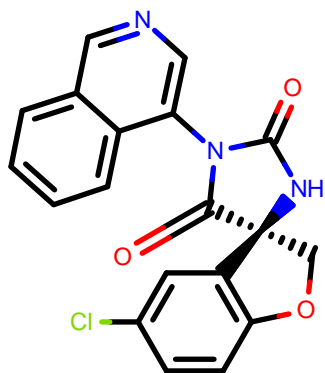
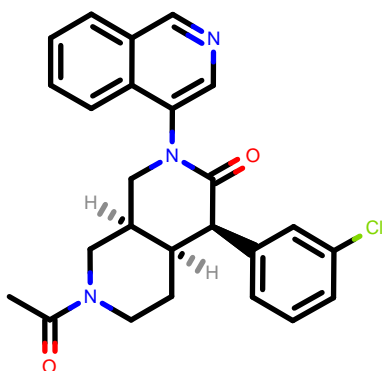


VLA-UNK-83c3754c-1_1



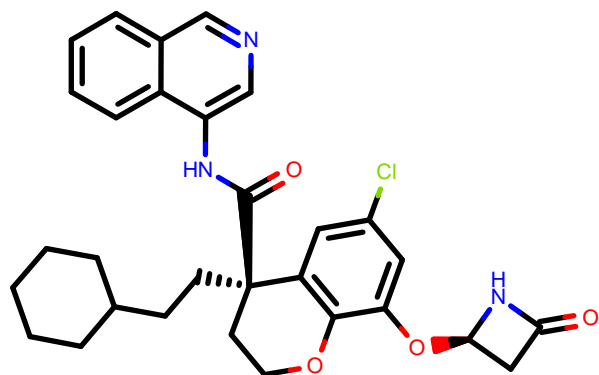
CID:	VLA-UNK-83c3754c-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@@]4(COCc5c4cc(cc5)Cl)NC3=O</chem>
RUN:	RUN2122
DDG (kcal/mol):	-7.04
dDDG (kcal/mol):	0.24

MIC-UNK-9582b2c5-1_6



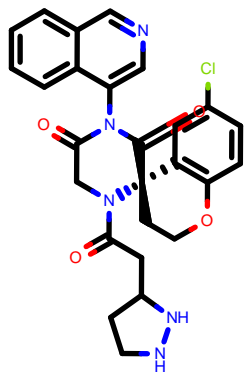
CID:	MIC-UNK-9582b2c5-1_6
SMILES:	<chem>CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4ncc5c4cccc5</chem>
RUN:	RUN200
DDG (kcal/mol):	-6.90
dDDG (kcal/mol):	0.24

VLA-UCB-50c39ae8-9_1_1



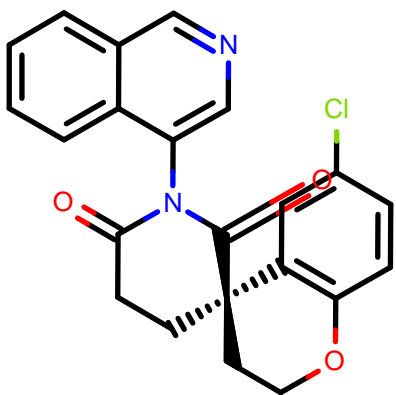
CID:	VLA-UCB-50c39ae8-9_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@@]3(COCc4c3cc(cc4O)[C@@H]5CC(=O)N5)Cl)COC6CCCCC6</chem>
RUN:	RUN2706
DDG (kcal/mol):	-6.42
dDDG (kcal/mol):	0.44

VLA-UCB-34f3ed0c-16_1



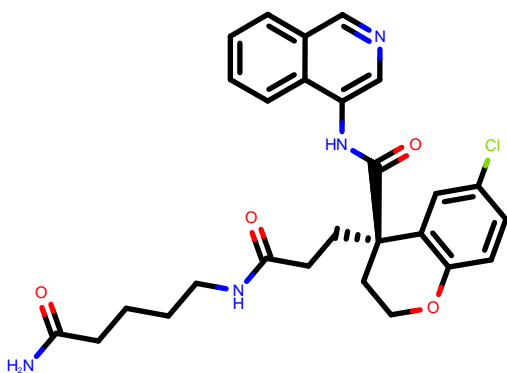
CID:	VLA-UCB-34f3ed0c-16_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)CN[C@@]4(C3=O)COCc5c4cc(cc5)Cl)C(=O)C6cccn[nH]6</chem>
RUN:	RUN544
DDG (kcal/mol):	-6.15
dDDG (kcal/mol):	0.28

VLA-UCB-50c39ae8-3_1



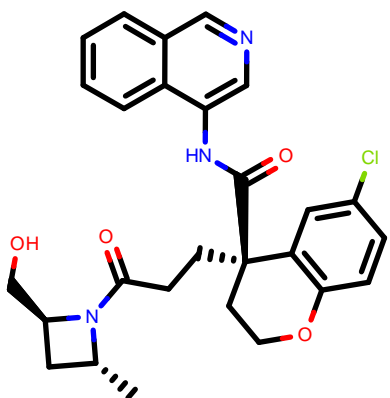
CID:	VLA-UCB-50c39ae8-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)CC[C@@]4(C3=O)CCOC5c4cc(cc5)Cl</chem>
RUN:	RUN277
DDG (kcal/mol):	-5.84
dDDG (kcal/mol):	0.22

EN300-125143_2_1_1



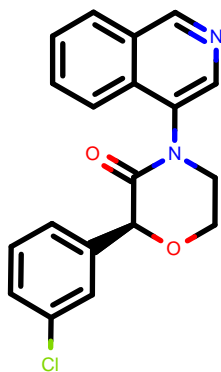
CID:	EN300-125143_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCCCC(=O)N</chem>
RUN:	RUN6629
DDG (kcal/mol):	-5.48
dDDG (kcal/mol):	0.29

EN300-1709410_2_3_1



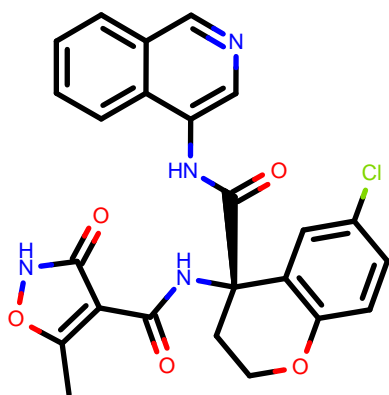
CID:	EN300-1709410_2_3_1
SMILES:	<chem>C[C@@]1[C@H]1[C@H](N1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO</chem>
RUN:	RUN7095
DDG (kcal/mol):	-5.10
dDDG (kcal/mol):	0.26

PET-UNK-431b3bfb-1_1



CID:	PET-UNK-431b3bfb-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCO[C@H](C3=O)c4cccc(c4)Cl</chem>
RUN:	RUN174
DDG (kcal/mol):	-5.06
dDDG (kcal/mol):	0.22

EN300-110423_1_1_1



CID: EN300-110423_1_1_1

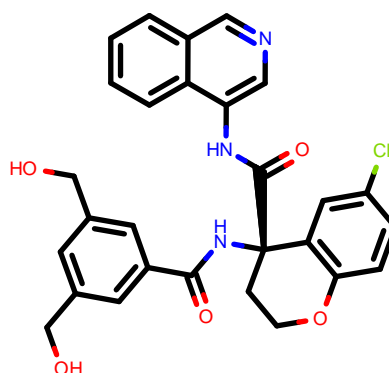
SMILES: Cc1c(c(=O)[nH]o1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN2721

DDG (kcal/mol): -4.96

dDDG (kcal/mol): 0.24

EN300-211158_1_1_1



CID: EN300-211158_1_1_1

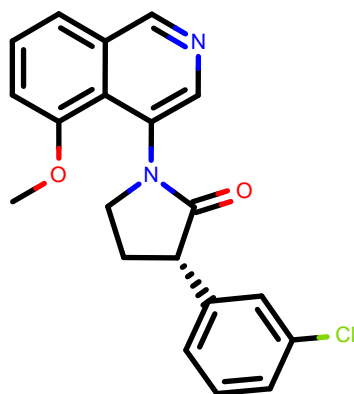
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cc(c5)CO)CO

RUN: RUN3995

DDG (kcal/mol): -4.95

dDDG (kcal/mol): 0.31

MIC-UNK-50cce87d-8_2



CID: MIC-UNK-50cce87d-8_2

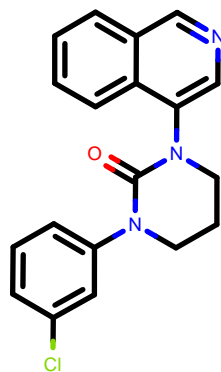
SMILES: COc1cccc2c1c(cnc2)N3CC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN554

DDG (kcal/mol): -4.91

dDDG (kcal/mol): 0.26

PET-UNK-7be94445-1_1



CID: PET-UNK-7be94445-1_1

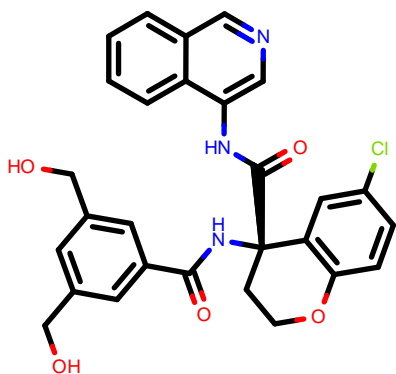
SMILES: c1ccc2c(c1)cncc2N3CCCN(C3=O)c4cccc(c4)Cl

RUN: RUN39

DDG (kcal/mol): -4.83

dDDG (kcal/mol): 0.19

EDJ-MED-6864a934-1_1



CID: EDJ-MED-6864a934-1_1

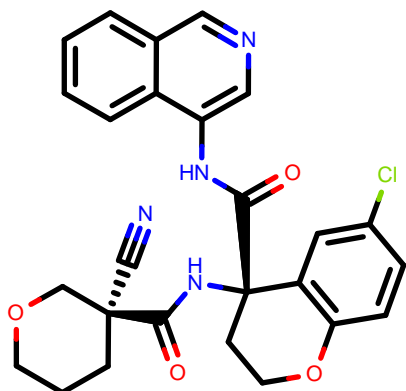
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc(c4)Cl)NC(=O)c5cc(cc(c5)CO)CO

RUN: RUN2422

DDG (kcal/mol): -4.33

dDDG (kcal/mol): 0.25

EN300-301925_1_2_1



CID: EN300-301925_1_2_1

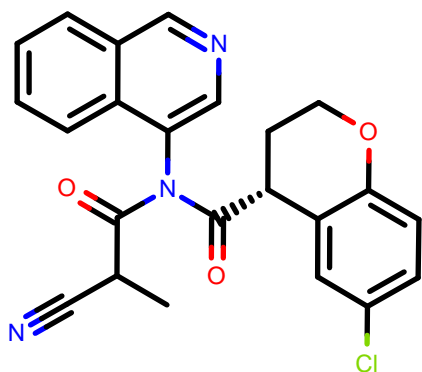
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc(c4)Cl)NC(=O)[C@]5(CCCOC5)C#N

