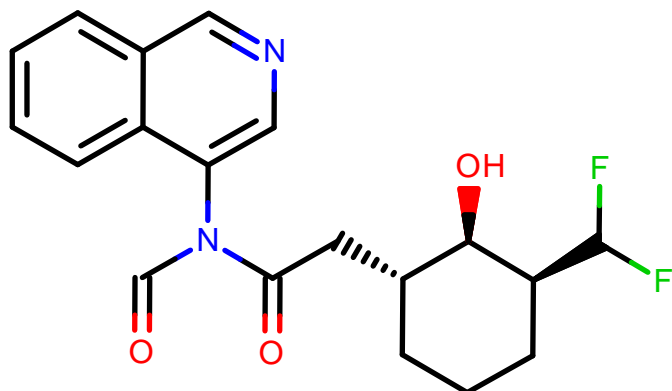
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](CC5CCOCC5)O

RUN: RUN5889

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.43

MAK-UNK-c749d764-28_2



CID: MAK-UNK-c749d764-28_2

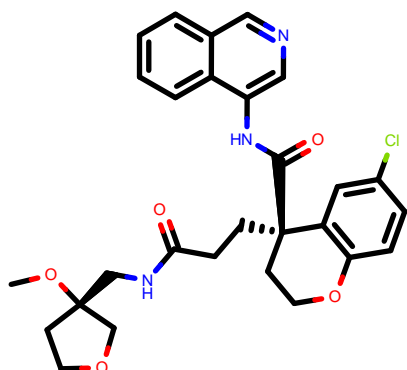
SMILES: c1ccc2c(c1)cncc2N(C=O)C(=O)[C@H]3CCC[C@@H]([C@@H]3O)C(F)F

RUN: RUN978

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.28

EN300-137255_2_2_1



CID: EN300-137255_2_2_1

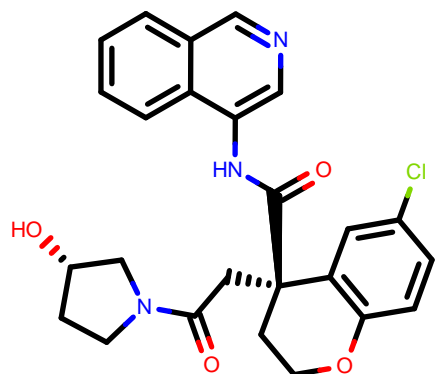
SMILES: CO[C@@]1(CCOc1)CNC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5

RUN: RUN7812

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.30

EN300-295515_1_1_1



CID: EN300-295515_1_1_1

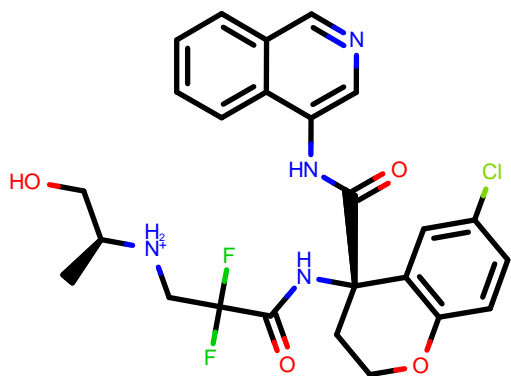
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)O

RUN: RUN6845

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.27

EDG-MED-90036822-39_1



CID: EDG-MED-90036822-39_1

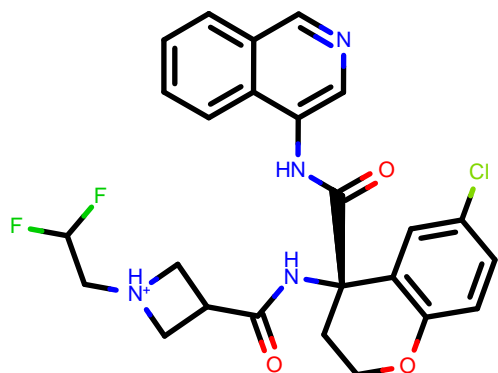
SMILES: C[C@@H](CO)NCC(C(=O)N[C@@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)F)F

RUN: RUN1621

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.32

EDG-MED-90036822-64_1



CID: EDG-MED-90036822-64_1

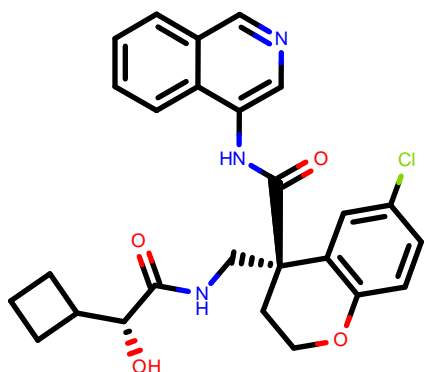
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CN(C5)CC(F)F

RUN: RUN1649

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.26

EN300-249764_2_1_1



CID: EN300-249764_2_1_1

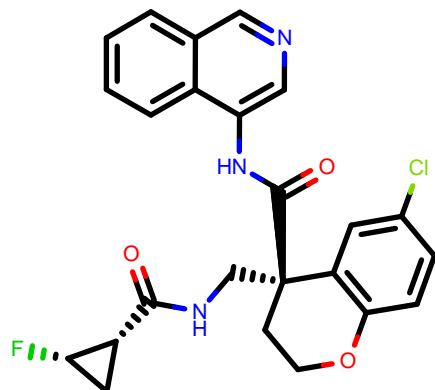
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C5CC5)O

RUN: RUN5962

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.31

EN300-1654606_2_1_1



CID: EN300-1654606_2_1_1

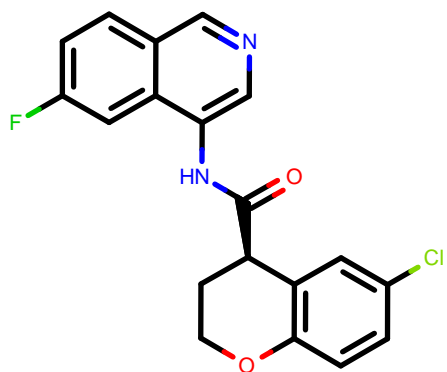
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C5C5)F

RUN: RUN6562

DDG (kcal/mol): -0.26

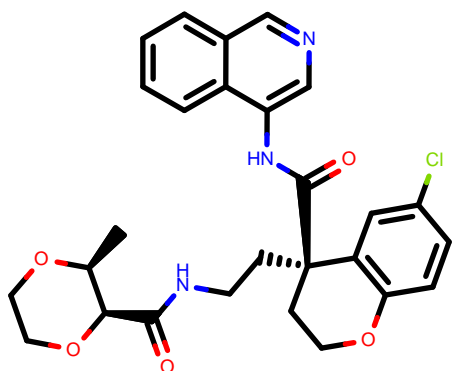
dDDG (kcal/mol): 0.20

ALP-POS-ce760d3f-7_1



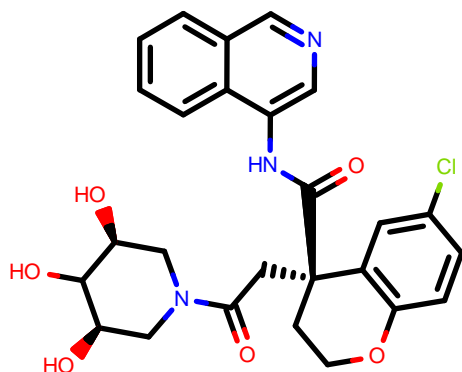
CID:	ALP-POS-ce760d3f-7_1
SMILES:	<chem>c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN1300
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.04

EN300-299215_3_1_1



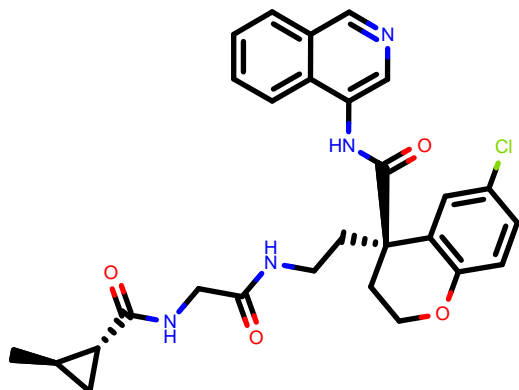
CID:	EN300-299215_3_1_1
SMILES:	<chem>C[C@H]1[C@H](OCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5</chem>
RUN:	RUN3305
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.25

EN300-299920_1_1_1



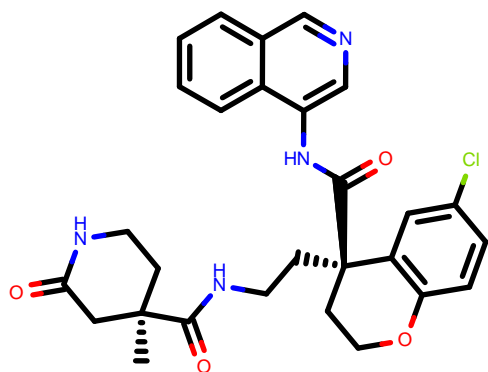
CID:	EN300-299920_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2N(C(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(O)N5C[C@H](C)[C@H]5O)O</chem>
RUN:	RUN5485
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.45

EN300-30768_3_3_1



CID:	EN300-30768_3_3_1
SMILES:	<chem>C[C@H]1[C@H](C[C@H]1C(=O)NCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5</chem>
RUN:	RUN7425
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.31

EN300-315854_3_2_1



CID: EN300-315854_3_2_1

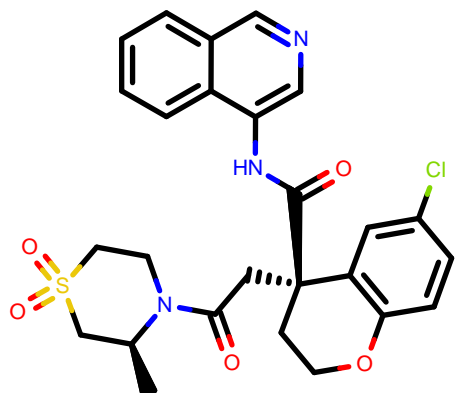
SMILES: C[C@H]1(CNC(=O)C1)C(=O)NCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN7089

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.31

EN300-171215_1_2_1



CID: EN300-171215_1_2_1

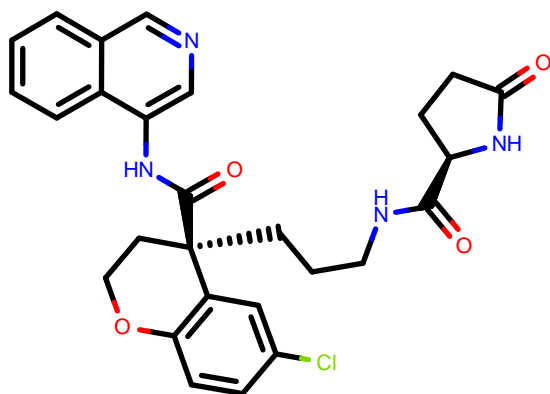
SMILES: C[C@H]1CS(=O)(=O)CCN1C(=O)C[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN6969

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.33

EN300-54541_4_1_1



CID: EN300-54541_4_1_1

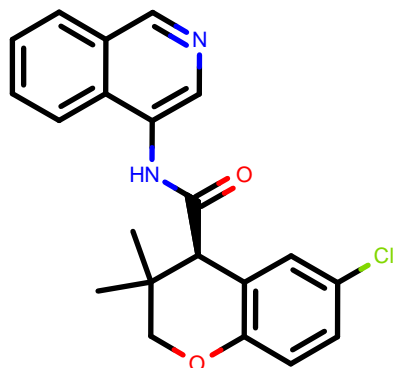
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)N5

RUN: RUN6638

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-3_1_1



CID: DAR-DIA-0d514e7d-3_1_1

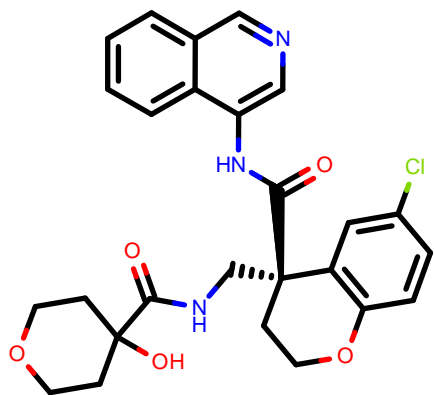
SMILES: CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cnc4c3cccc4)Cl)C

RUN: RUN7167

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.22

EN300-69368_2_1_1



CID: EN300-69368_2_1_1

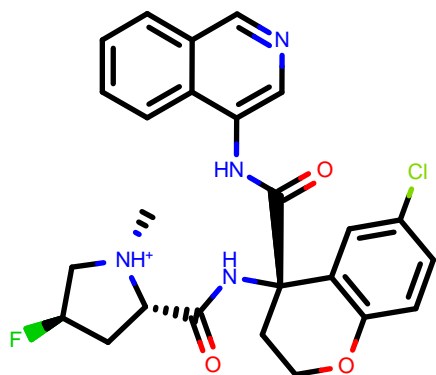
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4cc3cc(c4)C)CNC(=O)C5(C)COCOC5O

RUN: RUN6903

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.32

EDG-MED-90036822-74_6



CID: EDG-MED-90036822-74_6

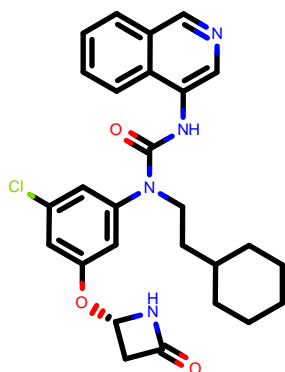
SMILES: C[N@H+]1C[C@@H](C[C@H]1C(=O)N[C@@]2(C)COCc3cc(cc3)C)C(=O)Nc4ccc5c4ccc5F

RUN: RUN1628

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.32

MAT-POS-53907a1c-3_2



CID: MAT-POS-53907a1c-3_2

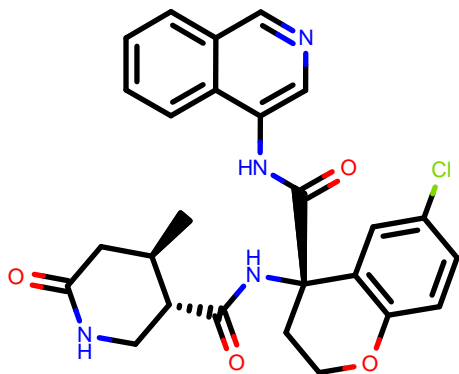
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(CCC3CCCC3)c4cc(cc(c4)Cl)O[C@H]5CC(=O)N5

RUN: RUN500

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.61

EN300-95698_1_3_1



CID: EN300-95698_1_3_1

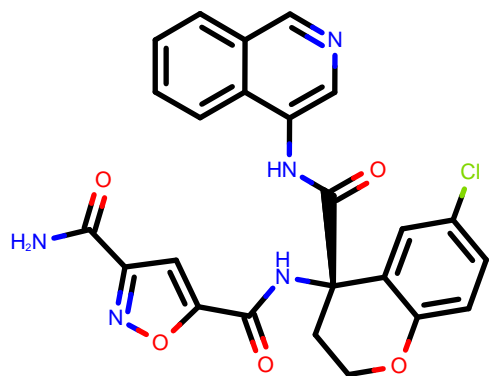
SMILES: C[C@@H]1CC(=O)NC[C@H]1C(=O)N[C@@]2(C)COCc3cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2853

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.22

EN300-127156_1_1_1



CID: EN300-127156_1_1_1

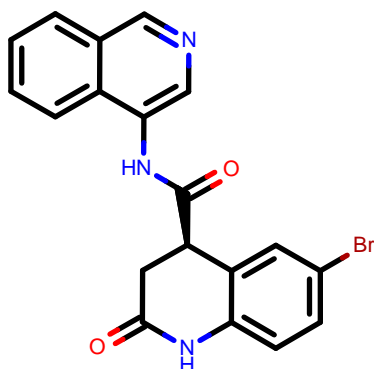
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(nc5)C(=O)N

RUN: RUN4342

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.25

MAT-POS-8d5af1ef-1_1



CID: MAT-POS-8d5af1ef-1_1

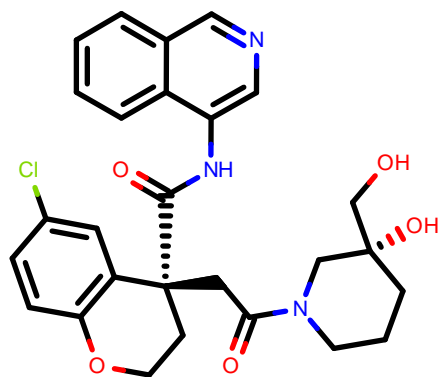
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4)Br

RUN: RUN1017

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.33

EN300-251396_1_1_1



CID: EN300-251396_1_1_1

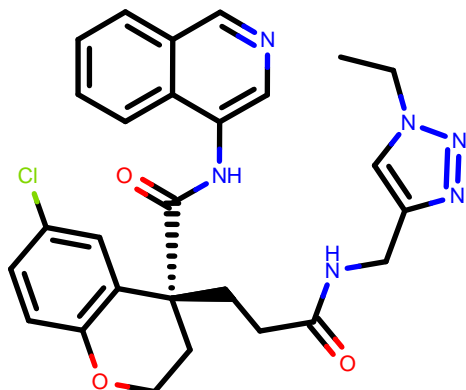
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@]3(C5)CO

RUN: RUN5351

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.50

EN300-300088_2_1_1



CID: EN300-300088_2_1_1

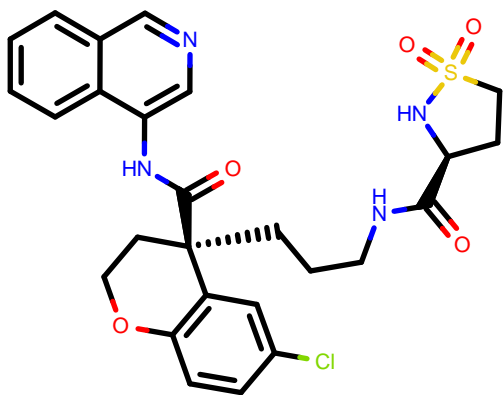
SMILES: CCn1cc(nn1)CNC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3265

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.23

EN300-45049_4_1_1



CID: EN300-45049_4_1_1

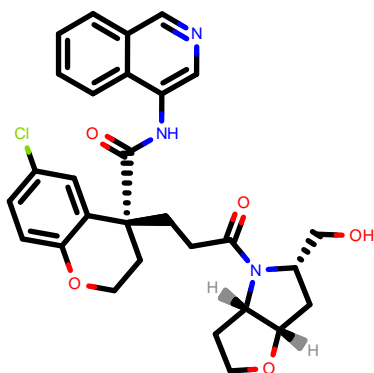
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@@@H5CCS(=O)(=O)N5

RUN: RUN7572

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.34

EN300-1588907_2_1_1



CID: EN300-1588907_2_1_1

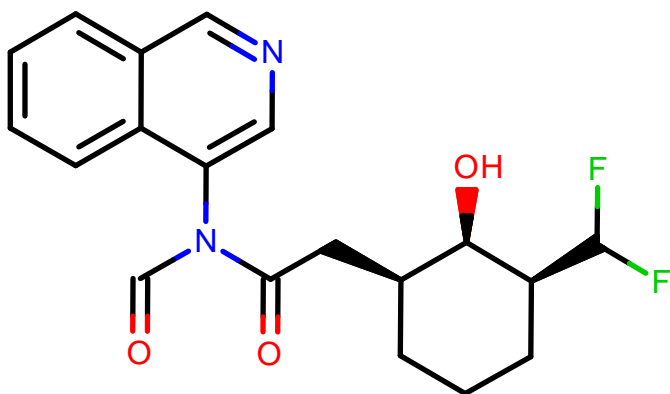
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]6C[C@@H]5CO

RUN: RUN5778

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.34

MAK-UNK-c749d764-28_1



CID: MAK-UNK-c749d764-28_1

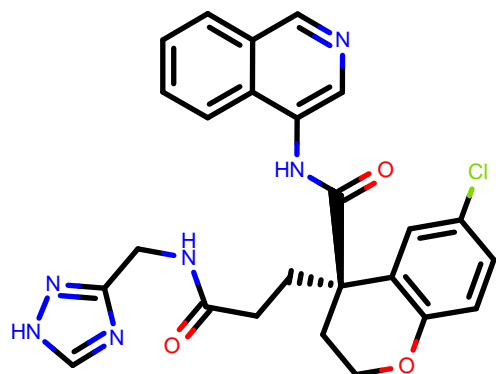
SMILES: c1ccc2c(c1)ncnc2N(C=O)C(=O)C[C@@@H]3CCCC[C@@@H]4[C@@H]3O[C@@]4(F)F

RUN: RUN1004

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.35

EN300-43972_2_1_1



CID: EN300-43972_2_1_1

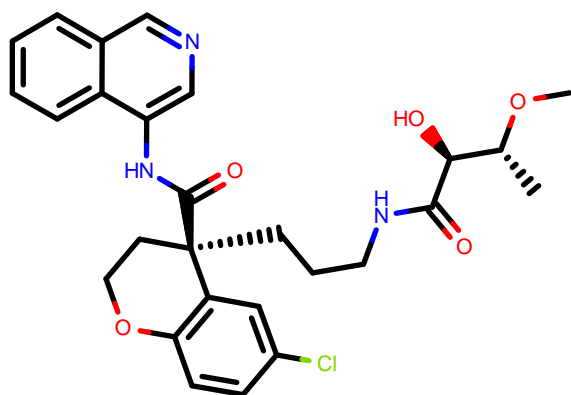
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5[nH]nns5

RUN: RUN5681

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.28

EN300-220194_4_2_1



CID: EN300-220194_4_2_1

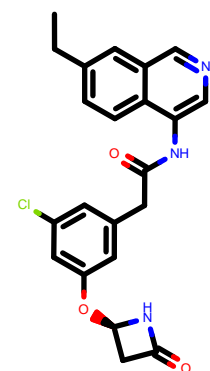
SMILES: C[C@H]([C@@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN5701

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.31

ALF-EVA-0b412456-4_1



CID: ALF-EVA-0b412456-4_1

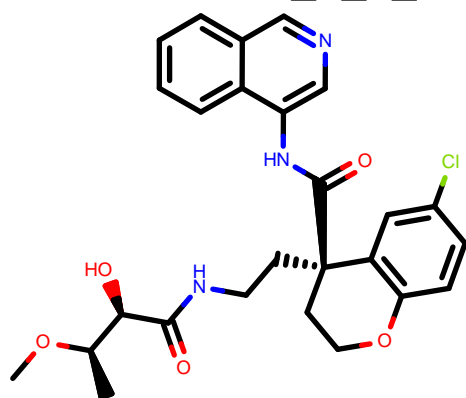
SMILES: CCc1ccc2c(c1)ncnc2NC(=O)Cc3cc(cc(c3)C)O[C@@H]4CC(=O)N4

RUN: RUN2581

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.42

EN300-220194_3_4_1



CID: EN300-220194_3_4_1

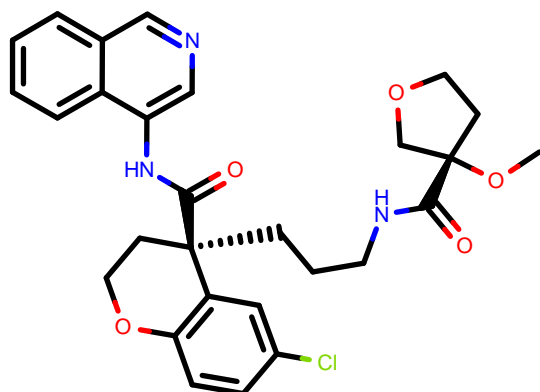
SMILES: C[C@H]([C@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN6093

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.35

EN300-174668_4_2_1



CID: EN300-174668_4_2_1

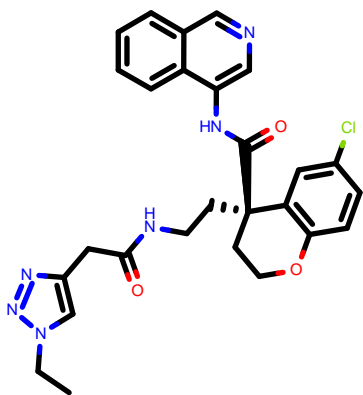
SMILES: CO[C@]1(CCOc1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN5012

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.40

EN300-717276_3_1_1



CID: EN300-717276_3_1_1

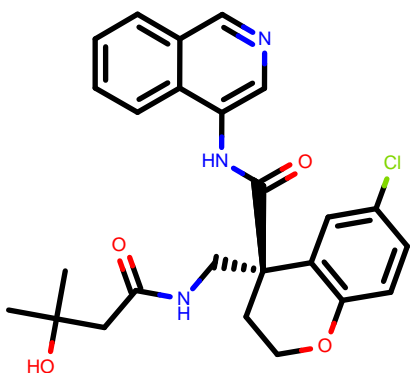
SMILES: CCn1cc(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN3378

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.29

EN300-117931_2_1_1



CID: EN300-117931_2_1_1

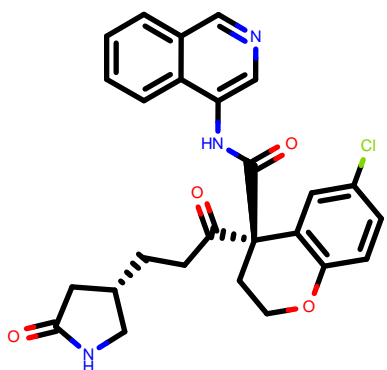
SMILES: CC(C)(CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4)O

RUN: RUN7187

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-21_2_1



CID: VLA-UCB-34f3ed0c-21_2_1

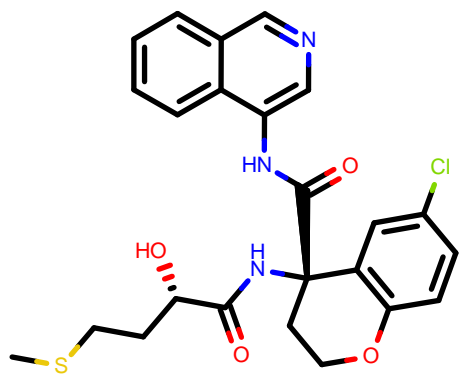
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NCS

RUN: RUN2994

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.30

EN300-103144_1_1_1



CID: EN300-103144_1_1_1

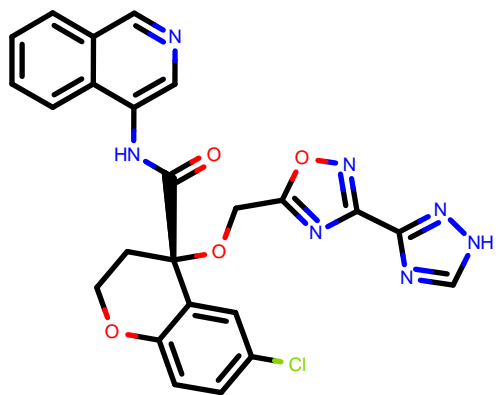
SMILES: CSCC[C@@H](C(=O)N[C@@]1(CCOc2c1ccc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4)O

RUN: RUN5969

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.29

EN300-92031_1_1_1



CID: EN300-92031_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)OCc5nc(no5)c6[nH]nc6

RUN:

RUN4704

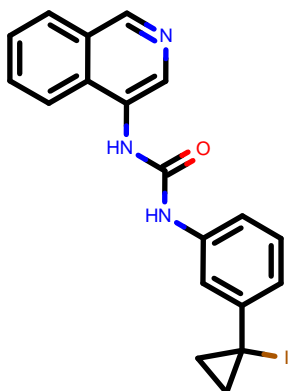
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.26

DAR-DIA-0cde14eb-53_1



CID: DAR-DIA-0cde14eb-53_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)Nc3cccc(c3)C4(CC4)I

RUN:

RUN5

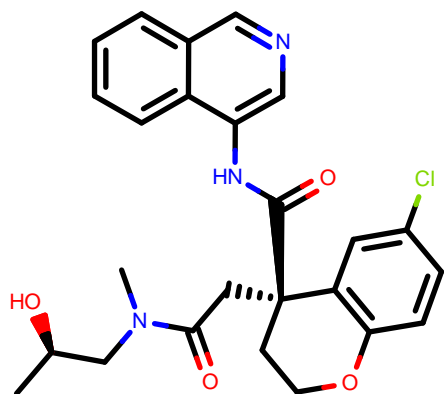
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.34

EN300-209068_1_1_1



CID: EN300-209068_1_1_1

SMILES:

C[C@@H](CN(C)C(=O)C)C@1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc3ccccc4O

RUN:

RUN5663

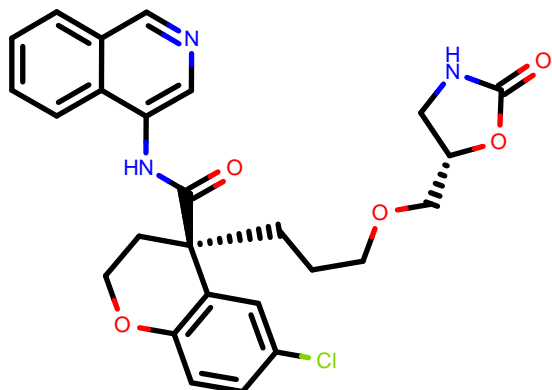
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.30

EN300-203293_4_1_1



CID: EN300-203293_4_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5NCC(=O)O5

RUN:

RUN4677

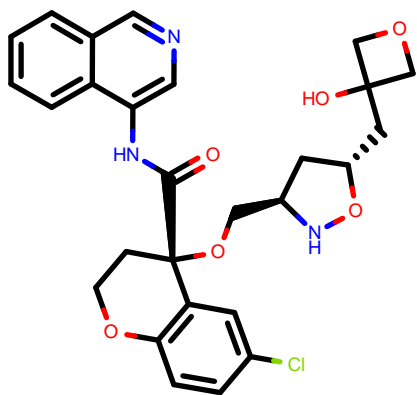
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.36

EN300-7457160_1_2_2



CID: EN300-7457160_1_2_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5OC5COC6OC6

RUN:

RUN5669

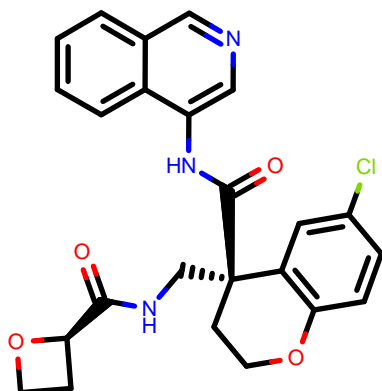
DDG (kcal/mol):

-0.24

dDDG (kcal/mol):

0.36

EN300-85760_2_2_1



CID: EN300-85760_2_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5OC5O5

RUN:

RUN5168

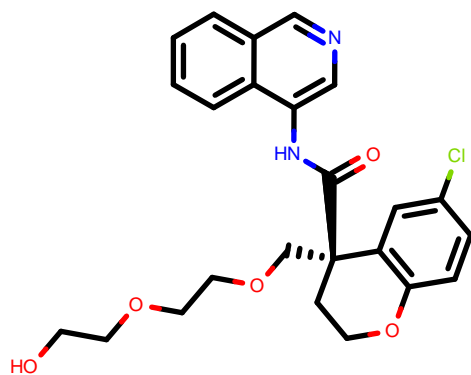
DDG (kcal/mol):

-0.24

dDDG (kcal/mol):

0.20

EN300-52467_2_1_1



CID: EN300-52467_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCOCOC

RUN:

RUN4976

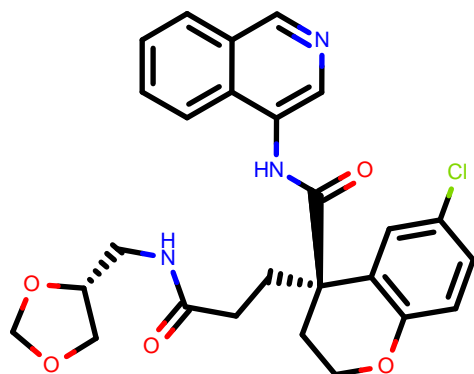
DDG (kcal/mol):

-0.24

dDDG (kcal/mol):

0.25

EN300-253187_2_1_1



CID: EN300-253187_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H]5OC5O5

RUN:

RUN7445

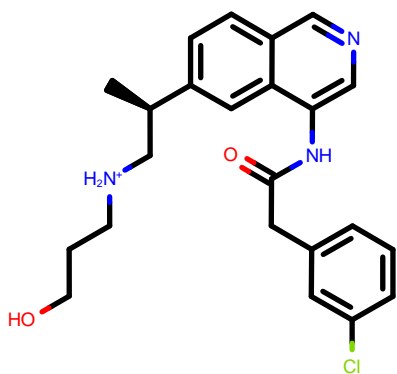
DDG (kcal/mol):

-0.24

dDDG (kcal/mol):

0.28

MAK-UNK-ffc90da7-6_2



CID: MAK-UNK-ffc90da7-6_2

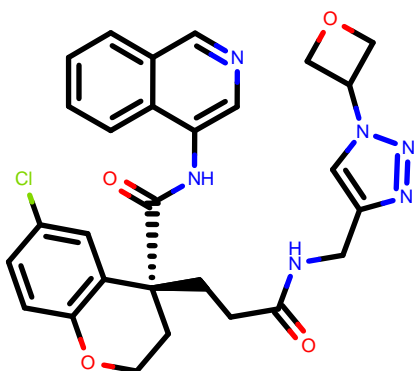
SMILES: C[C@H](C[NH2+])CCCO)c1ccc2nccc(c2c1)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN615

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.41

EN300-1709745_2_1_1



CID: EN300-1709745_2_1_1

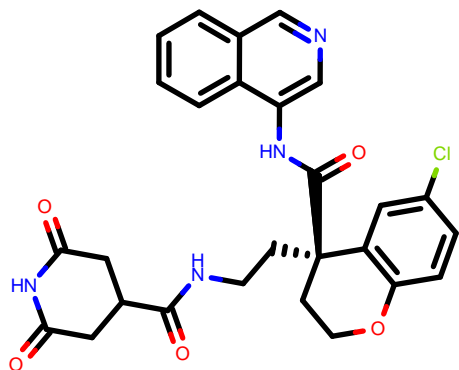
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5n(n5)C6OC6

RUN: RUN5715

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.24

EN300-62192_3_1_1



CID: EN300-62192_3_1_1

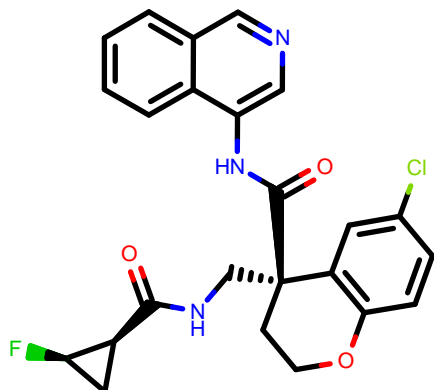
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC(=O)NC(=O)C5

RUN: RUN7805

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.33

EN300-6953121_2_1_1



CID: EN300-6953121_2_1_1

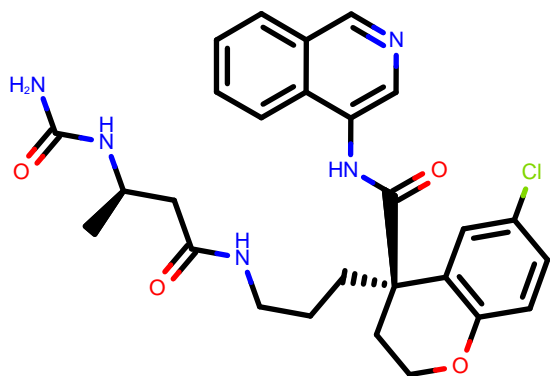
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5C[C@H]5F

RUN: RUN5432

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.16

EN300-268198_4_2_1



CID: EN300-268198_4_2_1

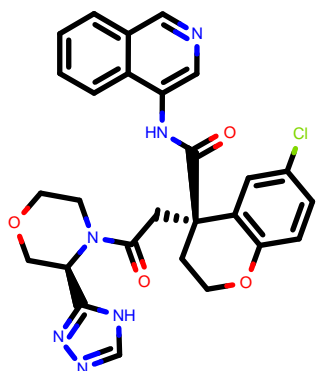
SMILES: C[C@H](CC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)N

RUN: RUN7778

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.35

EN300-205616_1_1_1



CID: EN300-205616_1_1_1

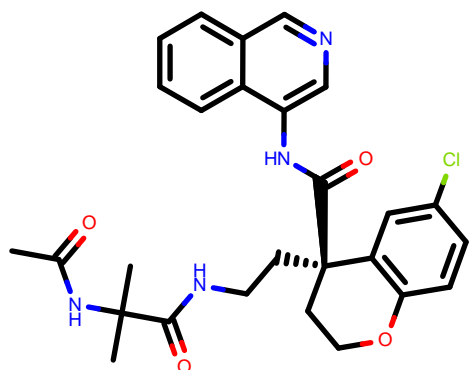
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@]5HJ5c6[nH]m6

RUN: RUN3569

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.34

EN300-65414_3_1_1



CID: EN300-65414_3_1_1

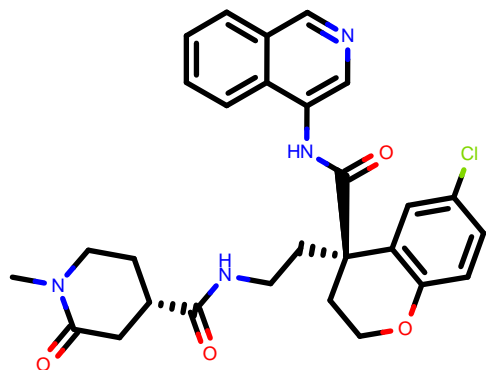
SMILES: CC(=O)NC(C)(C)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN3825

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.32

EN300-30458_3_1_1



CID: EN300-30458_3_1_1

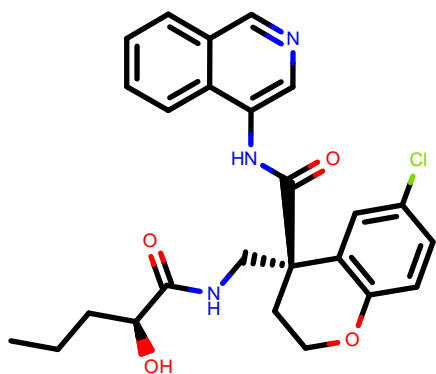
SMILES: CN1CC[C@@]1H(CC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7191

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.28

EN300-219531_2_1_1



CID: EN300-219531_2_1_1

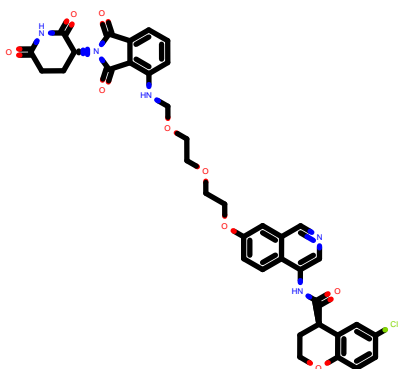
SMILES: CCC[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)O

RUN: RUN7822

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.34

DAR-DIA-9e4459de-11_1



CID: DAR-DIA-9e4459de-11_1

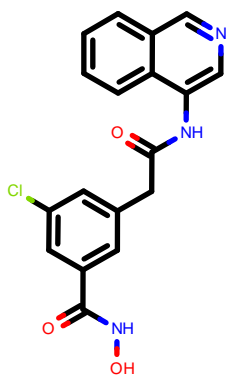
SMILES: c1cc2c(c1)NCOCCCCO3ccc4c(c3)ncn4NC(=O)[C@@H]5COC6c5cc(cc6)Cl)c7c(c2O)[C@@H]7C(C1=O)NC7=O)O

RUN: RUN1372

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.49

RAL-THA-1d44ff04-13_1



CID: RAL-THA-1d44ff04-13_1

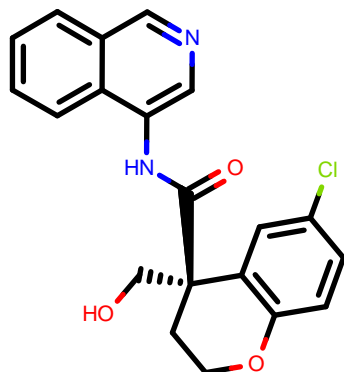
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(=O)NO

RUN: RUN389

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.29

EDG-MED-971238d3-2_1



CID: EDG-MED-971238d3-2_1

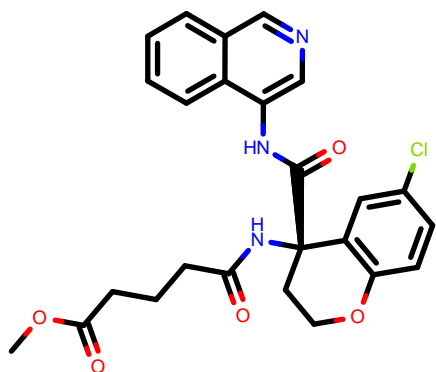
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO

RUN: RUN1288

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.14

EN300-24804_1_1_1



CID: EN300-24804_1_1_1

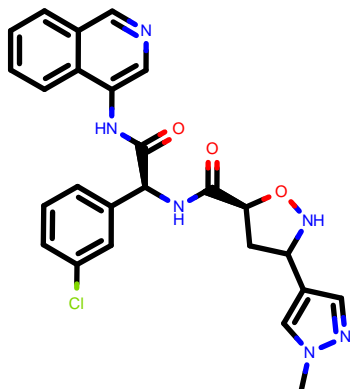
SMILES: COC(=O)CCCC(=O)N[C@@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5700

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.21

EDJ-MED-ee07cf00-6_1



CID: EDJ-MED-ee07cf00-6_1

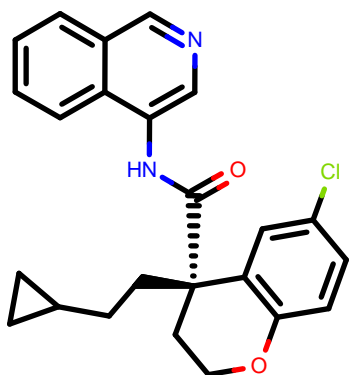
SMILES: Cn1cc(en1)C2=NO[C@@H](C2)C(=O)N[C@@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2670

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.48

ALP-POS-477dc5b7-3_2



CID: ALP-POS-477dc5b7-3_2

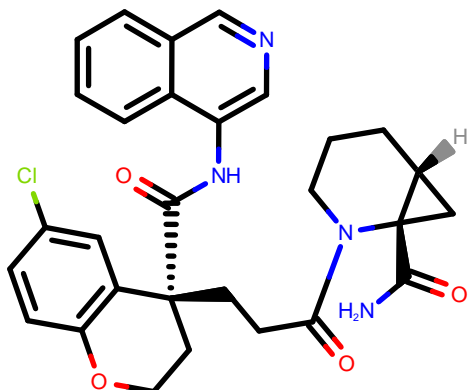
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CC5

RUN: RUN269

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.41

EN300-817777_2_1_1



CID: EN300-817777_2_1_1

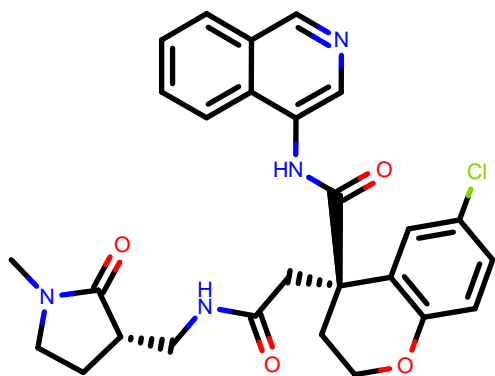
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C@H)(C@)5(C)C(C)=O

RUN: RUN6499

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.31

EN300-1264816_1_2_1



CID: EN300-1264816_1_2_1

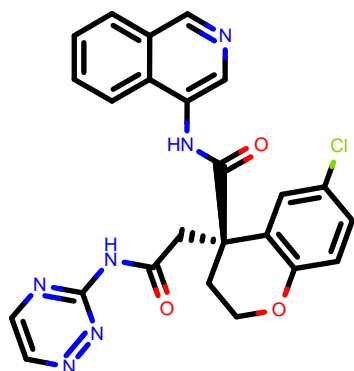
SMILES: CN1CC[C@H](C1=O)CNC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6396

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.26

EDJ-MED-d203f206-18_1



CID: EDJ-MED-d203f206-18_1

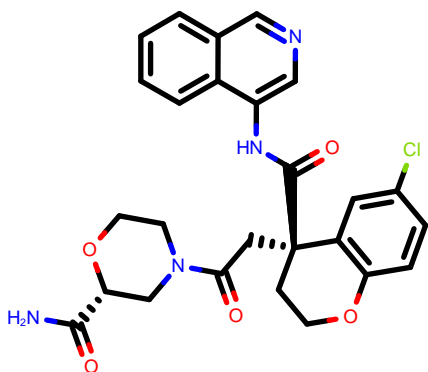
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5ncocn5

RUN: RUN2412

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EN300-60862_1_2_1



CID: EN300-60862_1_2_1

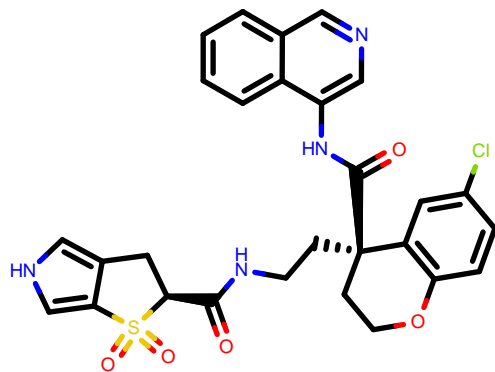
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@H](C5)C(=O)N

RUN: RUN6143

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-7445396_3_1_1



CID: EN300-7445396_3_1_1

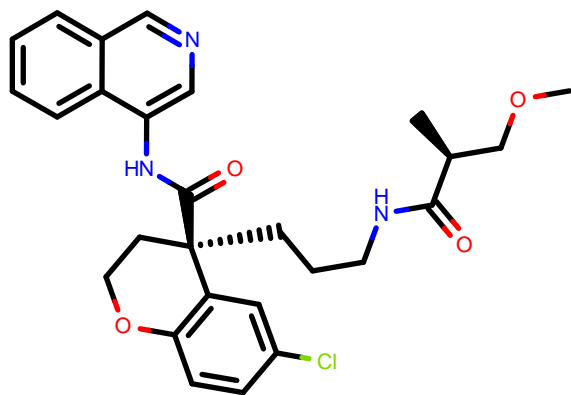
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5C6c6c[nH]c6c5S(=O)(=O)

RUN: RUN6982

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.53

EN300-69162_4_1_1



CID: EN300-69162_4_1_1

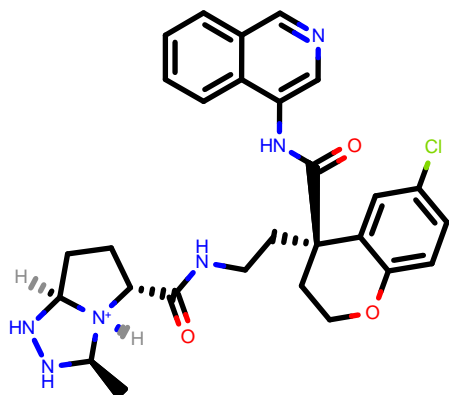
SMILES: C[C@@H](COC)C(=O)NCCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6803

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.32

EN300-6489289_3_2_2



CID: EN300-6489289_3_2_2

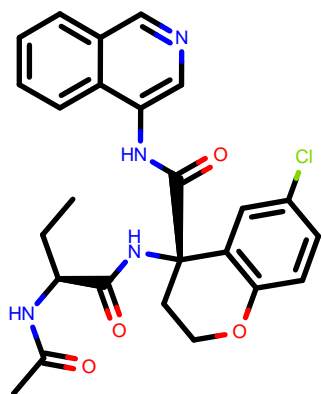
SMILES: C[C@H]1NN[C@@H]2[N@H]1[C@H](C2)Cl(=O)NC[C@H]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nccc6c5cccc6

RUN: RUN4678

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.55

EN300-332601_1_1_1



CID: EN300-332601_1_1_1

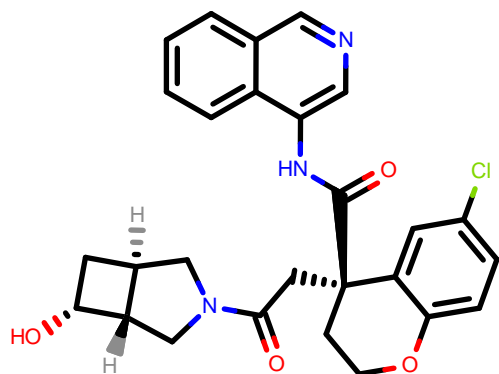
SMILES: CC[C@@H](C(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)NC(=O)C

RUN: RUN7235

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.23

EN300-305294_1_7_1



CID: EN300-305294_1_7_1

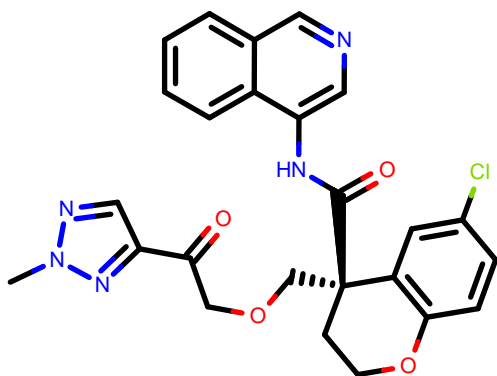
SMILES: c1cc2c(c1)nc2N[C@@H](C(=O)N[C@H]3(CCOc4c3cc(cc4)Cl)C(=O)N)C[C@@H]5C[C@H](C(=O)N)C5O

RUN: RUN6394

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EN300-204935_2_1_1



CID: EN300-204935_2_1_1

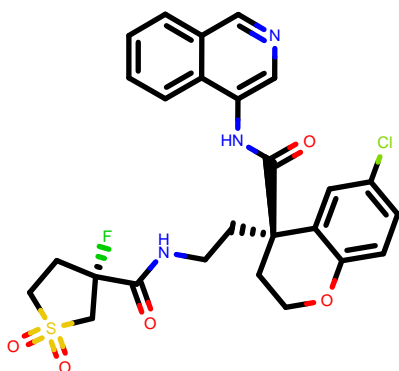
SMILES: Cn1ncc(n1)C(=O)COC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7711

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-311920_3_1_1



CID: EN300-311920_3_1_1

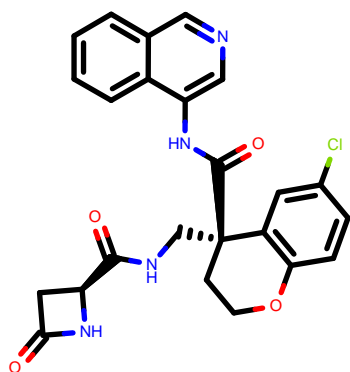
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(Cl)C)CNC(=O)[C@@]5(CCS(=O)=O)C5F

RUN: RUN7171

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.32

EN300-103219_2_1_1



CID: EN300-103219_2_1_1

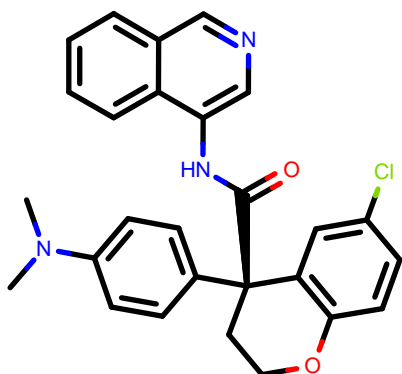
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(Cl)C)CNC(=O)[C@@]5CNC(=O)N5

RUN: RUN5947

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

FRA-DIA-13af2da5-2_1



CID: FRA-DIA-13af2da5-2_1

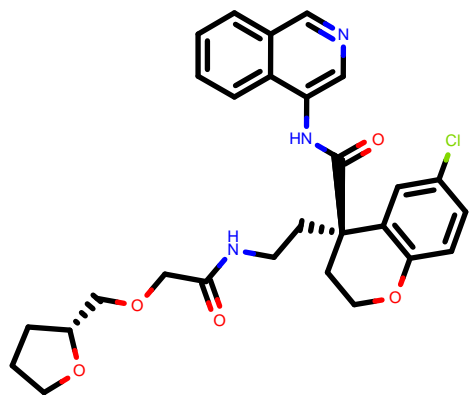
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN385

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.20

EN300-60033_3_2_1



CID: EN300-60033_3_2_1

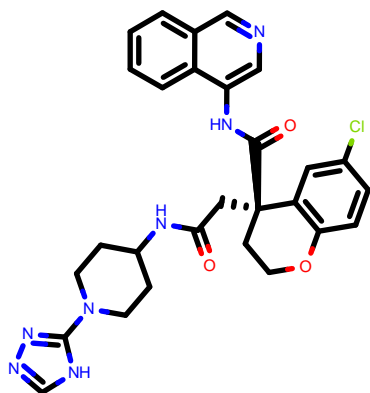
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@H]5CCOC5

RUN: RUN3813

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.31

EDJ-MED-d203f206-28_1



CID: EDJ-MED-d203f206-28_1

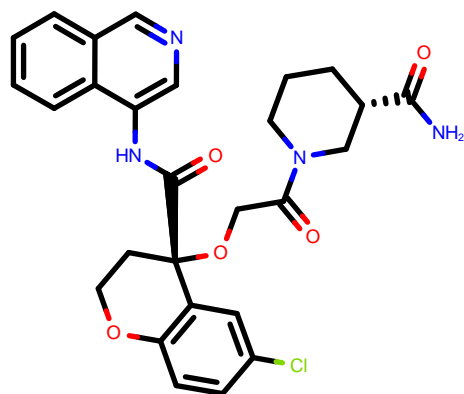
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)c6[nH]n6

RUN: RUN2446

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.29

CHO-MSK-5891c1ff-4_1



CID: CHO-MSK-5891c1ff-4_1

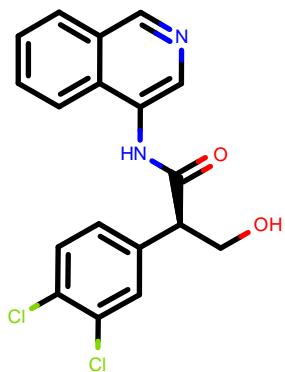
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CC[C@H](C5)C(=O)N

RUN: RUN1840

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.34

MAT-POS-fce787c2-11_1



CID: MAT-POS-fce787c2-11_1

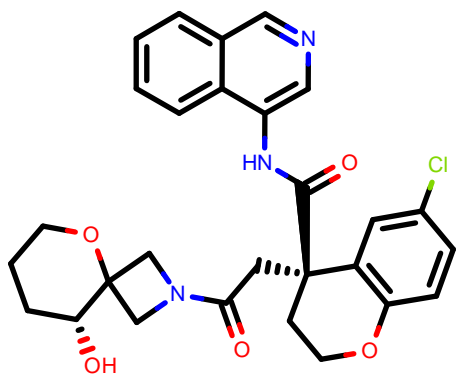
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CO)c3ccc(c(c3)Cl)Cl

RUN: RUN1981

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-7434114_1_1_1



CID: EN300-7434114_1_1_1

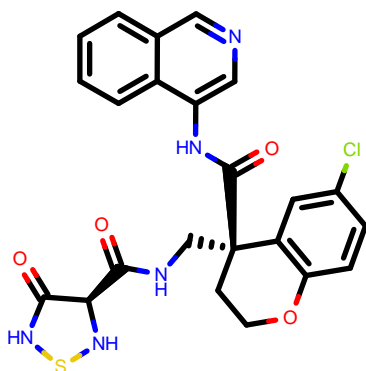
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)C@H(CCO6)O

RUN: RUN6062

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.24

EN300-261859_2_1_1



CID: EN300-261859_2_1_1

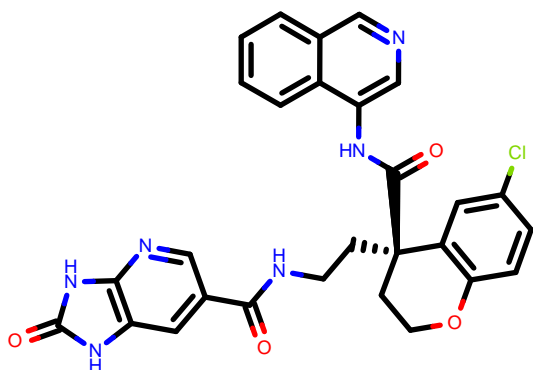
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C(=O)NS5

RUN: RUN6360

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

KAD-UNI-8a629cb0-22_1



CID: KAD-UNI-8a629cb0-22_1

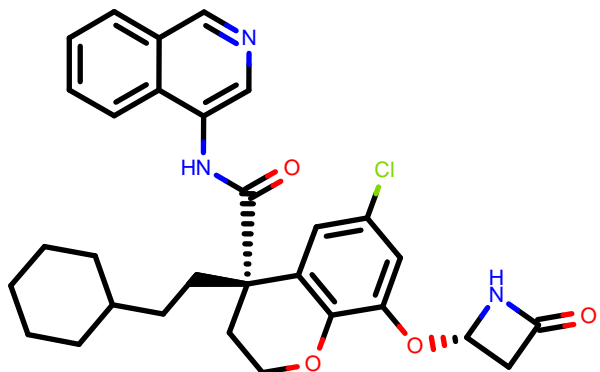
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc6c([nH]c(=O)[nH]6)nc5

RUN: RUN1992

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.29

VLA-UCB-05e51b3f-12_2



CID: VLA-UCB-05e51b3f-12_2

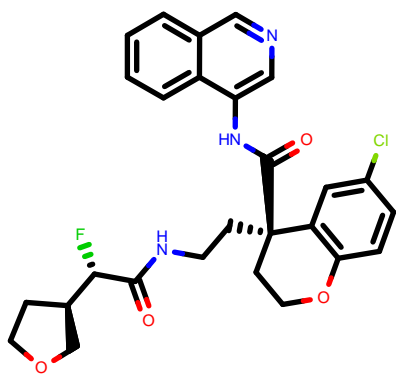
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C(=O)C6CCCC6

RUN: RUN353

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.43

EN300-783124_3_2_1



CID: EN300-783124_3_2_1

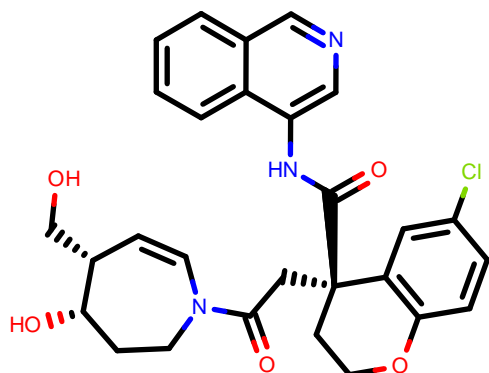
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]([C@@H]5CCOC5)F

RUN: RUN6488

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-7353672_1_4_1



CID: EN300-7353672_1_4_1

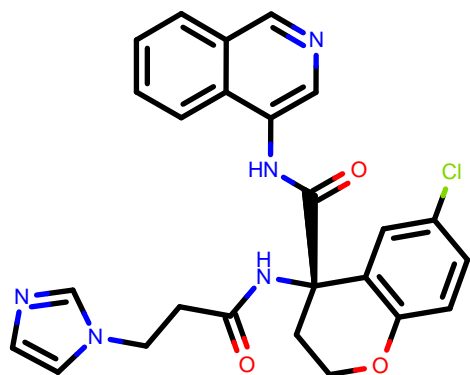
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(O)N(CO)C

RUN: RUN5916

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.37

EN300-75342_1_1_1



CID: EN300-75342_1_1_1

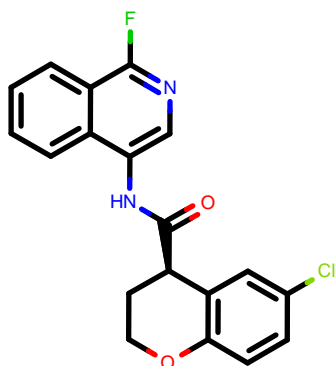
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5cnc5

RUN: RUN6431

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.23

JOH-SUS-a69c159d-2_1



CID: JOH-SUS-a69c159d-2_1

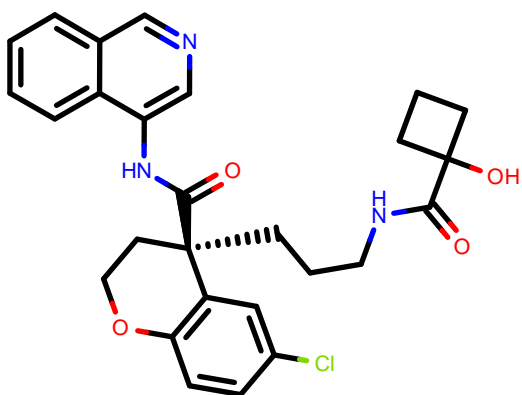
SMILES: c1ccc2c(c1)c(cnc2F)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C

RUN: RUN1047

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.05

EN300-52009_4_1_1



CID: EN300-52009_4_1_1

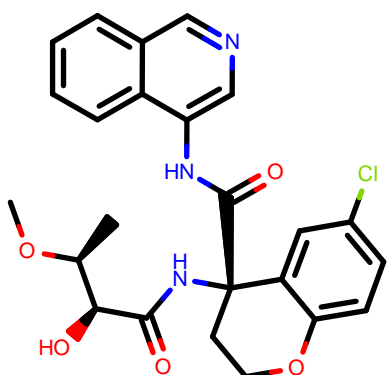
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)CCNC(=O)C5(CCC5)O

RUN: RUN7546

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.33

EN300-220194_1_1_1



CID: EN300-220194_1_1_1

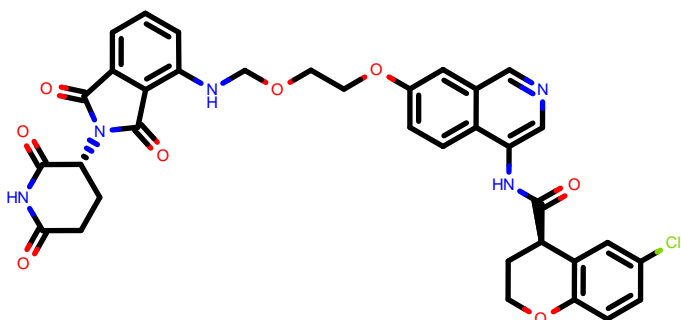
SMILES: C[C@@H]([C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN5324

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.29

DAR-DIA-9e4459de-13_2



CID: DAR-DIA-9e4459de-13_2

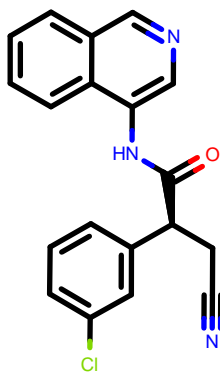
SMILES: c1cc2c(c1)NC(=O)C3C(=O)N(C3)C(=O)N[C@@H]4(CCOc5c4cc(cc5Cl)CCNC(=O)C6(CCC6)O

RUN: RUN1333

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.35

JOH-UNI-ee5ed7c8-6_1



CID: JOH-UNI-ee5ed7c8-6_1

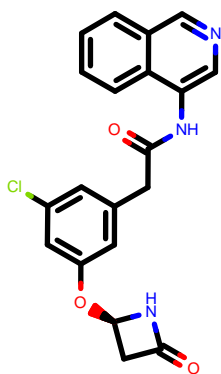
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C)C3(CCC3)Cl

RUN: RUN1711

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

ALP-POS-3b848b35-2_1



CID: ALP-POS-3b848b35-2_1

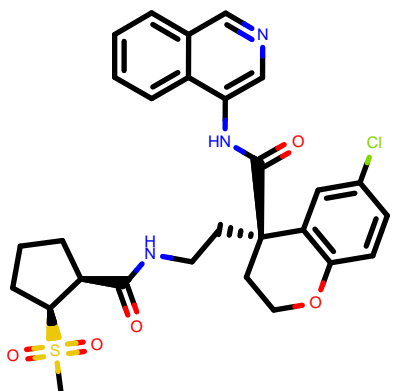
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@@H]4CC(=O)N4

RUN: RUN43

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.40

EN300-1387145_3_4_1



CID: EN300-1387145_3_4_1

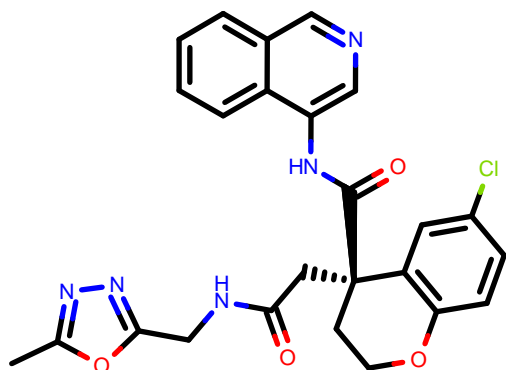
SMILES: CS(=O)(=O)C[C@@H]1CC[C@H]1C(=O)NC[C@@H]2(COCc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN5600

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.36

EN300-43090_1_1_1



CID: EN300-43090_1_1_1

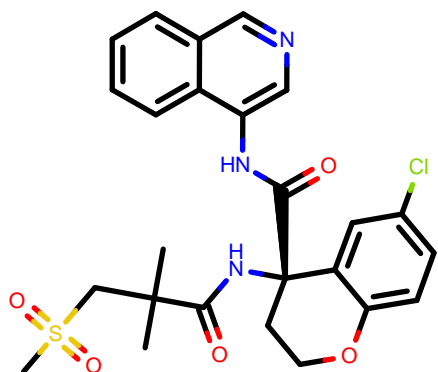
SMILES: Cc1nnc(o1)CNC(=O)C[C@@H]2(COCc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN7292

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.29

EN300-188217_1_1_1



CID: EN300-188217_1_1_1

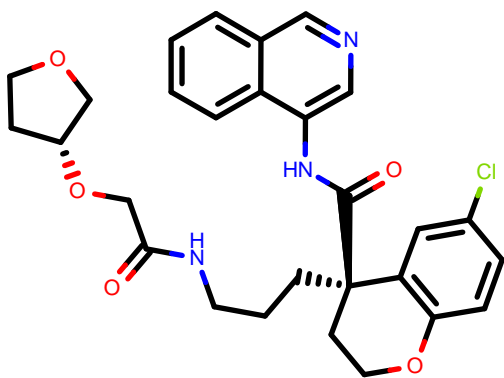
SMILES: CC(C)(CS(=O)(=O)C(=O)N)C[C@@H]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4

RUN: RUN6231

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-99391_4_1_1



CID: EN300-99391_4_1_1

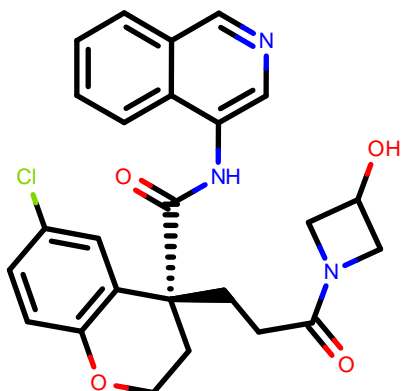
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN7228

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.32

EN300-65115_2_1_1



CID: EN300-65115_2_1_1

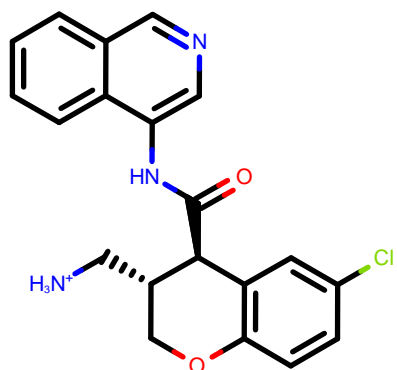
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)O

RUN: RUN7198

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

MAK-UNK-8be7dca9-3_2



CID: MAK-UNK-8be7dca9-3_2

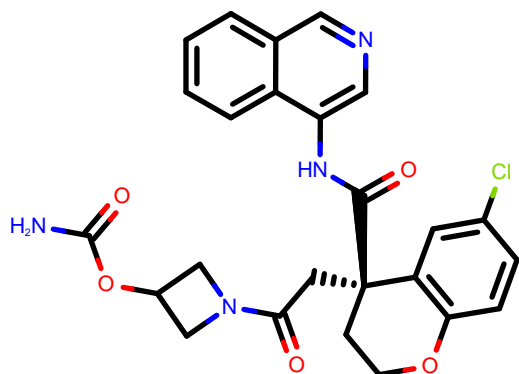
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4OC[C@@H]3C[NH3+])Cl

RUN: RUN414

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.12

EN300-1707774_1_1_1



CID: EN300-1707774_1_1_1

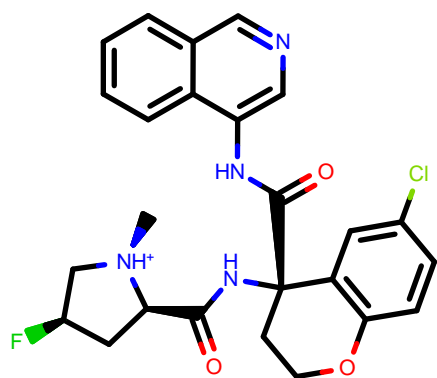
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)OC(=O)N

RUN: RUN4489

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.24

EDG-MED-90036822-74_1



CID: EDG-MED-90036822-74_1

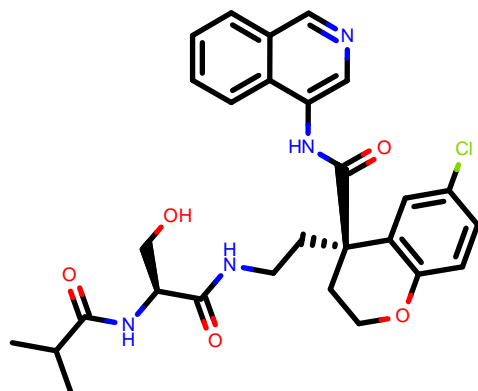
SMILES: CN1C(=O)N[C@@H](C1)C(=O)N[C@@H](C2=CC=CC=C2)C(=O)N3C4C(=O)C(=O)C4

RUN: RUN1630

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.23

EN300-212266_3_1_1



CID: EN300-212266_3_1_1

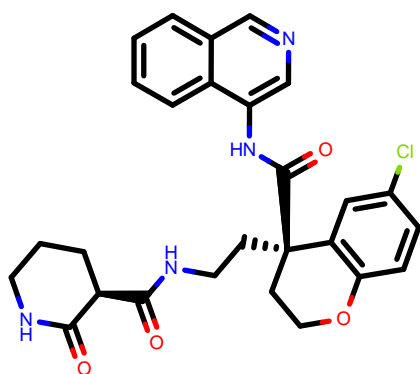
SMILES: CC(C)C(=O)N[C@@H](C1=CC=CC=C1)C(=O)N[C@@H](C2=CC=CC=C2)C(=O)N3C4C(=O)C(=O)C4

RUN: RUN7294

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.40

EN300-82616_3_1_1



CID: EN300-82616_3_1_1

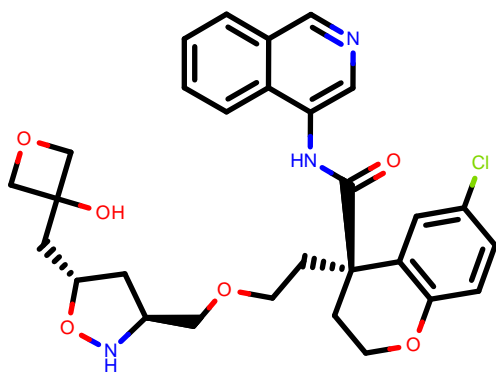
SMILES: C1CCC2C(=O)N[C@@H](C1)C(=O)N[C@@H](C2=CC=CC=C2)C(=O)N3C4C(=O)C(=O)C4

RUN: RUN5953

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.34

EN300-7457160_3_1_1



CID: EN300-7457160_3_1_1

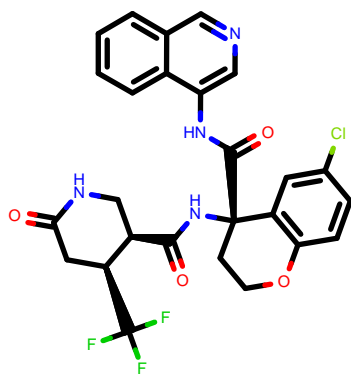
SMILES: C1CCC2C(=O)N[C@@H](C1)C(=O)N[C@@H](C2=CC=CC=C2)C(=O)N3C4C(=O)C(=O)C4

RUN: RUN3966

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.40

EN300-208959_1_1_1



CID: EN300-208959_1_1_1

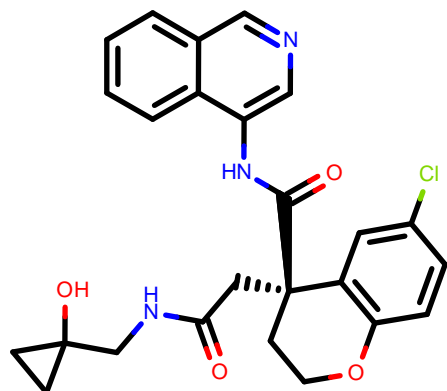
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@](O)(C(=O)C4=CC=CC=C4)C(=O)C@@H5CNC1=O)C[C@@H]5C(F)(F)F

RUN: RUN6524

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.29

EN300-1644703_1_1_1



CID: EN300-1644703_1_1_1

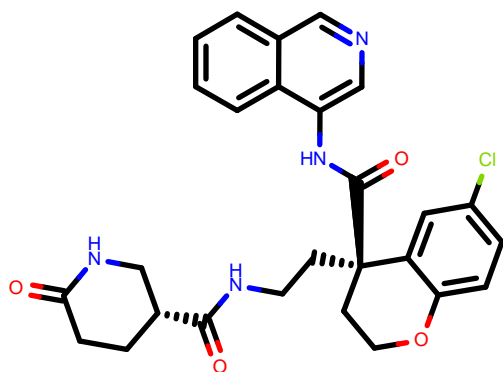
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@](O)(C(=O)C4=CC=CC=C4)C(=O)NCC5(C)CC5O

RUN: RUN6555

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.24

EN300-42819_3_1_1



CID: EN300-42819_3_1_1

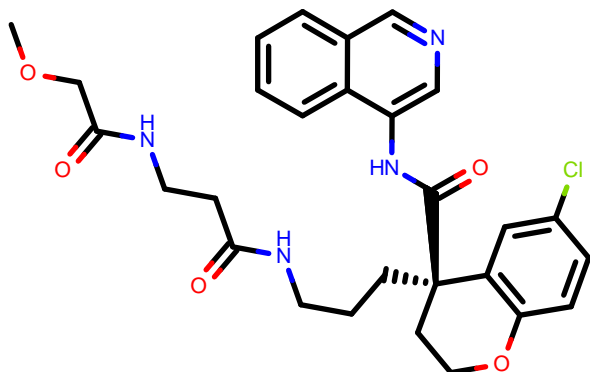
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@](O)(C(=O)C4=CC=CC=C4)C(=O)C@@H5CNC1=O)C[C@@H]5C(=O)NCC5

RUN: RUN4134

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.24

EN300-31242_4_1_1



CID: EN300-31242_4_1_1

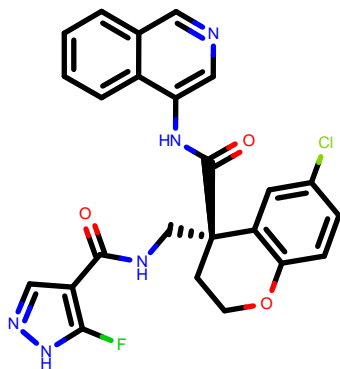
SMILES: COCC(=O)NCCC(=O)NCCC[C@@H]1(C(=O)C2=CC=CC=C2)C(=O)Nc3ccc4c3ccc4

RUN: RUN5973

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.32

EN300-7121836_2_1_1



CID: EN300-7121836_2_1_1

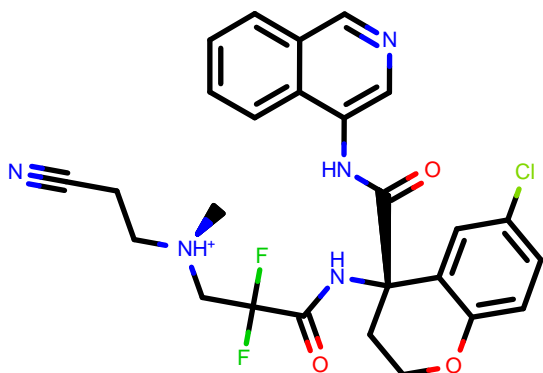
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CNC(=O)c5c[nH]c5F

RUN: RUN5803

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.21

EDG-MED-90036822-92_1



CID: EDG-MED-90036822-92_1

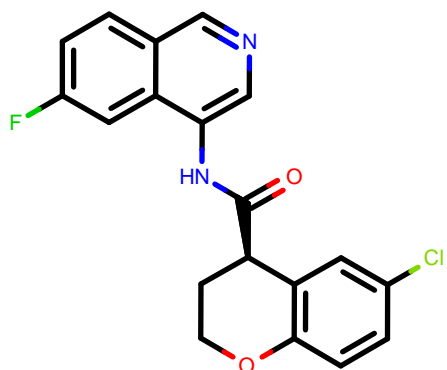
SMILES: C[N+](CCC#N)CC(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)F(F)

RUN: RUN1737

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.33

ALP-POS-696356e4-1_1_1



CID: ALP-POS-696356e4-1_1_1

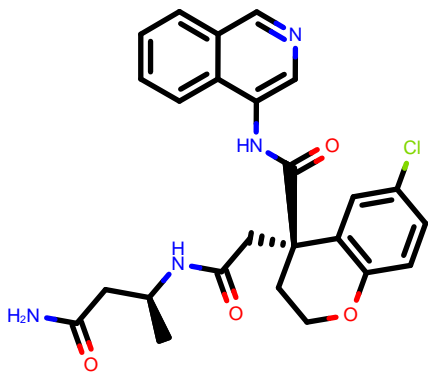
SMILES: c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN7511

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.04

EN300-84785_1_1_1



CID: EN300-84785_1_1_1

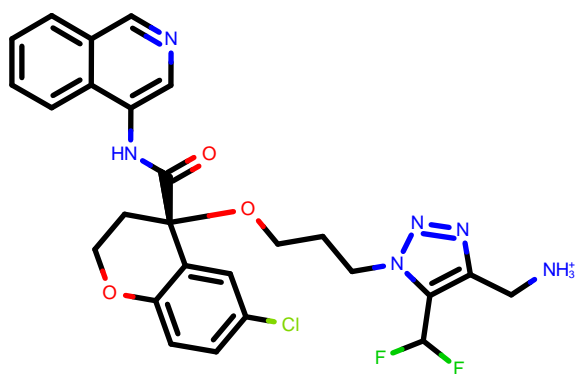
SMILES: C[C@@H](CC(=O)N)NC(=O)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN6868

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.26

ED_-GRI-5b13fbe2-54_1



CID: ED_-GRI-5b13fbe2-54_1

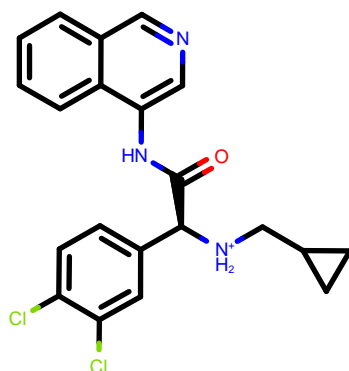
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](CCOC4c3cc(cc4)Cl)OCCc5c(c1nn5)C[NH3+](C(F)F)

RUN: RUN1523

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.39

MAT-POS-1f3f1a6f-4_2



CID: MAT-POS-1f3f1a6f-4_2

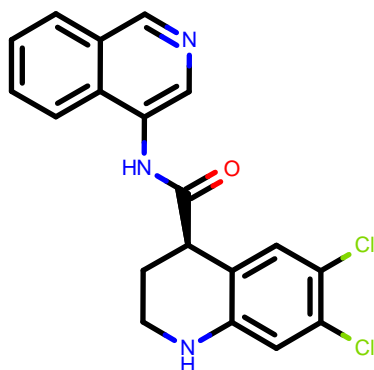
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)[NH2+](CC4CC4)

RUN: RUN2155

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.44

ALP-UNI-3735e77e-4_1



CID: ALP-UNI-3735e77e-4_1

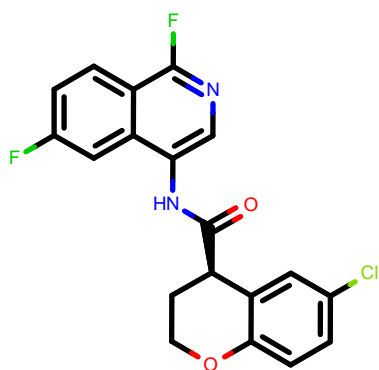
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNC4c3cc(c(c4)Cl)Cl

RUN: RUN1790

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.26

JOH-SUS-a69c159d-5_1



CID: JOH-SUS-a69c159d-5_1

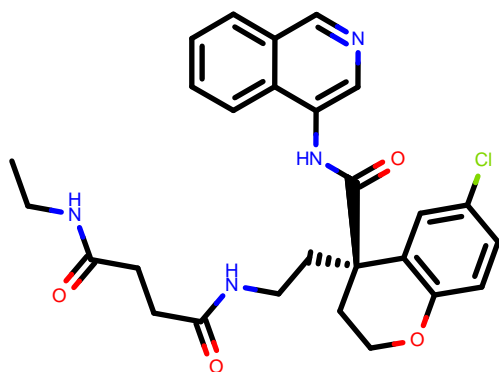
SMILES: c1cc2c(cc1F)c(cnc2F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1043

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.05

EN300-68889_3_1_1



CID: EN300-68889_3_1_1

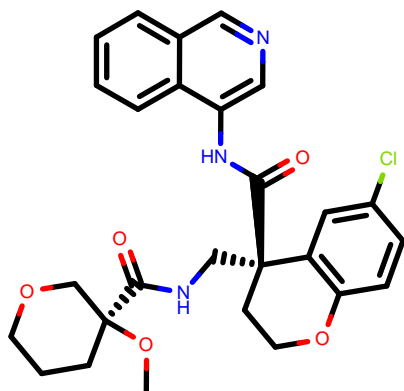
SMILES: CCNC(=O)CCC(=O)NCC[C@@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6164

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.30

EN300-1072199_2_2_1



CID: EN300-1072199_2_2_1

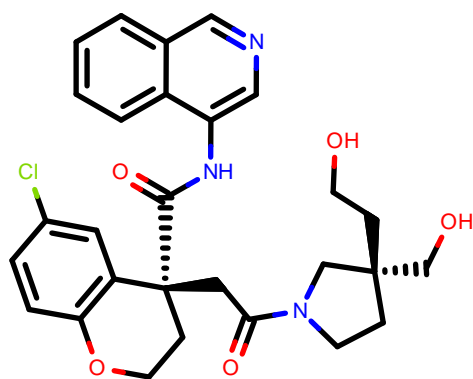
SMILES: CO[C@@]1(CCCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4774

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.33

EN300-1707870_1_1_1



CID: EN300-1707870_1_1_1

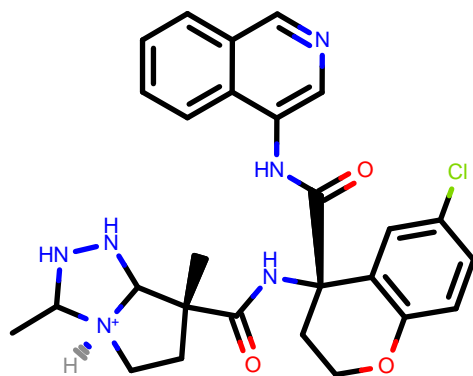
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)Cl)CC(=O)N5CC[C@]3(C5)(COC)CO

RUN: RUN7635

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.43

EN300-7431629_1_1_1



CID: EN300-7431629_1_1_1

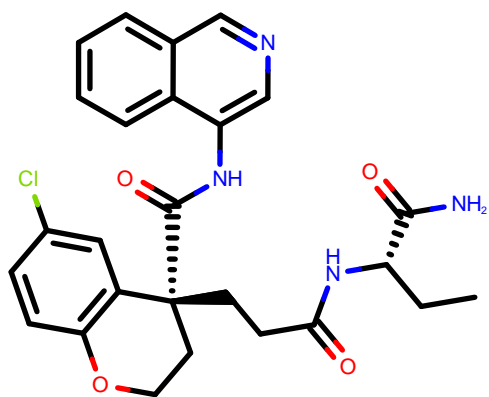
SMILES: Cc1nnc2n1CC[C@@]2(C)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN3742

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-7375395_2_1_1



CID: EN300-7375395_2_1_1

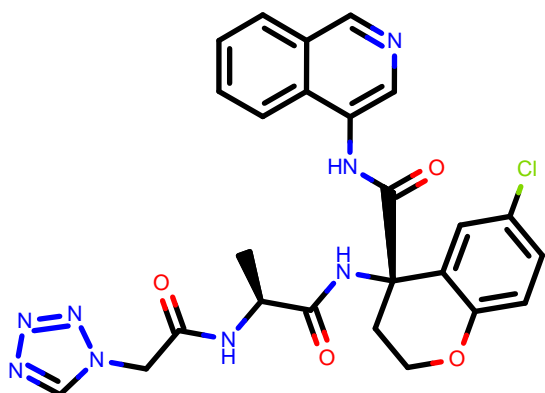
SMILES: CC[C@@H](C(=O)N)NC(=O)CC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7371

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-651177_1_1_1



CID: EN300-651177_1_1_1

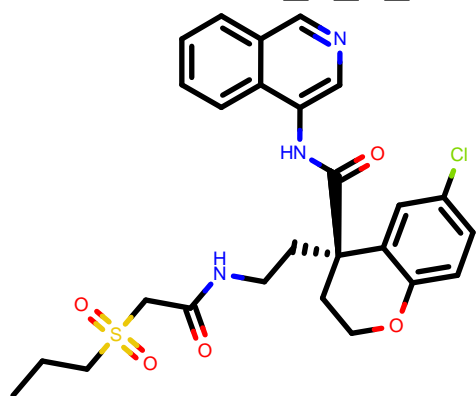
SMILES: C[C@@H](C(=O)N)C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)Cn5nnn5