RUN: RUN3762

DDG (kcal/mol): -4.33

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-1_1



CID: VLA-UCB-34f3ed0c-1_1

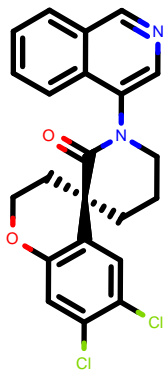
SMILES: C=C(C#N)C(=O)N(c1ncnc2c1cccc2)C(=O)[C@@H]3CCOc4cc3cc(c4)Cl

RUN: RUN592

DDG (kcal/mol): -4.32

dDDG (kcal/mol): 0.14

ALP-POS-e0fe77e5-4_1



CID: ALP-POS-e0fe77e5-4_1

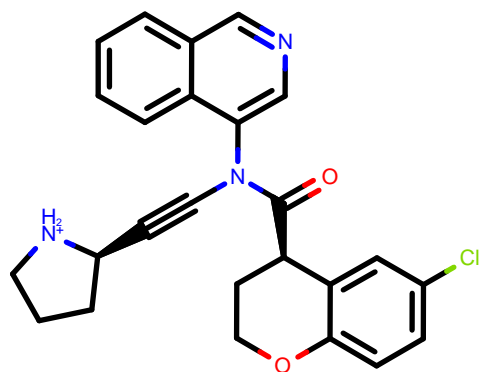
SMILES: c1ccc2c(c1)ncnc2N3CCC[C@]4(C3=O)CCOc5c4cc(c(c5)Cl)Cl

RUN: RUN2141

DDG (kcal/mol): -4.27

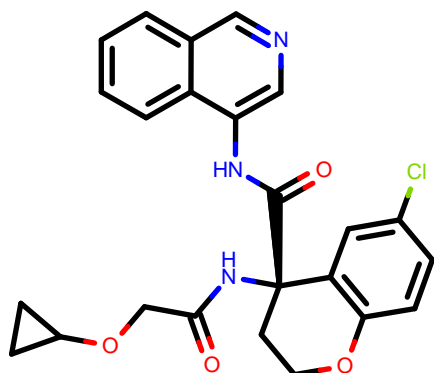
dDDG (kcal/mol): 0.24

DAR-DIA-5ff57136-12_2



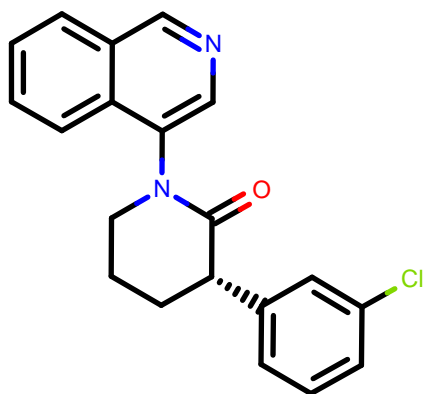
CID:	DAR-DIA-5ff57136-12_2
SMILES:	<chem>c1ccc2c(c1)cnc2N(C#C[C@H]3CCCC[NH2+])3)C(=O)[C@@H]4CCOCc5ccc(cc5)Cl</chem>
RUN:	RUN1259
DDG (kcal/mol):	-4.20
dDDG (kcal/mol):	0.22

EN300-378373_1_1_1



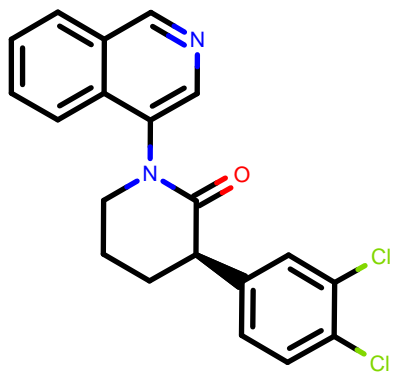
CID:	EN300-378373_1_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CO)c4ccc(cc4)Cl)NC(=O)COC5CC5</chem>
RUN:	RUN2794
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.18

PET-UNK-c9c1e0d8-3_2



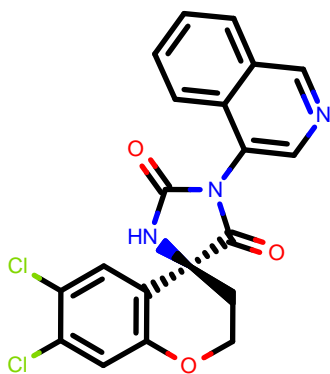
CID:	PET-UNK-c9c1e0d8-3_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3CCCC[C@H](C3=O)c4cccc(c4)Cl</chem>
RUN:	RUN33
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.31

ALP-UNI-3735e77e-1_1



CID:	ALP-UNI-3735e77e-1_1
SMILES:	<chem>c1ccc2c(c1)cnc2N3CCCC[C@H](C3=O)c4ccc(c(c4)Cl)Cl</chem>
RUN:	RUN1763
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.23

VLA-UNK-56836b69-2_1



CID: VLA-UNK-56836b69-2_1

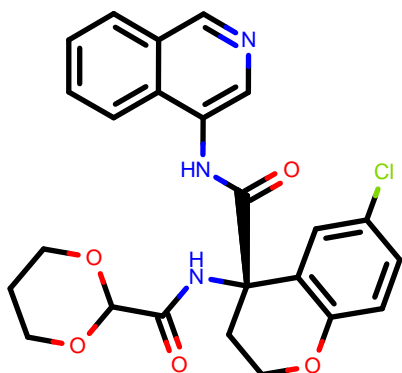
SMILES: c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O

RUN: RUN2096

DDG (kcal/mol): -4.15

dDDG (kcal/mol): 0.22

EN300-170985_1_1_1



CID: EN300-170985_1_1_1

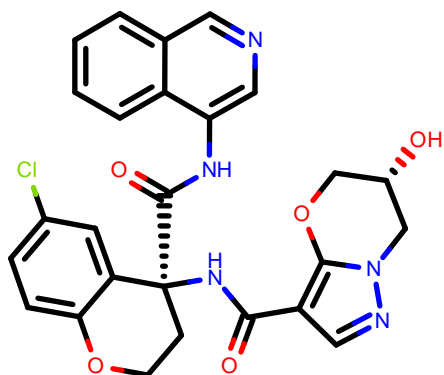
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCCC5

RUN: RUN2765

DDG (kcal/mol): -4.14

dDDG (kcal/mol): 0.24

EN300-6497444_1_1_1



CID: EN300-6497444_1_1_1

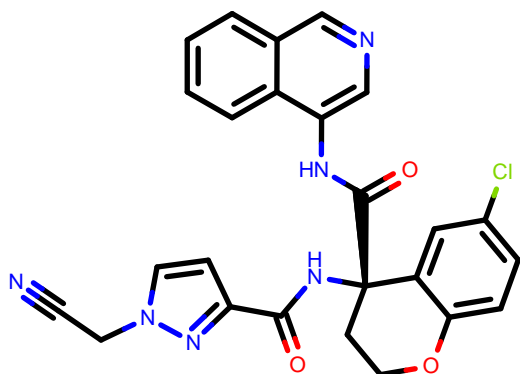
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5OC[C@@H](C6)O

RUN: RUN2775

DDG (kcal/mol): -4.13

dDDG (kcal/mol): 0.25

EDJ-MED-6864a934-9_1



CID: EDJ-MED-6864a934-9_1

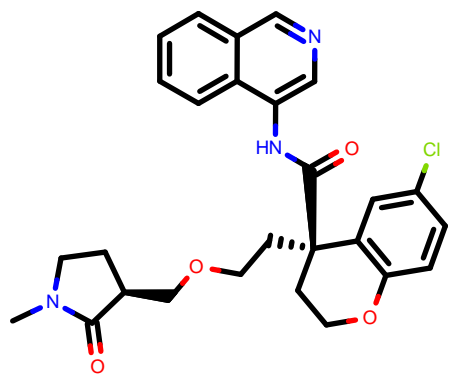
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncn(c5)C#N

RUN: RUN2455

DDG (kcal/mol): -4.13

dDDG (kcal/mol): 0.28

EN300-260816_3_2_1



CID: EN300-260816_3_2_1

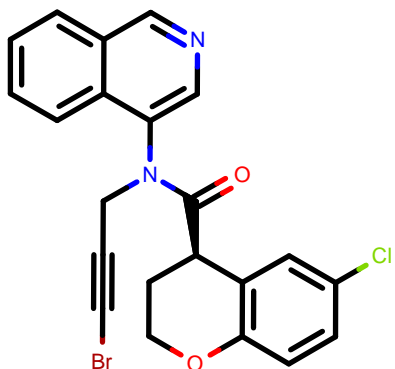
SMILES: CN1CC[C@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

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

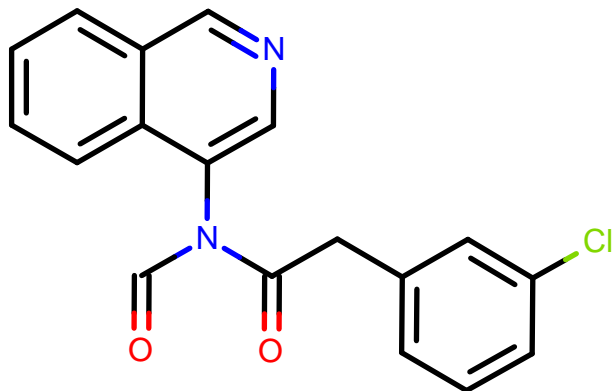
SMILES: c1ccc2c(c1)cncc2N(CC#CBr)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN3438

DDG (kcal/mol): -4.10

dDDG (kcal/mol): 0.18

PET-UNK-12d8d43f-1_1



CID: PET-UNK-12d8d43f-1_1

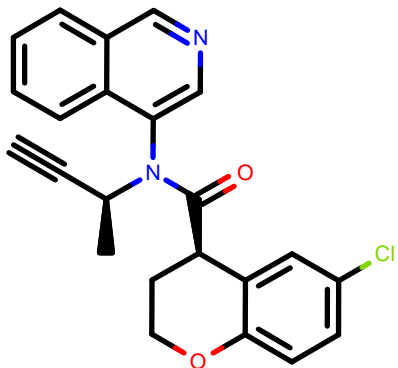
SMILES: c1ccc2c(c1)cncc2N(C=O)C(=O)Cc3cccc(c3)Cl

RUN: RUN1319

DDG (kcal/mol): -4.08

dDDG (kcal/mol): 0.22

DAR-DIA-5ff57136-16_1



CID: DAR-DIA-5ff57136-16_1

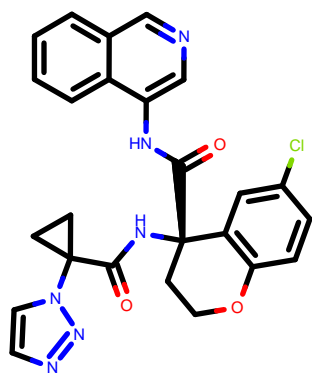
SMILES: C[C@@H](C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN1228