RUN: RUN6842

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.37

EN300-52325_3_1_1



CID: EN300-52325_3_1_1

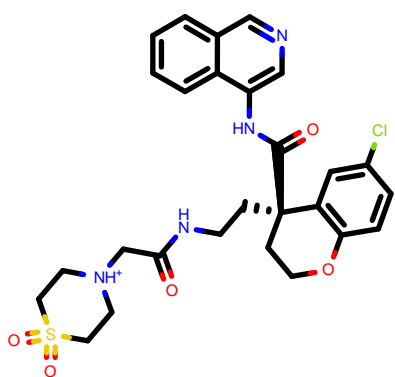
SMILES: CCCS(=O)(=O)CC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4457

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.46

EN300-39305_3_1_1



CID: EN300-39305_3_1_1

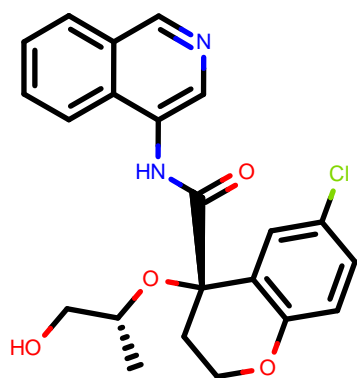
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCS(=O)(=O)CC5

RUN: RUN6875

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.27

EN300-175186_1_2_1



CID: EN300-175186_1_2_1

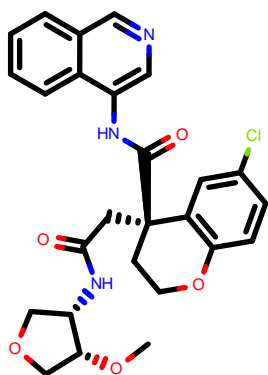
SMILES: C[C@H](CO)OC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN7539

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.26

EN300-252683_1_1_1



CID: EN300-252683_1_1_1

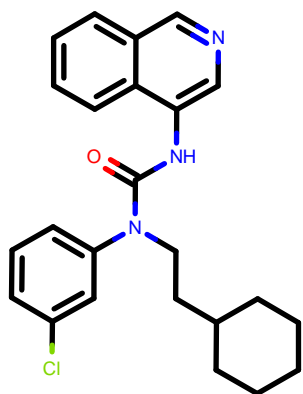
SMILES: CO[C@@H]1COC[C@@H]1NC(=O)C[C@]2(CCOC3c2cc(cc3)O)C(=O)Nc4ccc5c4cccc5

RUN: RUN4566

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.26

VLA-UCB-05e51b3f-14_1



CID: VLA-UCB-05e51b3f-14_1

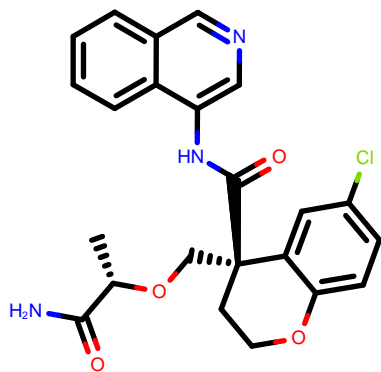
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cccc(c4)Cl

RUN: RUN295

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.34

EN300-17381_2_1_1



CID: EN300-17381_2_1_1

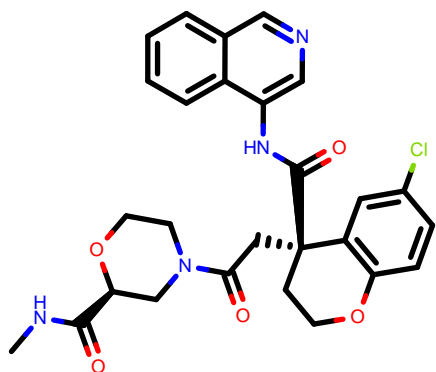
SMILES: C[C@@H](C(=O)N)OC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN6092

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.21

EN300-130644_1_1_1



CID: EN300-130644_1_1_1

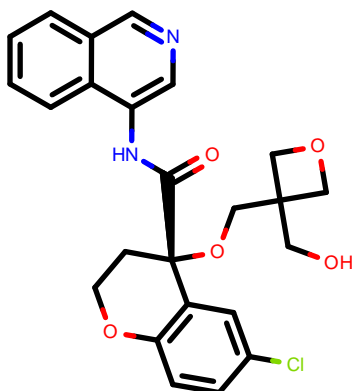
SMILES: CNC(=O)C@@H1CN(CCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7284

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.31

EN300-102347_1_1_1



CID: EN300-102347_1_1_1

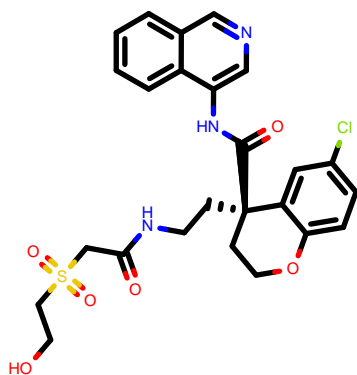
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)OCC5(COC5)CO

RUN: RUN7014

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.24

EN300-4293814_3_1_1



CID: EN300-4293814_3_1_1

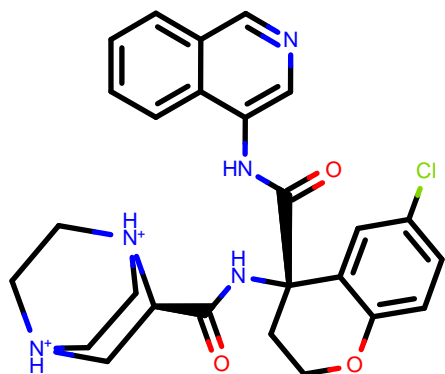
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)CO

RUN: RUN3104

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.50

EN300-1605566_1_2_1



CID: EN300-1605566_1_2_1

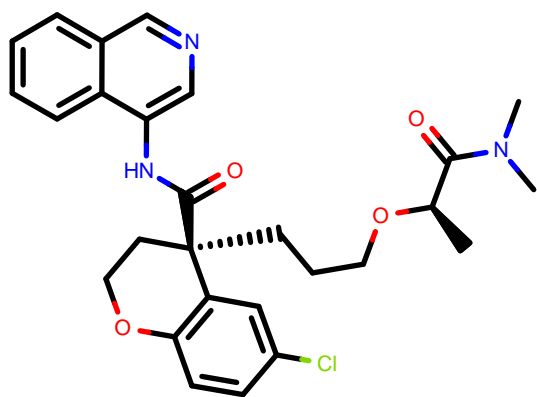
SMILES: c1ccc2c(c1)cncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CN6CC[NH+]5CC6

RUN: RUN7675

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.34

EN300-14458_4_2_1



CID: EN300-14458_4_2_1

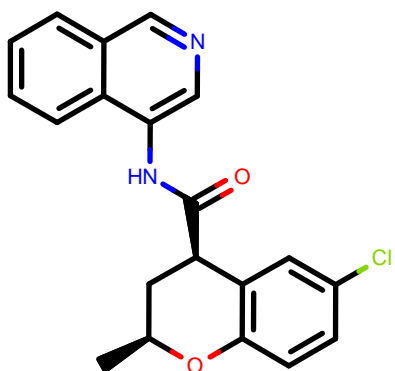
SMILES: C[C@H](C(=O)N(C)C)OCCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6682

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.31

ALP-POS-d3acb8cc-1_1_1



CID: ALP-POS-d3acb8cc-1_1_1

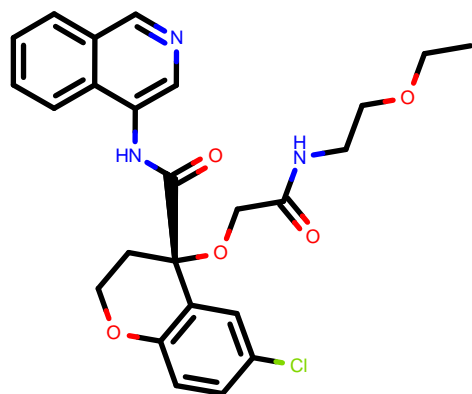
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5524

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.09

EN300-103187_1_1_1



CID: EN300-103187_1_1_1

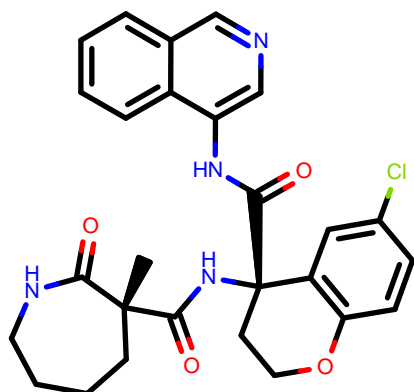
SMILES: CCOCCNC(=O)CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5563

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.22

EN300-6745081_1_2_1



CID: EN300-6745081_1_2_1

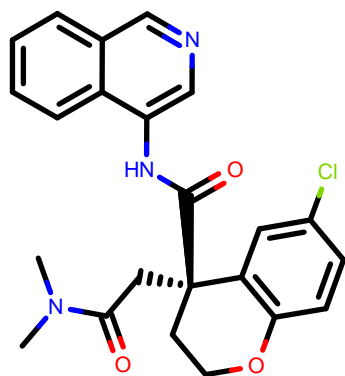
SMILES: C[C@]1(CCCNC1=O)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5698

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.26

MAT-POS-f9802937-4_1



CID: MAT-POS-f9802937-4_1

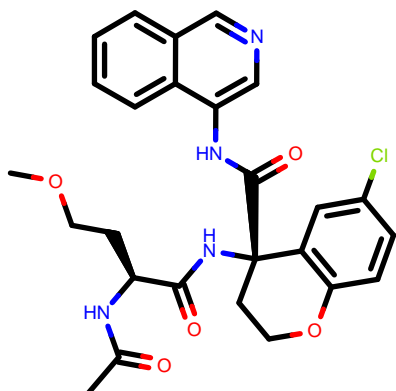
SMILES: CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2221

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.22

EN300-62074_1_1_1



CID: EN300-62074_1_1_1

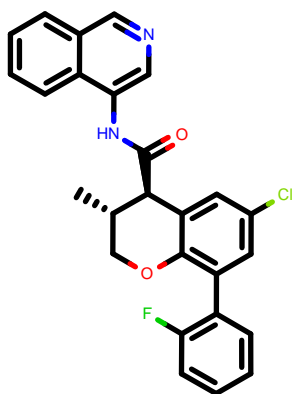
SMILES: CC(=O)N[C@@H](CCOC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4278

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.28

DAR-DIA-0d514e7d-16_1



CID: DAR-DIA-0d514e7d-16_1

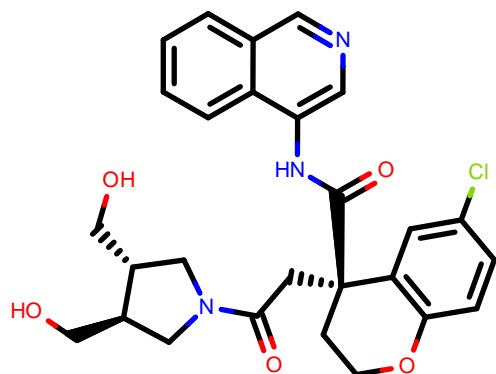
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3ncc4c3cccc4)Cl)c5ccccc5F

RUN: RUN796

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.21

EN300-314088_1_1_1



CID: EN300-314088_1_1_1

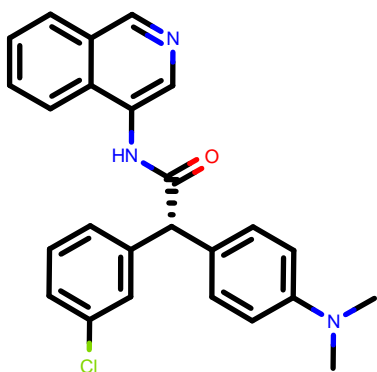
SMILES: c1ccc2c1)nc2NCl(=O)[C@@H](C)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5c(C[C@@H](C)[C@@H](C)CO)CO

RUN: RUN5707

DDG (kcal/mol): -0.20

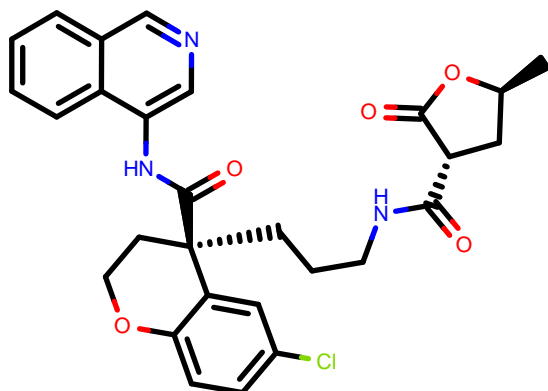
dDDG (kcal/mol): 0.30

MIC-UNK-d36ab305-4_2



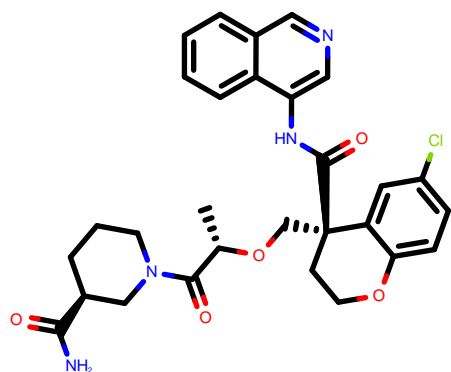
CID:	MIC-UNK-d36ab305-4_2
SMILES:	<chem>CN(C)c1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN141
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.36

EN300-7444533_4_2_1



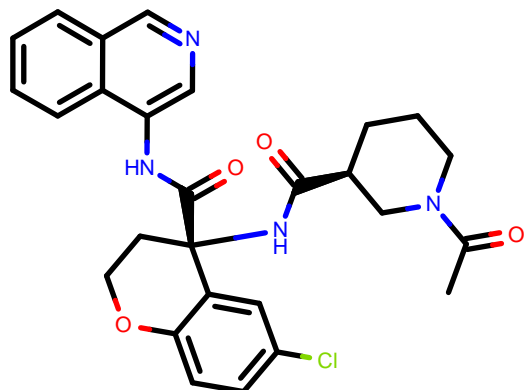
CID:	EN300-7444533_4_2_1
SMILES:	<chem>C[C@@H]1[C@@H](C)[C@@H](C)O1[C@@H](C)O1NCCC[C@@]2(C)COC3C2cc(c3)C[C@@]4O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN6979
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.30

EN300-28177_2_1_1



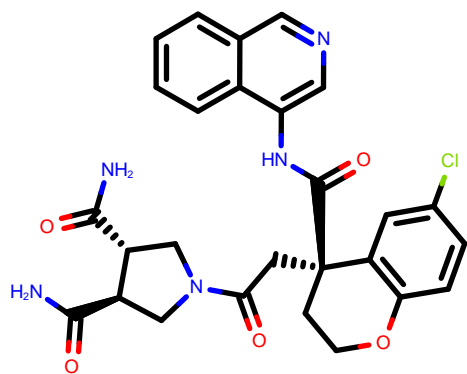
CID:	EN300-28177_2_1_1
SMILES:	<chem>C[C@@]1(C)[C@@H](C)O1NCCC[C@@]2(C)COC3C2cc(c3)C[C@@]4O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN5283
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.38

EN300-14752_1_1_1



CID:	EN300-14752_1_1_1
SMILES:	<chem>CC(=O)N1CCC[C@@]1(C)[C@@H](C)O1NCCC[C@@]2(C)COC3C2cc(c3)C[C@@]4O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN2739
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.16

EN300-7444316_1_1_1



CID: EN300-7444316_1_1_1

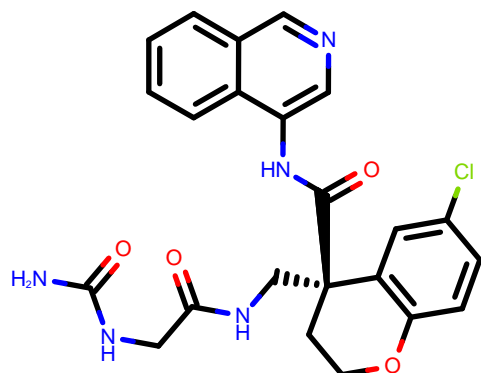
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc(c4)Cl)CC(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N

RUN: RUN6303

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.37

EN300-10397_2_1_1



CID: EN300-10397_2_1_1

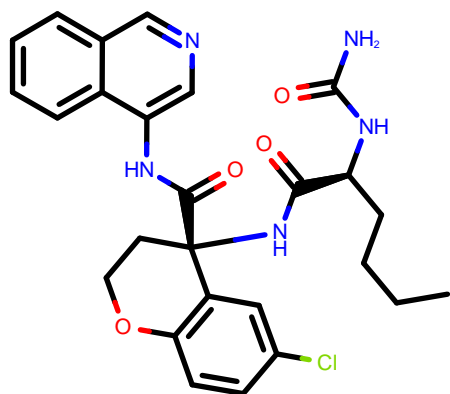
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc(c4)Cl)CNC(=O)CNC(=O)N

RUN: RUN4253

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.23

EN300-55744_1_1_1



CID: EN300-55744_1_1_1

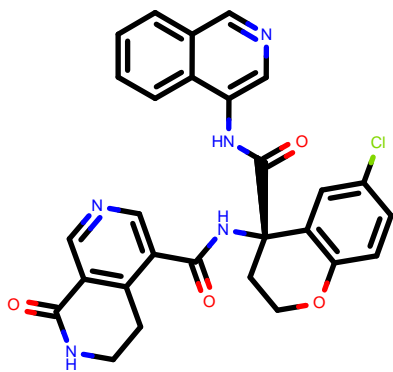
SMILES: CCCC[C@@H](C)C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4NC(=O)N

RUN: RUN7700

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-314274_1_1_1



CID: EN300-314274_1_1_1

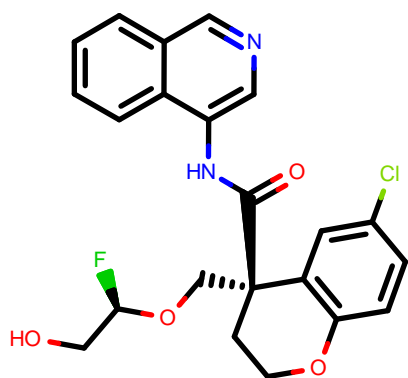
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc(c4)Cl)NC(=O)c5ccc6c5CCNC6=O

RUN: RUN4015

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.35

EN300-861925_2_1_1



CID: EN300-861925_2_1_1

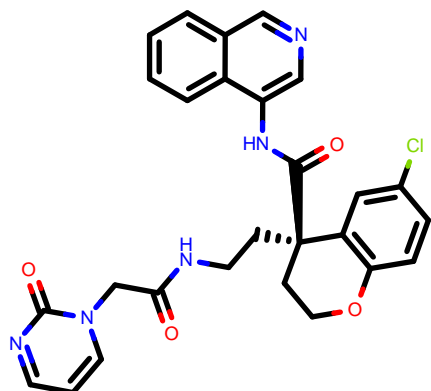
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H](CO)F

RUN: RUN7310

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.24

EN300-35789_3_1_1



CID: EN300-35789_3_1_1

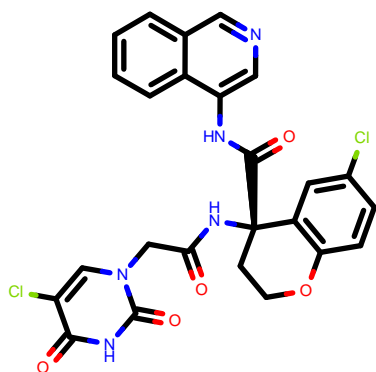
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccnc5=O

RUN: RUN5257

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.31

ALP-UNI-dbbfd3db-10_1



CID: ALP-UNI-dbbfd3db-10_1

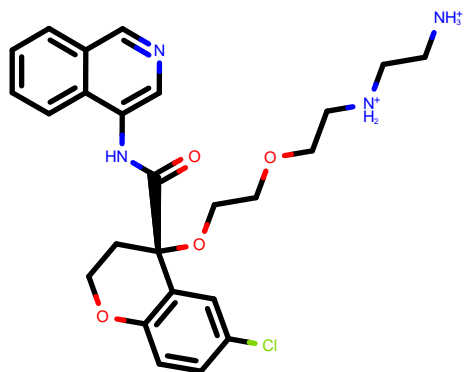
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Cn5cc(c1=O)[nH]5=O)Cl

RUN: RUN2610

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-8_1



CID: ED_-GRI-5b13fbe2-8_1

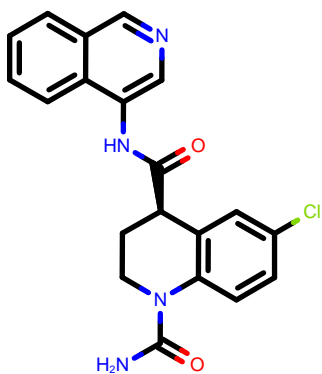
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCC[NH2+][CCN]

RUN: RUN1408

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.66

RAL-THA-4aa06b95-1_1



CID: RAL-THA-4aa06b95-1_1

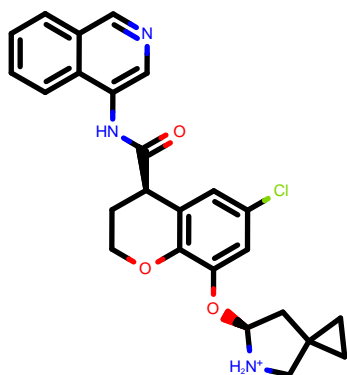
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)C(=O)N

RUN: RUN1120

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.25

DAR-DIA-23e5a6a0-4_2



CID: DAR-DIA-23e5a6a0-4_2

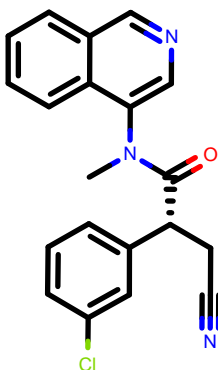
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCO(c4c3cc(cc4O)[C@H]5CC6(CC6)C[NH2+]5)Cl

RUN: RUN372

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.30

JOH-UNI-3fc3434e-7_2



CID: JOH-UNI-3fc3434e-7_2

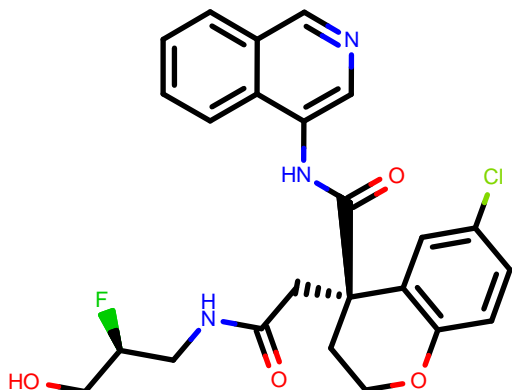
SMILES: CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl

RUN: RUN1778

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.23

EN300-7353973_1_1_1



CID: EN300-7353973_1_1_1

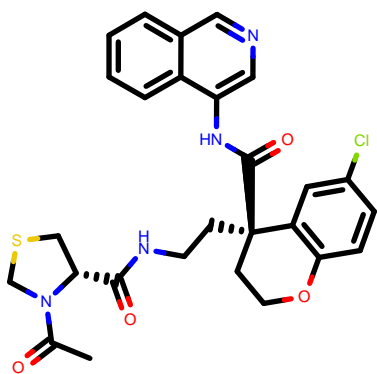
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H](CO)F

RUN: RUN6458

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-761220_3_1_1



CID: EN300-761220_3_1_1

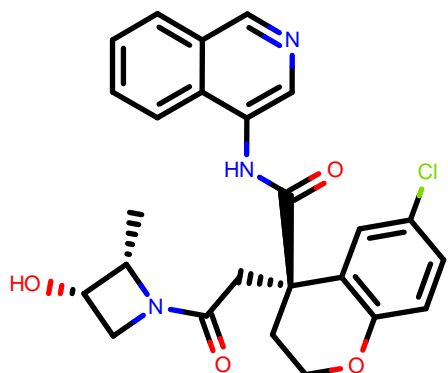
SMILES: CC(=O)N1CSC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3659

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.31

EN300-7471076_1_4_1



CID: EN300-7471076_1_4_1

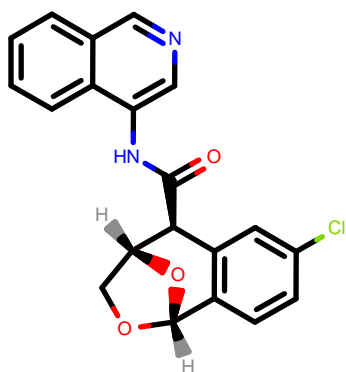
SMILES: C[C@H]1[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN5724

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

RAL-THA-c9f97604-2_1



CID: RAL-THA-c9f97604-2_1

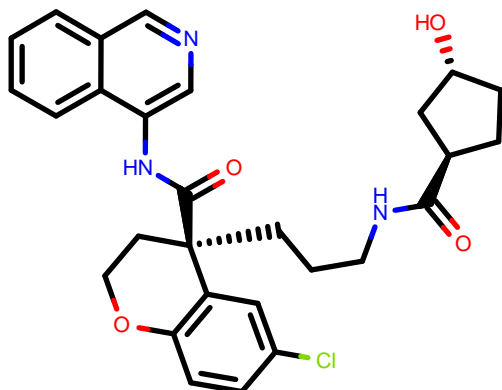
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4[C@@H]3)OC[C@H]3O5Cl

RUN: RUN457

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.21

EN300-321597_4_1_1



CID: EN300-321597_4_1_1

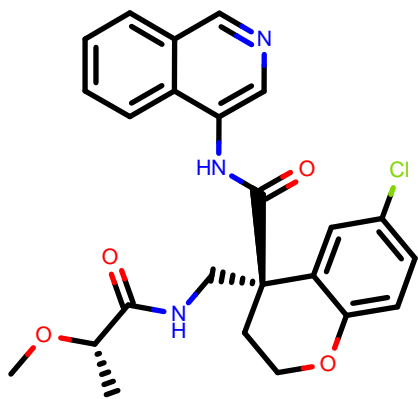
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@H](C5)O

RUN: RUN6169

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.36

EN300-51257_2_1_1



CID: EN300-51257_2_1_1

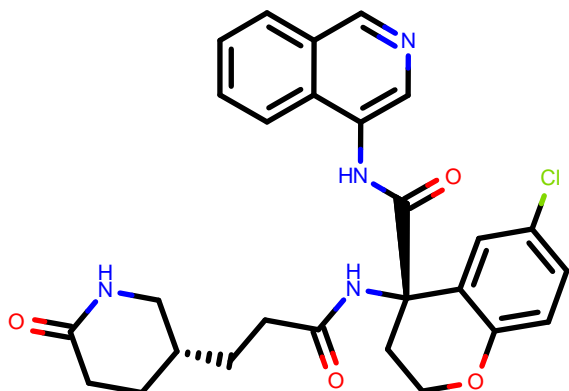
SMILES: C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)OC

RUN: RUN5473

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

EN300-1215738_1_1_1



CID: EN300-1215738_1_1_1

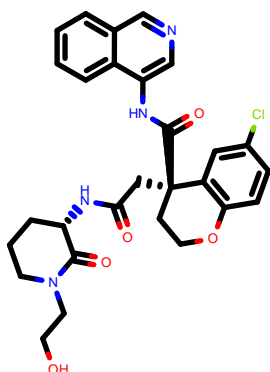
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)CC[C@@H]5CCC(=O)NC5

RUN: RUN7784

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

EN300-141480_1_2_1



CID: EN300-141480_1_2_1

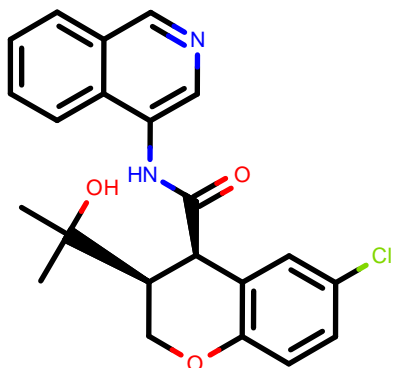
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N[C@@H]5CCCN(C5=O)CO

RUN: RUN6338

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.33

BEN-BAS-5c03e89e-1_1_1



CID: BEN-BAS-5c03e89e-1_1_1

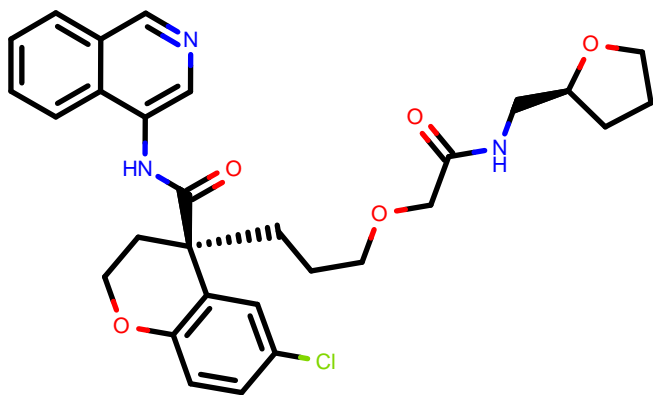
SMILES: CC(C)(C)[C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3ncc4c3ccc4)ClO

RUN: RUN6469

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.25

EN300-01527_4_1_1



CID: EN300-01527_4_1_1

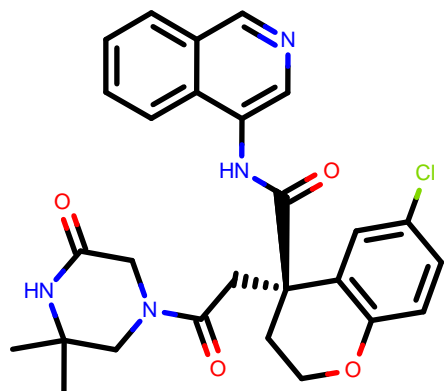
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC(=O)NC[C@@H]5CCOC5

RUN: RUN4707

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.34

EN300-7493939_1_1_1



CID: EN300-7493939_1_1_1

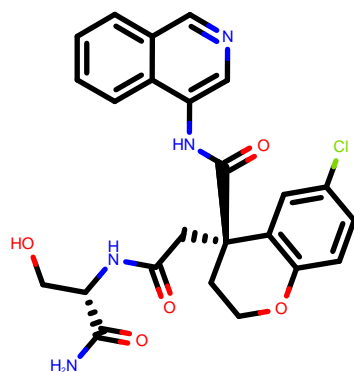
SMILES: CC1(CN(CC(=O)N1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)C

RUN: RUN4797

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

EN300-208204_1_1_1



CID: EN300-208204_1_1_1

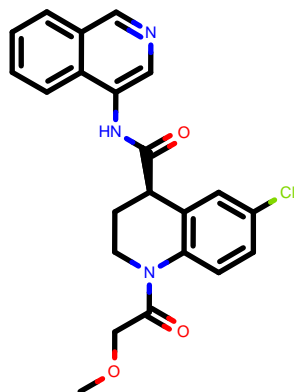
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)C(=O)N

RUN: RUN6233

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

RAL-THA-4aa06b95-5_2



CID: RAL-THA-4aa06b95-5_2

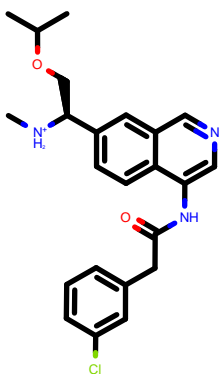
SMILES: COCC(=O)N1CC[C@H](c2c1ccc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN1169

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

MAK-UNK-ffc90da7-3_1



CID: MAK-UNK-ffc90da7-3_1

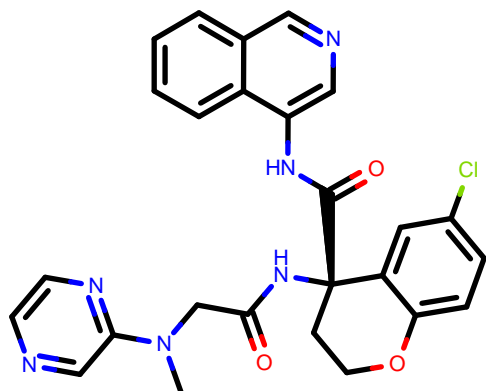
SMILES: CC(C)OC[C@@H](c1ccc2c(c1)cnc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C

RUN: RUN633

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-36855_1_1_1



CID: EN300-36855_1_1_1

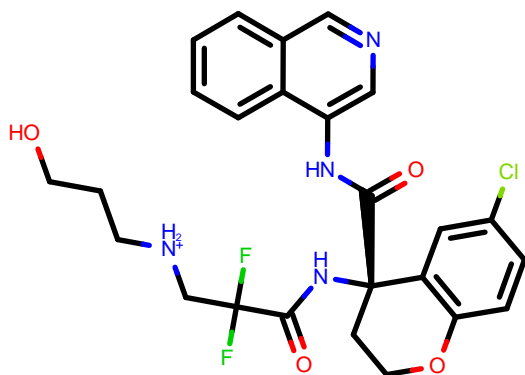
SMILES: CN(CC(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)c5nccn5

RUN: RUN5342

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

EDG-MED-90036822-52_1



CID: EDG-MED-90036822-52_1

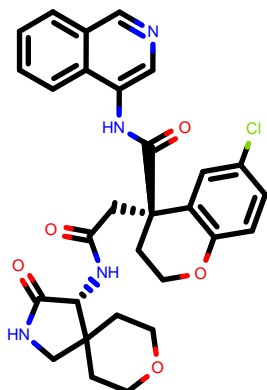
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CNCCCC)F

RUN: RUN1638

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.31

EN300-310254_1_2_1



CID: EN300-310254_1_2_1

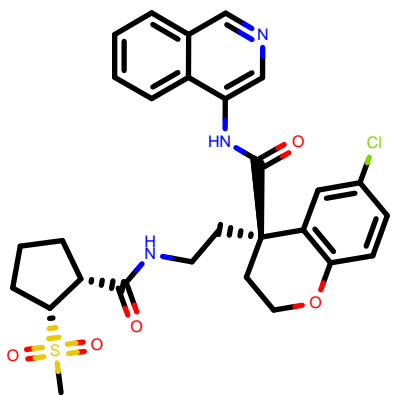
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(C)NCC5CCCCC6

RUN: RUN7716

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.45

EN300-1387145_3_1_1



CID: EN300-1387145_3_1_1

SMILES:

CS(=O)(=O)C@@H1CC[C@@H]1C(=O)NC[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5

RUN:

RUN5475

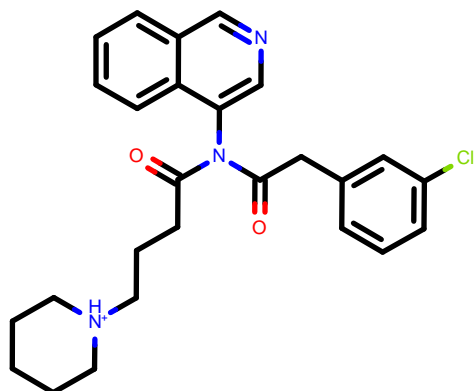
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.31

DAR-DIA-076fb6ea-12_1



CID: DAR-DIA-076fb6ea-12_1

SMILES:

c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)C=C/C[NH+]4CCCCC4

RUN:

RUN1309

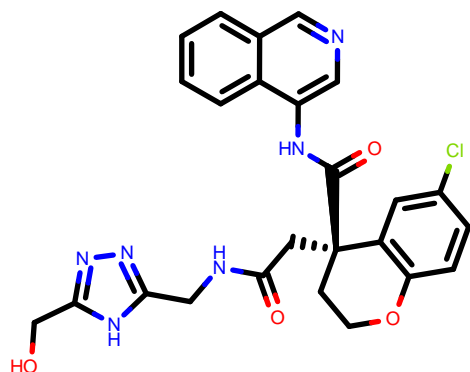
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.64

EN300-312662_1_1_1



CID: EN300-312662_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5[nH]nc(n5)CO

RUN:

RUN7750

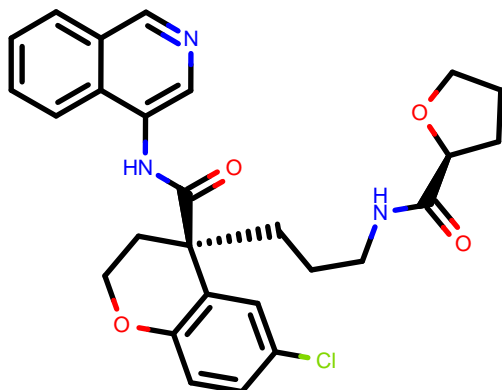
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.36

EN300-104395_4_1_1



CID: EN300-104395_4_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCO5

RUN:

RUN6115

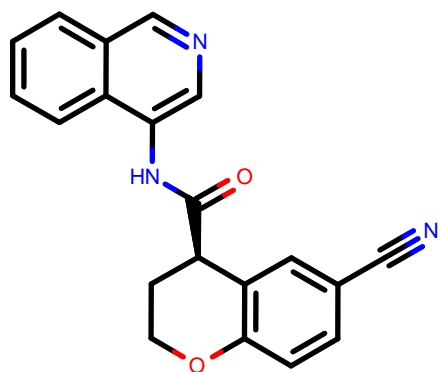
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.29

DAR-DIA-6a508060-3_1_1



CID: DAR-DIA-6a508060-3_1_1

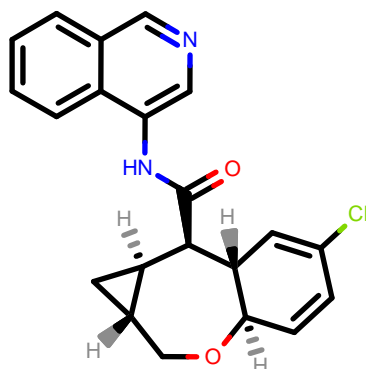
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C#N

RUN: RUN6892

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.05

DAR-DIA-0d514e7d-32_29



CID: DAR-DIA-0d514e7d-32_29

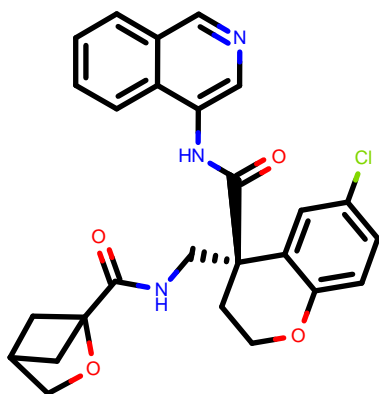
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H]4[C@H]4C[C@H]5[C@H]3C=C(C=C5)Cl

RUN: RUN781

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.23

EN300-2007648_2_1_1



CID: EN300-2007648_2_1_1

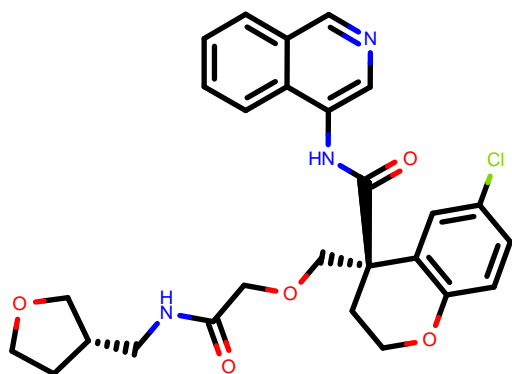
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CC(C5)C6

RUN: RUN4971

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.26

EN300-46832_2_1_1



CID: EN300-46832_2_1_1

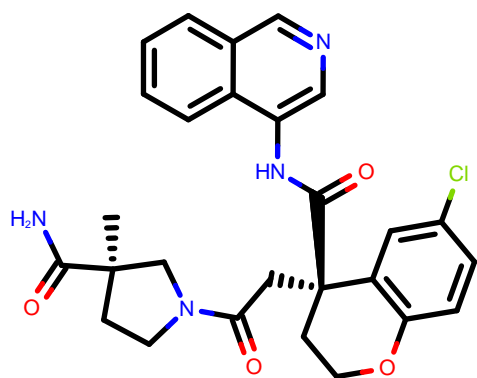
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@@H]5CCOC5

RUN: RUN6723

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.26

EN300-194442_1_2_1



CID: EN300-194442_1_2_1

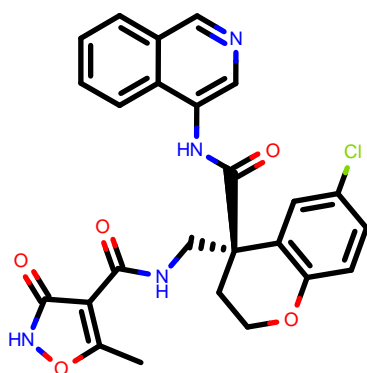
SMILES: C[C@@]1(CCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)C(=O)N

RUN: RUN4750

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.36

EN300-110423_2_1_1



CID: EN300-110423_2_1_1

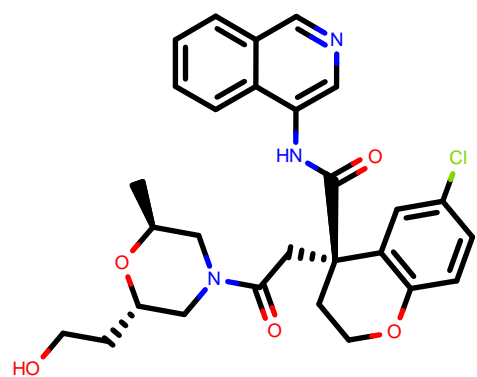
SMILES: Cc1c(c(=O)[nH]o1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN6359

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.20

EN300-212814_1_2_1



CID: EN300-212814_1_2_1

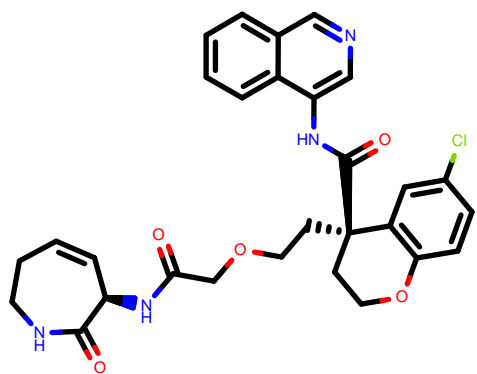
SMILES: C[C@@H]1CN(C[C@@H]1O)CCO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4975

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.36

EN300-37195_3_1_1



CID: EN300-37195_3_1_1

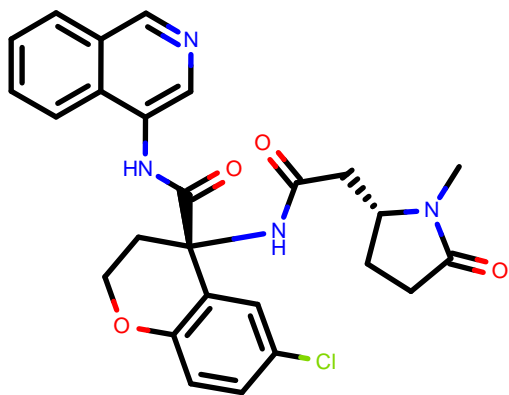
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CCCCNC5=O

RUN: RUN4744

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-207765_1_2_1



CID: EN300-207765_1_2_1

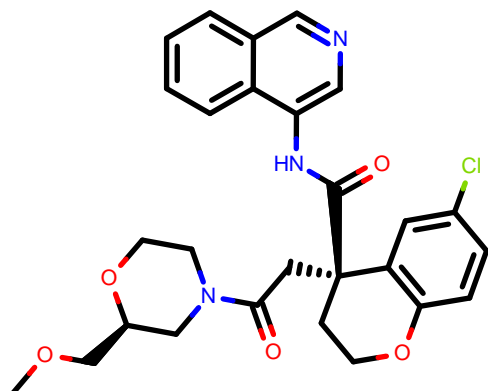
SMILES: CN1C@H](CCC1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4455

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.17

EN300-85707_1_1_1



CID: EN300-85707_1_1_1

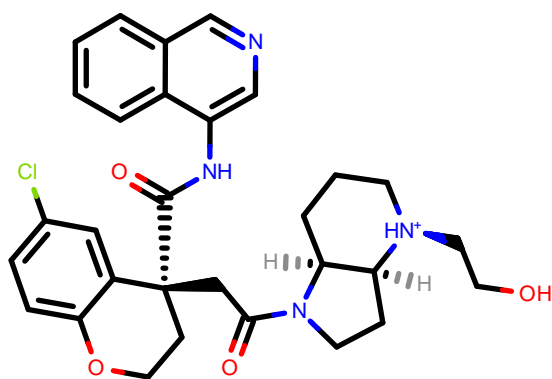
SMILES: COC[C@]H1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5204

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.44

ALP-UNI-3496895b-2_6



CID: ALP-UNI-3496895b-2_6

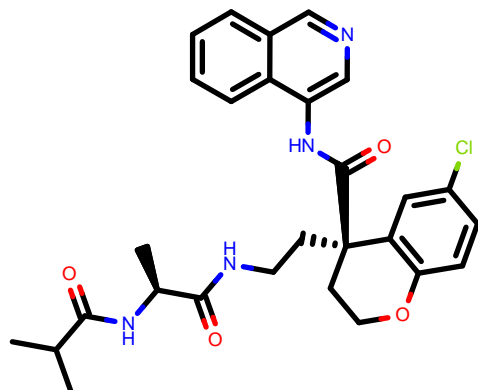
SMILES: c1ccc2c(c1)ccc2N[C@@]3(C)C(=O)C4=CC(=C4)C[C@@]3(O)N5C[C@@]H(C)C@H5O

RUN: RUN2367

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.51

EN300-31184_3_1_1



CID: EN300-31184_3_1_1

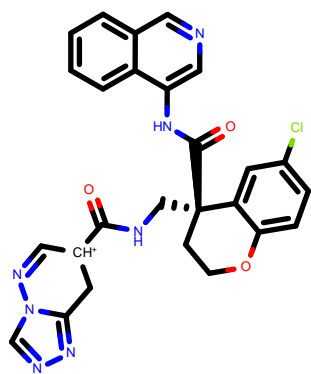
SMILES: C[C@@]H(C(=O)NCC[C@]1(C)C(=O)C2=CC(=C2)C)C(=O)Nc3ccc4c3ccc4)NC(=O)C(C)C

RUN: RUN7227

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.30

ALP-UNI-0676e700-15_1



CID: ALP-UNI-0676e700-15_1

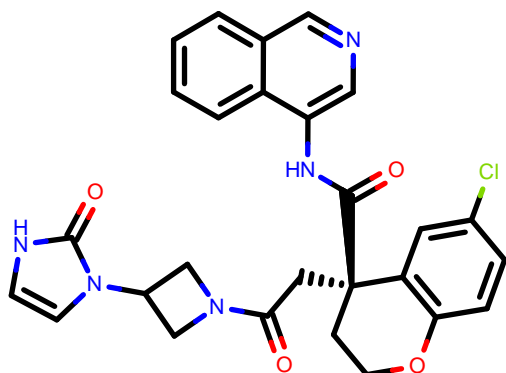
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CNC(=O)c5cc6nncn6c5

RUN: RUN2311

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.29

EN300-208993_1_1_1



CID: EN300-208993_1_1_1

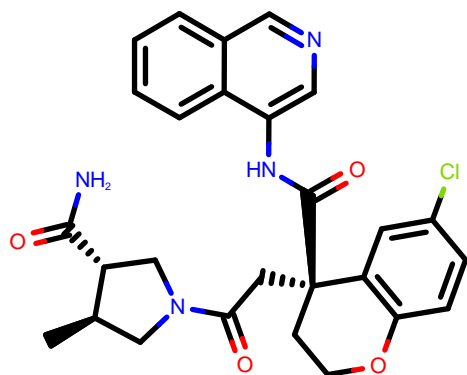
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)N5CC(5)N6CNC6=O

RUN: RUN5667

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.25

EN300-244842_1_1_1



CID: EN300-244842_1_1_1

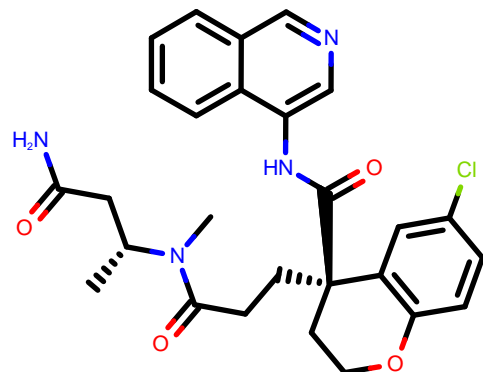
SMILES: C[C@@H]1CN(C[C@@H]1C(=O)N)C(=O)C[C@@2](CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN6838

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.25

EN300-1688974_2_2_1



CID: EN300-1688974_2_2_1

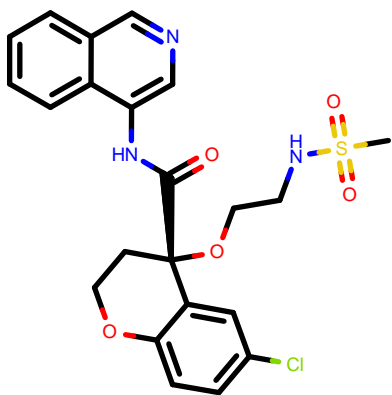
SMILES: C[C@@H](CC(=O)N)N(C)C(=O)CC[C@@1](CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccc4

RUN: RUN4266

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.29

EN300-1238839_1_1_1



CID: EN300-1238839_1_1_1

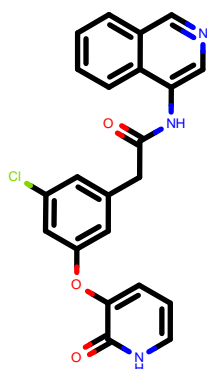
SMILES: CS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN: RUN7254

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.26

RAL-THA-1d44ff04-12_1



CID: RAL-THA-1d44ff04-12_1

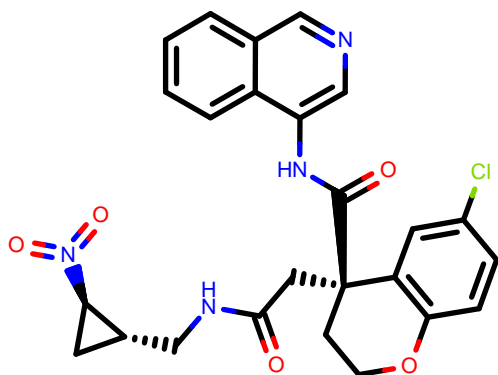
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Oc4ccc[nH]c4=O

RUN: RUN381

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.47

EN300-7465222_1_1_1



CID: EN300-7465222_1_1_1

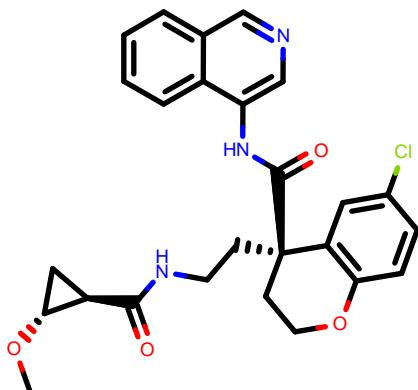
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]5[N+](=O)[O-]

RUN: RUN5526

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.20

EN300-650518_3_1_1



CID: EN300-650518_3_1_1

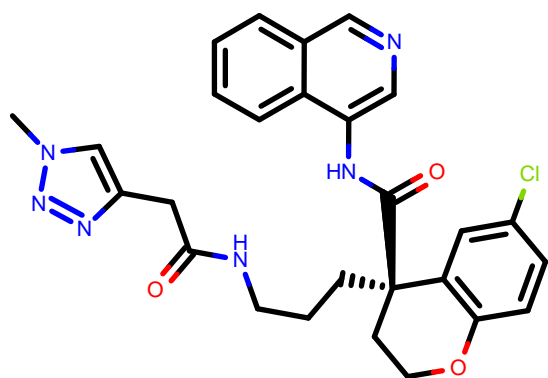
SMILES: CO[C@@H]1C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN4493

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.22

EN300-1073264_4_1_1



CID: EN300-1073264_4_1_1

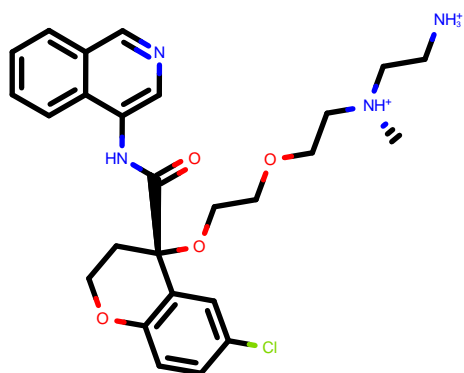
SMILES: Cn1cc(nn1)CC(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN6854

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.36

ED_-GRI-5b13fbe2-15_2



CID: ED_-GRI-5b13fbe2-15_2

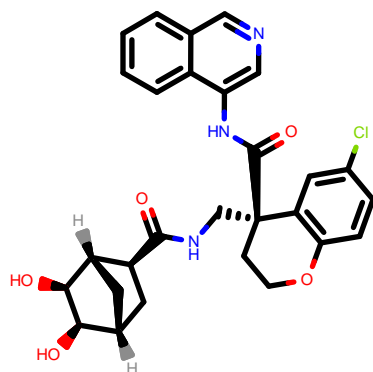
SMILES: C[NH2+][C][C][NH3+][C]COCOC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4

RUN: RUN1441

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.43

EN300-6744028_2_2_1



CID: EN300-6744028_2_2_1

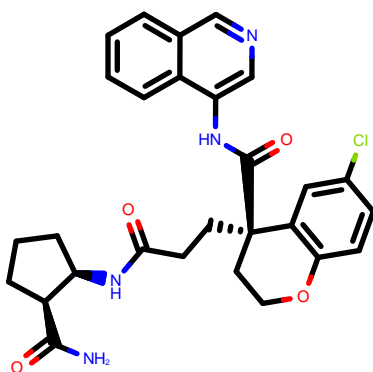
SMILES: c1ccc2c(c1)ncnc2NCl(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC1=O[C@@H]5C[C@@H]6[C@@]3([C@@H]5)C[C@@H]6O

RUN: RUN6204

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.32

EN300-90531_2_1_1



CID: EN300-90531_2_1_1

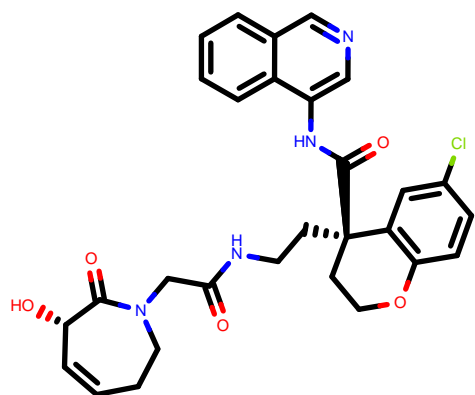
SMILES: c1ccc2c(c1)ncnc2NCl(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]5(C)C[C@@]5O

RUN: RUN6434

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.38

EN300-259849_3_1_1



CID: EN300-259849_3_1_1

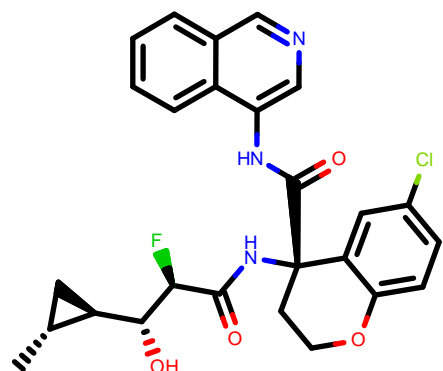
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc4ccc(cc4)C(C)CNC(=O)CNSCOC[C@@H](C)C5=O

RUN: RUN4231

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.38

EDG-MED-90036822-94_15



CID: EDG-MED-90036822-94_15

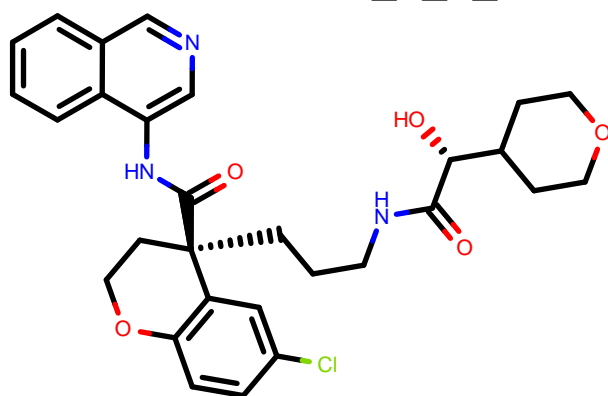
SMILES: C[C@@H](C)[C@@H](C)[C@@H](C)C(=O)NC[C@@H](C)COCc4ccc(cc4)C(C)CNC(=O)C5=O

RUN: RUN1680

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-7443878_4_1_1



CID: EN300-7443878_4_1_1

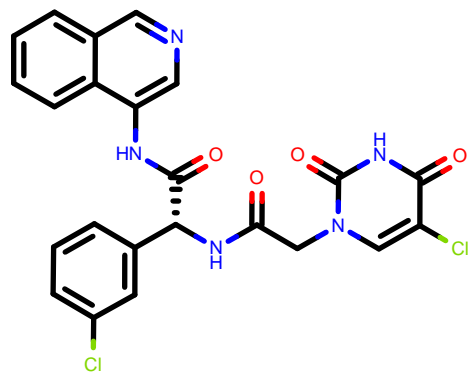
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc4ccc(cc4)C(C)CNC(=O)[C@@H](C)C5=O

RUN: RUN5802

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.44

EDJ-MED-ee07cf00-16_1



CID: EDJ-MED-ee07cf00-16_1

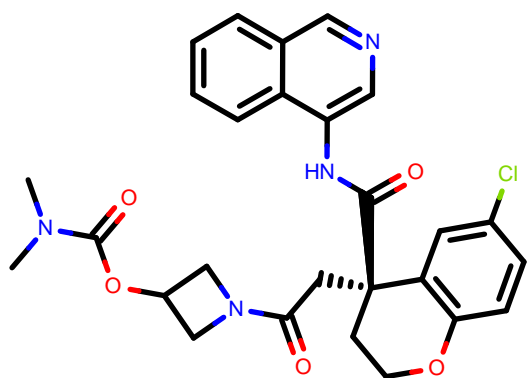
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)COCc4ccc(cc4)C(C)CNC(=O)Cn4cc(c(=O)[nH]4=O)Cl

RUN: RUN2673

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.47

EN300-1272529_1_1_1



CID: EN300-1272529_1_1_1

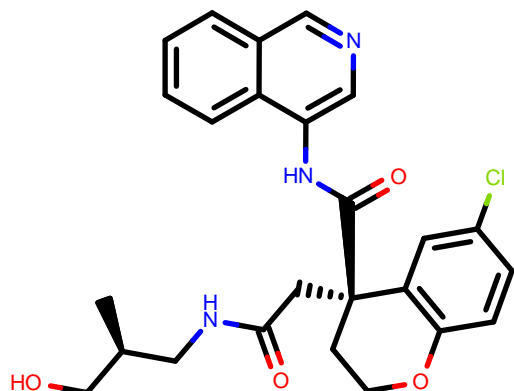
SMILES: CN(C)C(=O)OC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5ccccc5

RUN: RUN6777

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.26

EN300-108430_1_1_1



CID: EN300-108430_1_1_1

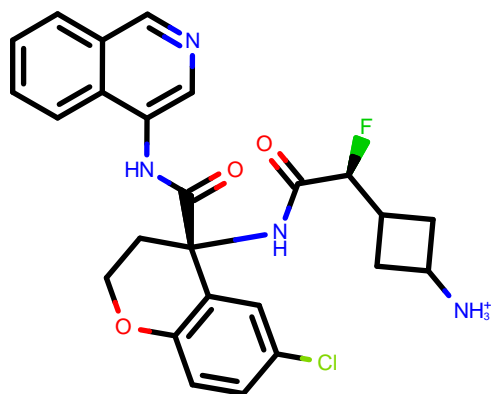
SMILES: C[C@@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)CO

RUN: RUN7608

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.22

EDG-MED-90036822-35_1



CID: EDG-MED-90036822-35_1

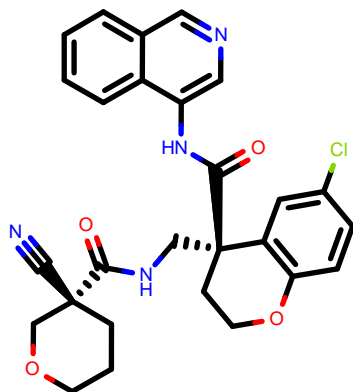
SMILES: c1cc2c(cnc2)NC(=O)[C@@]3(c4ccc5c4)C(OCC3)NC(=O)[C@@H](F)[C@@H]5C[C@H](C5)N3+

RUN: RUN1554

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.25

EN300-301925_2_1_1



CID: EN300-301925_2_1_1

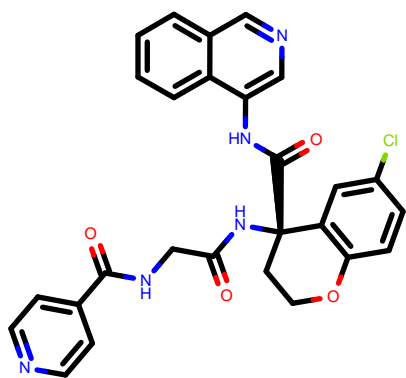
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCCCOC5)C#N

RUN: RUN3535

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.25

EN300-36089_1_1_1



CID: EN300-36089_1_1_1

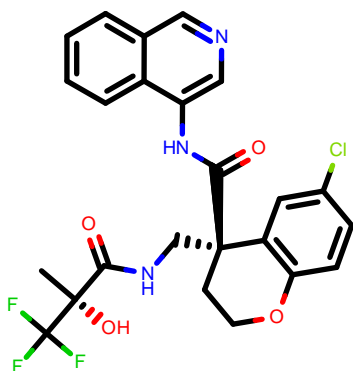
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)c5ccncc5

RUN: RUN5924

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.27

EN300-159633_2_1_1



CID: EN300-159633_2_1_1

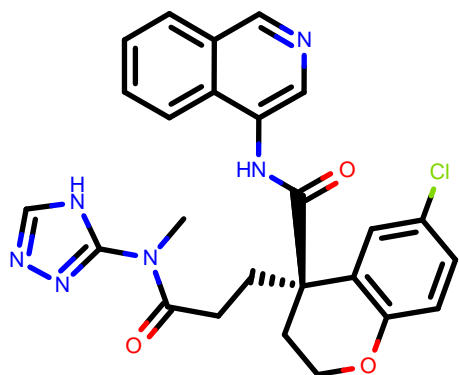
SMILES: C[C@@]([C](O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)(C(F)(F)F)O

RUN: RUN4344

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-1699100_2_1_1



CID: EN300-1699100_2_1_1

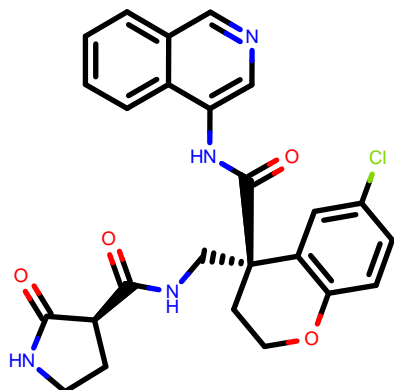
SMILES: CN(c1[nH]ncc1)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN7714

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.24

EN300-94945_2_2_1



CID: EN300-94945_2_2_1

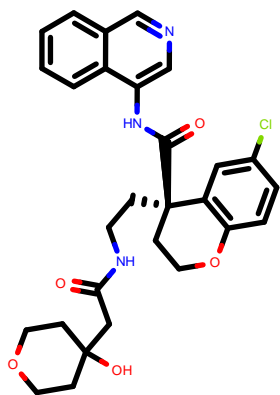
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CCNC5=O

RUN: RUN6239

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.24

EN300-151423_3_1_1



CID: EN300-151423_3_1_1

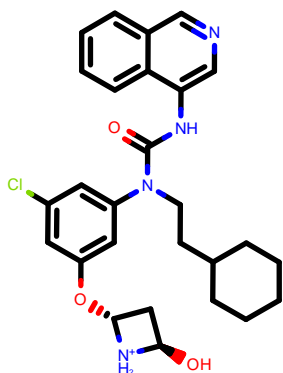
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CCOCC5)O

RUN: RUN2869

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.35

MAT-POS-53907a1c-3_1



CID: MAT-POS-53907a1c-3_1

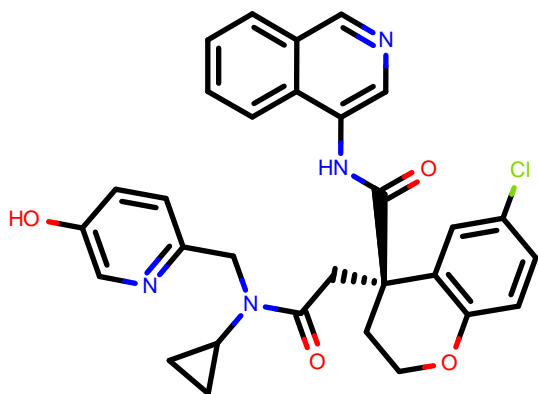
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(CCC3CCCCC3)c4cc(cc(c4)O)C@H]5CC(=O)N5

RUN: RUN492

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.66

EDG-MED-ba1ac7b9-29_1



CID: EDG-MED-ba1ac7b9-29_1

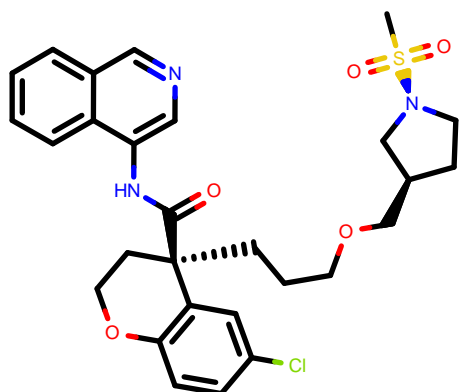
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(Cc5ccc(cn5)O)C6CC6

RUN: RUN2635

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.28

EN300-261986_4_2_1



CID: EN300-261986_4_2_1

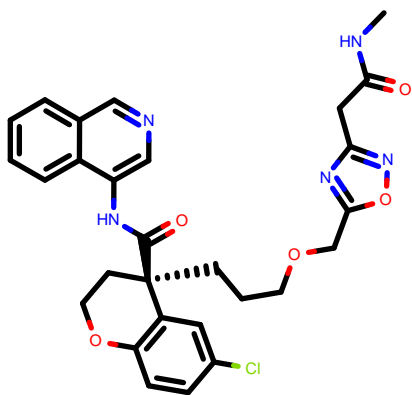
SMILES: CS(=O)(=O)N@]1CC[C@H](C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN7259

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.43

EN300-99983_4_1_1



CID: EN300-99983_4_1_1

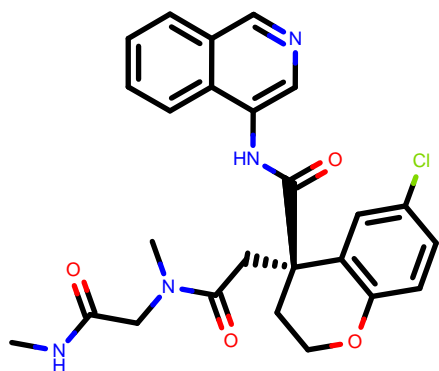
SMILES: CNC(=O)Cc1nc(on1)COC[C@]2(C)COCc3c2cc(cc3Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4679

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

EN300-34491_1_1_1



CID: EN300-34491_1_1_1

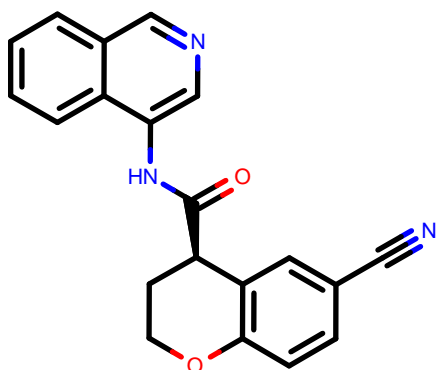
SMILES: CNC(=O)CN(C)C(=O)C[C@]1(C)COCc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6074

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.29

RAL-THA-05e671eb-7_1



CID: RAL-THA-05e671eb-7_1

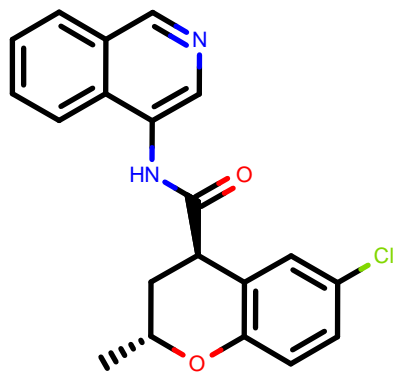
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C#N

RUN: RUN1871

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.09

MAT-POS-8a69d52e-1_3_1



CID: MAT-POS-8a69d52e-1_3_1

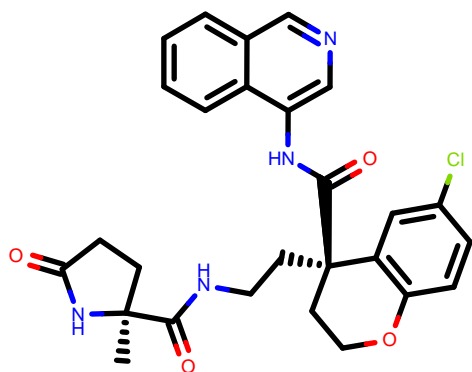
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7557

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.04

EN300-370280_3_1_1



CID: EN300-370280_3_1_1

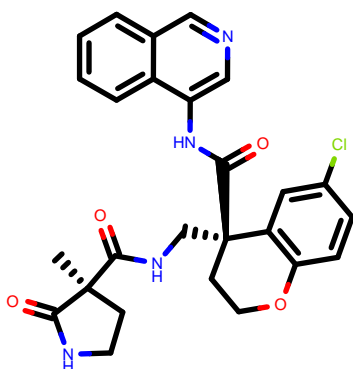
SMILES: C[C@]1(CCC(=O)N)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4474

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

EN300-207959_2_1_1



CID: EN300-207959_2_1_1

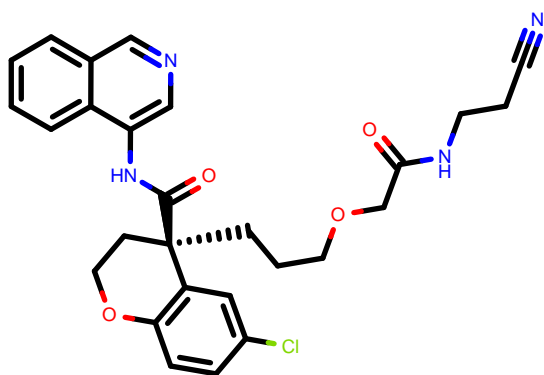
SMILES: C[C@@]1(CCN(C1=O)C(=O)N)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5014

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-10895_4_1_1



CID: EN300-10895_4_1_1

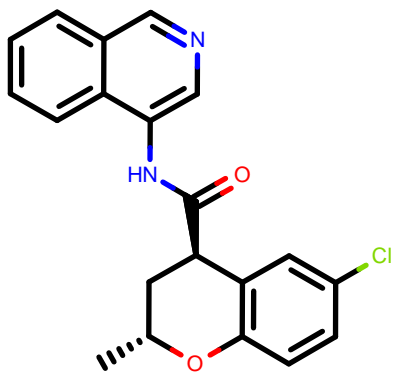
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NCCC#N

RUN: RUN7129

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.36

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

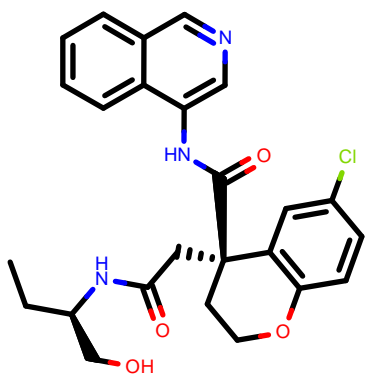
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN980

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.04

EN300-19709_1_2_1



CID: EN300-19709_1_2_1

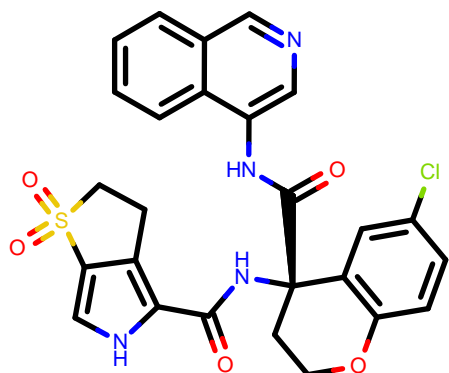
SMILES: CC[C@H](CO)NC(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5221

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.39

EN300-205047_1_1_1



CID: EN300-205047_1_1_1

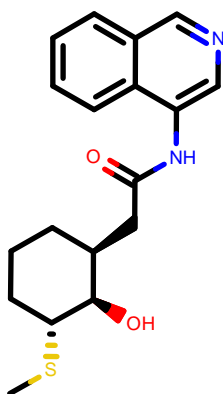
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c(c[nH]5)S(=O)(=O)CC6

RUN: RUN4568

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

MAK-UNK-c749d764-4_7



CID: MAK-UNK-c749d764-4_7

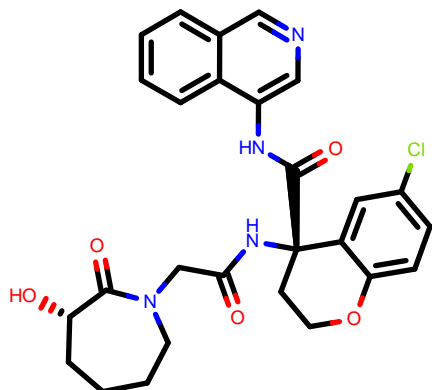
SMILES: CS[C@@H]1CCC[C@H]([C@H]1O)CC(=O)Nc2cncc3c2cccc3

RUN: RUN840

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-259849_1_1_1



CID: EN300-259849_1_1_1

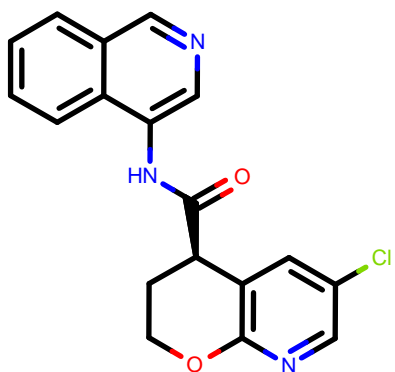
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCCC[C@@H](C5=O)O

RUN: RUN7273

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.39

EDJ-MED-12f7f543-1_1



CID: EDJ-MED-12f7f543-1_1

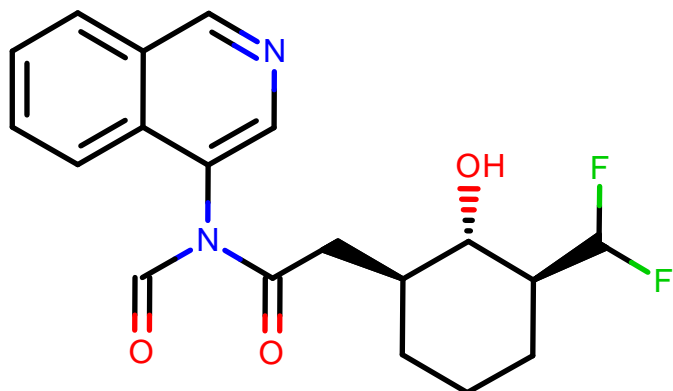
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cn4)Cl

RUN: RUN1227

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.22

MAK-UNK-c749d764-5_5



CID: MAK-UNK-c749d764-5_5

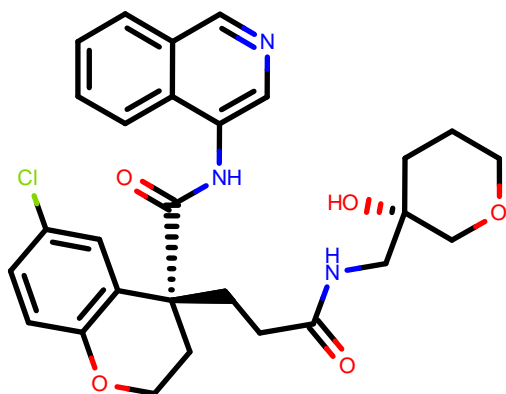
SMILES: c1ccc2c(c1)cncc2N(CO)C(=O)C@@H]3CCC[C@@H]([C@H]3O)C(F)F

RUN: RUN874

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.39

EN300-193679_2_2_1



CID: EN300-193679_2_2_1

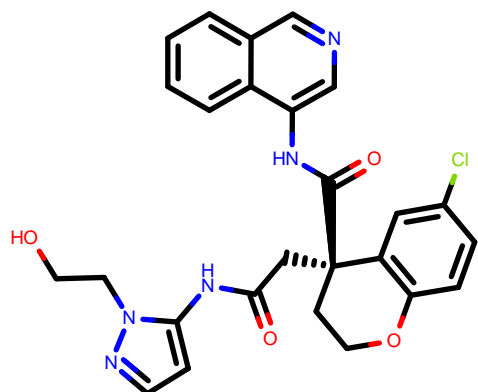
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCCC(=O)NC[C@@H]5(CCCOC5)O

RUN: RUN4063

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-134536_1_1_1



CID: EN300-134536_1_1_1

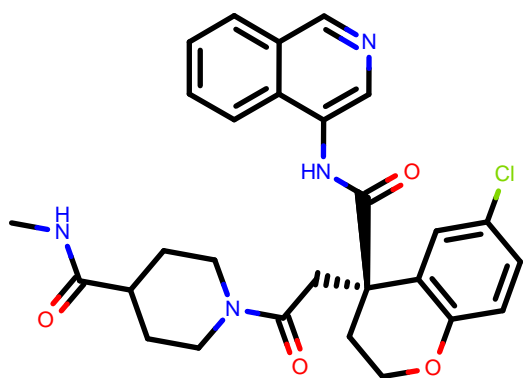
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cnn5CCO

RUN: RUN5938

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

EN300-24653_1_1_1



CID: EN300-24653_1_1_1

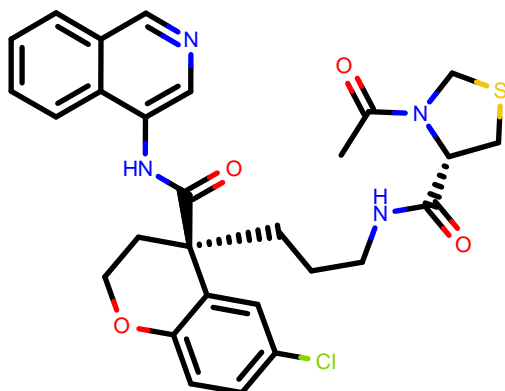
SMILES: CNC(=O)C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3250

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.34

EN300-56202_4_1_1



CID: EN300-56202_4_1_1

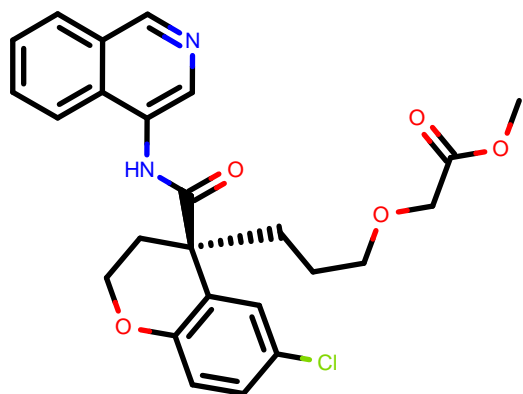
SMILES: CC(=O)N1CSC[C@@H]1C(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7116

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.36

EN300-19700_4_1_1



CID: EN300-19700_4_1_1

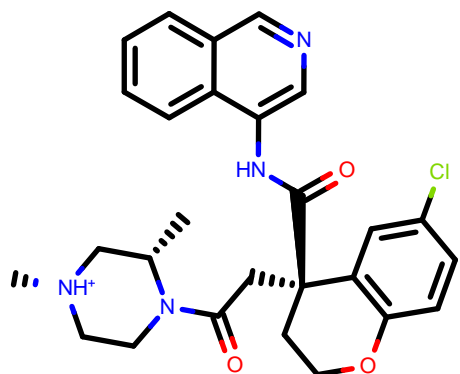
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4733

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

EDG-MED-ba1ac7b9-15_8



CID: EDG-MED-ba1ac7b9-15_8

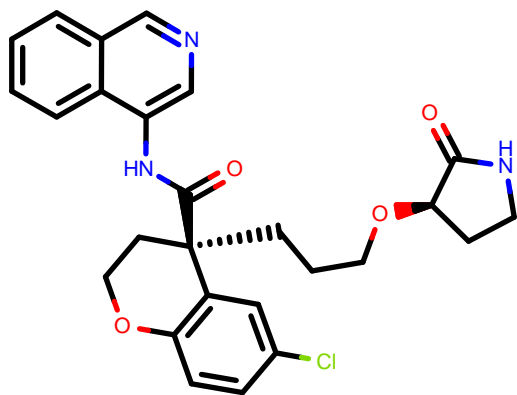
SMILES: C[C@H]1CN([H+])(CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)C

RUN: RUN2494

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.34

EN300-6736413_4_1_1



CID: EN300-6736413_4_1_1

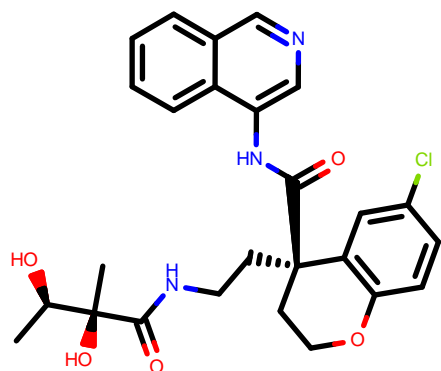
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN4192

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

EN300-202922_3_4_1



CID: EN300-202922_3_4_1

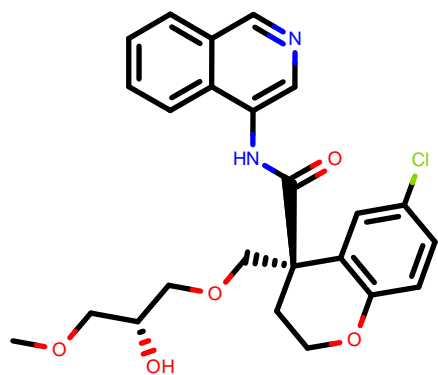
SMILES: C[C@H]([C@@](C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O)O

RUN: RUN6918

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-1915260_2_2_1



CID: EN300-1915260_2_2_1

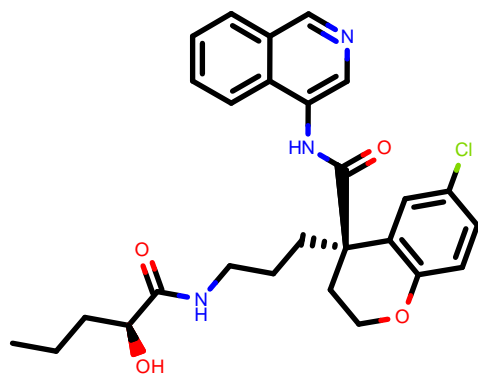
SMILES: COC[C@H](COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN7037

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.32

EN300-300217_4_2_1



CID: EN300-300217_4_2_1

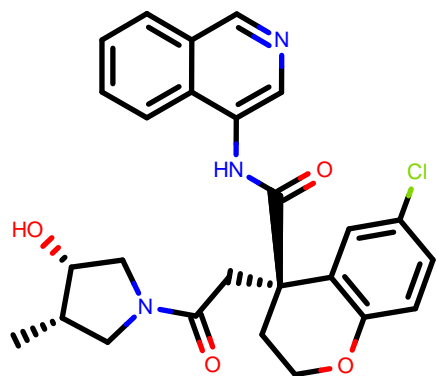
SMILES: C/C=C/[C@@H]([C@@](C(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O)O

RUN: RUN7653

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.38

EN300-124052_1_4_1



CID: EN300-124052_1_4_1

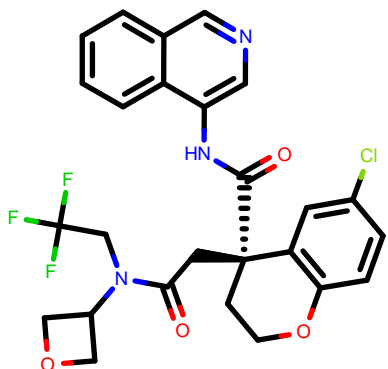
SMILES: C[C@H]1CN(C[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN4863

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.35

EDG-MED-ba1ac7b9-24_2



CID: EDG-MED-ba1ac7b9-24_2

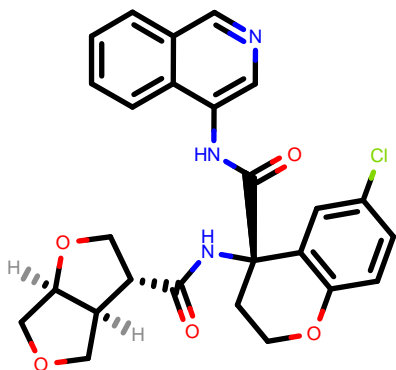
SMILES: c1ccc2c(c1)encc2NC(=O)[C@]3(CCOc4c3cc(cc4Cl)CC(=O)N(C)C(F)F)C5COO5

RUN: RUN2567

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.34

EN300-6482296_1_4_1



CID: EN300-6482296_1_4_1

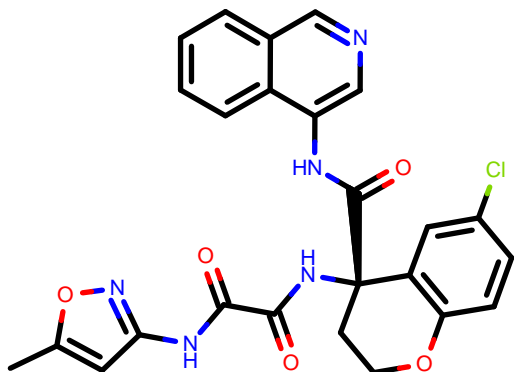
SMILES: c1ccc2c(c1)encc2NC(=O)[C@]3(CCOc4c3cc(cc4Cl)N(C)O)C@H5CO[C@H]3[C@]5H5COO6