DDG (kcal/mol): -4.07

dDDG (kcal/mol): 0.14

EN300-658559_1_1_1



CID: EN300-658559_1_1_1

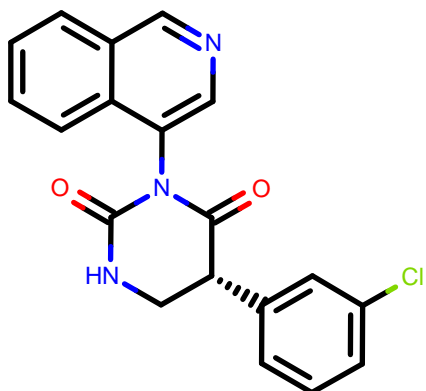
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)n6ccnn6

RUN: RUN3087

DDG (kcal/mol): -3.99

dDDG (kcal/mol): 0.28

PET-UNK-abc197b8-1_1



CID: PET-UNK-abc197b8-1_1

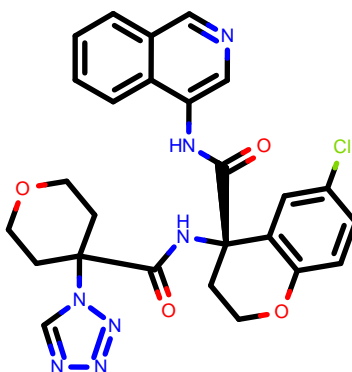
SMILES: c1ccc2c(c1)ncnc2N3C(=O)[C@@H](CNC3=O)c4cccc(c4)Cl

RUN: RUN334

DDG (kcal/mol): -3.98

dDDG (kcal/mol): 0.27

EN300-254908_1_1_1



CID: EN300-254908_1_1_1

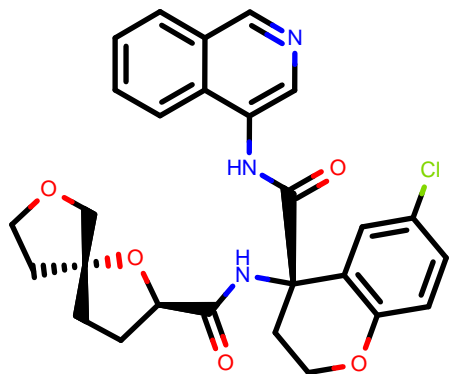
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COCC5)n6ccnn6

RUN: RUN2738

DDG (kcal/mol): -3.97

dDDG (kcal/mol): 0.26

EN300-3031933_1_2_1



CID: EN300-3031933_1_2_1

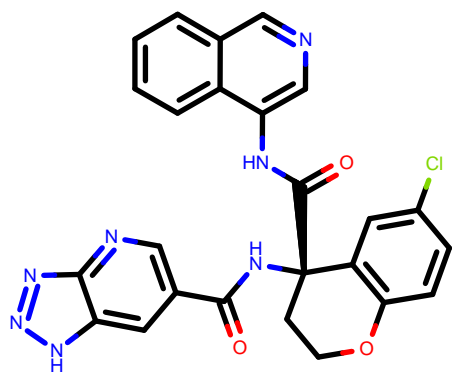
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC[C@@]3(O)5)CCOC6

RUN: RUN2768

DDG (kcal/mol): -3.97

dDDG (kcal/mol): 0.26

EN300-124555_1_1_1



CID: EN300-124555_1_1_1

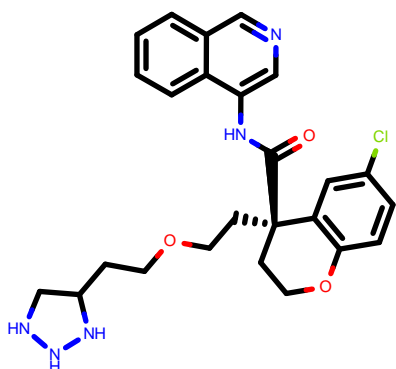
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(nc5)n[nH]n6

RUN: RUN2829

DDG (kcal/mol): -3.94

dDDG (kcal/mol): 0.22

EN300-222357_3_1_1



CID: EN300-222357_3_1_1

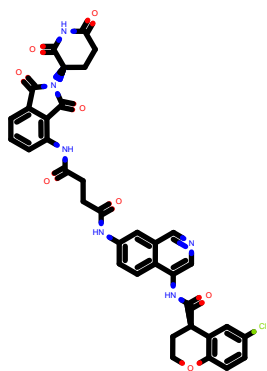
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5cn[nH]n5

RUN: RUN2719

DDG (kcal/mol): -3.93

dDDG (kcal/mol): 0.27

DAR-DIA-9e4459de-15_4



CID: DAR-DIA-9e4459de-15_4

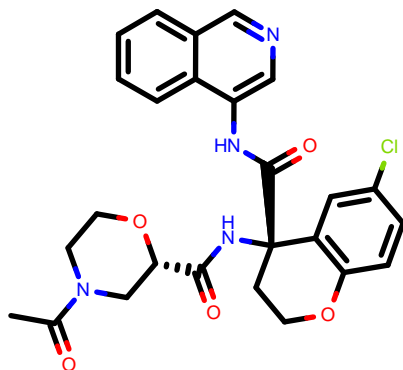
SMILES: c1cc2c(c1)NC(=O)CCCl(=O)Nc3ccc4c(c3)ncnc4NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)c5c[nH]n5C(=O)[C@@]6(C)CCCl(=O)NC7=O)O

RUN: RUN1321

DDG (kcal/mol): -3.93

dDDG (kcal/mol): 0.36

EN300-100689_1_1_1



CID: EN300-100689_1_1_1

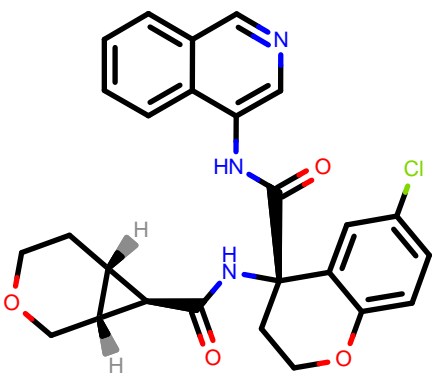
SMILES: CC(=O)N1CCO[C@@]2(C)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN2763

DDG (kcal/mol): -3.90

dDDG (kcal/mol): 0.25

EN300-1644723_1_5_1



CID: EN300-1644723_1_5_1

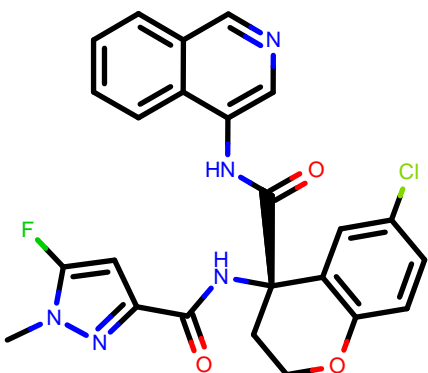
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3[C@@]4COC(=O)C1N(C1)C@H5[C@@H]6[C@@H]COC65

RUN: RUN2832

DDG (kcal/mol): -3.87

dDDG (kcal/mol): 0.22

EN300-243465_1_1_1



CID: EN300-243465_1_1_1

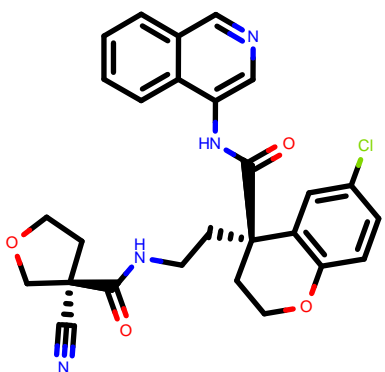
SMILES: Cn1c(cc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)F

RUN: RUN2753

DDG (kcal/mol): -3.77

dDDG (kcal/mol): 0.21

EN300-261210_3_1_1



CID: EN300-261210_3_1_1

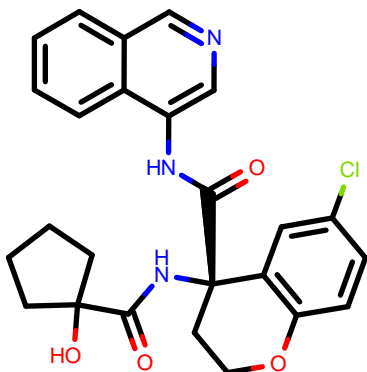
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3[C@@]4COC(=O)C1N(C1)CCNC(=O)[C@@]5[C@@]6COC65)C#N

RUN: RUN4146

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.32

EN300-25960_1_1_1



CID: EN300-25960_1_1_1

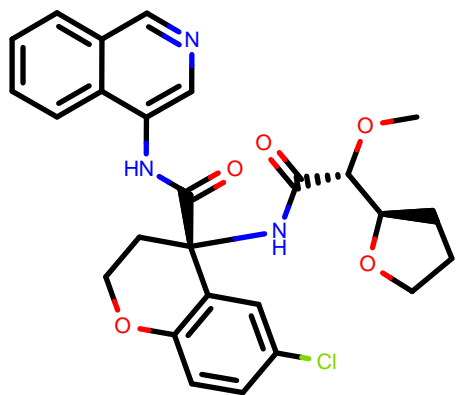
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3[C@@]4COC(=O)C1N(C1)C(=O)C5(CCCC5)O

RUN: RUN3171

DDG (kcal/mol): -3.73

dDDG (kcal/mol): 0.36

EN300-6277108_1_4_1



CID: EN300-6277108_1_4_1

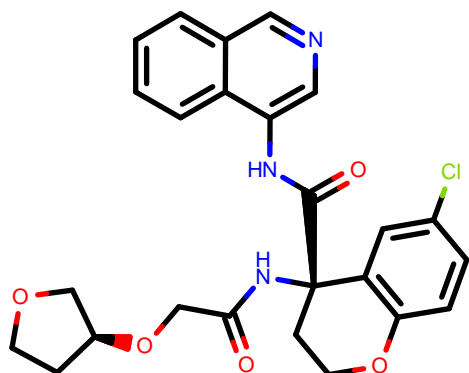
SMILES: CO[C@H]([C@H]1CCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3230

DDG (kcal/mol): -3.71

dDDG (kcal/mol): 0.25

EN300-99391_1_2_1



CID: EN300-99391_1_2_1

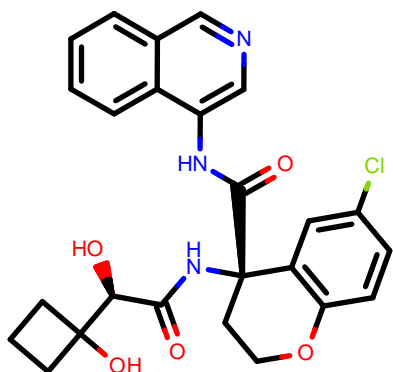
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@H]5CCOC5