RUN: RUN3841

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.30

EN300-36938_1_1_1



CID: EN300-36938_1_1_1

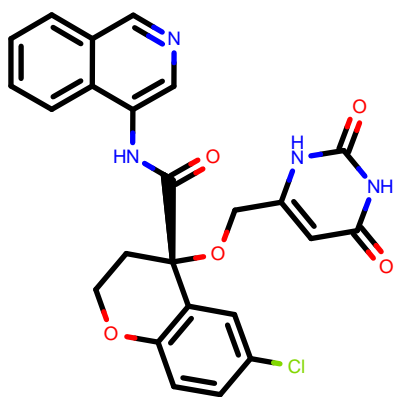
SMILES: Cc1cc(nc1)NC(=O)C(=O)N[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN6421

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.23

EN300-11300_1_1_1



CID: EN300-11300_1_1_1

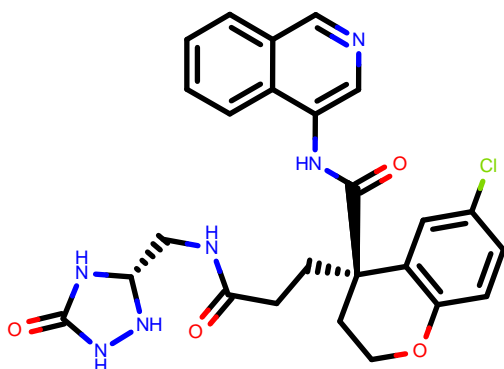
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4c3cc(cc4O)OCc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN7652

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.28

EN300-98038_2_1_2



CID: EN300-98038_2_1_2

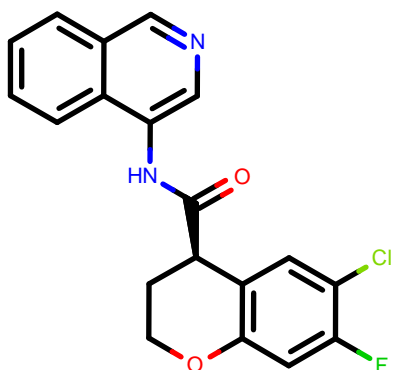
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4c3cc(cc4O)COC(=O)NC[C@@H]5[nH+]NC1=O]N5

RUN: RUN5862

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.25

RAL-THA-05e671eb-10_1



CID: RAL-THA-05e671eb-10_1

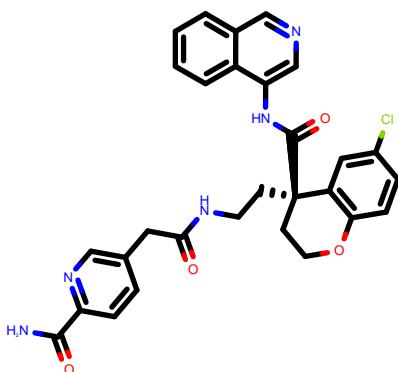
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4c3cc(cc4O)C(F)

RUN: RUN1906

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.04

EN300-322332_3_1_1



CID: EN300-322332_3_1_1

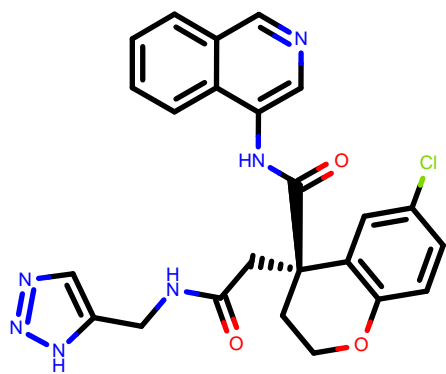
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@O]c4c3cc(cc4O)CCNC(=O)C5c5cc(nc5)C(=O)N

RUN: RUN4398

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.33

EN300-98429_1_1_1



CID: EN300-98429_1_1_1

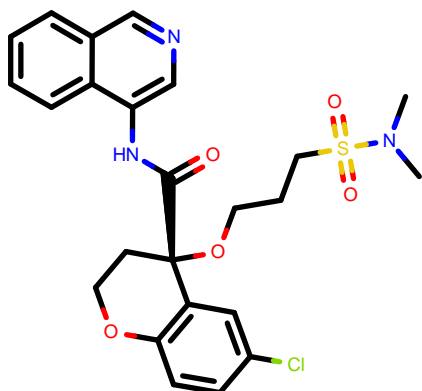
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5cn[nH]n5

RUN: RUN6681

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.37

EN300-66432_1_1_1



CID: EN300-66432_1_1_1

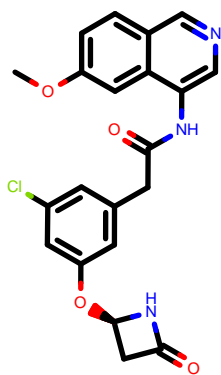
SMILES: CN(C)S(=O)(=O)CCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5206

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.35

ALF-EVA-0b412456-2_1



CID: ALF-EVA-0b412456-2_1

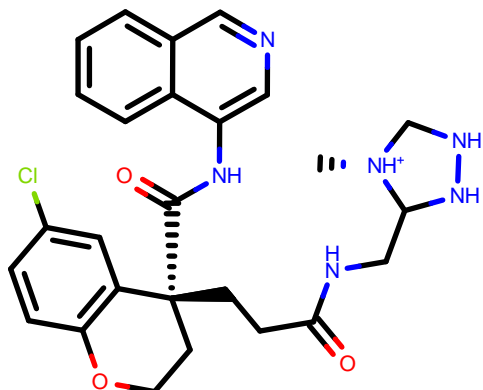
SMILES: COc1ccc2ncnc(c2c1)NC(=O)Cc3cc(cc3)Cl)O[C@@]4C(=O)N4

RUN: RUN2563

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.40

EN300-30859_2_1_1



CID: EN300-30859_2_1_1

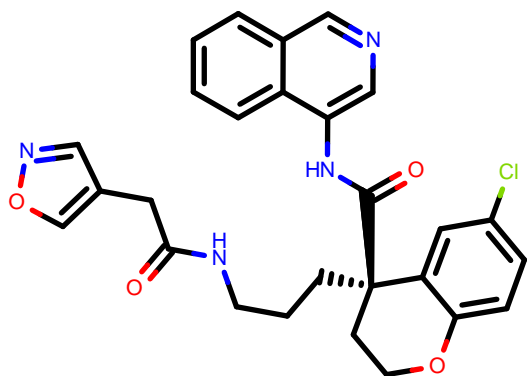
SMILES: Cn1cnc1CNC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6761

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-315963_4_1_1



CID: EN300-315963_4_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5ncoc5

RUN:

RUN4735

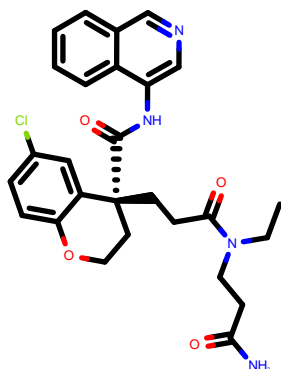
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

0.34

EN300-6766477_2_1_1



CID: EN300-6766477_2_1_1

SMILES:

CCN(CCC(=O)N)C(=O)CC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4

RUN:

RUN5985

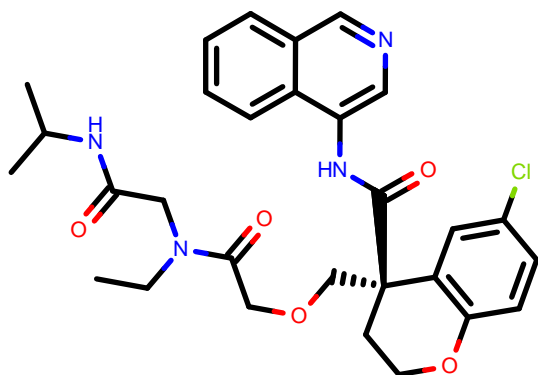
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

0.31

EN300-07936_2_1_1



CID: EN300-07936_2_1_1

SMILES:

CCN(CC(=O)NC(C)C(=O)COC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4

RUN:

RUN5025

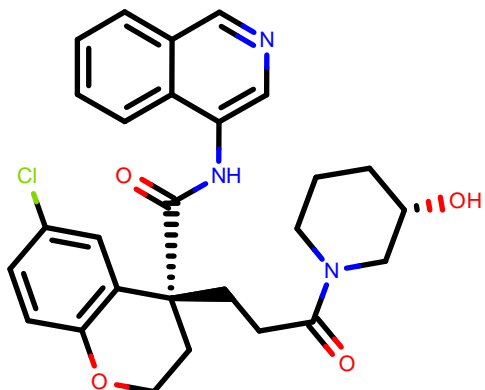
DDG (kcal/mol):

-0.14

dDDG (kcal/mol):

0.36

EN300-188582_2_1_1



CID: EN300-188582_2_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCC[C@@H]3C5O

RUN:

RUN6418

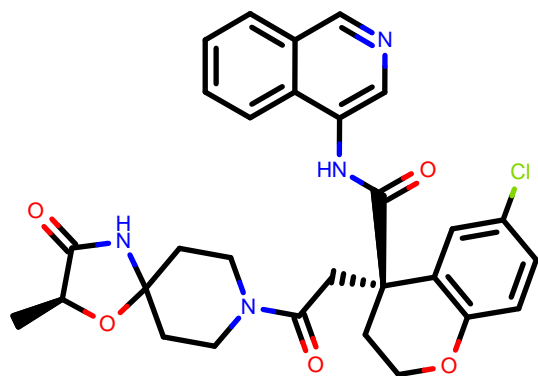
DDG (kcal/mol):

-0.14

dDDG (kcal/mol):

0.25

EN300-6478789_1_2_1



CID: EN300-6478789_1_2_1

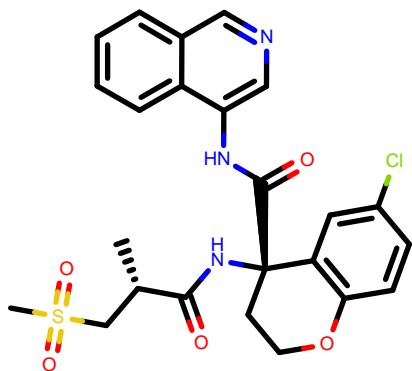
SMILES: C[C@H]1C(=O)NC2(O1)CCN(CC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN6167

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.32

EN300-97699_1_1_1



CID: EN300-97699_1_1_1

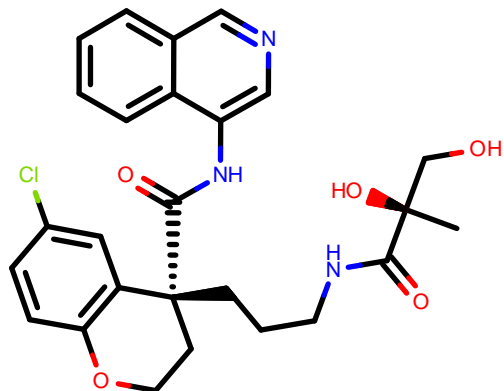
SMILES: C[C@@H](CS(=O)(=O)C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN7024

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.36

EN300-89418_4_1_1



CID: EN300-89418_4_1_1

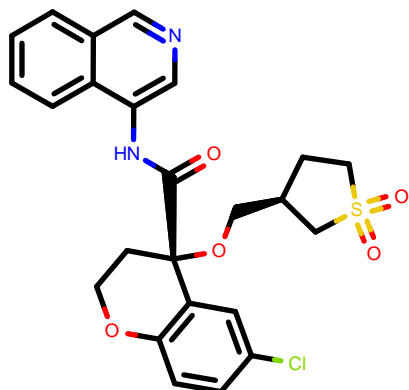
SMILES: C[C@@]([CO](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6921

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.67

EN300-1448603_1_2_1



CID: EN300-1448603_1_2_1

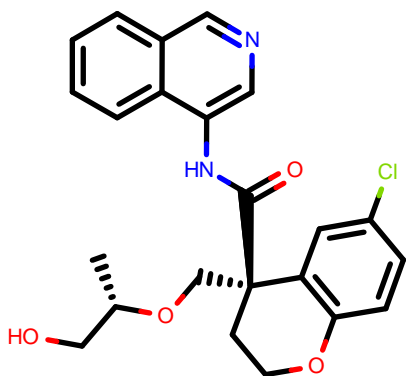
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5SCCS(=O)(=O)C5

RUN: RUN6215

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.32

EN300-175186_2_1_1



CID: EN300-175186_2_1_1

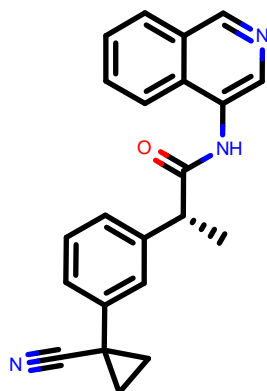
SMILES: C[C@@H](CO)OC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6325

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.23

DAR-DIA-0cde14eb-60_2



CID: DAR-DIA-0cde14eb-60_2

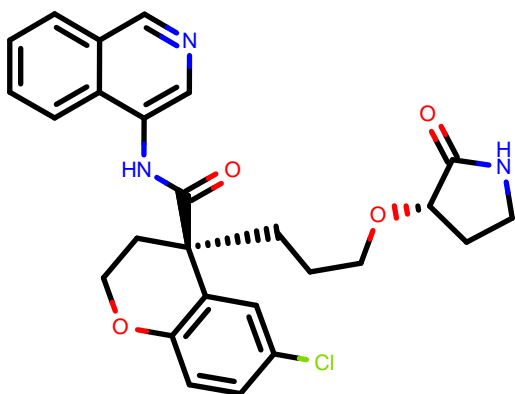
SMILES: C[C@H](c1cccc(c1)C2(CC2)C#N)C(=O)Nc3cncc4c3cccc4

RUN: RUN23

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.33

EN300-6736413_4_2_1



CID: EN300-6736413_4_2_1

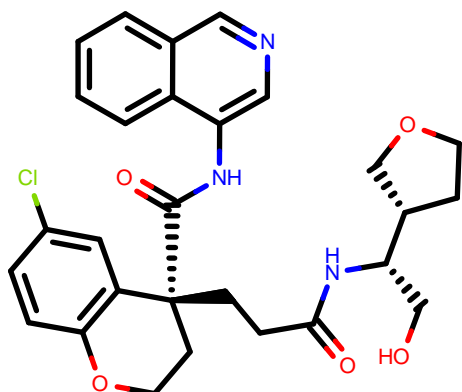
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN5815

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.31

EN300-104493_2_3_1



CID: EN300-104493_2_3_1

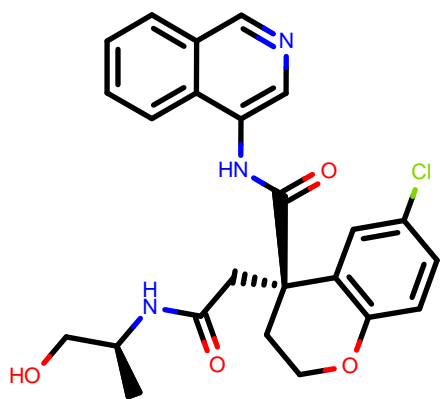
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H](CO)[C@@H]5CCOC5

RUN: RUN7126

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.41

EN300-86282_1_1_1



CID: EN300-86282_1_1_1

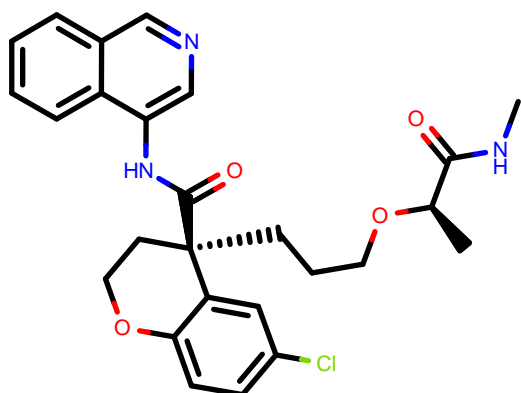
SMILES: C[C@@H](CO)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6403

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.25

EN300-211482_4_2_1



CID: EN300-211482_4_2_1

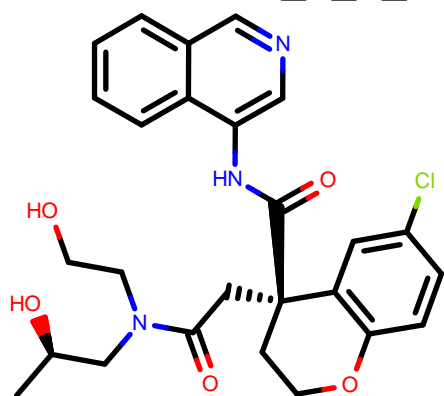
SMILES: C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6366

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.36

EN300-214038_1_2_1



CID: EN300-214038_1_2_1

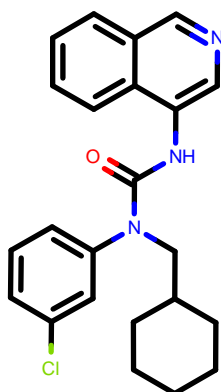
SMILES: C[C@H](CN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)O

RUN: RUN4808

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.35

MIC-UNK-bcd487e9-2_1



CID: MIC-UNK-bcd487e9-2_1

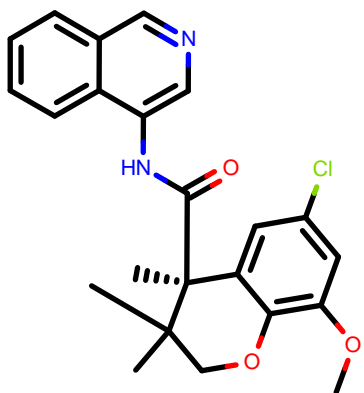
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CC3CCCCC3)c4cccc(c4)Cl

RUN: RUN487

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.36

DAR-DIA-0d514e7d-27_1_1



CID: DAR-DIA-0d514e7d-27_1_1

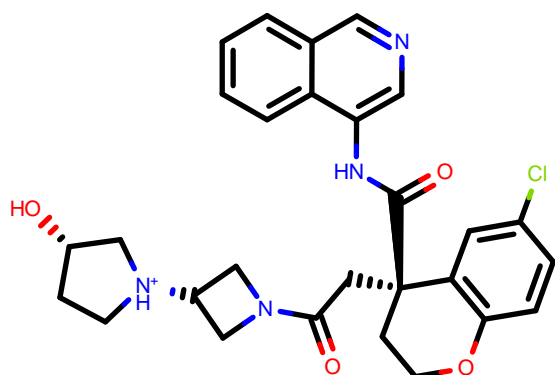
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)OC)C(=O)Nc3ccc4c3ccc4

RUN: RUN7441

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.28

EDG-MED-ba1ac7b9-4_1



CID: EDG-MED-ba1ac7b9-4_1

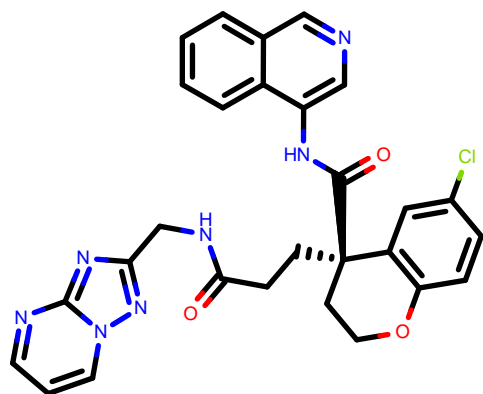
SMILES: c1ccc2c(c1)cnc2NC(=O)C[C@@]3(CCCO4c3ccc4)C(C)OC(=O)N5CC(C5)[N+]([H])C[C@@]6H[C@H]6O

RUN: RUN2482

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.30

EN300-250416_2_1_1



CID: EN300-250416_2_1_1

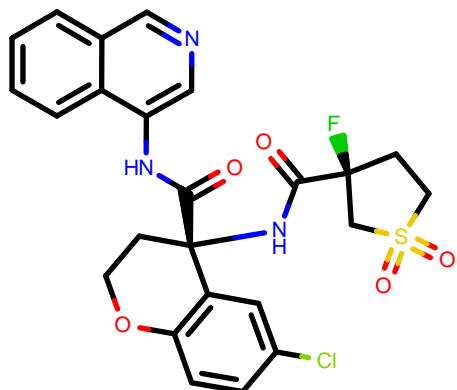
SMILES: c1ccc2c(c1)cnc2NC(=O)C[C@@]3(CCCO4c3ccc4)C(C)OC(=O)NC5nc6ncccn65

RUN: RUN6696

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.29

EN300-311920_1_1_1



CID: EN300-311920_1_1_1

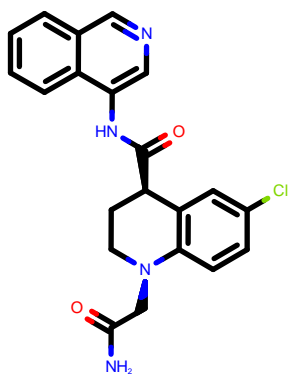
SMILES: c1ccc2c(c1)cnc2NC(=O)C[C@@]3(CCO4c3ccc4)C(C)NC(=O)C[C@@]5(CCS(=O)(=O)C5)F

RUN: RUN6735

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.29

RAL-THA-8416115c-8_3



CID: RAL-THA-8416115c-8_3

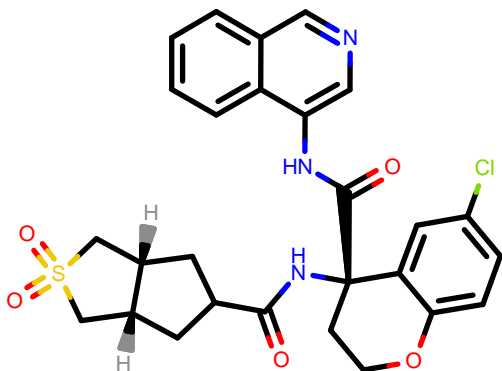
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)CC(=O)N

RUN: RUN1176

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.32

EN300-7438088_1_1_1



CID: EN300-7438088_1_1_1

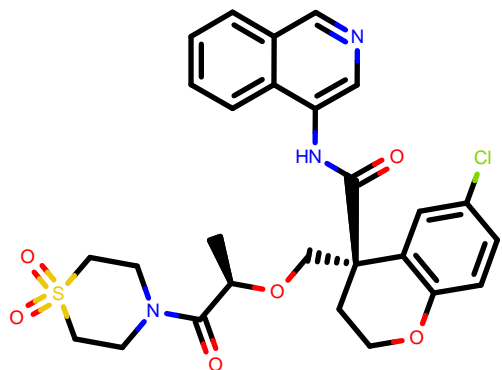
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOC43cc(cc4)C1NC(=O)CS[C@@H]6C(S(=O)(=O)O)C@H]6C5

RUN: RUN5441

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.34

EN300-1265949_2_2_1



CID: EN300-1265949_2_2_1

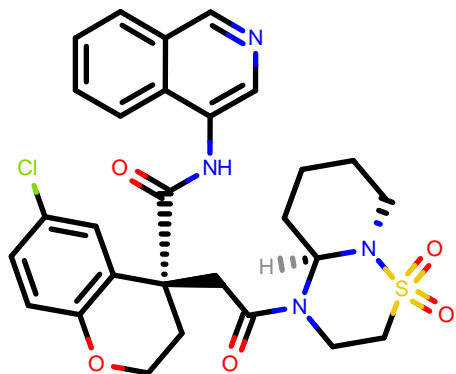
SMILES: C[C@H](C(=O)N1CCS(=O)(=O)CC1)OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c6ccc5

RUN: RUN5054

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.41

ALP-UNI-3496895b-1_1



CID: ALP-UNI-3496895b-1_1

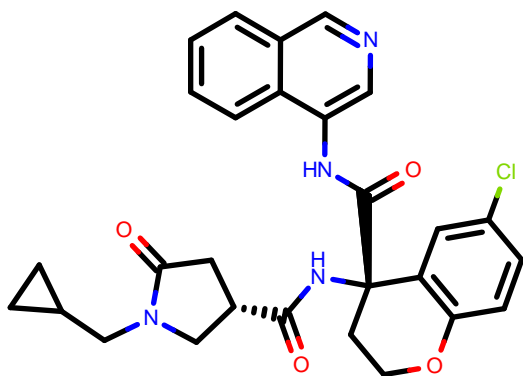
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@]4(CO3)CC(=O)N5CCS(=O)(=O)N@H]C@H]5CCCC6

RUN: RUN2333

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.35

EN300-31969_1_2_1



CID: EN300-31969_1_2_1

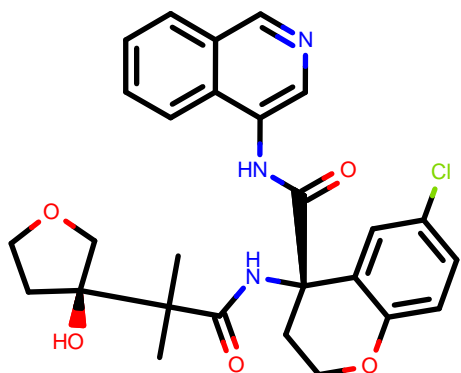
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC(=O)N(C5)CC6CC6

RUN: RUN5112

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.32

EN300-1630093_1_1_1



CID: EN300-1630093_1_1_1

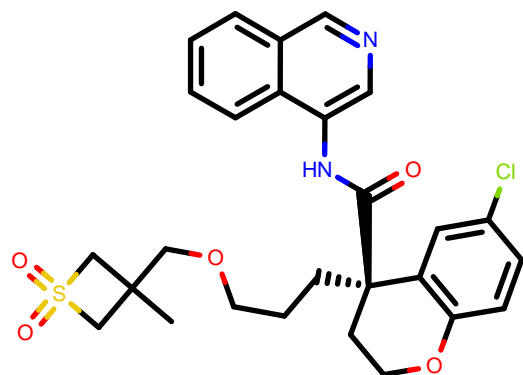
SMILES: CC(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)O)C(=O)Nc3nccc4c3ccc4)[C@@]5(CCOc5)O

RUN: RUN5762

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.35

EN300-1705754_4_1_1



CID: EN300-1705754_4_1_1

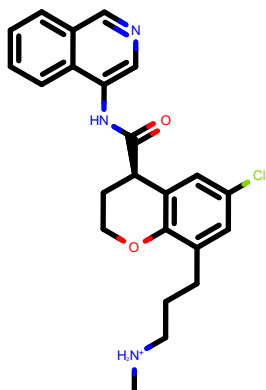
SMILES: CC1(CS(=O)(=O)C1)COC(C)C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5

RUN: RUN5624

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.48

LAU-MED-88a3970a-11_1



CID: LAU-MED-88a3970a-11_1

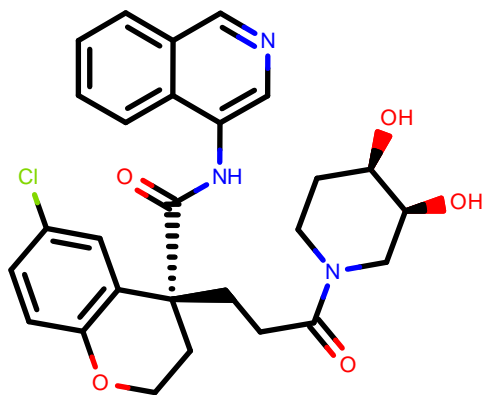
SMILES: C[NH2+]CCc1cc(cc2c1OCC[C@H]2C(=O)Nc3nccc4c3ccc4)Cl

RUN: RUN1356

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.25

EN300-349304_2_1_1



CID: EN300-349304_2_1_1

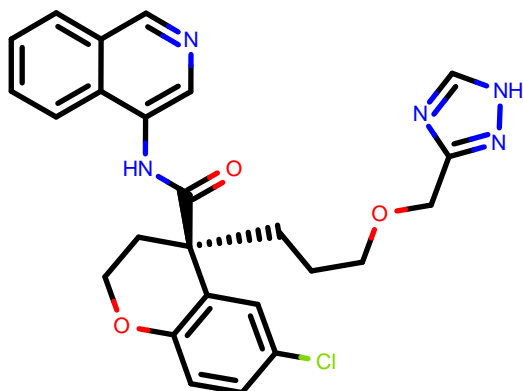
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC@H(C5)O)O

RUN: RUN4078

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.32

EN300-306316_4_1_1



CID: EN300-306316_4_1_1

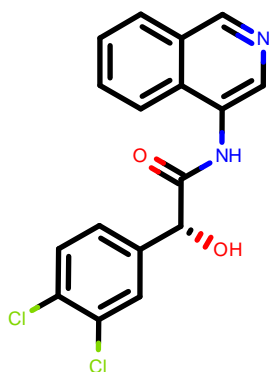
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]nnc5

RUN: RUN3589

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.33

MAT-POS-fce787c2-4_1



CID: MAT-POS-fce787c2-4_1

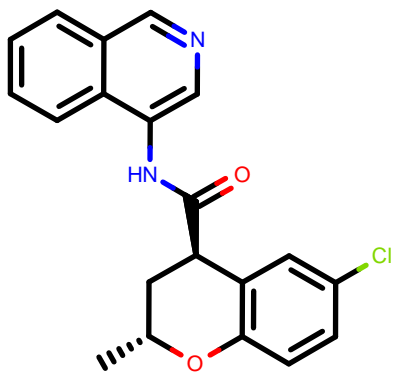
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccc(c(c3)Cl)Cl)O

RUN: RUN1940

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.32

EDJ-MED-e4b030d8-2_1_1



CID: EDJ-MED-e4b030d8-2_1_1

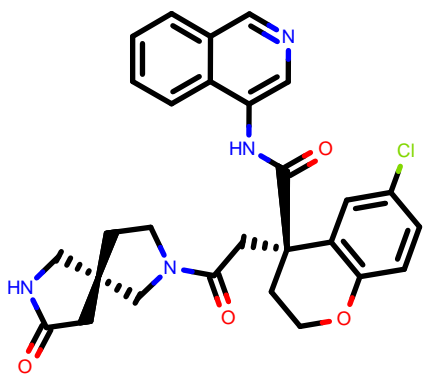
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7571

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.05

EN300-187998_1_1_1



CID: EN300-187998_1_1_1

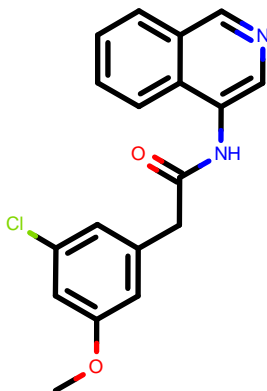
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CC(=O)N5CC[C@@]6(C5)CC(=O)NC6

RUN: RUN7526

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.32

MAT-POS-3b92565d-2_1



CID: MAT-POS-3b92565d-2_1

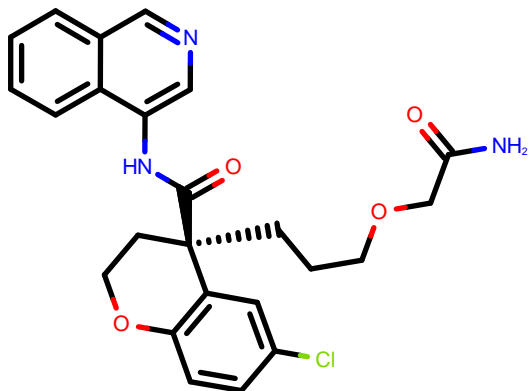
SMILES: COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3

RUN: RUN29

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-18249_4_1_1



CID: EN300-18249_4_1_1

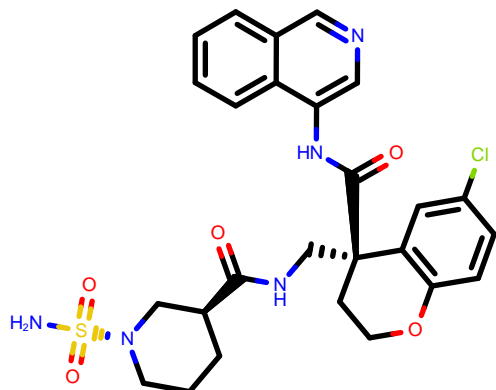
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCOCC(=O)N

RUN: RUN3944

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.30

EN300-219496_2_2_1



CID: EN300-219496_2_2_1

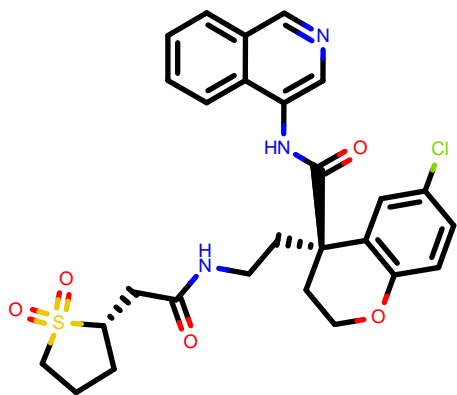
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)O)CNC(=O)[C@H]5CCC[N@]5(S(=O)(=O)N)

RUN: RUN6807

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.30

EN300-155176_3_1_1



CID: EN300-155176_3_1_1

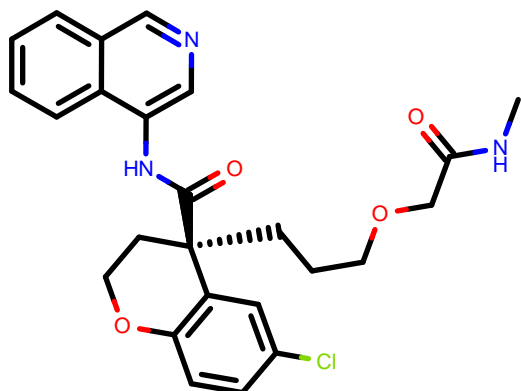
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOC4c3cc(cc4)C)CCNC(=O)C[C@@H]5CCCS5(=O)=O

RUN: RUN6889

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.36

EN300-2977549_4_1_1



CID: EN300-2977549_4_1_1

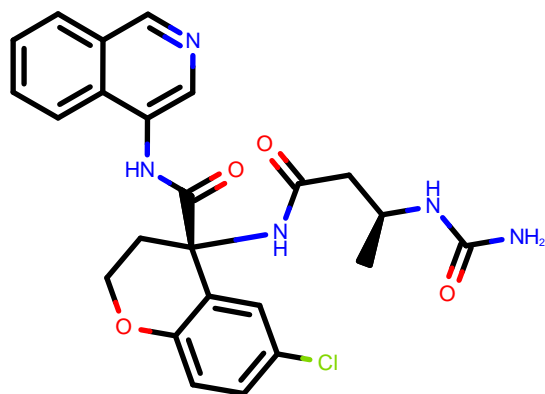
SMILES: CNC(=O)COCC[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN7272

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.31

EN300-268198_1_1_1



CID: EN300-268198_1_1_1

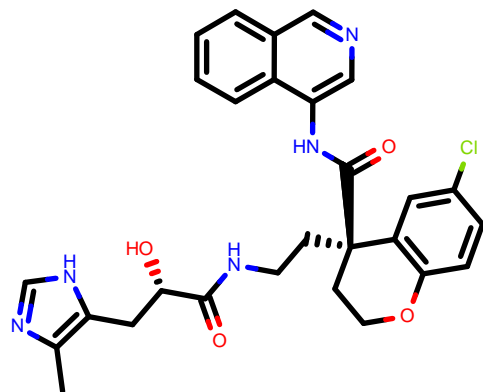
SMILES: C[C@@H](C(=O)N)C@@1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4NC(=O)N

RUN: RUN3967

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.26

EN300-7494324_3_1_1



CID: EN300-7494324_3_1_1

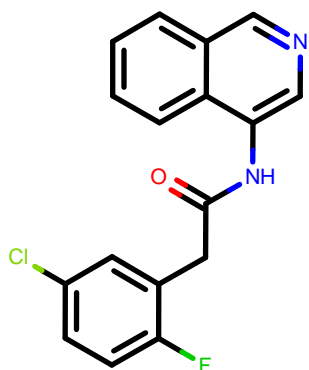
SMILES: Cc1c[nH]1)C[C@@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7674

DDG (kcal/mol): -0.12

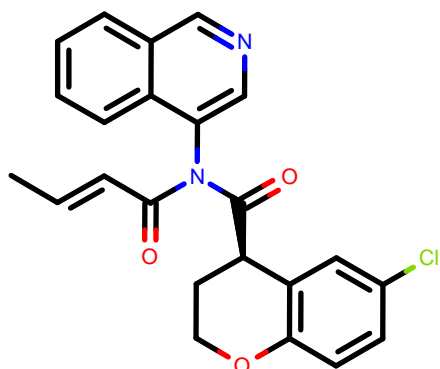
dDDG (kcal/mol): 0.34

PET-UNK-dd44aeb6-1_1



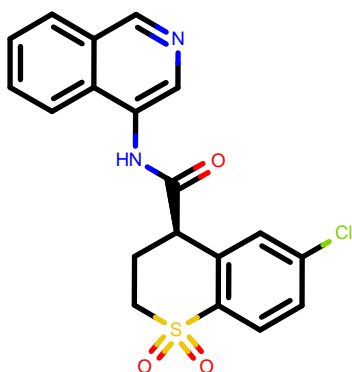
CID:	PET-UNK-dd44aeb6-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(ccc3F)Cl</chem>
RUN:	RUN345
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.24

DAR-DIA-5ff57136-11_1_2



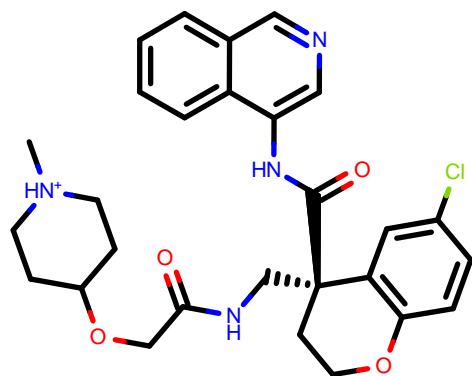
CID:	DAR-DIA-5ff57136-11_1_2
SMILES:	<chem>C/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN2764
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.24

MIC-UNK-91acba05-3_1



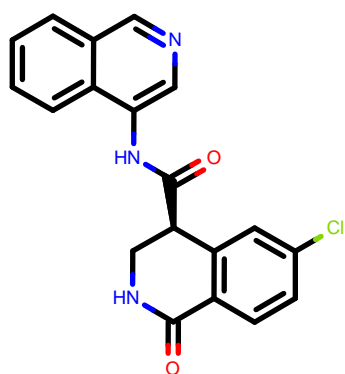
CID:	MIC-UNK-91acba05-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(cc4)Cl</chem>
RUN:	RUN367
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.20

EN300-237224_2_1_1



CID:	EN300-237224_2_1_1
SMILES:	<chem>C[NH+]1CCC(CC1)OCC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5</chem>
RUN:	RUN7019
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.32

MIC-UNK-91acba05-1_1



CID: MIC-UNK-91acba05-1_1

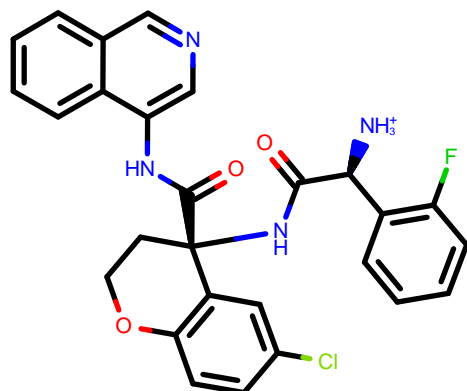
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CNC(=O)c4c3cc(cc4)Cl

RUN: RUN363

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.22

EDG-MED-90036822-90_2



CID: EDG-MED-90036822-90_2

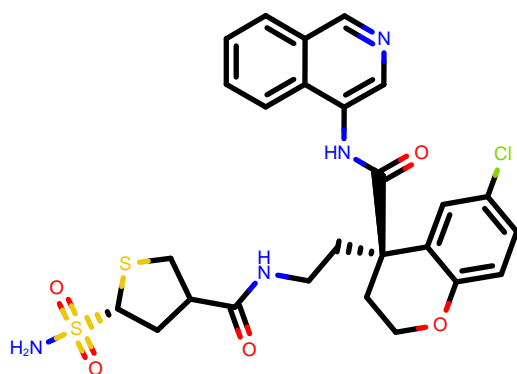
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)N(C(=O)[C@H](c5ccccc5F)[NH3+])

RUN: RUN1671

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.30

KAD-UNI-8a629cb0-3_1



CID: KAD-UNI-8a629cb0-3_1

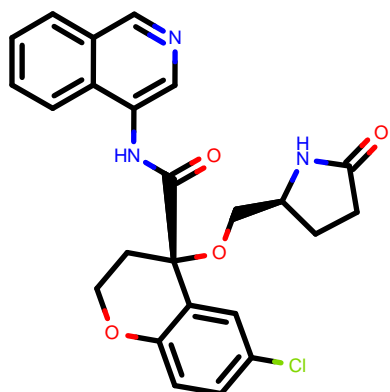
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(s5)S(=O)(=O)N

RUN: RUN2004

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.32

EN300-195756_1_1_1



CID: EN300-195756_1_1_1

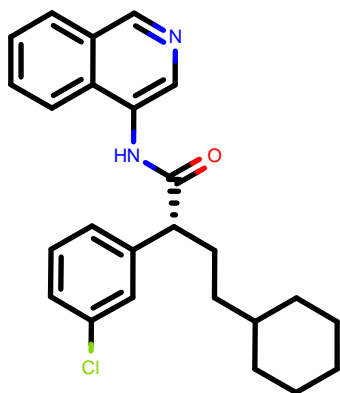
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCCC(=O)N5

RUN: RUN4938

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.21

ALP-POS-3b848b35-4_2



CID: ALP-POS-3b848b35-4_2

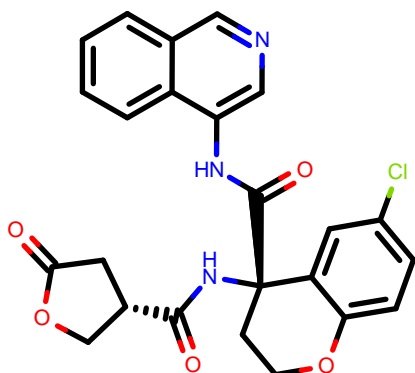
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl

RUN: RUN47

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.35

EN300-113234_1_2_1



CID: EN300-113234_1_2_1

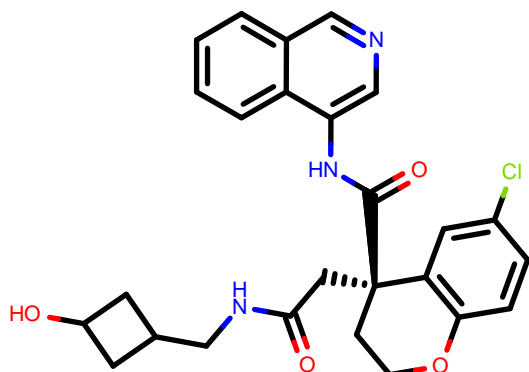
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)[C@H]5CC(=O)OC5