RUN: RUN2870

DDG (kcal/mol): -3.68

dDDG (kcal/mol): 0.21

EDJ-MED-6864a934-10_1



CID: EDJ-MED-6864a934-10_1

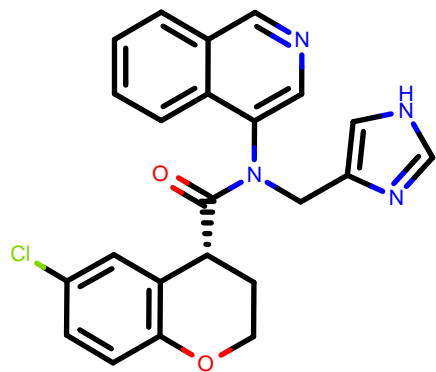
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5(CCC5)O

RUN: RUN2454

DDG (kcal/mol): -3.67

dDDG (kcal/mol): 0.25

ALP-UNI-44c99a80-2_1_1



CID: ALP-UNI-44c99a80-2_1_1

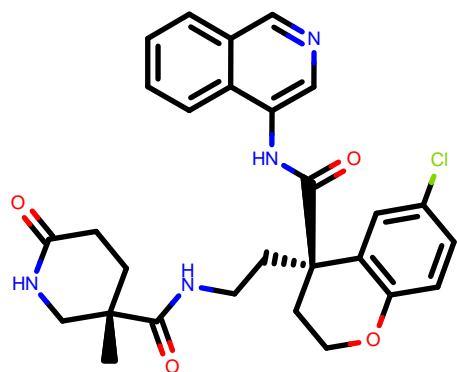
SMILES: c1ccc2c(c1)ncnc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN: RUN2949

DDG (kcal/mol): -3.66

dDDG (kcal/mol): 0.19

EN300-195924_3_1_1



CID: EN300-195924_3_1_1

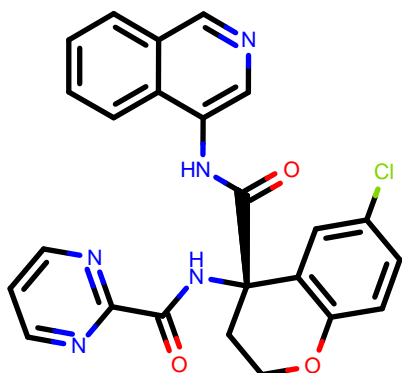
SMILES: C[C@@]1(CCC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN4401

DDG (kcal/mol): -3.66

dDDG (kcal/mol): 0.29

EN300-80230_1_1_1



CID: EN300-80230_1_1_1

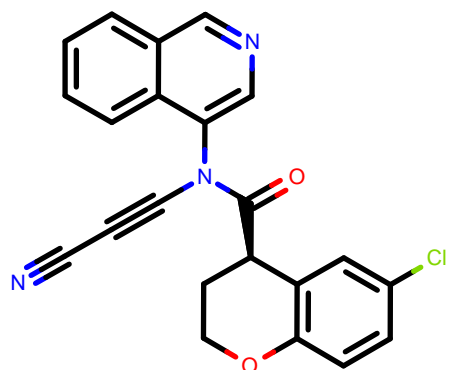
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccc5

RUN: RUN3124

DDG (kcal/mol): -3.65

dDDG (kcal/mol): 0.20

DAR-DIA-5ff57136-10_1_1



CID: DAR-DIA-5ff57136-10_1_1

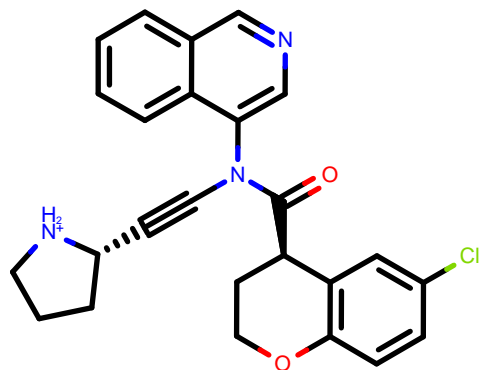
SMILES: c1ccc2c(c1)cnc2N(C#CC#N)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN2801

DDG (kcal/mol): -3.64

dDDG (kcal/mol): 0.13

DAR-DIA-5ff57136-12_1



CID: DAR-DIA-5ff57136-12_1

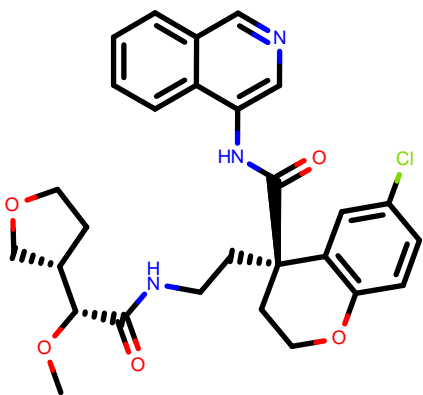
SMILES: c1ccc2c(c1)cnc2N(C#C[C@@H]3CC[C@H]3)C(=O)[C@@H]4CCOc5c4ccc(cc5)Cl

RUN: RUN1270

DDG (kcal/mol): -3.63

dDDG (kcal/mol): 0.20

EN300-298552_3_4_1



CID: EN300-298552_3_4_1

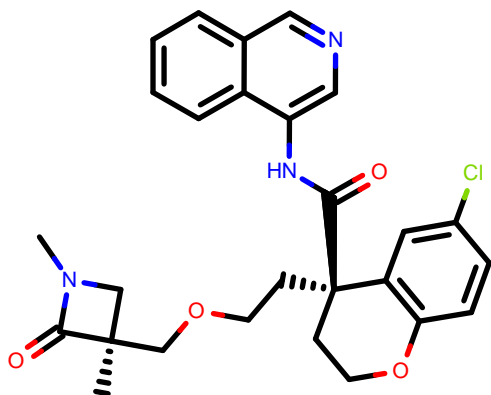
SMILES: CO[C@H]([C@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccoc5

RUN: RUN5290

DDG (kcal/mol): -3.63

dDDG (kcal/mol): 0.23

EN300-1273362_3_2_1



CID: EN300-1273362_3_2_1

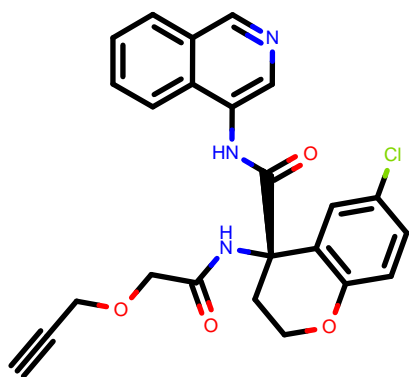
SMILES: C[C@]1(CN(C1=O)C)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccoc5

RUN: RUN2779

DDG (kcal/mol): -3.62

dDDG (kcal/mol): 0.37

EN300-106432_1_1_1



CID: EN300-106432_1_1_1

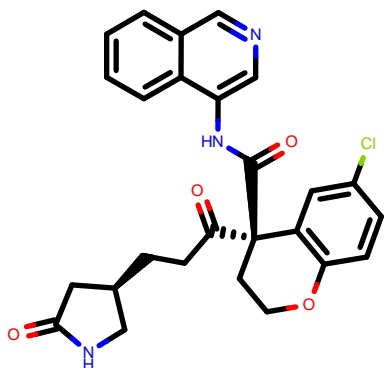
SMILES: C#CCOCC(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nc4c3ccoc4

RUN: RUN4022

DDG (kcal/mol): -3.60

dDDG (kcal/mol): 0.19

VLA-UCB-34f3ed0c-21_1



CID: VLA-UCB-34f3ed0c-21_1

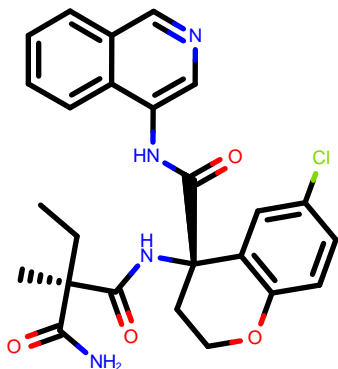
SMILES: c1cc2c(c1)nc2NC(=O)[C@]3(CCOc4c3cc(cc4)C)C(=O)CC[C@]4H5CC(=O)NCS

RUN: RUN589

DDG (kcal/mol): -3.60

dDDG (kcal/mol): 0.35

EN300-2908024_1_2_1



CID: EN300-2908024_1_2_1

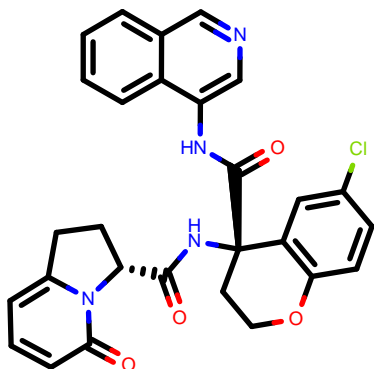
SMILES: CC(C@H)(C(=O)N)C(=O)N[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN3388

DDG (kcal/mol): -3.59

dDDG (kcal/mol): 0.31

EN300-332002_1_2_1



CID: EN300-332002_1_2_1

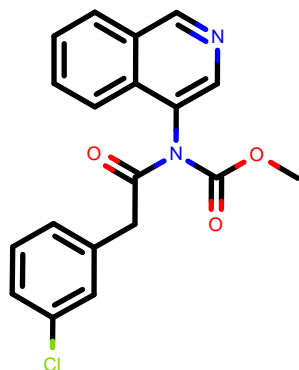
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCc6n5c(=O)ccc6

RUN: RUN2761

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.33

PET-UNK-12d8d43f-2_1



CID: PET-UNK-12d8d43f-2_1

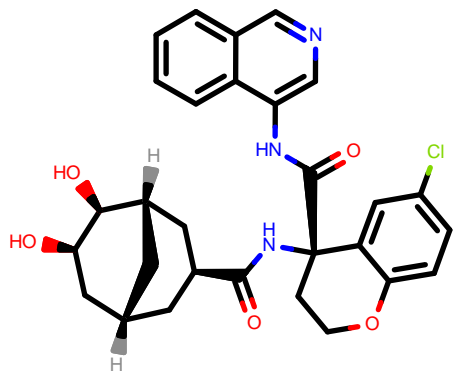
SMILES: COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl

RUN: RUN1313

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.26

EN300-6487755_1_1_1



CID: EN300-6487755_1_1_1

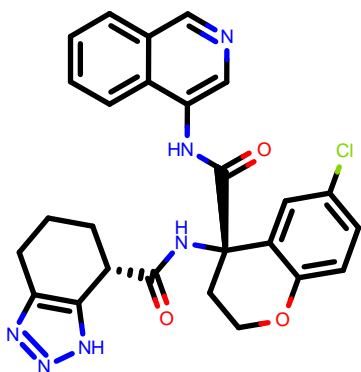
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H]6[C@@H](C5)C[C@@H]6(C5)O

RUN: RUN3399

DDG (kcal/mol): -3.56

dDDG (kcal/mol): 0.29

EDJ-MED-6864a934-6_1



CID: EDJ-MED-6864a934-6_1

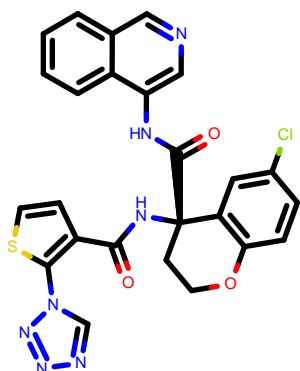
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCOc6c5n[nH]n6

RUN: RUN2440

DDG (kcal/mol): -3.55

dDDG (kcal/mol): 0.31

EN300-6744029_1_1_1



CID: EN300-6744029_1_1_1

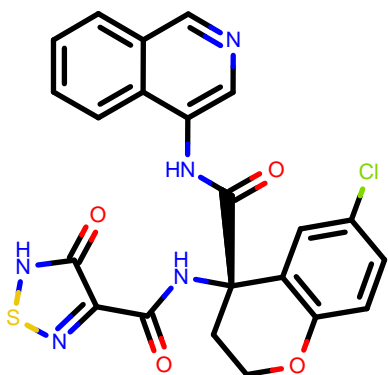
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc5n6nnn6

RUN: RUN2735

DDG (kcal/mol): -3.54

dDDG (kcal/mol): 0.26

EN300-261859_1_1_1



CID: EN300-261859_1_1_1

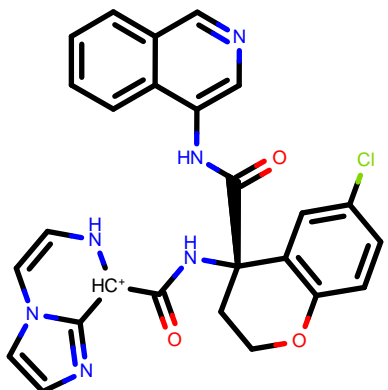
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(=O)[nH]sn5

RUN: RUN2804

DDG (kcal/mol): -3.53

dDDG (kcal/mol): 0.20

EDJ-MED-6864a934-4_1



CID: EDJ-MED-6864a934-4_1

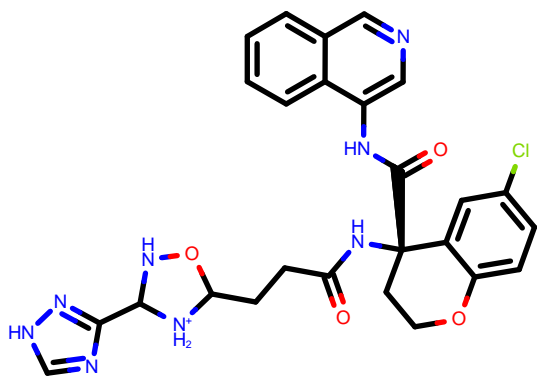
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6nccn6ccn5

RUN: RUN2448

DDG (kcal/mol): -3.51

dDDG (kcal/mol): 0.24

EN300-61140_1_1_1



CID: EN300-61140_1_1_1

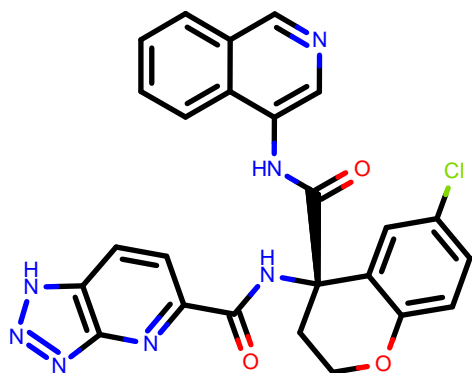
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5nc(nc5)c6[nH]n6

RUN: RUN4161

DDG (kcal/mol): -3.47

dDDG (kcal/mol): 0.26

EN300-133058_1_1_1



CID: EN300-133058_1_1_1

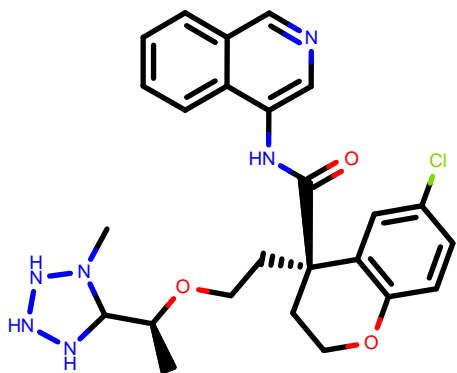
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)[nH]n6

RUN: RUN2918

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.21

EN300-173006_3_1_1



CID: EN300-173006_3_1_1

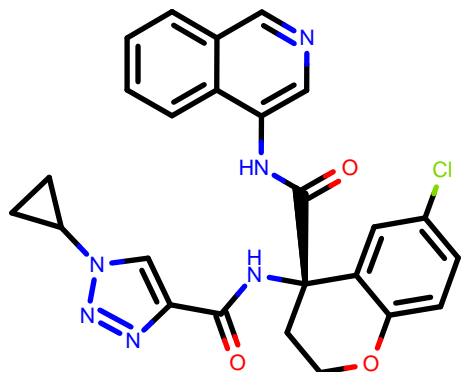
SMILES: C[C@@H](c1nncn1C)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3655

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.24

EN300-210110_1_1_1



CID: EN300-210110_1_1_1

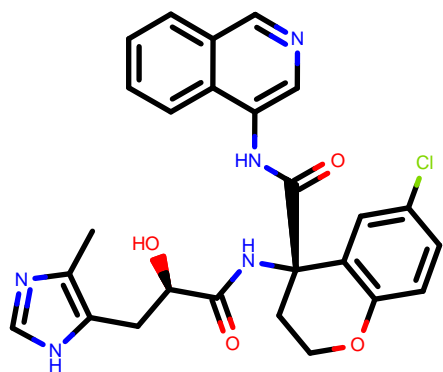
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nc5)n6C6C6

RUN: RUN5972

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.23

EN300-7494324_1_2_1



CID: EN300-7494324_1_2_1

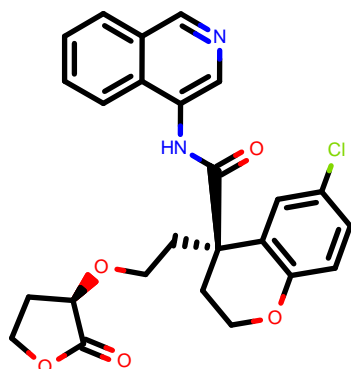
SMILES: Cc1c(nc[nH]1)C[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)O

RUN: RUN4567

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.25

EN300-20496_3_1_1



CID: EN300-20496_3_1_1

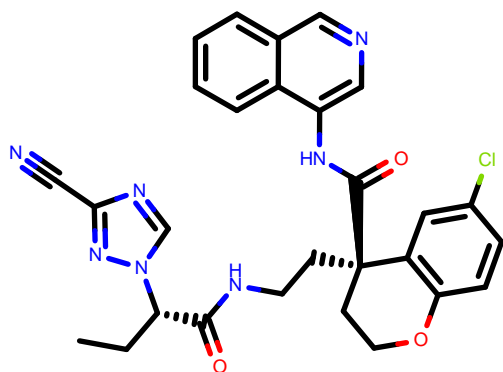
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCOC5=O

RUN: RUN2834

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.22

EN300-245264_3_1_1



CID: EN300-245264_3_1_1

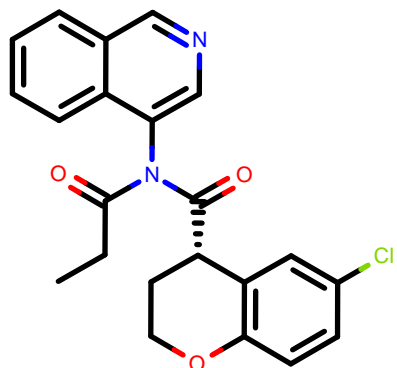
SMILES: CC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)n5nc(n5)C#N

RUN: RUN4065

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.34

VLA-UCB-05e51b3f-10_1



CID: VLA-UCB-05e51b3f-10_1

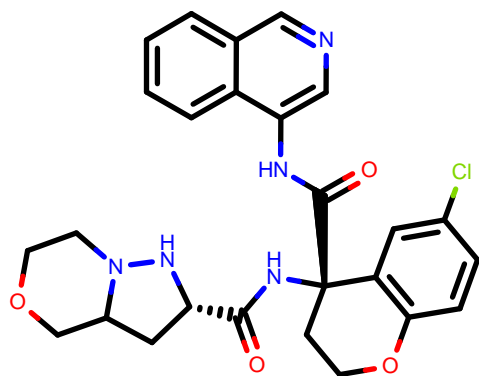
SMILES: C=CC(=O)N(c1cnc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN260

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.34

EN300-244278_1_1_1



CID: EN300-244278_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](COCc3cc(ccc3)C)N(C=O)[C@@H](C)C5CCOCCN5

RUN:

RUN2961

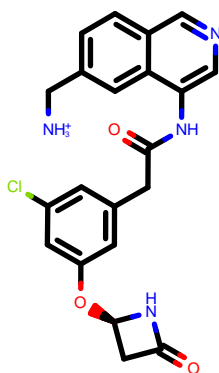
DDG (kcal/mol):

-3.42

dDDG (kcal/mol):

0.34

ALF-EVA-0b412456-5_1



CID: ALF-EVA-0b412456-5_1

SMILES:

c1cc2cnc(c2cc1C[NH3+])NC(=O)[C@@H](COCc3cc(ccc3)C)O[C@@H](C)C(=O)N4

RUN:

RUN2582

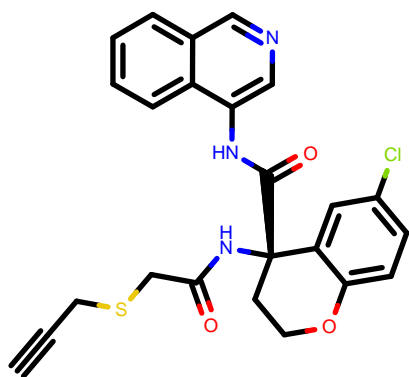
DDG (kcal/mol):

-3.41

dDDG (kcal/mol):

0.59

EN300-86878_1_1_1



CID: EN300-86878_1_1_1

SMILES:

C#CCSCC(=O)N[C@@H]1(COCc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccccc4

RUN:

RUN2762

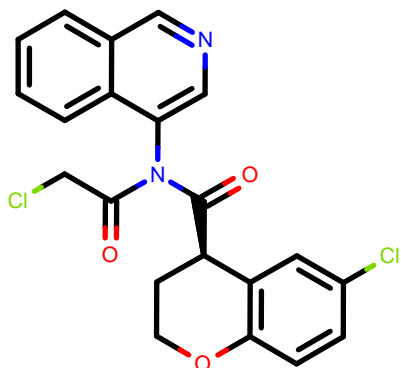
DDG (kcal/mol):

-3.39

dDDG (kcal/mol):

0.24

VLA-UCB-50c39ae8-6_1



CID: VLA-UCB-50c39ae8-6_1

SMILES:

c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H](C)C3CCOC4C3cc(c4)Cl

RUN:

RUN329

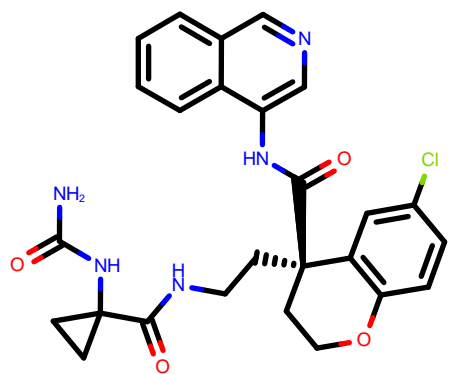
DDG (kcal/mol):

-3.38

dDDG (kcal/mol):

0.21

EN300-123614_3_1_1



CID: EN300-123614_3_1_1

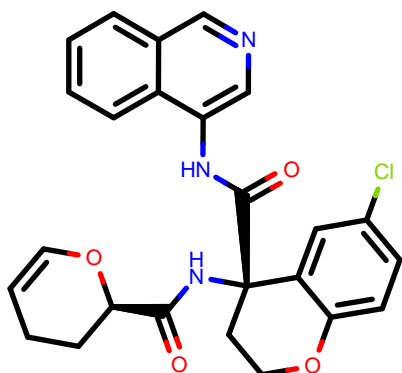
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5NC(=O)N

RUN: RUN5741

DDG (kcal/mol): -3.37

dDDG (kcal/mol): 0.31

EN300-378044_1_2_1



CID: EN300-378044_1_2_1

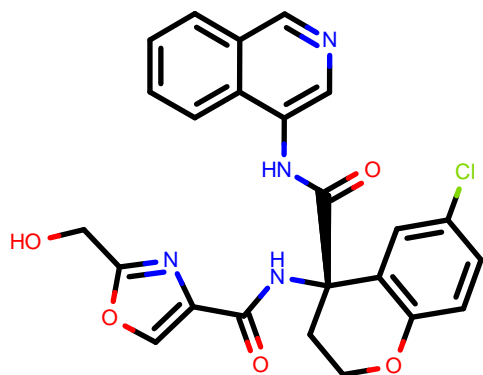
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N[C@@H]5CC=CCO5

RUN: RUN3525

DDG (kcal/mol): -3.36

dDDG (kcal/mol): 0.24

EN300-7549555_1_1_1



CID: EN300-7549555_1_1_1

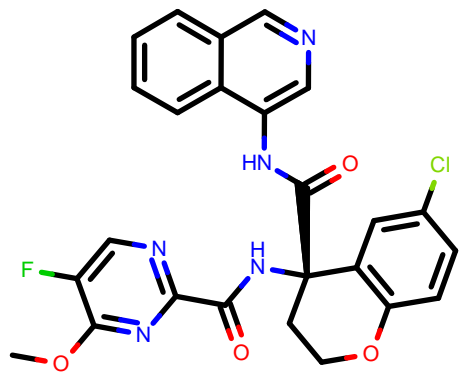
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ocnc5CO

RUN: RUN3756

DDG (kcal/mol): -3.35

dDDG (kcal/mol): 0.18

EN300-1703711_1_1_1



CID: EN300-1703711_1_1_1

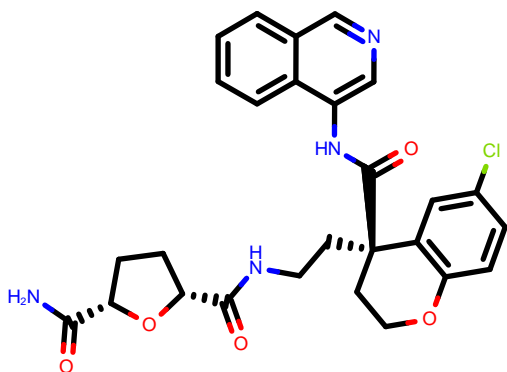
SMILES: COc1c(nc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5)F

RUN: RUN2813

DDG (kcal/mol): -3.34

dDDG (kcal/mol): 0.23

EN300-315238_3_1_1



CID: EN300-315238_3_1_1

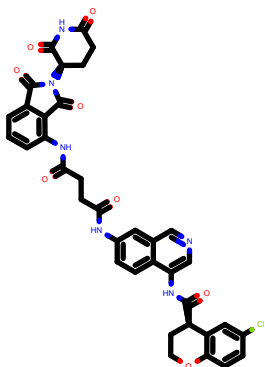
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)CCOC4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@@H](O5)Cl=O

RUN: RUN3079

DDG (kcal/mol): -3.34

dDDG (kcal/mol): 0.29

DAR-DIA-9e4459de-15_1



CID: DAR-DIA-9e4459de-15_1

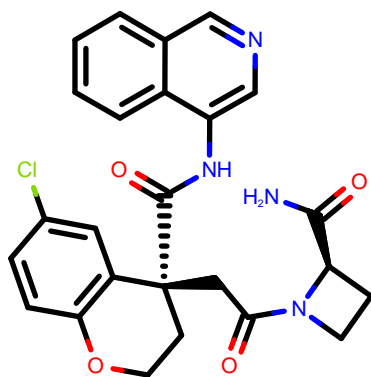
SMILES: c1cc2c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cnc4NC(=O)[C@@H](C)CCOC5c6cc(cc5)Cl)c7c(c2O)[C@@H]7CC(=O)NC7=O

RUN: RUN1382

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.26

EN300-862094_1_1_1



CID: EN300-862094_1_1_1

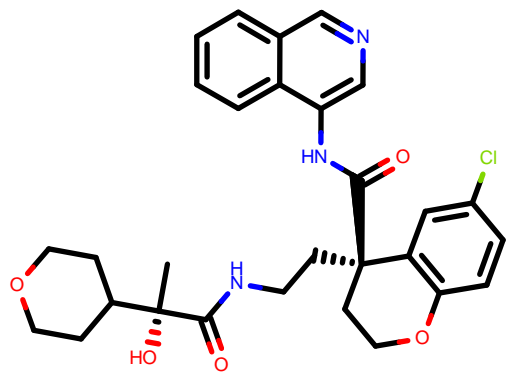
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)CCOC4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5Cl=O

RUN: RUN2836

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.26

EN300-217499_3_2_1



CID: EN300-217499_3_2_1

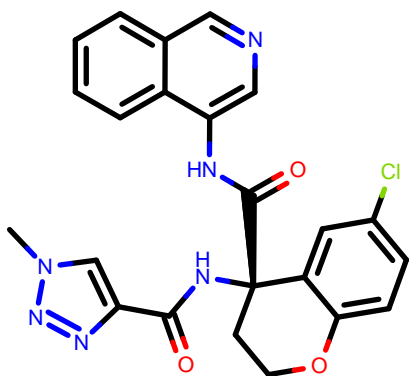
SMILES: C[C@@H](C1CCOCC1)C(=O)NCC[C@@H](C)CCOC3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5O

RUN: RUN4777

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.44

EN300-86357_1_1_1



CID: EN300-86357_1_1_1

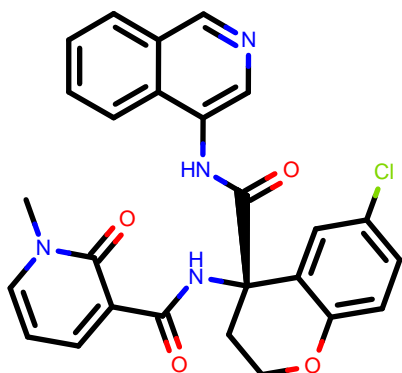
SMILES: Cn1cc(nn1)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4674

DDG (kcal/mol): -3.30

dDDG (kcal/mol): 0.22

EN300-69811_1_1_1



CID: EN300-69811_1_1_1

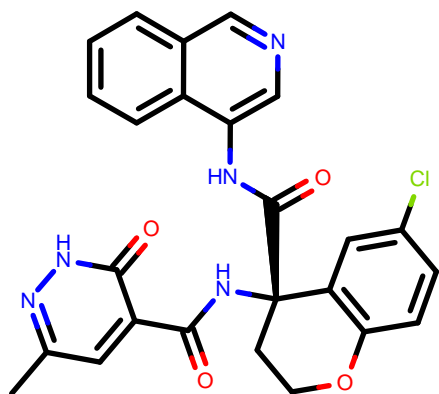
SMILES: Cn1cccc(c1=O)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3117

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.32

EN300-147499_1_1_1



CID: EN300-147499_1_1_1

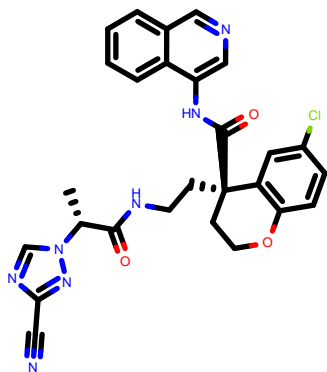
SMILES: Cc1cc(c(=O)[nH]n1)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2722

DDG (kcal/mol): -3.27

dDDG (kcal/mol): 0.26

EN300-198515_3_2_1



CID: EN300-198515_3_2_1

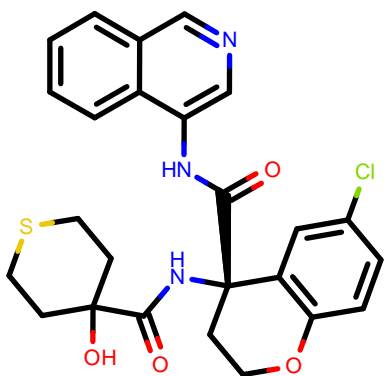
SMILES: C[C@H](C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3encc4c3cccc4)n5nc(n5)C#N

RUN: RUN3001

DDG (kcal/mol): -3.25

dDDG (kcal/mol): 0.33

EN300-122340_1_1_1



CID: EN300-122340_1_1_1

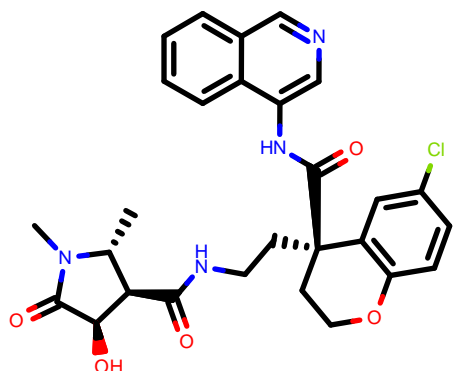
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCSC5)O

RUN: RUN2895

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.28

EN300-378828_3_1_1



CID: EN300-378828_3_1_1

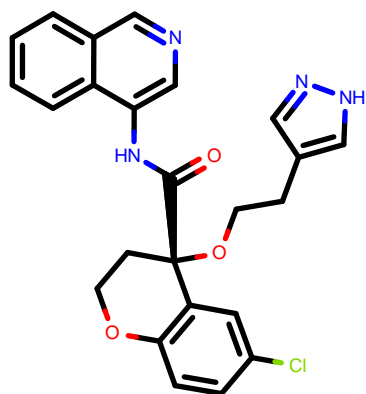
SMILES: C[C@@H]1[C@@H](C[C@@H](C1=O)N1C)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN3599