RUN: RUN5597

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.21

EN300-94856_1_1_1



CID: EN300-94856_1_1_1

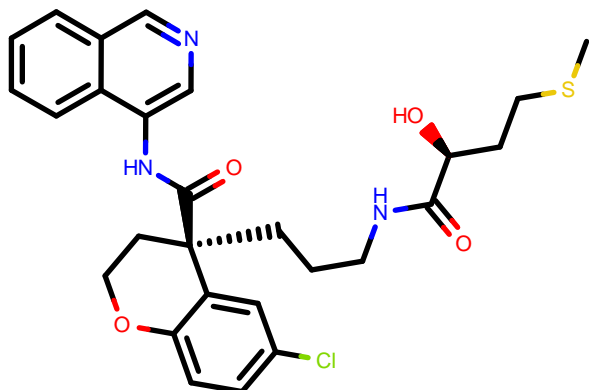
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)NCC5CC(O)O5

RUN: RUN6675

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.27

EN300-103144_4_1_1



CID: EN300-103144_4_1_1

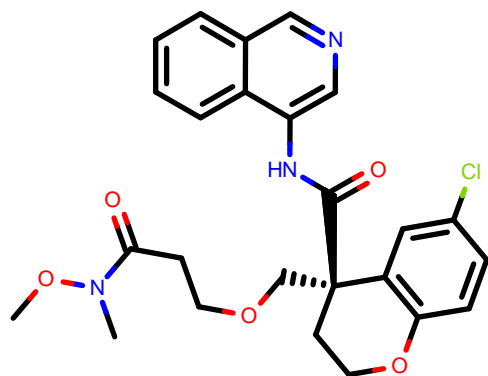
SMILES: CSCC[C@@H](C(=O)NCCC[C@@]1(CCOc2c1cc(c2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN2943

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.43

EN300-174603_2_1_1



CID: EN300-174603_2_1_1

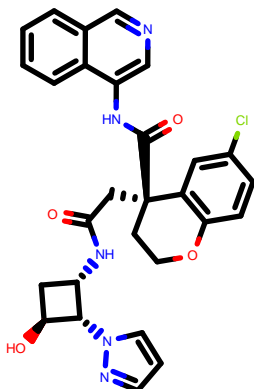
SMILES: CN(C(=O)CCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OC

RUN: RUN5582

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.26

EN300-260696_1_6_1



CID: EN300-260696_1_6_1

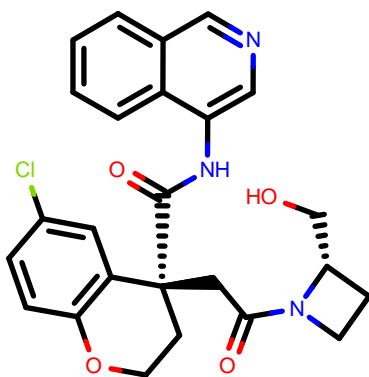
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3ccc4)C(C)C(=O)N[C@@H]5C[C@@H]J[C@@H]5n6cccc6O

RUN: RUN5768

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.34

EDG-MED-ba1ac7b9-2_3



CID: EDG-MED-ba1ac7b9-2_3

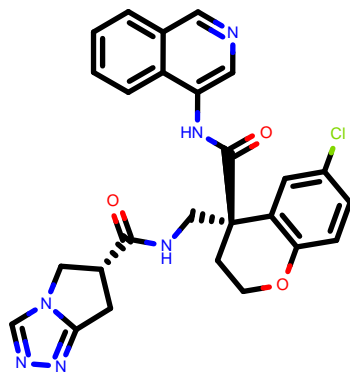
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CC(=O)N5CC[C@@H]5CO

RUN: RUN2465

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.30

EN300-6745453_2_1_1



CID: EN300-6745453_2_1_1

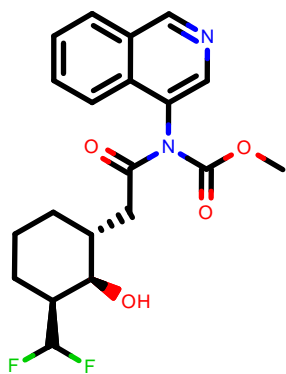
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CNC(=O)[C@@]5[C@@H]5C6nncn6C5

RUN: RUN6604

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.28

MAK-UNK-c749d764-25_2



CID: MAK-UNK-c749d764-25_2

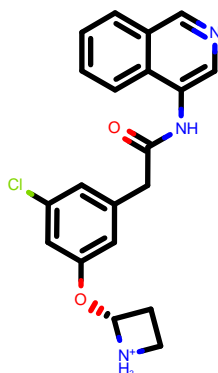
SMILES: COC(=O)N(c1cnc2c1cccc2)C(=O)C[C@H]3CC[C@@H]([C@@H]3O)C(F)F

RUN: RUN1001

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.31

PET-UNK-cf04cb02-1_1



CID: PET-UNK-cf04cb02-1_1

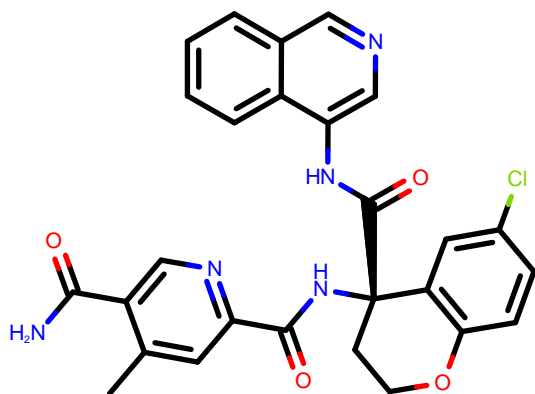
SMILES: c1ccc2c(c1)cnc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC[NH2+]4

RUN: RUN330

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.51

EN300-247617_1_1_1



CID: EN300-247617_1_1_1

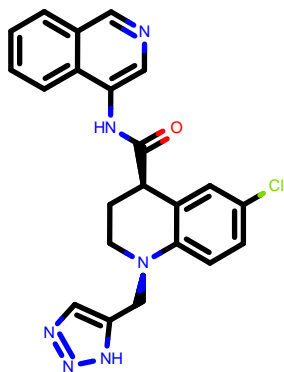
SMILES: Cc1cc(ncc1C(=O)N)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5o4cccc5

RUN: RUN4939

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.23

RAL-THA-8416115c-14_1



CID: RAL-THA-8416115c-14_1

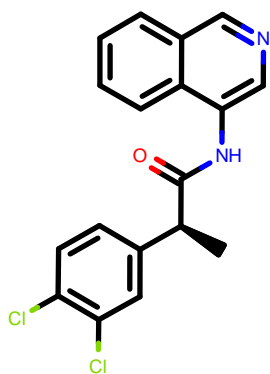
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)C5c[nH]n5

RUN: RUN1205

DDG (kcal/mol): -0.10

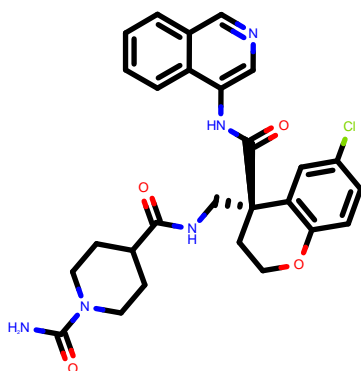
dDDG (kcal/mol): 0.35

MAT-POS-fce787c2-3_1



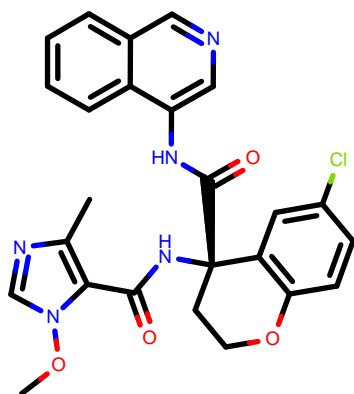
CID:	MAT-POS-fce787c2-3_1
SMILES:	<chem>C[C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN1936
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.31

EN300-13489_2_1_1



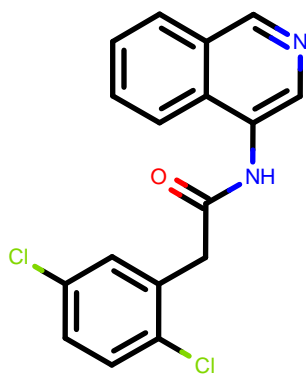
CID:	EN300-13489_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CCN(CC5)C(=O)N</chem>
RUN:	RUN7176
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.25

EN300-7442332_1_1_1



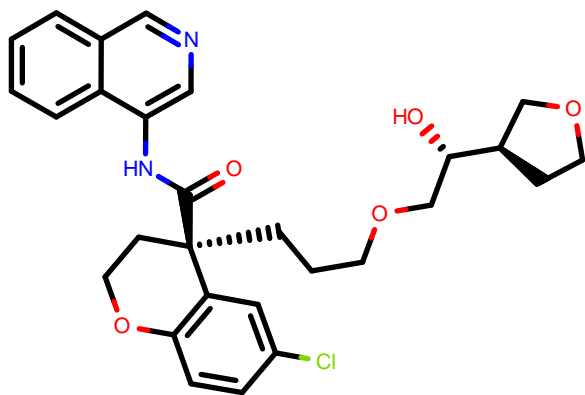
CID:	EN300-7442332_1_1_1
SMILES:	<chem>Cc1c(n(cn1)OC)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN7387
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

PET-UNK-dd44aeb6-2_1



CID:	PET-UNK-dd44aeb6-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(ccc3Cl)Cl</chem>
RUN:	RUN336
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.26

EN300-1911992_4_1_1



CID: EN300-1911992_4_1_1

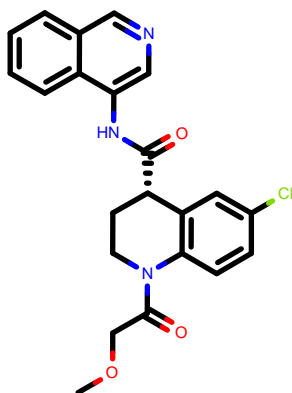
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H]([C@@H]5CCOC5)O

RUN: RUN5620

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.35

RAL-THA-4aa06b95-5_1



CID: RAL-THA-4aa06b95-5_1

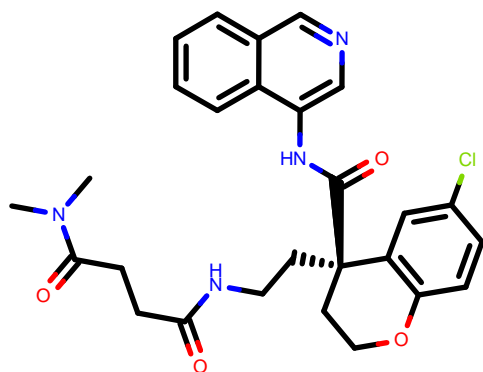
SMILES: COCC(=O)N1CC[C@@H]([C@H]2C=CC=C(Cl)C=C2)C(=O)Nc3ncc4c3ccoc4

RUN: RUN1133

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.36

EN300-176877_3_1_1



CID: EN300-176877_3_1_1

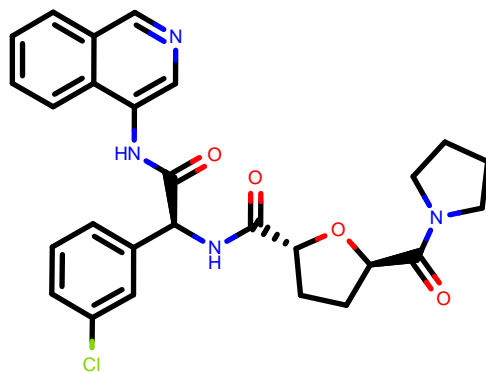
SMILES: CN(C)C(=O)CCC(=O)NCC[C@@H]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN7135

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.27

EDJ-MED-ee07cf00-11_4



CID: EDJ-MED-ee07cf00-11_4

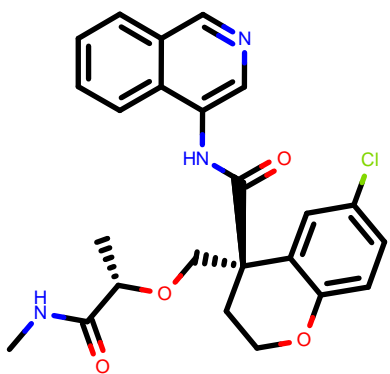
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]([C@@H]3CCOC3)C(=O)N[C@@H]4C[C@H]([C@@H]4)C5CCN5

RUN: RUN2694

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.56

EN300-211482_2_1_1



CID: EN300-211482_2_1_1

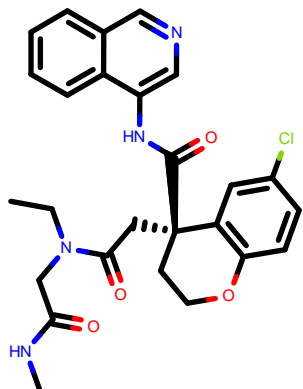
SMILES: C[C@@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6288

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.23

EN300-39007_1_1_1



CID: EN300-39007_1_1_1

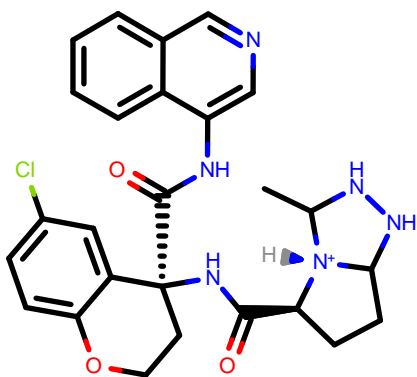
SMILES: CCN(CC(=O)NC)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5758

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.31

EN300-6489289_1_1_1



CID: EN300-6489289_1_1_1

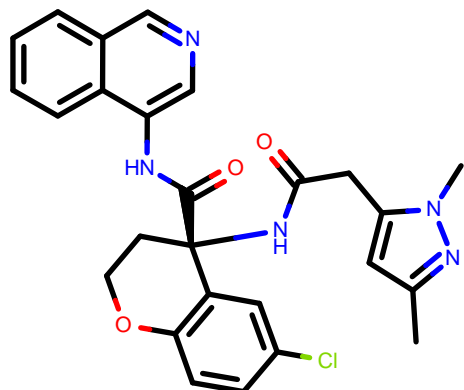
SMILES: Cc1nnc2n1[C@@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN4941

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.24

EN300-6499639_1_1_1



CID: EN300-6499639_1_1_1

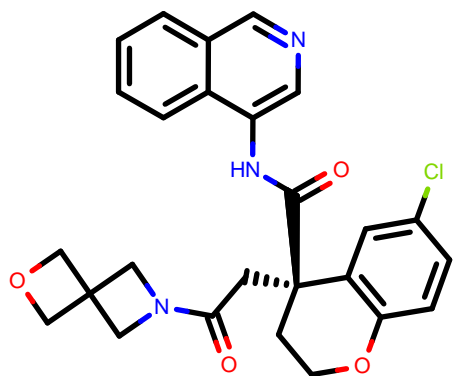
SMILES: CC1=N[N@@]([C@@H](C1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN5611

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.27

EN300-81038_1_1_1



CID: EN300-81038_1_1_1

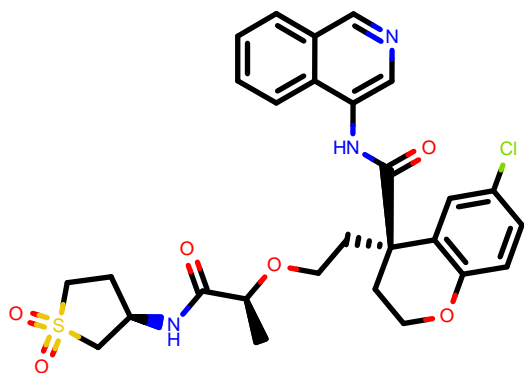
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6(C5)COC6

RUN: RUN6422

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.27

EN300-23318_3_1_1



CID: EN300-23318_3_1_1

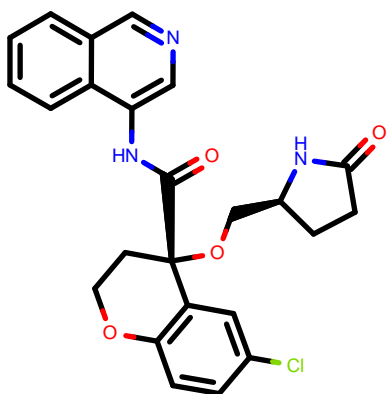
SMILES: C[C@@]1H[C@@]2(CO)N[C@@]1(CS(=O)(=O)O)O[C@@]3(CCOc4c3cc(cc4)C)C[C@@]2O[N]6c4ccc5c4ccc5

RUN: RUN5588

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.40

EN300-264301_1_1_1



CID: EN300-264301_1_1_1

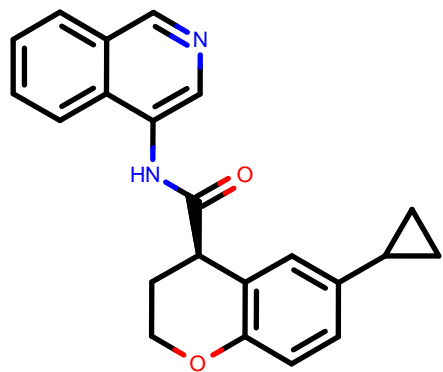
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@]4H5CCC(=O)N5

RUN: RUN7788

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.30

DAR-DIA-6a508060-8_1



CID: DAR-DIA-6a508060-8_1

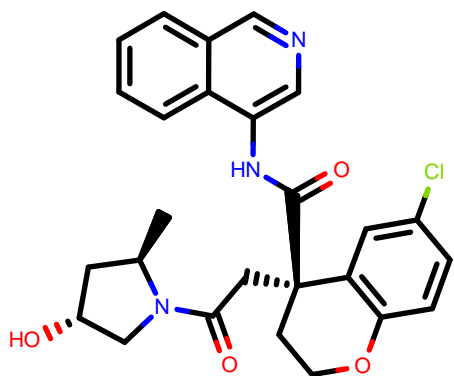
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C5CC5

RUN: RUN259

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.09

EN300-173562_1_3_1



CID: EN300-173562_1_3_1

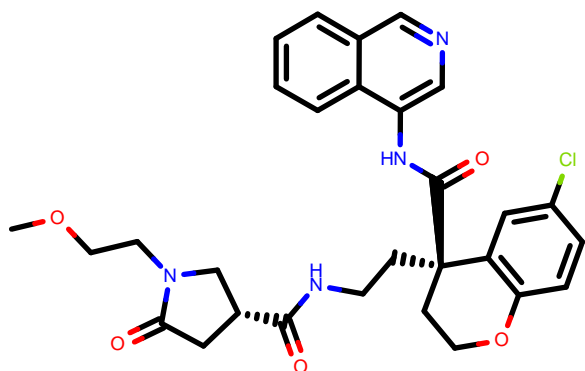
SMILES: C[C@@H]1C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3990

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.29

EN300-31845_3_1_1



CID: EN300-31845_3_1_1

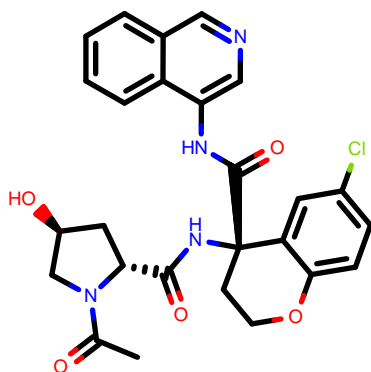
SMILES: COCCN1C[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5873

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.40

EN300-158274_1_1_1



CID: EN300-158274_1_1_1

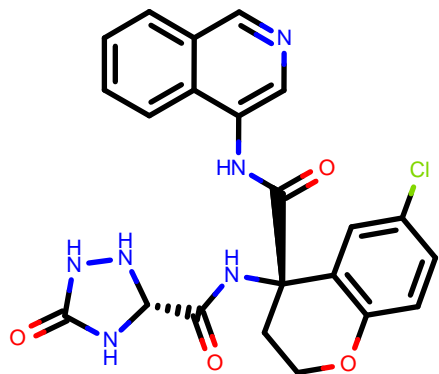
SMILES: CC(=O)N1C[C@H](C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN4914

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.34

EN300-35843_1_1_1



CID: EN300-35843_1_1_1

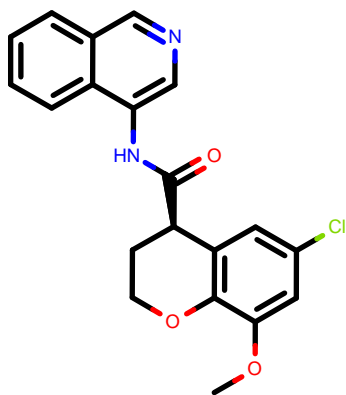
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@]5C(=O)Nc6[nH]n[nH]6

RUN: RUN4207

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.25

EDJ-MED-e4b030d8-7_1



CID: EDJ-MED-e4b030d8-7_1

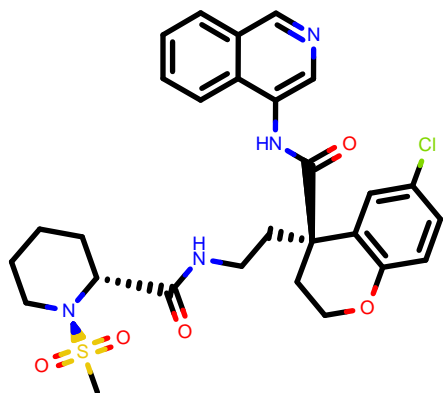
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN235

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.11

EN300-24014_3_1_1



CID: EN300-24014_3_1_1

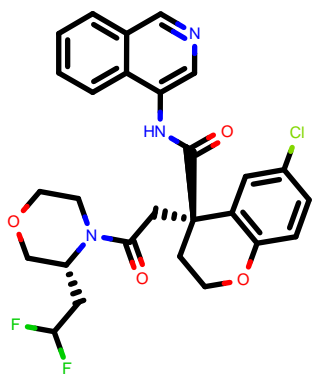
SMILES: CS(=O)(=O)N1CCCC1C@H2[C@@H]1C(=O)NCC[C@H]2[C@@H]3COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7626

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.42

EDG-MED-ba1ac7b9-20_3



CID: EDG-MED-ba1ac7b9-20_3

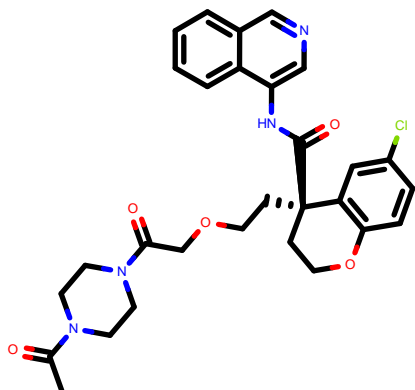
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](COCc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5C(F)F

RUN: RUN2557

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.29

EN300-1724771_3_1_1



CID: EN300-1724771_3_1_1

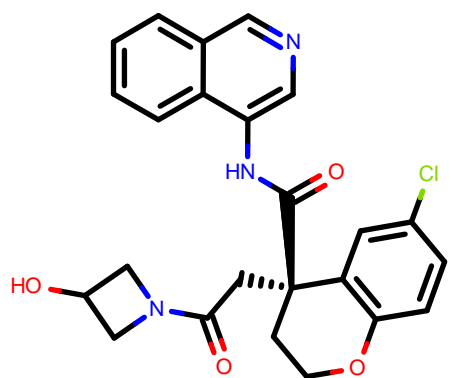
SMILES: CC(=O)N1CCN(CC1)C(=O)COCC[C@H]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6894

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.30

EN300-65115_1_1_1



CID: EN300-65115_1_1_1

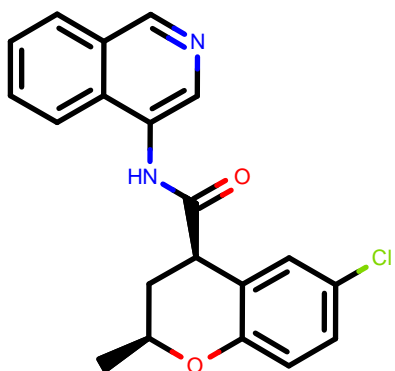
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)O

RUN: RUN6863

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.21

MAT-POS-8a69d52e-1_4_1



CID: MAT-POS-8a69d52e-1_4_1

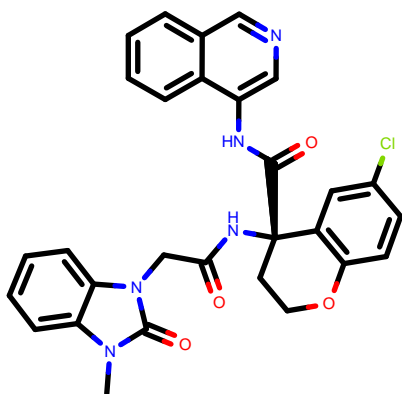
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5786

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.09

EN300-26603_1_1_1



CID: EN300-26603_1_1_1

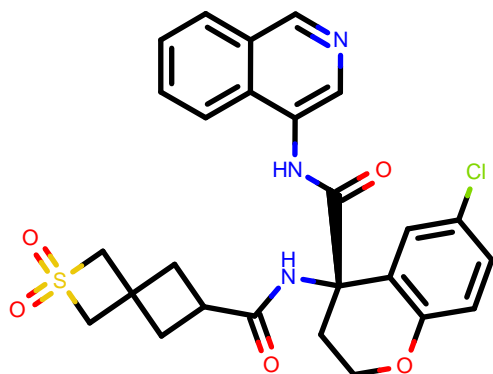
SMILES: Cn1c2cccc2n(c1=O)CC(=O)N[C@@]3(CCOc4c3cc(cc4)O)C(=O)Nc5ncc6c5cccc6

RUN: RUN4301

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.32

EN300-318305_1_1_1



CID: EN300-318305_1_1_1

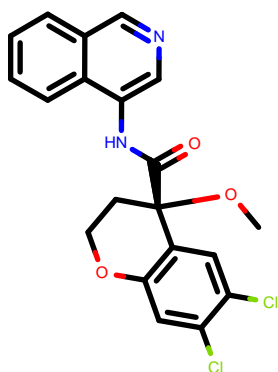
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC6(C5)CS(=O)(=O)C6

RUN: RUN7736

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.23

EDJ-MED-d08626de-4_1



CID: EDJ-MED-d08626de-4_1

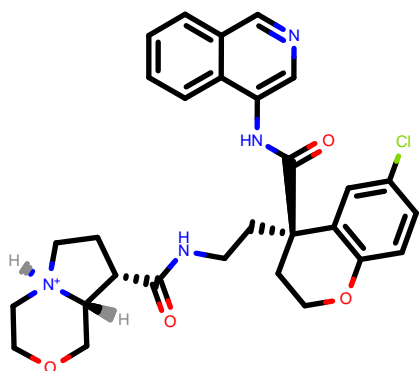
SMILES: CO[C@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2172

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.12

EN300-1588613_3_4_1



CID: EN300-1588613_3_4_1

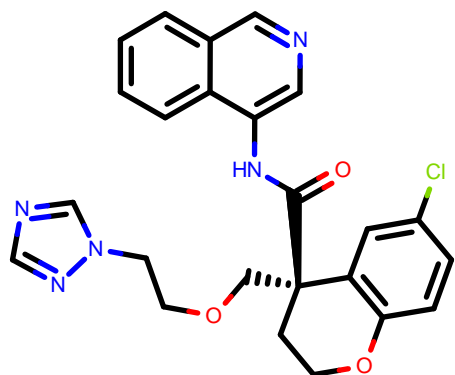
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3ccc(c4)Cl)CCN(C=O)[C@@H]5C[C@H]6C#N5C6

RUN: RUN5876

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.46

EN300-6255179_2_1_1



CID: EN300-6255179_2_1_1

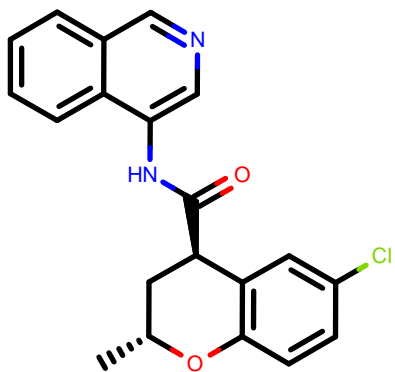
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5n5cn5

RUN: RUN7654

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.25

MAT-POS-8a69d52e-1_3



CID: MAT-POS-8a69d52e-1_3

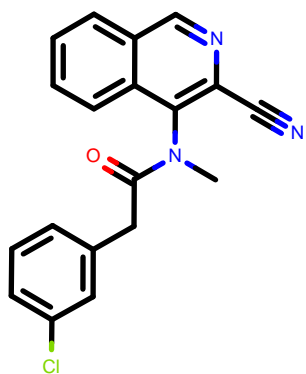
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN272

DDG (kcal/mol): -0.08

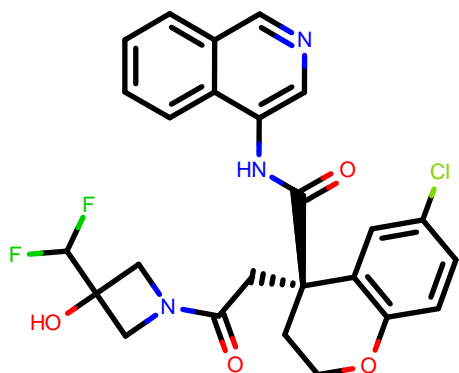
dDDG (kcal/mol): 0.04

JOH-UNI-ee5ed7c8-9_1



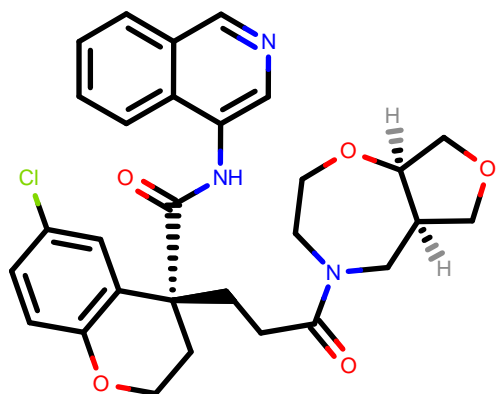
CID:	JOH-UNI-ee5ed7c8-9_1
SMILES:	<chem>CN(c1c2ccccc2cnc1C#N)C(=O)Cc3ccccc(c3)Cl</chem>
RUN:	RUN1732
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.33

EN300-249245_1_1_1



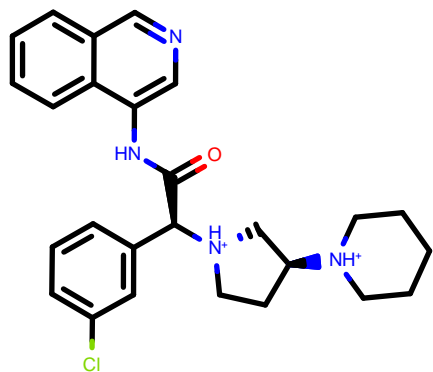
CID:	EN300-249245_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4=C3C(=O)C1CC(=O)N5CC(C5)(C(F)F)O</chem>
RUN:	RUN7640
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.24

EN300-395719_2_1_1



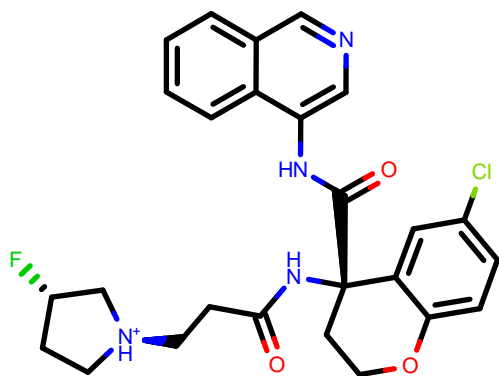
CID:	EN300-395719_2_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4=C3C(=O)C1CC(=O)N5CC(C1)C@H6COC(C@H)6C5</chem>
RUN:	RUN5134
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.30

MIC-UNK-5a93dd5f-12_4



CID:	MIC-UNK-5a93dd5f-12_4
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C1N@H(C)C[C@@]3(C)N[C@@H]4C1CCN4</chem>
RUN:	RUN737
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.51

EDG-MED-90036822-109_2



CID: EDG-MED-90036822-109_2

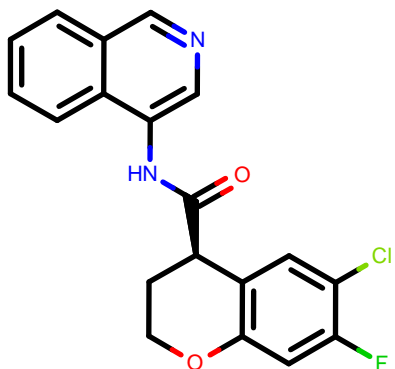
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)NC(=O)CC[N@H]5CC[C@@H](C5)F

RUN: RUN1748

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.31

ALP-POS-d91e0300-1_1



CID: ALP-POS-d91e0300-1_1

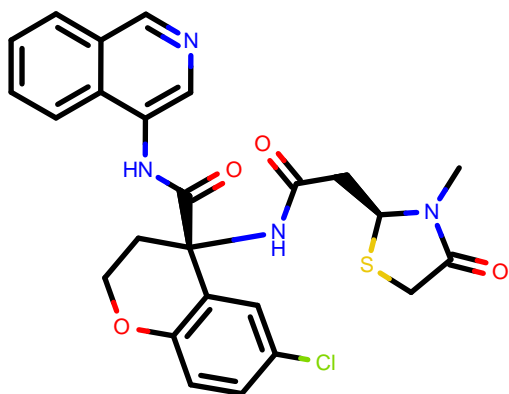
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(c(c4)F)Cl

RUN: RUN1965

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.04

EN300-143564_1_2_1



CID: EN300-143564_1_2_1

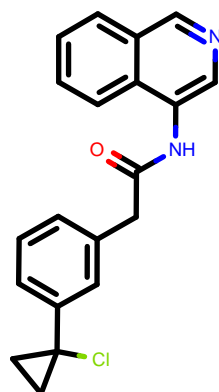
SMILES: CN1[C@@H](SCC1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2948

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.19

DAR-DIA-0cde14eb-47_1



CID: DAR-DIA-0cde14eb-47_1

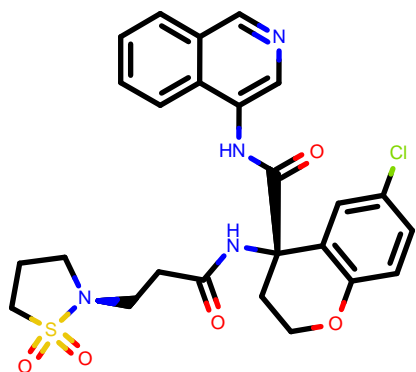
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)C4(CC4)Cl

RUN: RUN6

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.34

EN300-44873_1_1_1



CID: EN300-44873_1_1_1

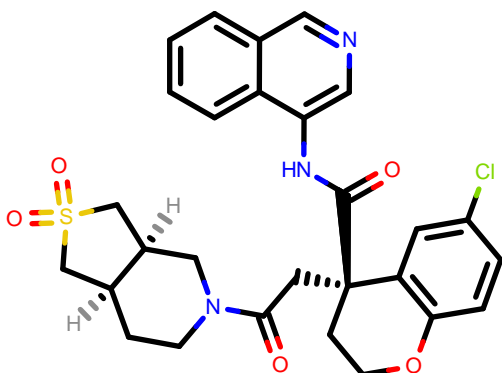
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC[N@@]5SCCS5(=O)=O

RUN: RUN3828

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.36

KAD-UNI-80f122c8-3_7



CID: KAD-UNI-80f122c8-3_7

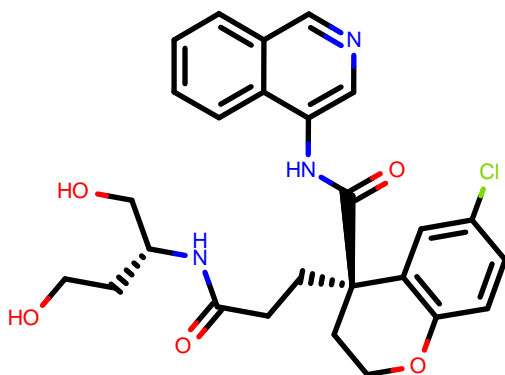
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C=O)NSC[C@@H]6CS(=O)(=O)C[C@@H]6C5

RUN: RUN2190

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.30

EN300-297144_2_2_1



CID: EN300-297144_2_2_1

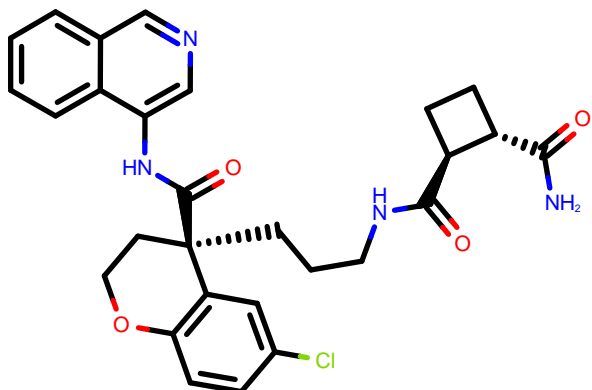
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H](CO)CO

RUN: RUN5440

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.27

EN300-217107_4_2_1



CID: EN300-217107_4_2_1

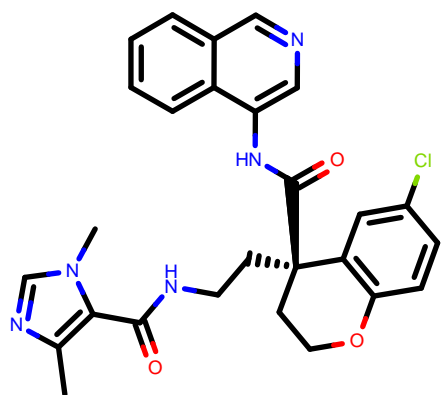
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCN(C(=O)[C@@H]5CC[C@@H]5)C1=CN

RUN: RUN7631

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.37

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

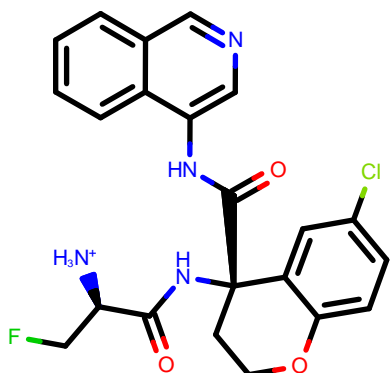
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6753

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.35

EDG-MED-90036822-5_1



CID: EDG-MED-90036822-5_1

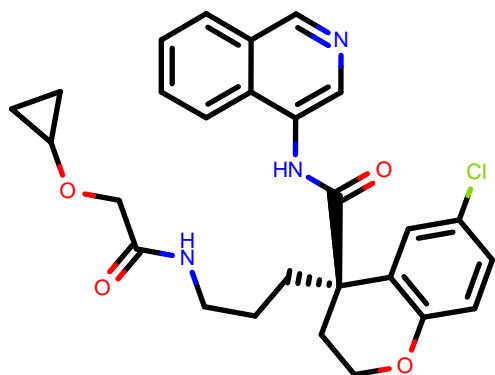
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](Cl)(N3+)

RUN: RUN1517

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.26

EN300-378373_4_1_1



CID: EN300-378373_4_1_1

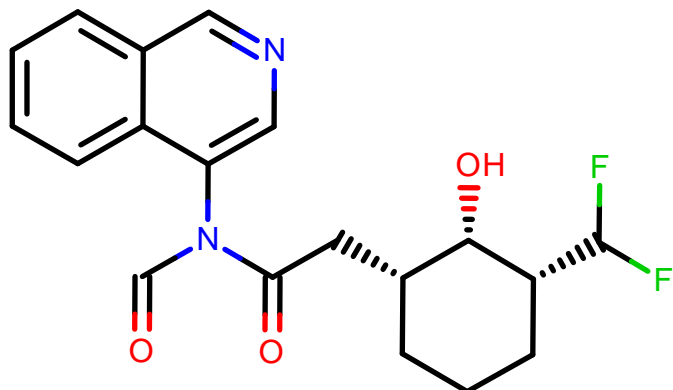
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC5OC5

RUN: RUN3937

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.31

MAK-UNK-c749d764-28_8



CID: MAK-UNK-c749d764-28_8

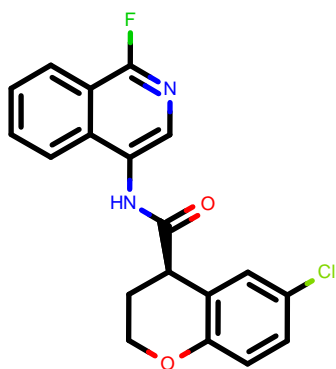
SMILES: c1ccc2c(c1)cncc2N(C(=O)C(=O)C[C@@H]3CCCC[C@H]3O)C(F)F

RUN: RUN992

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.36

JOH-SUS-a69c159d-2_1_1



CID: JOH-SUS-a69c159d-2_1_1

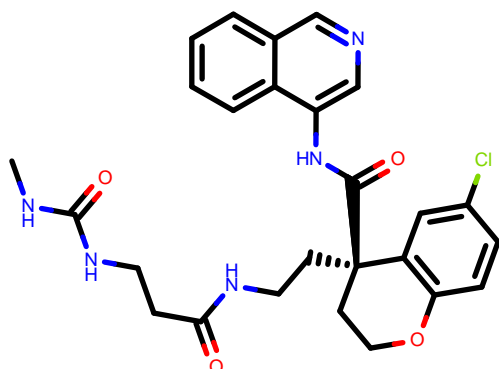
SMILES: c1ccc2c(c1)c(cnc2F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN5404

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.05

EN300-66494_3_1_1



CID: EN300-66494_3_1_1

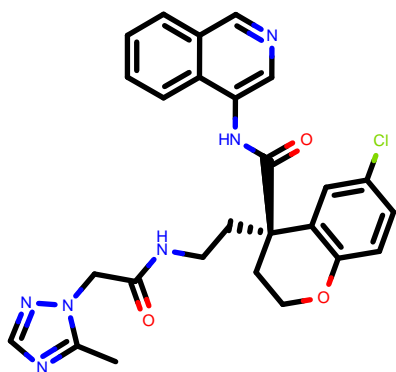
SMILES: CNC(=O)NCCC(=O)NCC[C@]1(C)CCOCc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4

RUN: RUN5644

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.31

EN300-7536177_3_1_1



CID: EN300-7536177_3_1_1

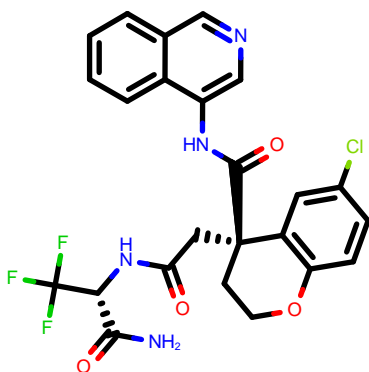
SMILES: Cc1nncn1CC(=O)NCC[C@]2(C)CCOCc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5