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.46

EDJ-MED-28ec730d-5_1



CID: EDJ-MED-28ec730d-5_1

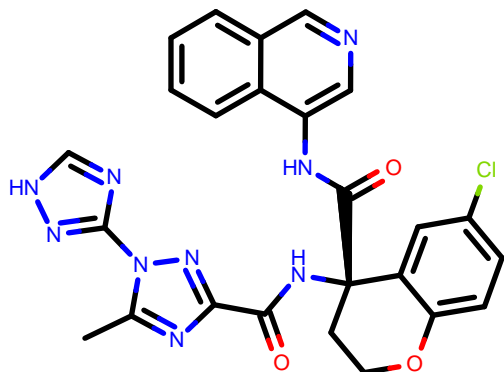
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5

RUN: RUN582

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.22

EN300-26973_1_1_1



CID: EN300-26973_1_1_1

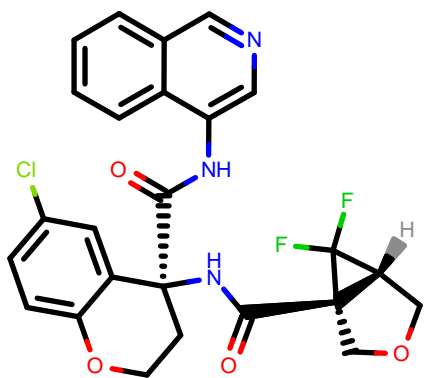
SMILES: Cc1nc(mn1c2[nH]ncn2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccc6

RUN: RUN2940

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.24

EN300-6738732_1_1_1



CID: EN300-6738732_1_1_1

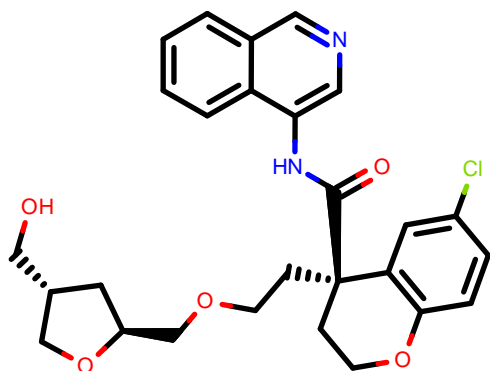
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56COC[C@H]5C6(F)F

RUN: RUN2783

DDG (kcal/mol): -3.21

dDDG (kcal/mol): 0.21

EN300-6494158_3_3_1



CID: EN300-6494158_3_3_1

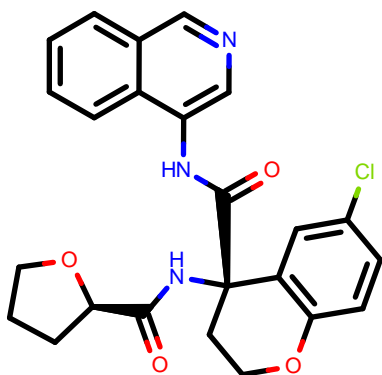
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5C[C@H](CO)5CO

RUN: RUN7125

DDG (kcal/mol): -3.20

dDDG (kcal/mol): 0.32

EN300-21009_1_2_1



CID: EN300-21009_1_2_1

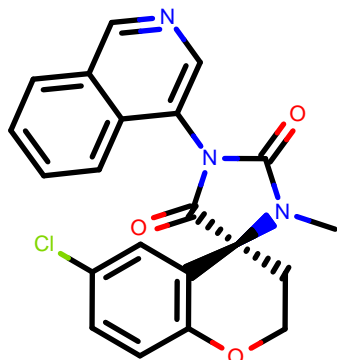
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C5COCO5

RUN: RUN3145

DDG (kcal/mol): -3.20

dDDG (kcal/mol): 0.25

BEN-BAS-c2bc0d80-7_1



CID: BEN-BAS-c2bc0d80-7_1

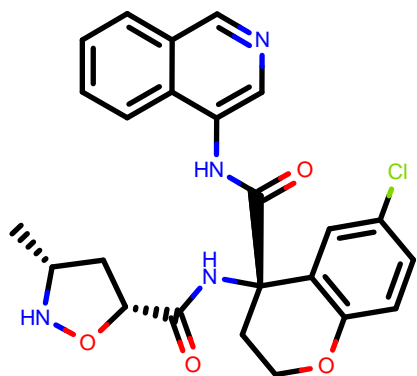
SMILES: CN1C(=O)N(C(=O)[C@@]12CCOC3c2cc(cc3)Cl)c4cnc5c4ccc5

RUN: RUN1000

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.28

EN300-92447_1_2_1



CID: EN300-92447_1_2_1

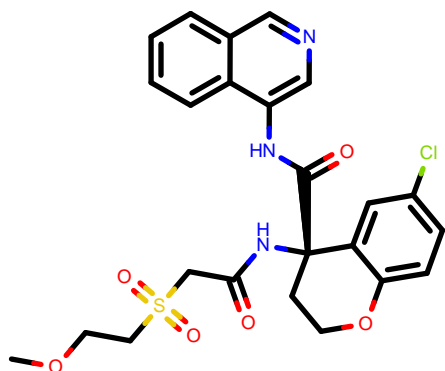
SMILES: C[C@@H]1C[C@@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3464

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.26

EN300-39501_1_1_1



CID: EN300-39501_1_1_1

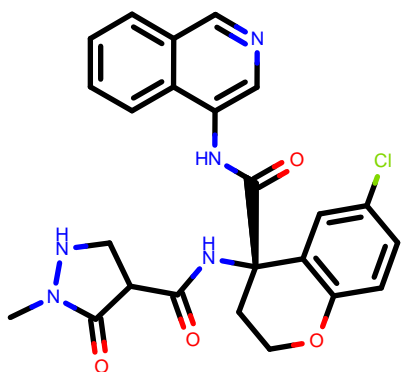
SMILES: COCCS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3300

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.41

EN300-7437779_1_1_1



CID: EN300-7437779_1_1_1

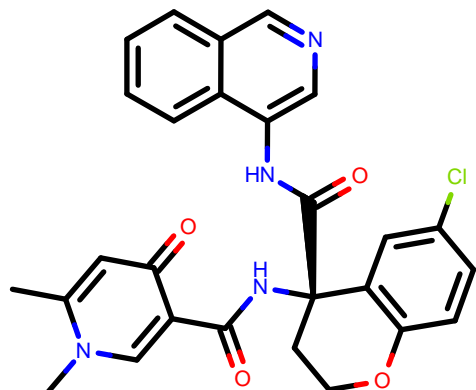
SMILES: Cn1c(=O)c(c[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2685

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.26

EN300-199991_1_1_1



CID: EN300-199991_1_1_1

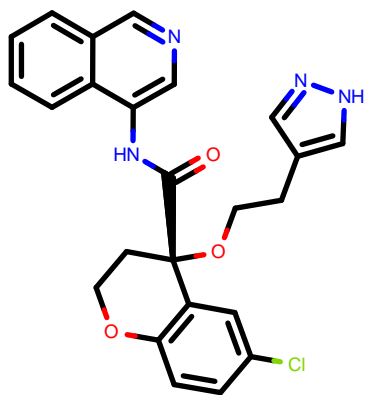
SMILES: Cc1cc(=O)c(c[n1]C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3446

DDG (kcal/mol): -3.18

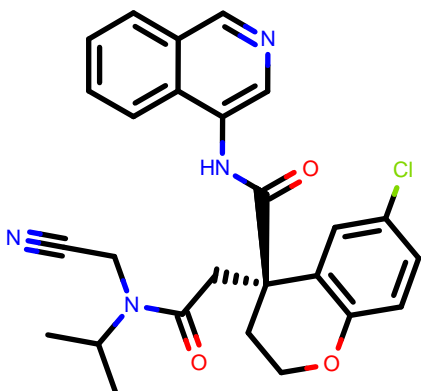
dDDG (kcal/mol): 0.32

CHO-MSK-5891c1ff-12_1



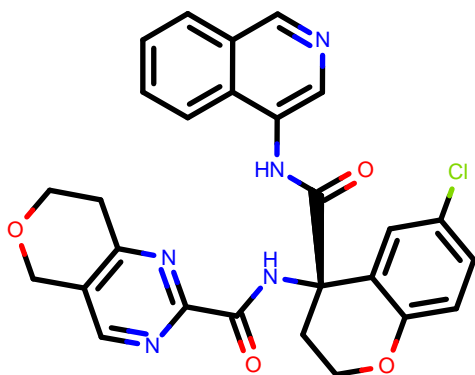
CID:	CHO-MSK-5891c1ff-12_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5</chem>
RUN:	RUN1735
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.22

EDG-MED-ba1ac7b9-6_2



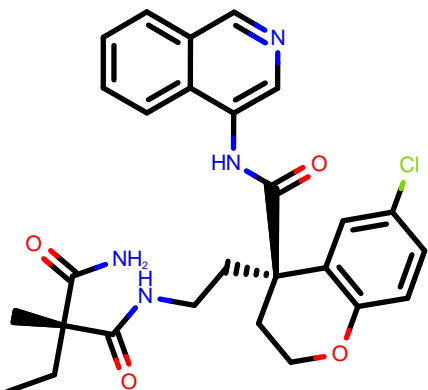
CID:	EDG-MED-ba1ac7b9-6_2
SMILES:	<chem>CC(C)N(CC#N)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN2483
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.27

EN300-7435929_1_1_1



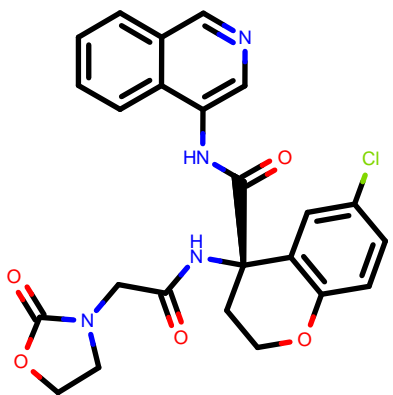
CID:	EN300-7435929_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncc6c(n5)CCO6</chem>
RUN:	RUN3106
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.27

EN300-2908024_3_2_1



CID:	EN300-2908024_3_2_1
SMILES:	<chem>CC[C@@](C)(C(=O)N)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN4298
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.29

EN300-172179_1_1_1



CID: EN300-172179_1_1_1

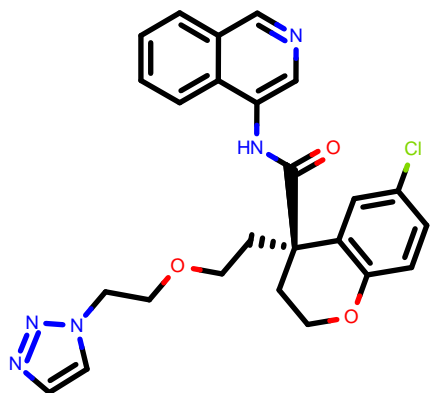
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCOC5=O