RUN: RUN5570

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.34

EN300-6763470_1_2_1



CID: EN300-6763470_1_2_1

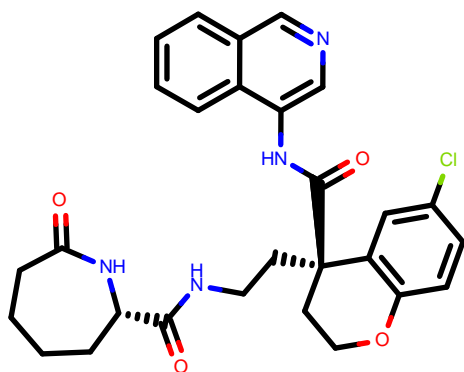
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOCc4c3cc(cc4)Cl)CC(=O)N[C@@H](C(=O)N)C(F)(F)F

RUN: RUN7231

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.23

EN300-80083_3_1_1



CID: EN300-80083_3_1_1

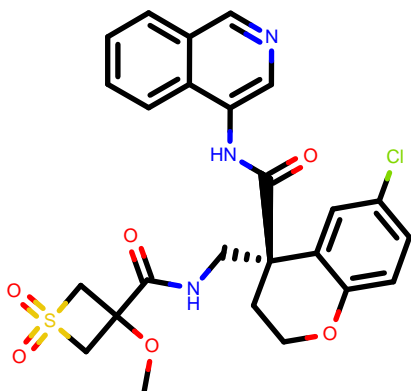
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]H5CCCCC(=O)N5

RUN: RUN3621

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.38

EN300-704025_2_1_1



CID: EN300-704025_2_1_1

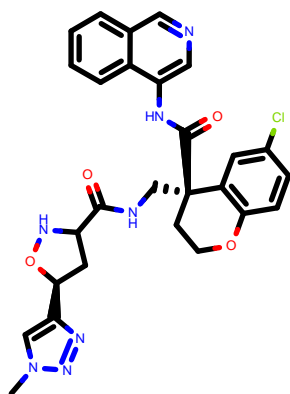
SMILES: COC1(CS(=O)(=O)C1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccccc5

RUN: RUN4921

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.32

EN300-1789253_2_1_1



CID: EN300-1789253_2_1_1

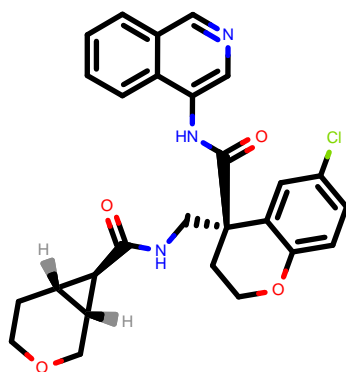
SMILES: Cn1cc(nn1)c2cc(n2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cnc6c5ccccc6

RUN: RUN4614

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.30

EN300-1644723_2_5_1



CID: EN300-1644723_2_5_1

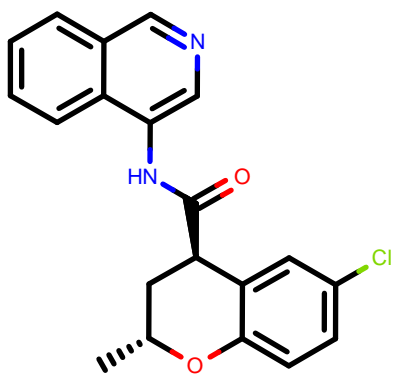
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]H5[C@@]H6[C@@]H5CCCC6

RUN: RUN6272

DDG (kcal/mol): -0.07

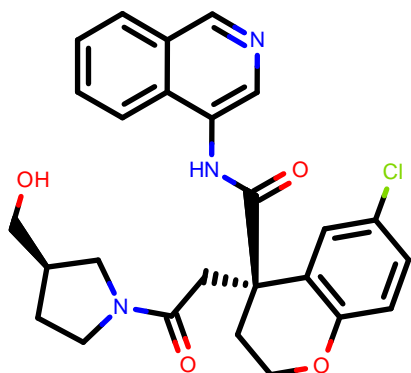
dDDG (kcal/mol): 0.29

EDJ-MED-e4b030d8-2_1



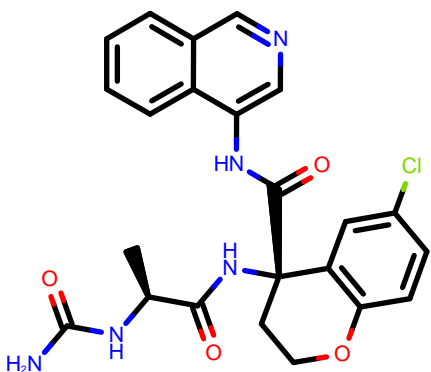
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN234
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.04

EN300-144970_1_1_1



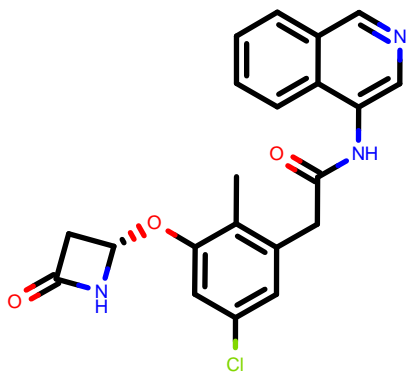
CID:	EN300-144970_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](C)COC(=O)N5CC[C@H](C5)CO</chem>
RUN:	RUN4554
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.27

EN300-152705_1_1_1



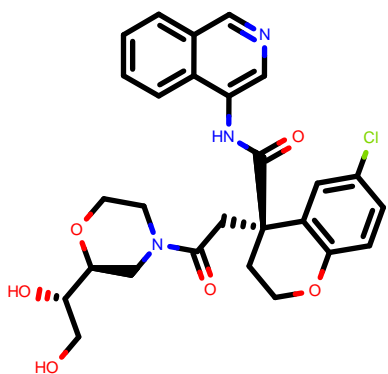
CID:	EN300-152705_1_1_1
SMILES:	<chem>C[C@@H](C(=O)N[C@@H]1(C)COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4NC(=O)N</chem>
RUN:	RUN5652
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.22

EDJ-MED-50011917-2_2



CID:	EDJ-MED-50011917-2_2
SMILES:	<chem>Cc1c(cc(cc1O[C@H]2CC(=O)N2)Cl)CC(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN340
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.37

EN300-373446_1_1_1



CID: EN300-373446_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](Cl)COC(=O)C1=CC=C(C=C1)N

RUN:

RUN6185

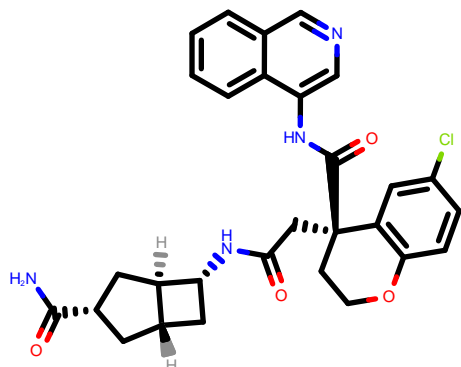
DDG (kcal/mol):

-0.07

dDDG (kcal/mol):

0.58

EN300-1268016_1_15_1



CID: EN300-1268016_1_15_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](Cl)COC(=O)C1=CC=C(C=C1)N

RUN:

RUN6337

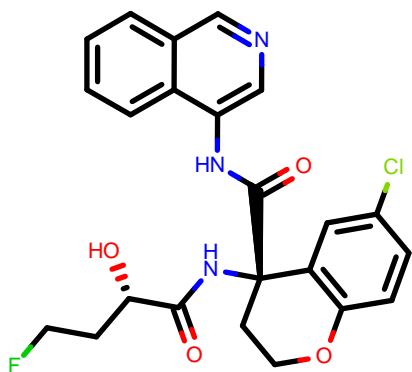
DDG (kcal/mol):

-0.07

dDDG (kcal/mol):

0.32

EDG-MED-90036822-51_2



CID: EDG-MED-90036822-51_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](Cl)COC(=O)C1=CC=C(C=C1)N

RUN:

RUN1619

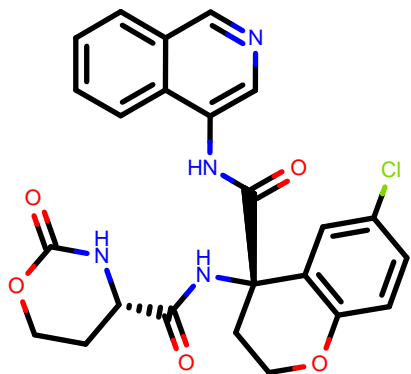
DDG (kcal/mol):

-0.07

dDDG (kcal/mol):

0.29

EN300-249804_1_1_1



CID: EN300-249804_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](Cl)COC(=O)C1=CC=C(C=C1)N

RUN:

RUN7798

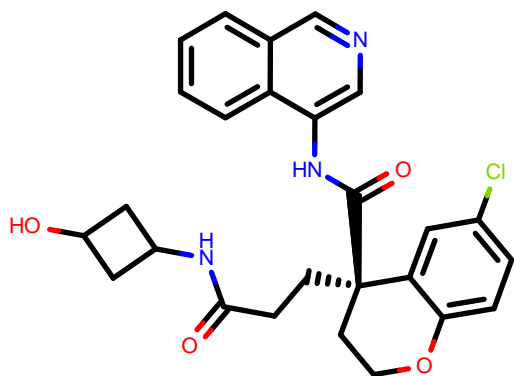
DDG (kcal/mol):

-0.06

dDDG (kcal/mol):

0.22

EN300-307592_2_1_1



CID: EN300-307592_2_1_1

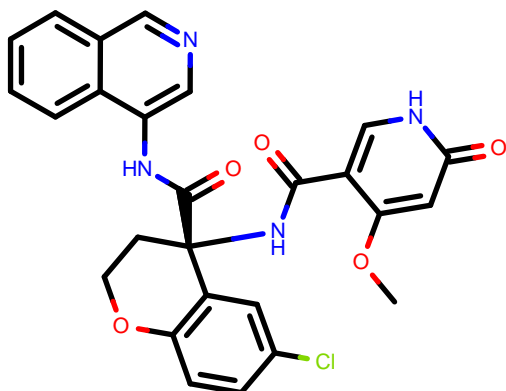
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)Cl)CCC(=O)NC5CC(C5)O

RUN: RUN7619

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.23

EN300-734638_1_1_1



CID: EN300-734638_1_1_1

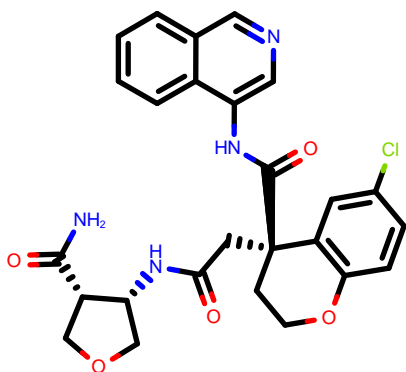
SMILES: COc1cc(=O)[nH]c1C(=O)N[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4ncce5c4ccc5

RUN: RUN7156

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.39

EN300-7435892_1_1_1



CID: EN300-7435892_1_1_1

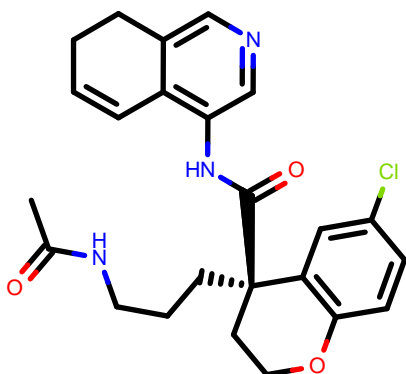
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)Cl)CC(=O)NC@@H5COC[C@@H]5Cl=O

RUN: RUN7554

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.31

EN300-18074_4_1_1



CID: EN300-18074_4_1_1

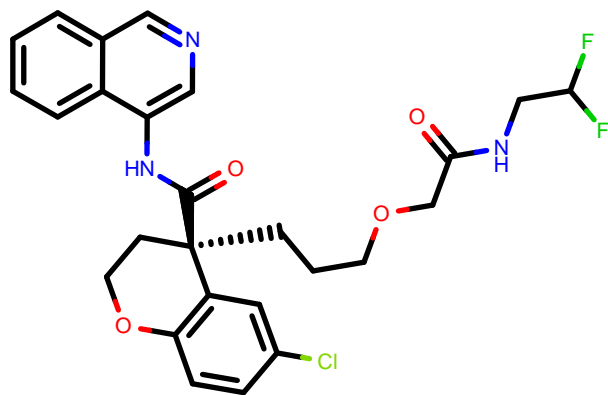
SMILES: CC(=O)NCCC[C@@1](CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccc4

RUN: RUN4302

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.28

EN300-120586_4_1_1



CID: EN300-120586_4_1_1

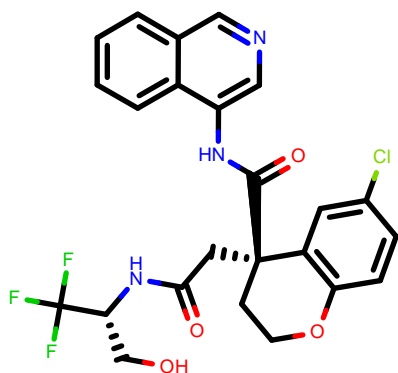
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCOC(=O)NCC(F)F

RUN: RUN5839

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.30

EN300-296237_1_2_1



CID: EN300-296237_1_2_1

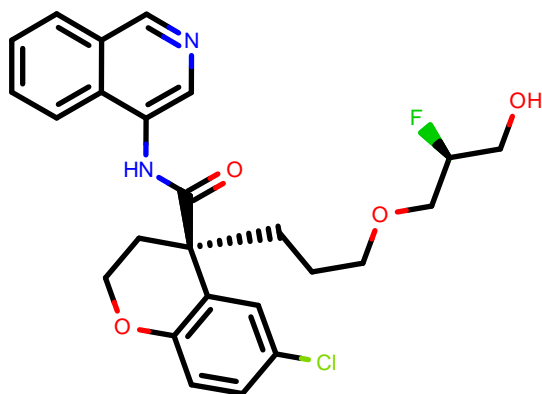
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)C(F)(F)F

RUN: RUN7464

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.43

EN300-1600517_4_2_1



CID: EN300-1600517_4_2_1

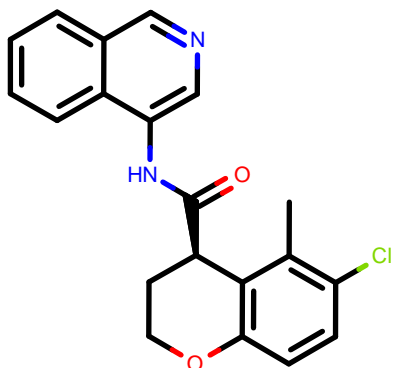
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCOC[C@H](CO)F

RUN: RUN5591

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.37

EDJ-MED-e4b030d8-8_1



CID: EDJ-MED-e4b030d8-8_1

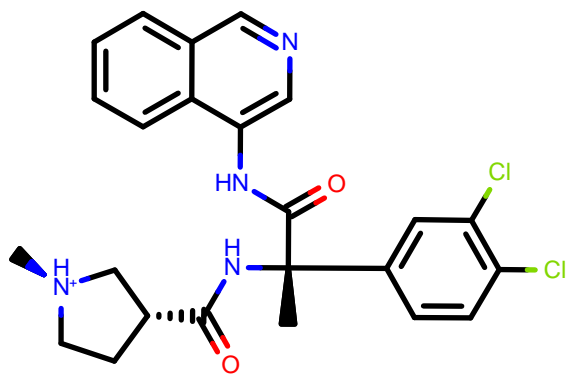
SMILES: Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN252

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.08

MAT-POS-e9e99895-13_6



CID: MAT-POS-e9e99895-13_6

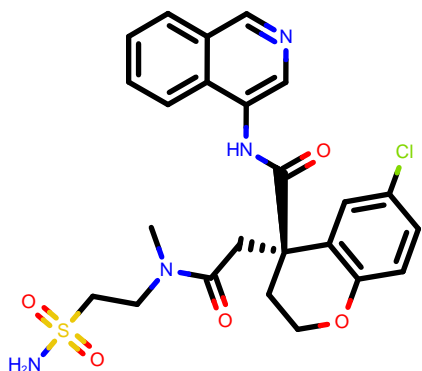
SMILES: C[C@](c1ccc(c1)Cl)C(=O)Nc2ncoc3c2ccc3NC(=O)C@@H4CC[N@H+](C4)C

RUN: RUN2147

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.53

EN300-366974_1_1_1



CID: EN300-366974_1_1_1

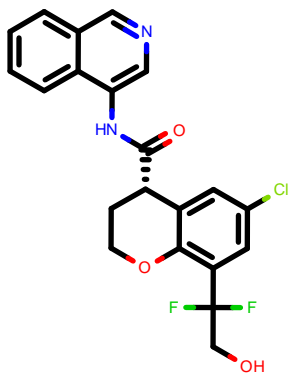
SMILES: CN(CCS(=O)=O)N(C=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5530

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.27

MIC-UNK-08fa0751-1_2



CID: MIC-UNK-08fa0751-1_2

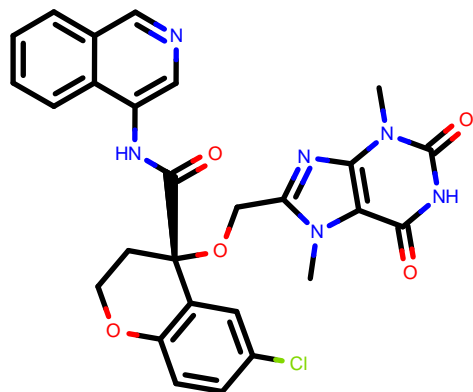
SMILES: c1ccc2c(c1)ncoc2NC(=O)C[C@H]3CCOC4c3cc(cc4C(CO)(F)F)Cl

RUN: RUN1369

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.38

EN300-52589_1_1_1



CID: EN300-52589_1_1_1

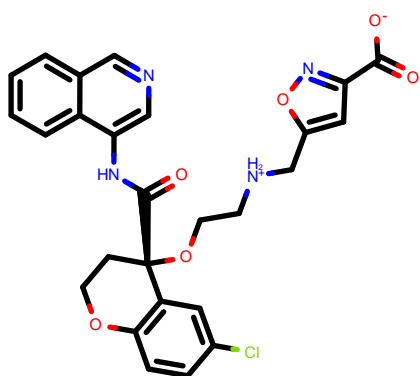
SMILES: Cn1c(nc2c1c(=O)[nH]c(=O)n2C)C[C@]3(CCO4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN4756

DDG (kcal/mol): -0.06

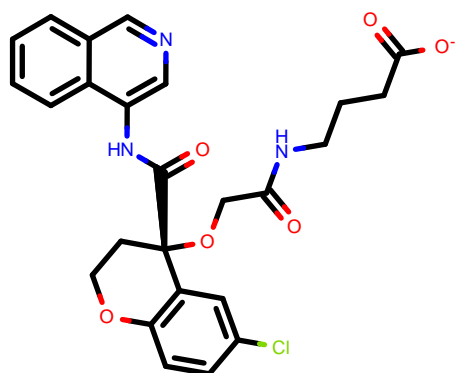
dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-1_1



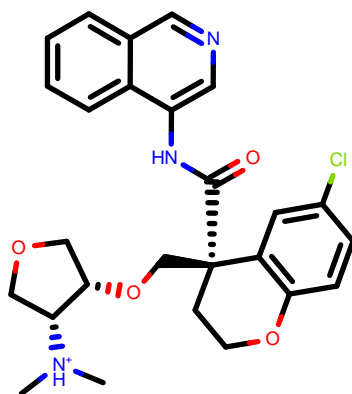
CID:	ED_-GRI-5b13fbe2-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+]Cc5cc(nc5)C(=O)[O-]</chem>
RUN:	RUN1392
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.49

EDG-MED-4c68219f-11_1



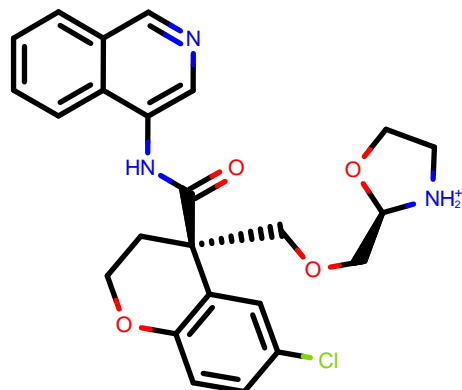
CID:	EDG-MED-4c68219f-11_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCC(=O)[O-]</chem>
RUN:	RUN1544
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.29

LEE-CAM-7ab9b158-1_1



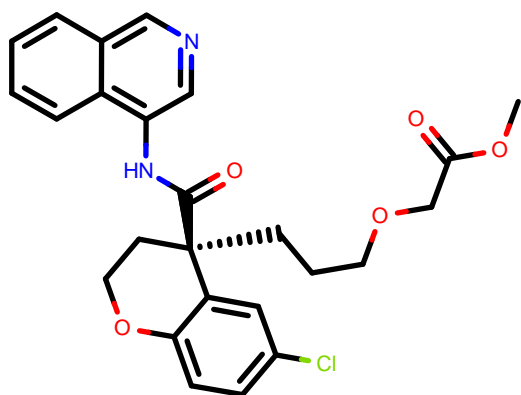
CID:	LEE-CAM-7ab9b158-1_1
SMILES:	<chem>C[NH+]C(C)[C@@]H1COC[C@@]H1OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN2027
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.39

EN300-317555_2_1_1



CID:	EN300-317555_2_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]H5[NH2+]CCO5</chem>
RUN:	RUN4957
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.28

EN300-19700_4_1_1



CID: EN300-19700_4_1_1

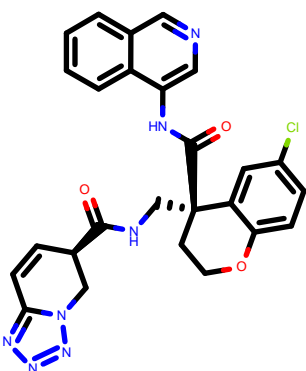
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5093

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.27

EN300-269453_2_1_1



CID: EN300-269453_2_1_1

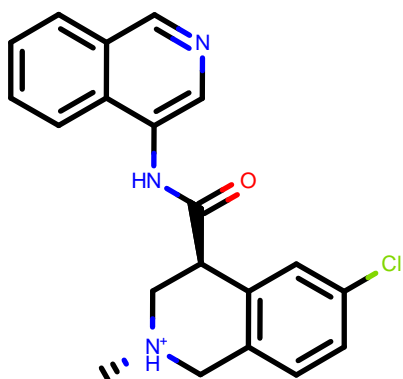
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5C6C6nncn6C5

RUN: RUN3598

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.28

BEN-DND-f2e727cd-6_2



CID: BEN-DND-f2e727cd-6_2

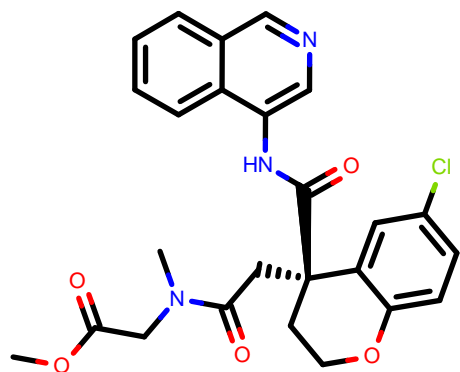
SMILES: C[N@H+]1Cc2ccc(cc2[C@@]H(C1)C(=O)Nc3ncc4c3cccc4)Cl

RUN: RUN1041

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-13000_1_1_1



CID: EN300-13000_1_1_1

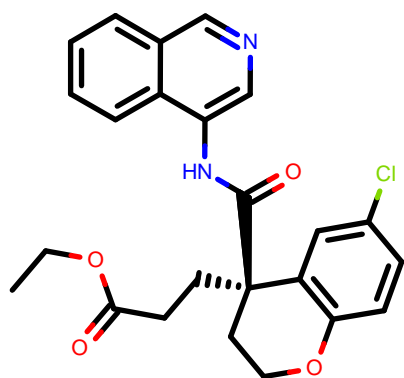
SMILES: CN(CC(=O)OC)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4454

DDG (kcal/mol): -0.05

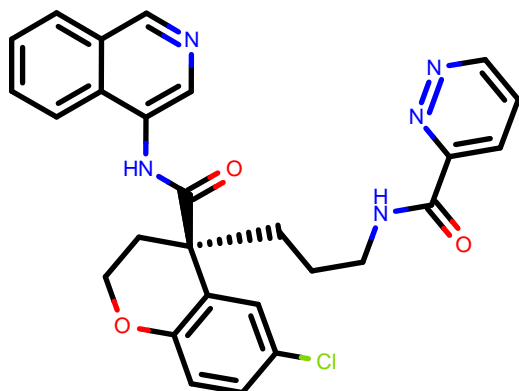
dDDG (kcal/mol): 0.29

JAG-UCB-706446eb-4_1_1



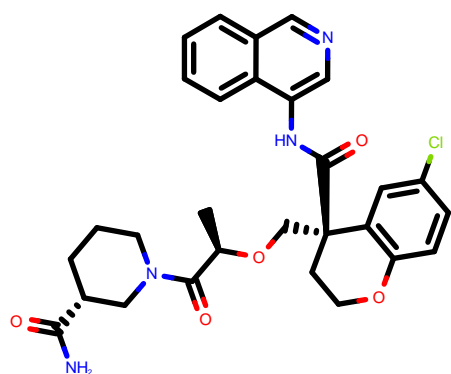
CID:	JAG-UCB-706446eb-4_1_1
SMILES:	<chem>CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4</chem>
RUN:	RUN5846
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.24

EN300-79022_4_1_1



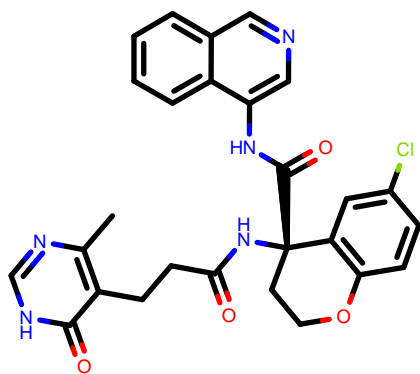
CID:	EN300-79022_4_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccnnc5</chem>
RUN:	RUN4667
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.32

EN300-28177_2_4_1



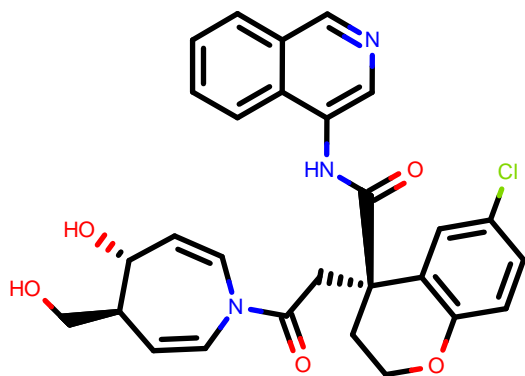
CID:	EN300-28177_2_4_1
SMILES:	<chem>C[C@@H](Cl=O)N1CCC[C@H](C1)C(=O)NOC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5</chem>
RUN:	RUN5345
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.37

EN300-33553_1_1_1



CID:	EN300-33553_1_1_1
SMILES:	<chem>Cc1c(c(=O)[nH]cn1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5</chem>
RUN:	RUN6996
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.26

EN300-7353672_1_2_1



CID: EN300-7353672_1_2_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4c3cc(c(c4)Cl)CC(=O)N5CC[C@@H](C5)CC5O)C

RUN:

RUN6158

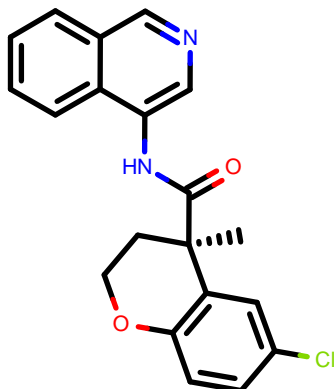
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

0.41

DAR-DIA-6a508060-10_2_1



CID: DAR-DIA-6a508060-10_2_1

SMILES:

C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN5557

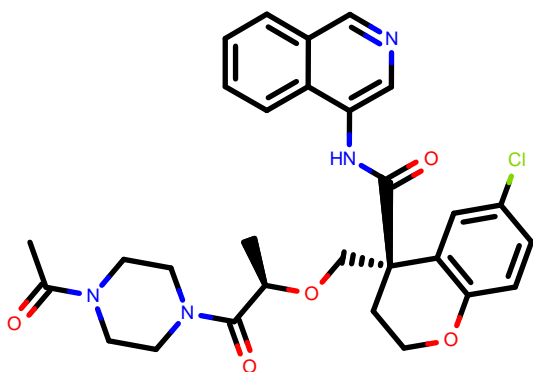
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

0.11

EN300-28106_2_2_1



CID: EN300-28106_2_2_1

SMILES:

C[C@@H](C(=O)N1CCN(CC1)C(=O)C)OC[C@@]2(C)CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN5673

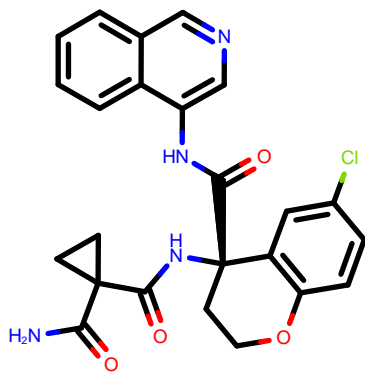
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

0.34

EN300-69070_1_1_1



CID: EN300-69070_1_1_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4c3cc(c(c4)Cl)NC(=O)C5(C)C5(=O)N

RUN:

RUN6617

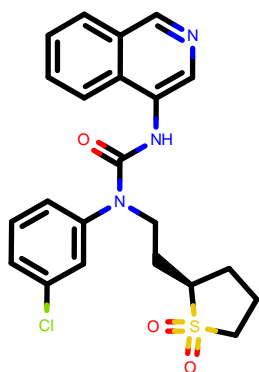
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

0.21

MIC-UNK-cdc2493e-15_2



CID: MIC-UNK-cdc2493e-15_2

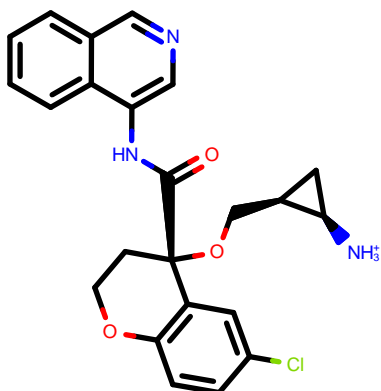
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CC[C@H]3CCCS3(=O)=O)c4cccc(c4)Cl

RUN: RUN534

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.34

ED_-GRI-5b13fbe2-70_1



CID: ED_-GRI-5b13fbe2-70_1

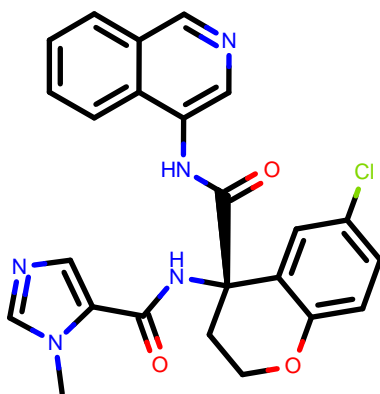
SMILES: c1ccc2c(c1)cncc2NC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@H]5[NH3+]

RUN: RUN1455

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-88417_1_1_1



CID: EN300-88417_1_1_1

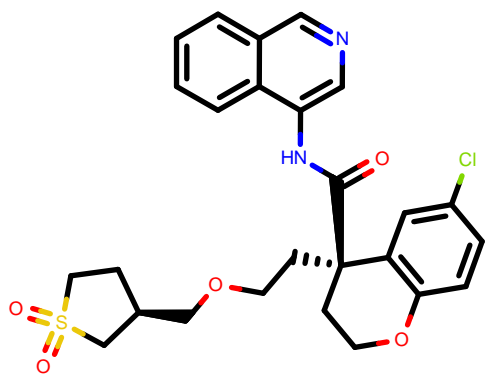
SMILES: Cn1cncc1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4680

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.23

EN300-1448603_3_1_1



CID: EN300-1448603_3_1_1

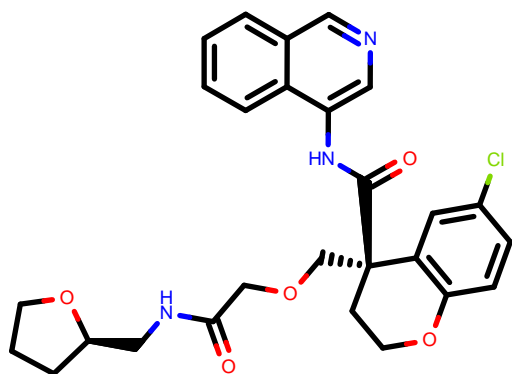
SMILES: c1ccc2c(c1)cncc2NC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5SCCS5(=O)=O)c5

RUN: RUN5446

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.35

EN300-01527_2_2_1



CID: EN300-01527_2_2_1

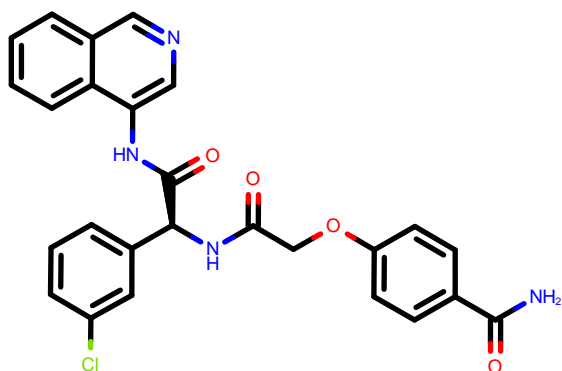
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)NC[C@@H]5CCOC5

RUN: RUN5629

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.29

EDJ-MED-ee07cf00-12_2



CID: EDJ-MED-ee07cf00-12_2

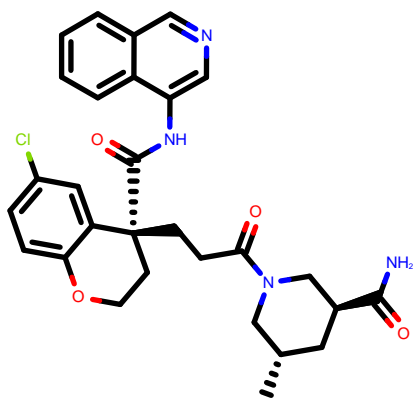
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H](c3ccccc3)C(=O)COc4ccc(cc4)C(=O)N

RUN: RUN2667

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.59

EN300-1724086_2_2_1



CID: EN300-1724086_2_2_1

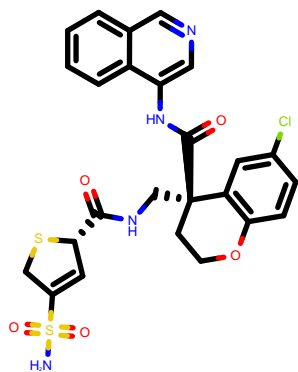
SMILES: C[C@@H]1C[C@@H](NC1C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccccc5)C(=O)N

RUN: RUN6692

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.19

EN300-98099_2_1_1



CID: EN300-98099_2_1_1

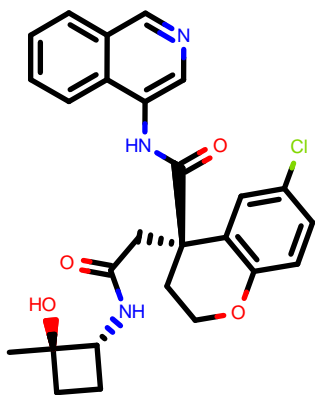
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cc(c5)S(=O)(=O)N

RUN: RUN6518

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.40

EN300-262389_1_1_1



CID: EN300-262389_1_1_1

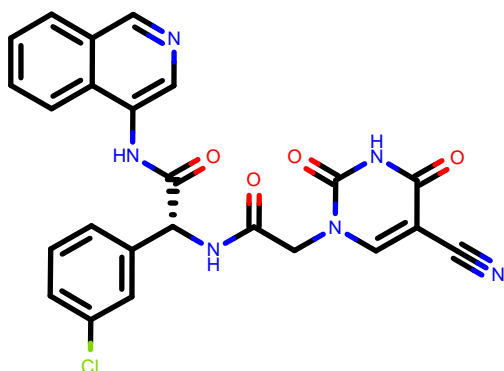
SMILES: C[C@]1(CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN6192

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.32

EDJ-MED-ee07cf00-8_1



CID: EDJ-MED-ee07cf00-8_1

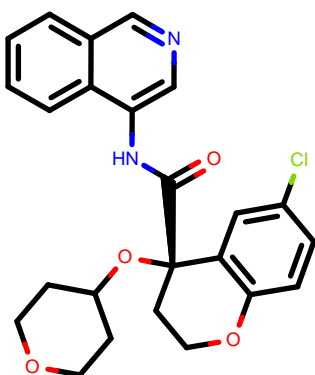
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]c4=O)C#N

RUN: RUN2632

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.53

EDJ-MED-28ec730d-3_1



CID: EDJ-MED-28ec730d-3_1

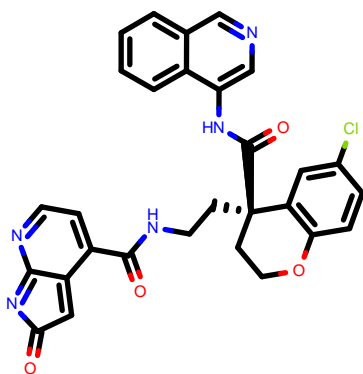
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5CCOCC5

RUN: RUN561

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

KAD-UNI-8a629cb0-19_1



CID: KAD-UNI-8a629cb0-19_1

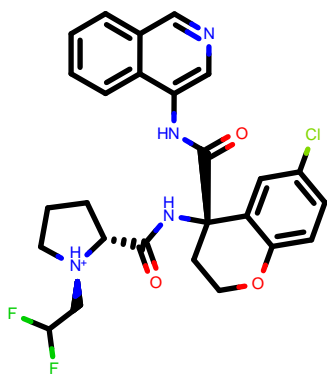
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnc6c5CC(=O)N6

RUN: RUN1991

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.28

EDG-MED-90036822-98_2



CID: EDG-MED-90036822-98_2

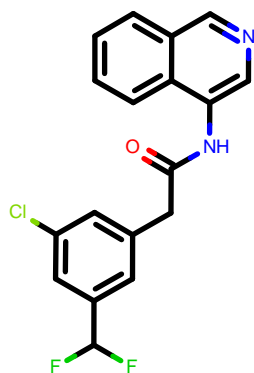
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@N]5C(F)F

RUN: RUN1744

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

MIC-UNK-16ccb665-3_1



CID: MIC-UNK-16ccb665-3_1

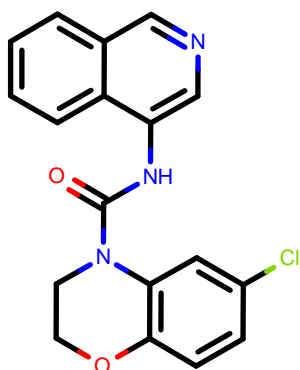
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(F)F

RUN: RUN2142

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.28

BEN-DND-f2e727cd-1_1



CID: BEN-DND-f2e727cd-1_1

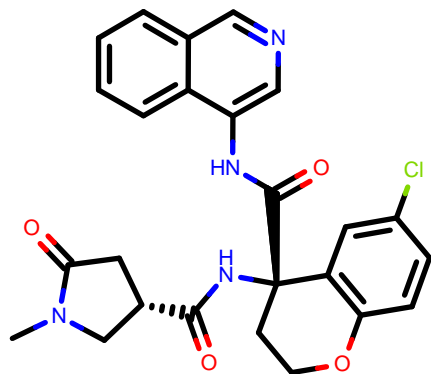
SMILES: c1ccc2c(c1)cncc2NC(=O)N3CCOc4c3cc(cc4)Cl

RUN: RUN1050

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

EN300-33601_1_2_1



CID: EN300-33601_1_2_1

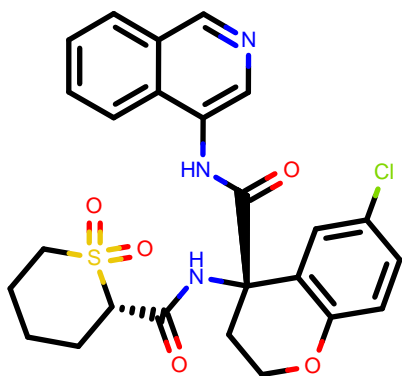
SMILES: CN1C[C@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4CCCC5C4CCCC5

RUN: RUN6155

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

EN300-107435_1_1_1



CID: EN300-107435_1_1_1

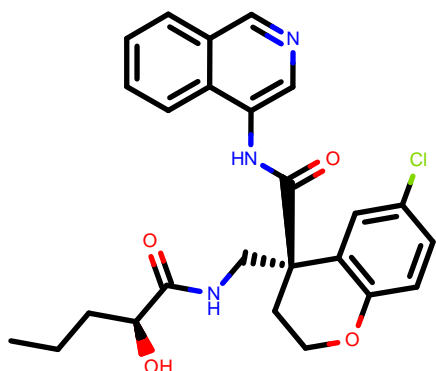
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)C@@H5CCCCS5(=O)=O

RUN: RUN7092

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.26

EN300-316679_2_1_1



CID: EN300-316679_2_1_1

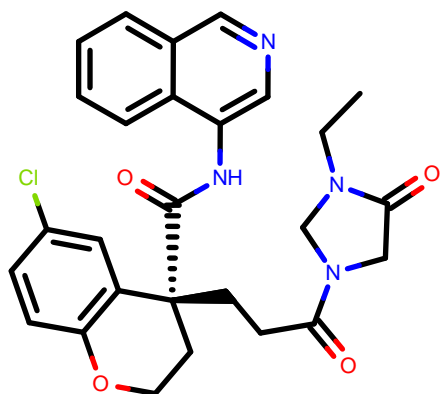
SMILES: CCC[C@@H](C(=O)NC)C@1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4O

RUN: RUN7373

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.34

KAD-UNI-8a629cb0-16_1



CID: KAD-UNI-8a629cb0-16_1

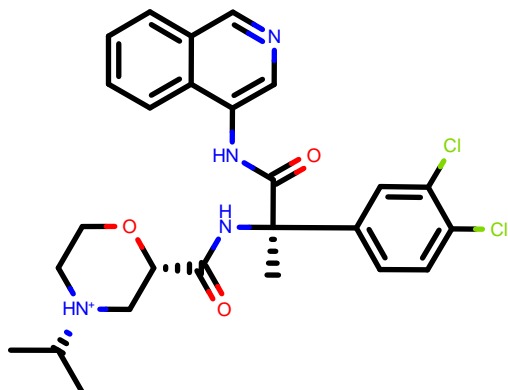
SMILES: CCN1CN(CC1=O)C(=O)CC[C@@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN1989

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

MAT-POS-e9e99895-2_5



CID: MAT-POS-e9e99895-2_5

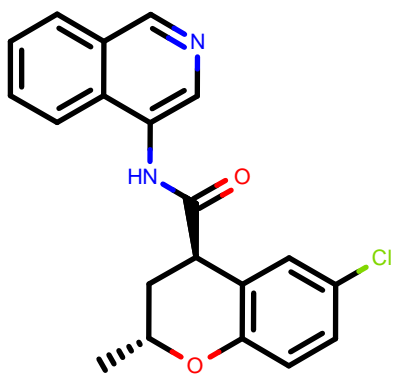
SMILES: CC(C)[N@@H+1]CCO[C@@H](C1C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN2143

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.64

ALP-POS-d3acb8cc-4_1_1



CID: ALP-POS-d3acb8cc-4_1_1

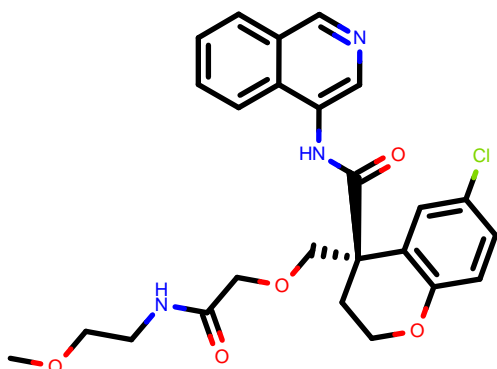
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7815

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.04

EN300-02015_2_1_1



CID: EN300-02015_2_1_1

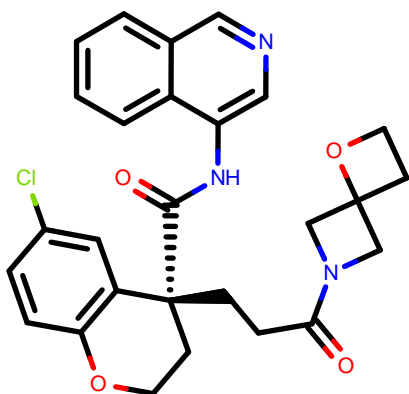
SMILES: COCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6384

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.36

KAD-UNI-8a629cb0-26_1



CID: KAD-UNI-8a629cb0-26_1

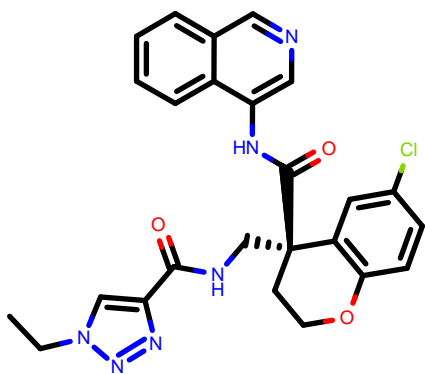
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6(C5)CCO6

RUN: RUN1944

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.22

EN300-262745_2_1_1



CID: EN300-262745_2_1_1

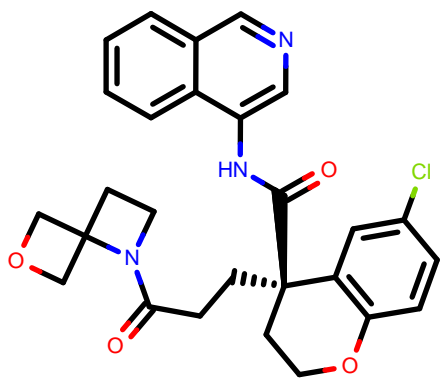
SMILES: CCn1cc(nn1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7589

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.20

EN300-247468_2_1_1



CID: EN300-247468_2_1_1

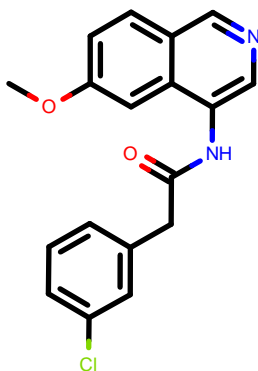
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOC4C3cc(c4)Cl)CCC(=O)N5CCCC56COC6

RUN: RUN7458

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

PET-UNK-8df914d1-1_1



CID: PET-UNK-8df914d1-1_1

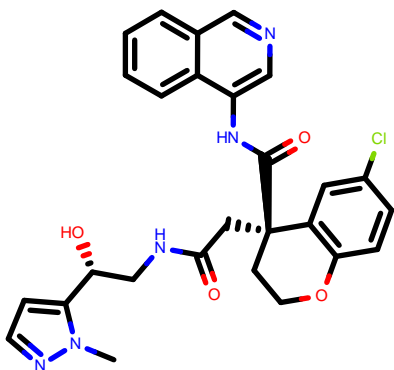
SMILES: COc1ccc2cncnc(c2c1)NC(=O)Cc3ccccc(c3)Cl

RUN: RUN71

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.29

EN300-716082_1_1_1



CID: EN300-716082_1_1_1

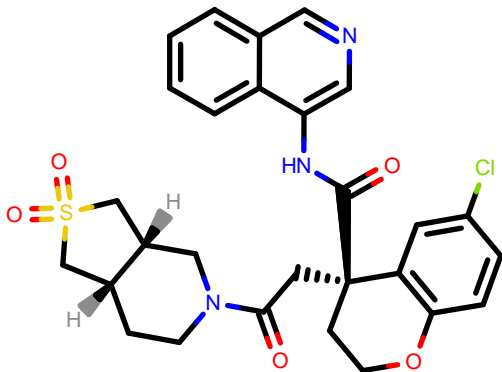
SMILES: C[n+]1c(cc[nH]1)[C@@H](CNC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4cncnc5c4cccc5)O

RUN: RUN6623

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.32

ALP-UNI-76695c4f-4_1



CID: ALP-UNI-76695c4f-4_1

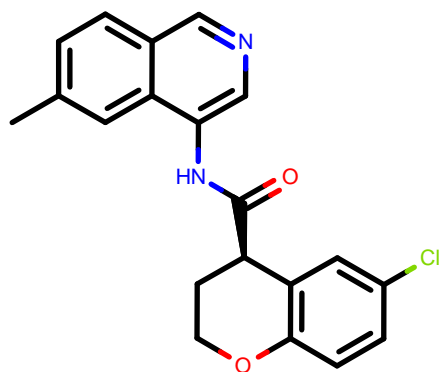
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOC4C3cc(c4)Cl)CC(=O)N5CC[C@@]6H[C@@]5(O)(=O)C[C@@]6H6C5

RUN: RUN2067

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.39

ALF-EVA-5b152d2f-2_1



CID: ALF-EVA-5b152d2f-2_1

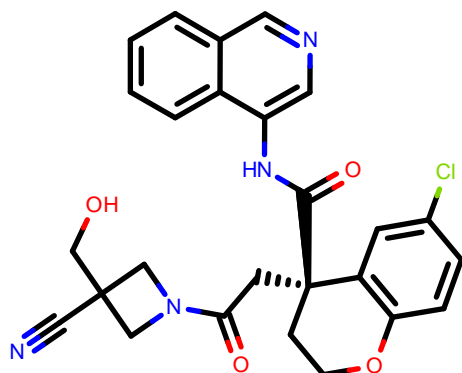
SMILES: Cc1ccc2cnc(c2c1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2209

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.05

EN300-227044_1_1_1



CID: EN300-227044_1_1_1

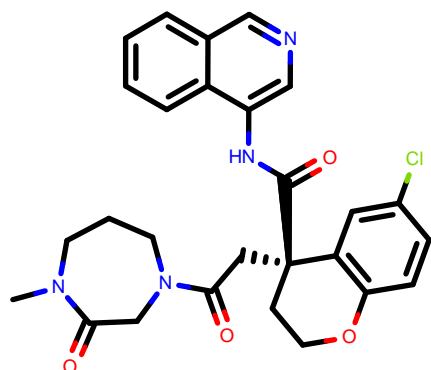
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)C#N

RUN: RUN6870

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

EN300-160143_1_1_1



CID: EN300-160143_1_1_1

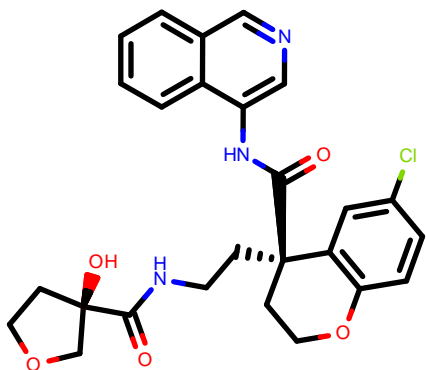
SMILES: CN1CCCN(CC1=O)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4cnc5c4ccccc5

RUN: RUN6130

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.26

EN300-148421_3_2_1



CID: EN300-148421_3_2_1

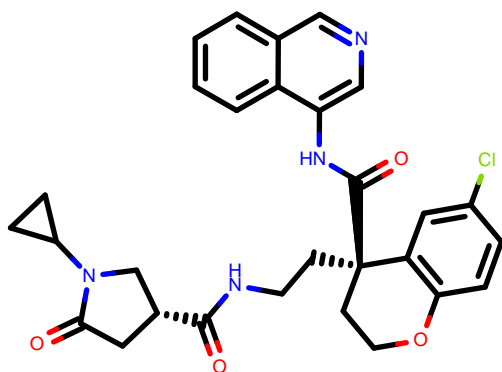
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOCC5)O

RUN: RUN7195

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.38

EN300-12440_3_1_1



CID: EN300-12440_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCN(C)C@H5CC(=O)N(C5)C6C6

RUN:

RUN7446

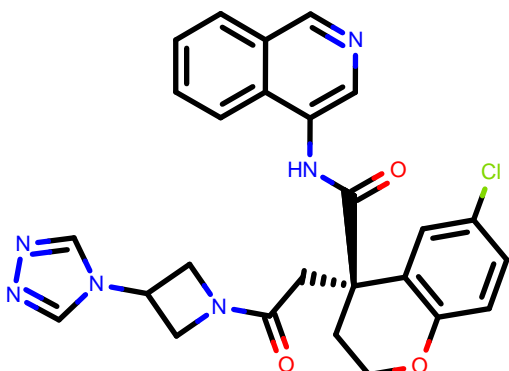
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.29

EN300-7427921_1_1_1



CID: EN300-7427921_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6nnn6

RUN:

RUN6795

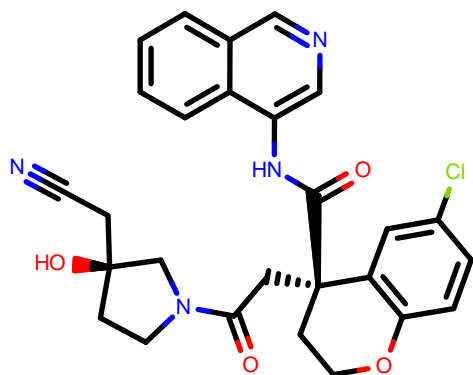
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.28

EN300-257405_1_1_1



CID: EN300-257405_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C@H)(C5)C#N

RUN:

RUN4131

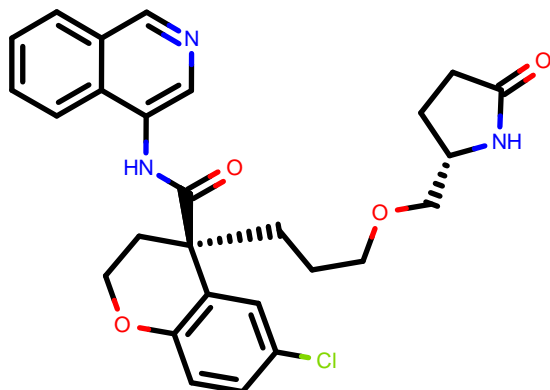
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.27

EN300-195756_4_1_1



CID: EN300-195756_4_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@]4H5CC(=O)N5

RUN:

RUN5300

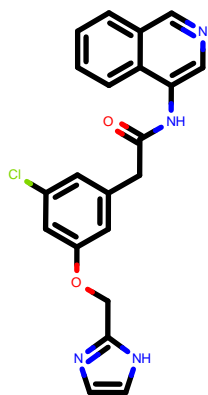
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.38

RAL-THA-1d44ff04-1_1



CID: RAL-THA-1d44ff04-1_1

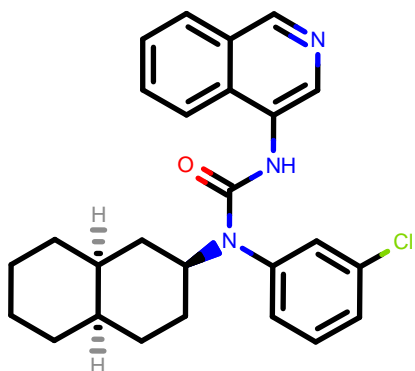
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCc4[nH]cn4

RUN: RUN402

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.43

MIC-UNK-cdc2493e-8_8



CID: MIC-UNK-cdc2493e-8_8

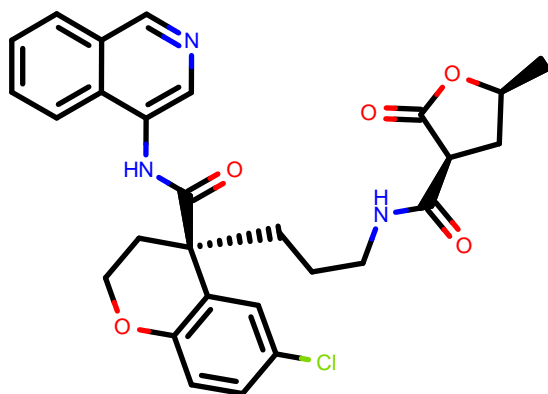
SMILES: c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C@H4CC[C@H]5CCCC[C@H]5C4

RUN: RUN512

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.42

EN300-7444533_4_4_1



CID: EN300-7444533_4_4_1

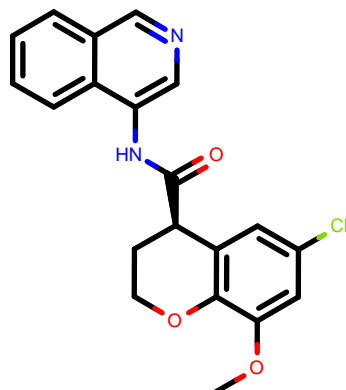
SMILES: C[C@H]1C[C@H](C(=O)O1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7322

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.36

DAR-DIA-6a508060-4_2



CID: DAR-DIA-6a508060-4_2

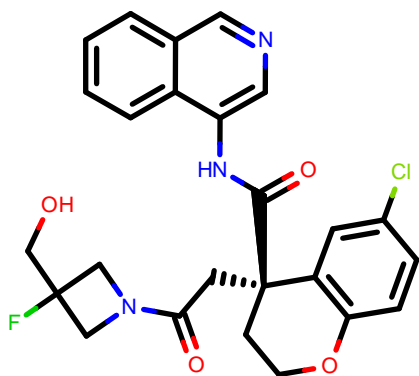
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN289

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.11

EN300-204507_1_1_1



CID: EN300-204507_1_1_1

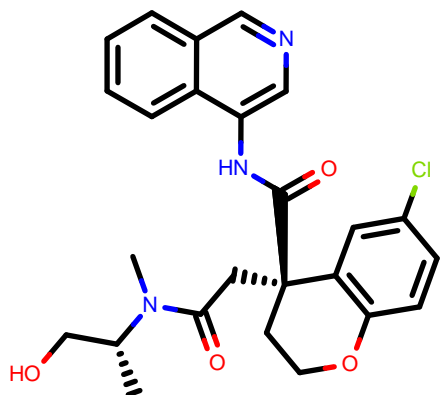
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F

RUN: RUN4822

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.32

EN300-117414_1_2_1



CID: EN300-117414_1_2_1

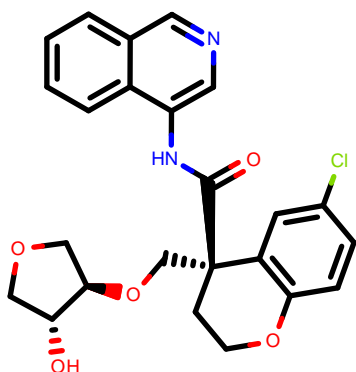
SMILES: C[C@H](CO)N(C)C(=O)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4187

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.36

EN300-331828_2_1_1



CID: EN300-331828_2_1_1

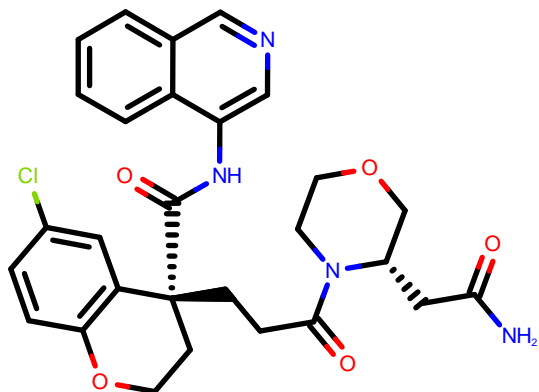
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@]5OCC[C@@H]5O

RUN: RUN4217

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.25

EN300-249093_2_1_1



CID: EN300-249093_2_1_1

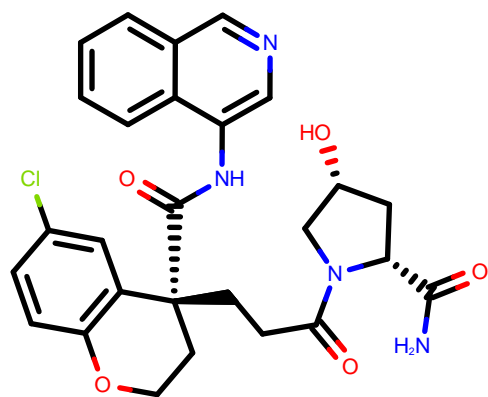
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@@]5C(=O)N

RUN: RUN3848

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.31

EN300-07752_2_1_1



CID: EN300-07752_2_1_1

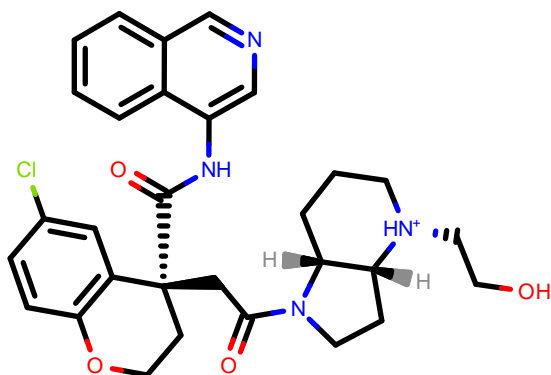
SMILES: c1ccc2c(c1)cnc2NC(=O)C@ @]3(CCOc4c3cc(cc4)C)C(=O)N5C[C@ @H]C[C@ @H]5C(=O)N5O

RUN: RUN7744

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.46

ALP-UNI-3496895b-2_3



CID: ALP-UNI-3496895b-2_3

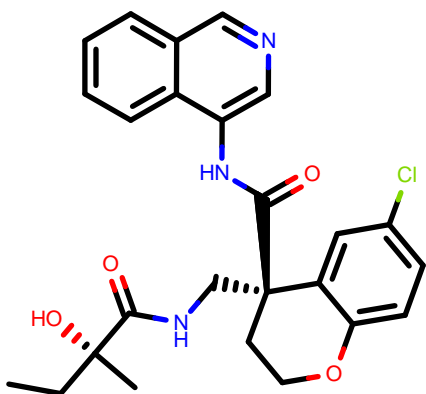
SMILES: c1ccc2c(c1)cnc2NC(=O)C@ @]3(CCOc4c3cc(cc4)C)C(=O)N5C[C@ @H]C@ @H]5C(=O)N5CO

RUN: RUN2372

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.62

EN300-248888_2_1_1



CID: EN300-248888_2_1_1

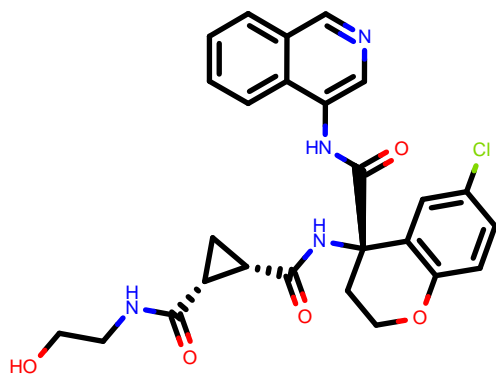
SMILES: C[C@ @](C=C)(C(=O)NC[C@ @]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4)O

RUN: RUN5105

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.32

EN300-6335413_1_1_1



CID: EN300-6335413_1_1_1

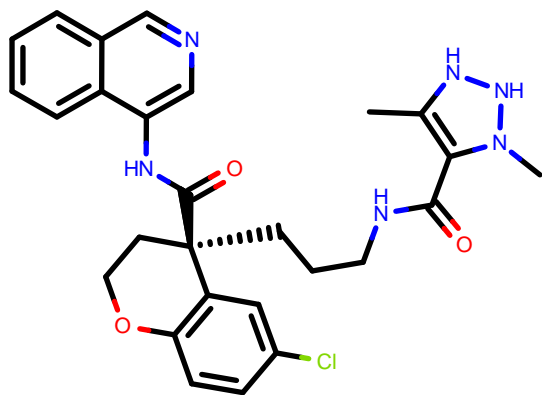
SMILES: c1ccc2c(c1)cnc2NC(=O)C@ @]3(CCOc4c3cc(cc4)C)NC(=O)C@ @H]5C[C@ @H]5C(=O)N5CO

RUN: RUN4985

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.35

EN300-649738_4_1_1



CID: EN300-649738_4_1_1

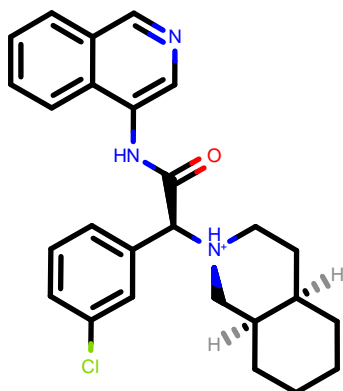
SMILES: Cc1c(n(n1)C)C(=O)NCCC[C@]2(CCOc3c2cc(c3)C)C(=O)Nc4nc5c4ccccc5

RUN: RUN7772

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.33

MIC-UNK-5a93dd5f-3_16



CID: MIC-UNK-5a93dd5f-3_16

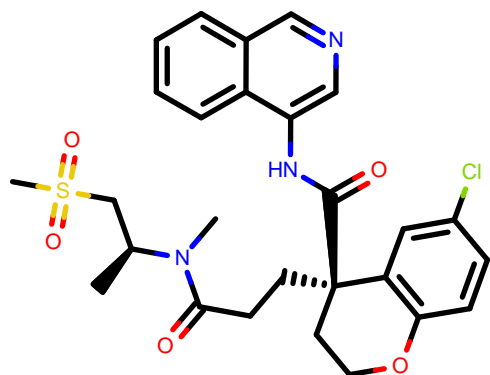
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)C)[N@H]4CC[C@H]5CCCC[C@H]5C4

RUN: RUN693

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.35

EN300-75209_2_1_1



CID: EN300-75209_2_1_1

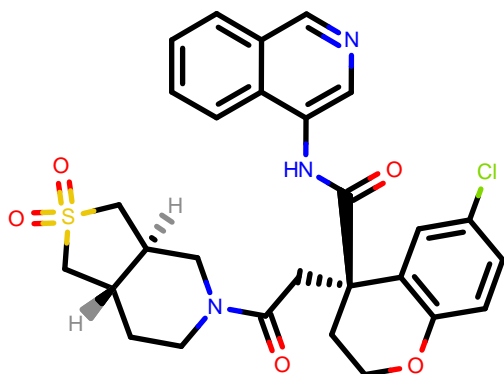
SMILES: C[C@]([H])(CS(=O)(=O)N)C(C(=O)CC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nc4c3ccccc4

RUN: RUN6293

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.33

ALP-UNI-76695c4f-4_3



CID: ALP-UNI-76695c4f-4_3

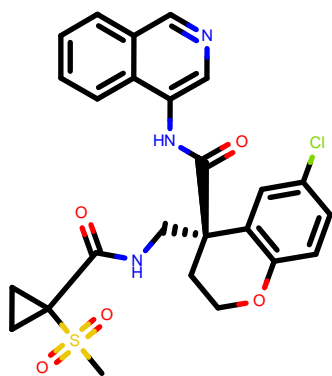
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]([H])(CS(=O)(=O)N)C5

RUN: RUN2046

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.37

EN300-191495_2_1_1



CID: EN300-191495_2_1_1

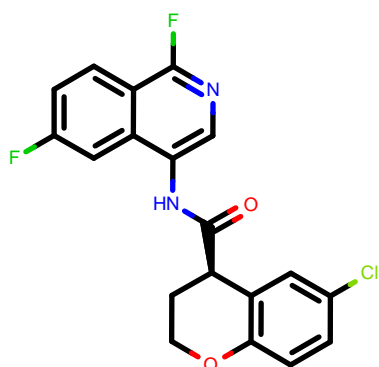
SMILES: CS(=O)(=O)C1(CC1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3782

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.43

JOH-SUS-a69c159d-5_1_1



CID: JOH-SUS-a69c159d-5_1_1

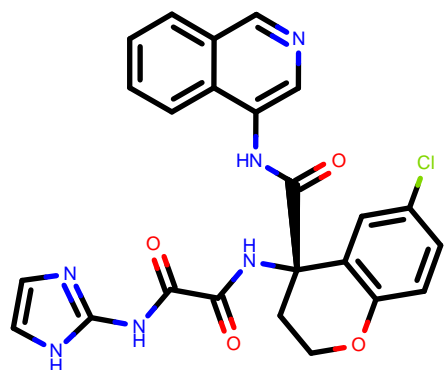
SMILES: c1cc2c(cc1F)c(cnc2F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN5194

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.06

EN300-1703015_1_1_1



CID: EN300-1703015_1_1_1

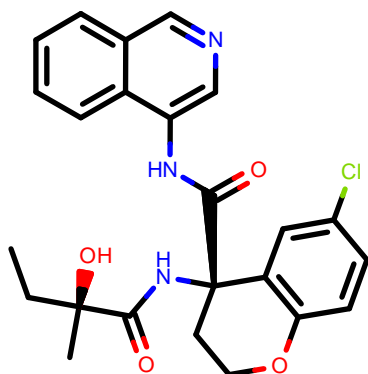
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)Nc5[nH]cnc5

RUN: RUN6959

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-104746_1_1_1



CID: EN300-104746_1_1_1

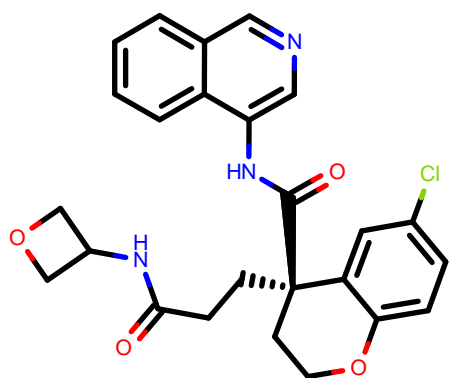
SMILES: CC[C@@](C)(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN7586

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-49064_2_1_1



CID: EN300-49064_2_1_1

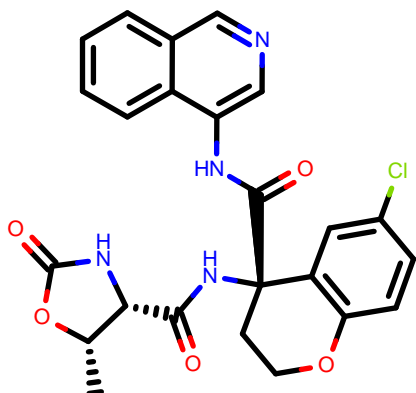
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5COC5

RUN: RUN6701

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.25

EN300-172640_1_4_1



CID: EN300-172640_1_4_1

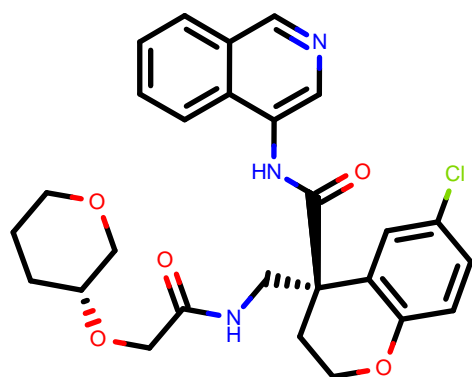
SMILES: C[C@H]1[C@H](NC(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN6577

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.23

EN300-1627945_2_1_1



CID: EN300-1627945_2_1_1

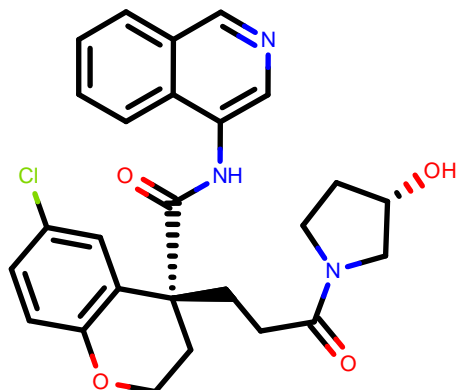
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CO[C@@H]5CCOC5

RUN: RUN7560

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.24

EN300-69312_2_1_1



CID: EN300-69312_2_1_1

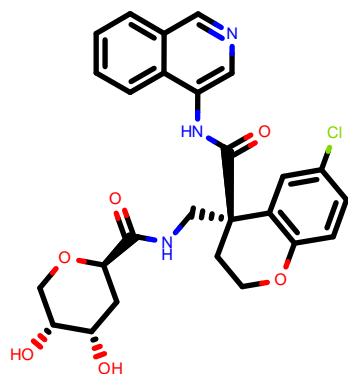
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](C5)O

RUN: RUN7374

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.27

EN300-7352736_2_1_1



CID: EN300-7352736_2_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C[C@@H](COCc4cc3ccc4O)CNC(=O)[C@@H](C[C@@H](CO)CO)O

RUN:

RUN6391

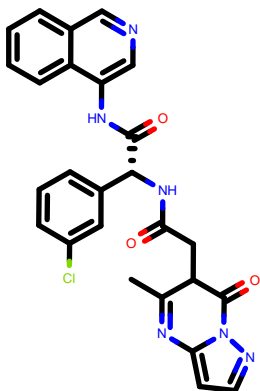
DDG (kcal/mol):

-0.02

dDDG (kcal/mol):

0.27

EDJ-MED-ee07cf00-2_2



CID: EDJ-MED-ee07cf00-2_2

SMILES:

Cc1c(c(O)n2c(n1)cd[nH]2)CC(=O)N[C@@H](c3ccccc3C)C(=O)Nc4ncoc5c4ccoc5

RUN:

RUN2642

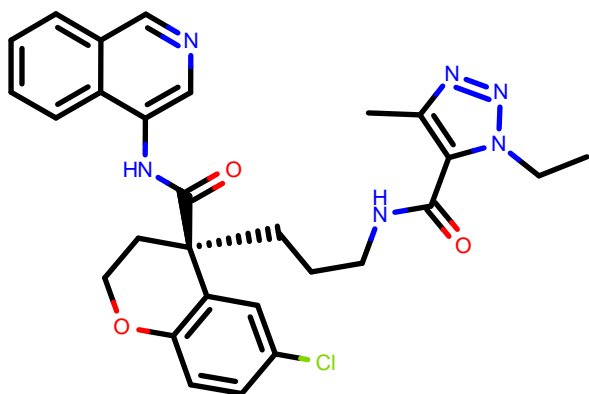
DDG (kcal/mol):

-0.02

dDDG (kcal/mol):

0.45

EN300-217526_4_1_1



CID: EN300-217526_4_1_1

SMILES:

CCn1c(c[nH]1)C(=O)NCCC[C@@H](COCc4cc3ccc4O)CNC(=O)[C@@H](COCc5c4ccoc5)

RUN:

RUN7223

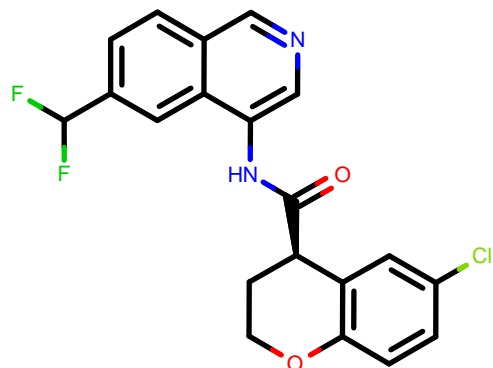
DDG (kcal/mol):

-0.02

dDDG (kcal/mol):

0.34

BEN-DND-c852c98b-7_1



CID: BEN-DND-c852c98b-7_1

SMILES:

c1cc2cnccc(c2cc1C(F)F)NC(=O)[C@@H](COCc4cc3ccc4O)Cl

RUN:

RUN1111

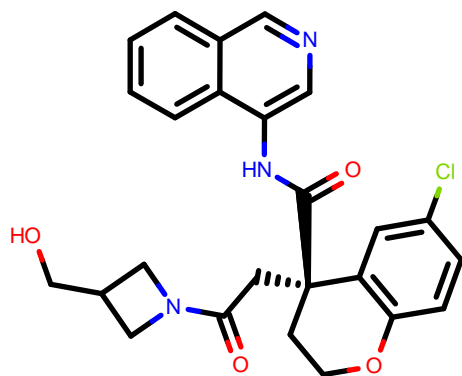
DDG (kcal/mol):

-0.02

dDDG (kcal/mol):

0.05

EN300-7370063_1_1_1



CID: EN300-7370063_1_1_1

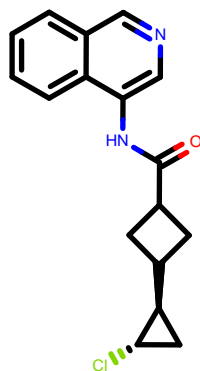
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(cc4O)CC(=O)N5CC(C5)CO

RUN: RUN5881

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.23

DAR-DIA-6a508060-11_2



CID: DAR-DIA-6a508060-11_2

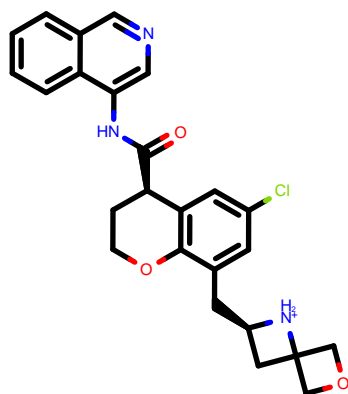
SMILES: c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@H]4C[C@@H]4Cl

RUN: RUN275

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.25

DAR-DIA-23e5a6a0-8_1_1



CID: DAR-DIA-23e5a6a0-8_1_1

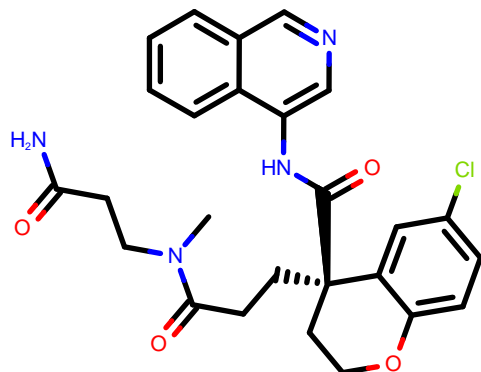
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4C)[C@@H]5CC6([NH2+][5])CO6)Cl

RUN: RUN7625

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.37

EN300-209532_2_1_1



CID: EN300-209532_2_1_1

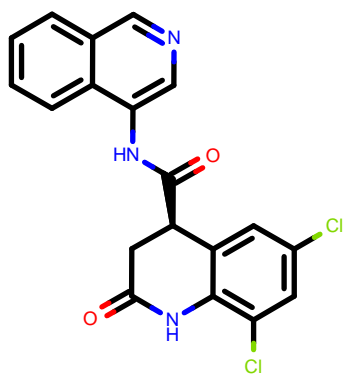
SMILES: CN(CCC(=O)N)C(=O)CC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4021

DDG (kcal/mol): -0.01

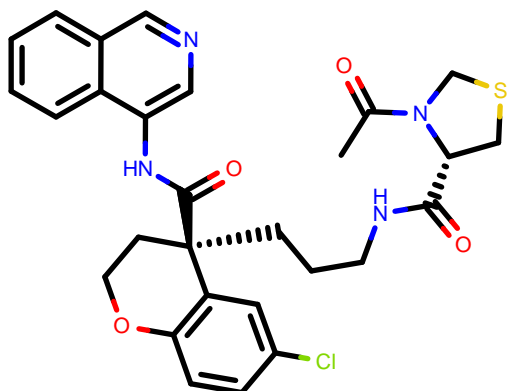
dDDG (kcal/mol): 0.29

MAT-POS-f39f51fd-1_1



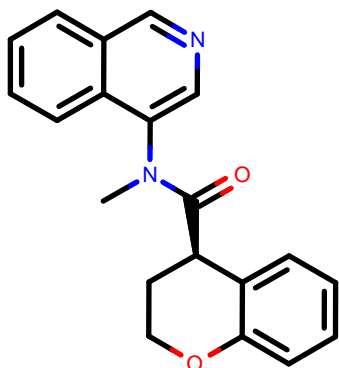
CID:	MAT-POS-f39f51fd-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4Cl)Cl</chem>
RUN:	RUN2203
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.32

EN300-761220_4_1_1



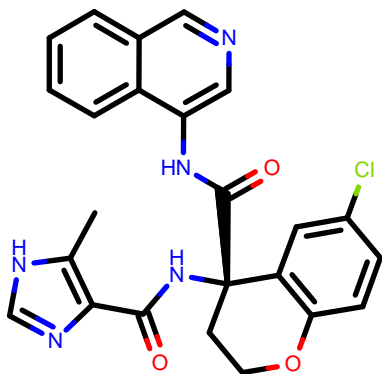
CID:	EN300-761220_4_1_1
SMILES:	<chem>CC(=O)N1CSC[C@@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN5222
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.27

MAK-UNK-3875bbc8-3_1



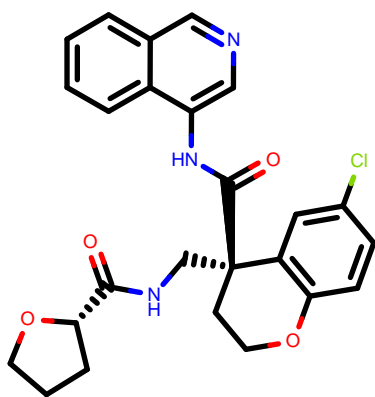
CID:	MAK-UNK-3875bbc8-3_1
SMILES:	<chem>CN(c1cnc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cccc4</chem>
RUN:	RUN706
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.10

EN300-266736_1_1_1



CID:	EN300-266736_1_1_1
SMILES:	<chem>Cc1c(nc[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN3630
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.20

EN300-21009_2_1_1



CID: EN300-21009_2_1_1

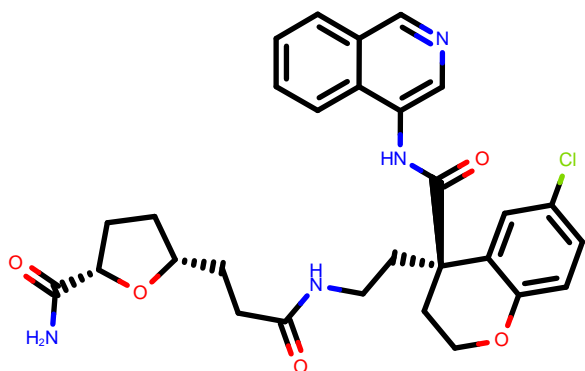
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCCO5

RUN: RUN5200

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.28

EN300-364992_3_1_1



CID: EN300-364992_3_1_1

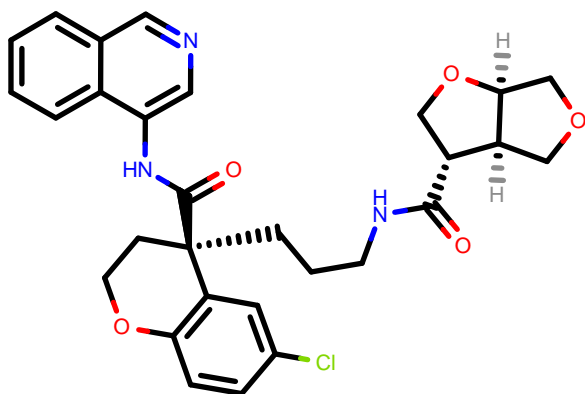
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CC[C@H]5OC[C@H]5C(=O)N

RUN: RUN6858

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.33

EN300-6482296_4_5_1



CID: EN300-6482296_4_5_1

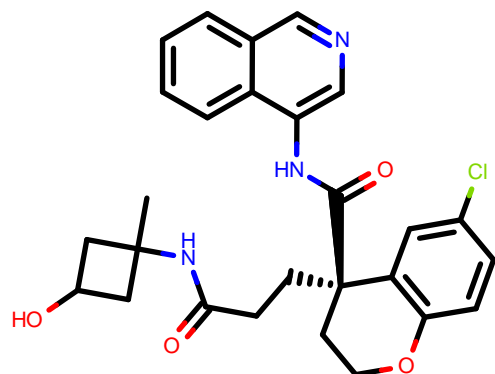
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5C[C@H]5C[C@H]5COC6

RUN: RUN6371

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.44

EN300-7396882_2_1_1



CID: EN300-7396882_2_1_1

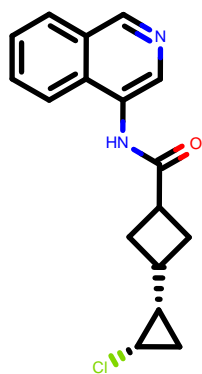
SMILES: CC1(CC(C1)O)NC(=O)CC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4795

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.27

DAR-DIA-6a508060-11_1



CID: DAR-DIA-6a508060-11_1

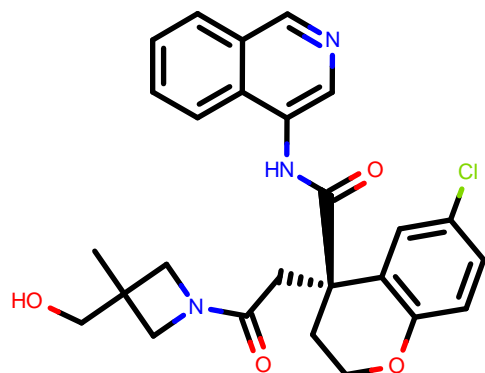
SMILES: c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@@H]4C[C@@H]4Cl

RUN: RUN270

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.21

EN300-244122_1_1_1



CID: EN300-244122_1_1_1

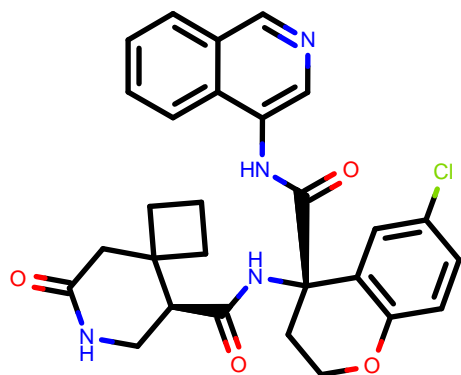
SMILES: CC1(CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)CO

RUN: RUN4490

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.29

EN300-1704404_1_2_1



CID: EN300-1704404_1_2_1

SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CNC(=O)CC56CCC6

RUN: RUN5327

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.27