RUN: RUN3218

DDG (kcal/mol): -3.12

dDDG (kcal/mol): 0.29

EN300-1715993_3_1_1



CID: EN300-1715993_3_1_1

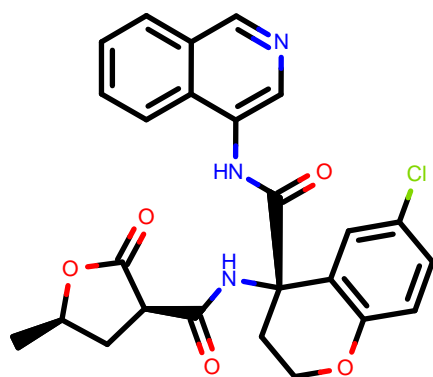
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnn5

RUN: RUN2879

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.22

EN300-7444533_1_1_1



CID: EN300-7444533_1_1_1

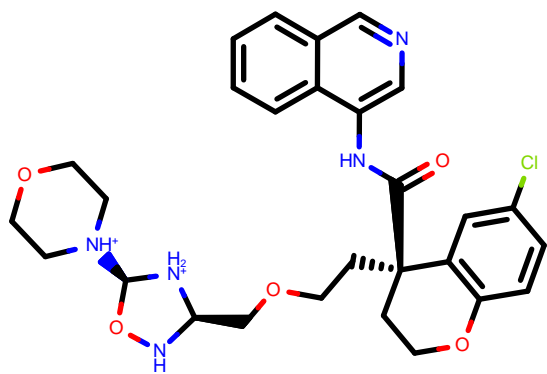
SMILES: C[C@@H]1C[C@@H](C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3936

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.27

EN300-1608590_3_1_1



CID: EN300-1608590_3_1_1

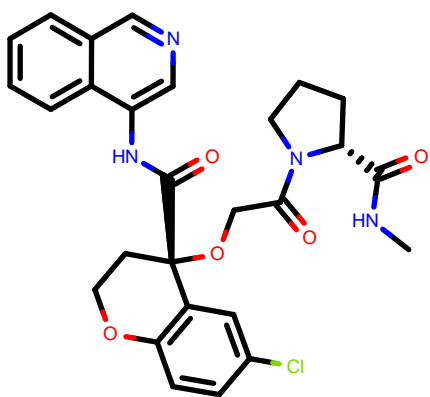
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5N[C@@H](O5)N+KCCOC6

RUN: RUN4648

DDG (kcal/mol): -3.08

dDDG (kcal/mol): 0.42

EN300-48902_1_2_1



CID: EN300-48902_1_2_1

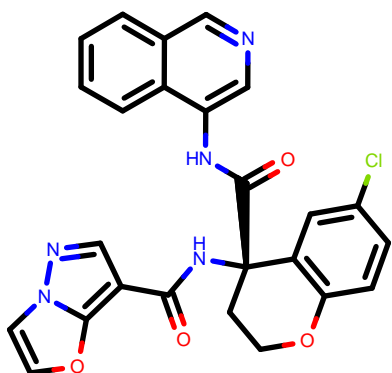
SMILES: CNC(=O)[C@H]1CCCN1C(=O)CO[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN6056

DDG (kcal/mol): -3.07

dDDG (kcal/mol): 0.34

EN300-303519_1_1_1



CID: EN300-303519_1_1_1

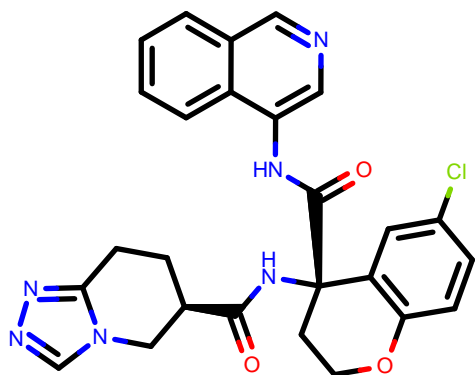
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5nnc6c5OCC6

RUN: RUN3842

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.20

EN300-51350_1_1_1



CID: EN300-51350_1_1_1

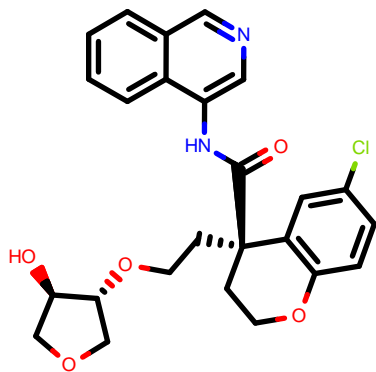
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@]5COC6nncn6C5

RUN: RUN3377

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.31

EN300-331828_3_1_1



CID: EN300-331828_3_1_1

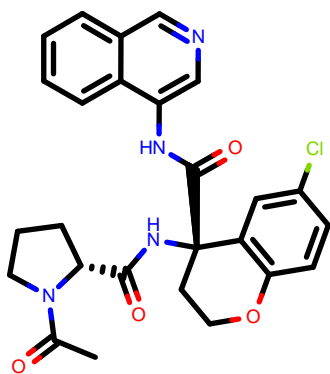
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCO[C@@]5COC[C@H]5O

RUN: RUN4515

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.25

EN300-12587_1_1_1



CID: EN300-12587_1_1_1

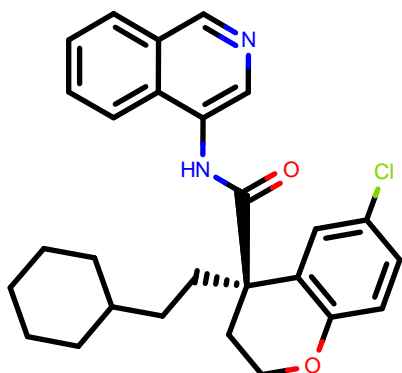
SMILES: CC(=O)N1CCC[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN2785

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.34

VLA-UCB-50c39ae8-10_1



CID: VLA-UCB-50c39ae8-10_1

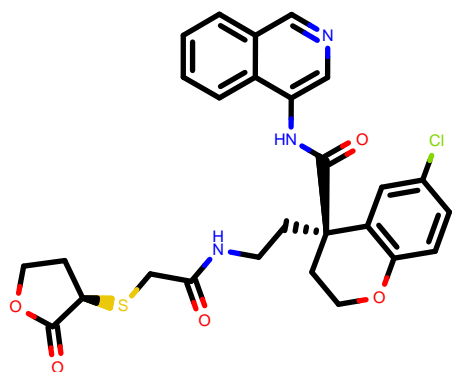
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCC5CCCC5

RUN: RUN315

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.26

EN300-113218_3_1_1



CID: EN300-113218_3_1_1

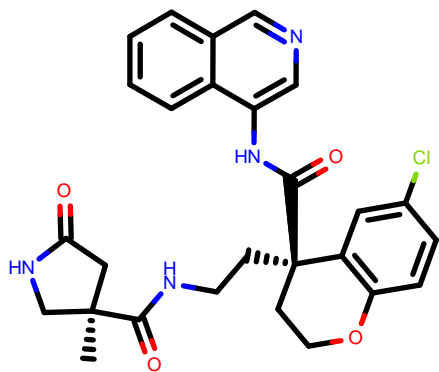
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5COC(=O)5=O

RUN: RUN3263

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.36

EN300-132157_3_2_1



CID: EN300-132157_3_2_1

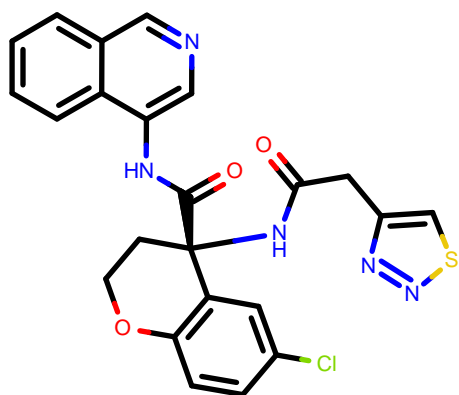
SMILES: C[C@]1(CC(=O)NC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN4724

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.34

EN300-300519_1_1_1



CID: EN300-300519_1_1_1

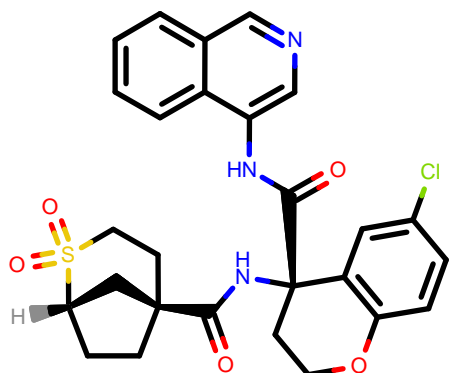
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5csnn5

RUN: RUN3407

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.20

EN300-6503702_1_1_1



CID: EN300-6503702_1_1_1

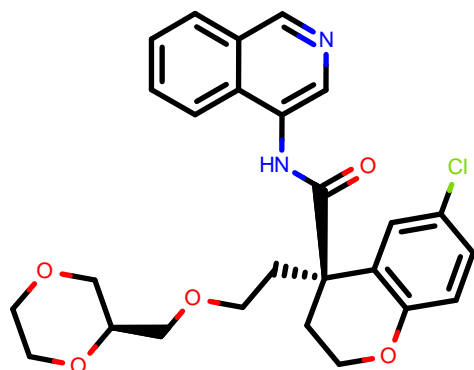
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5=CC(=O)N(S(=O)(=O)C)C5

RUN: RUN5125

DDG (kcal/mol): -3.03

dDDG (kcal/mol): 0.31

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

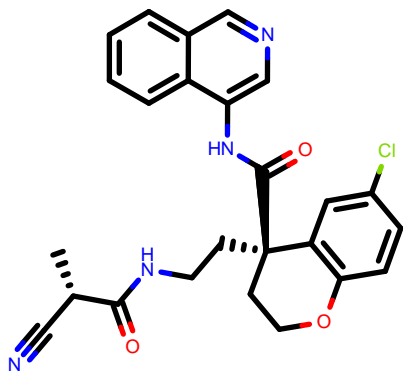
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(O)COC5

RUN: RUN3916

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.27

EN300-72730_3_1_1



CID: EN300-72730_3_1_1

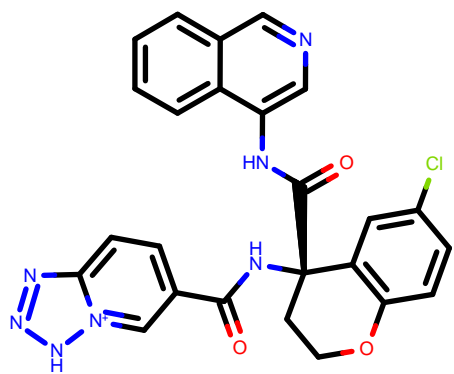
SMILES: C[C@@]5(O)COC5C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN3703

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.22

EN300-102853_1_1_1



CID: EN300-102853_1_1_1

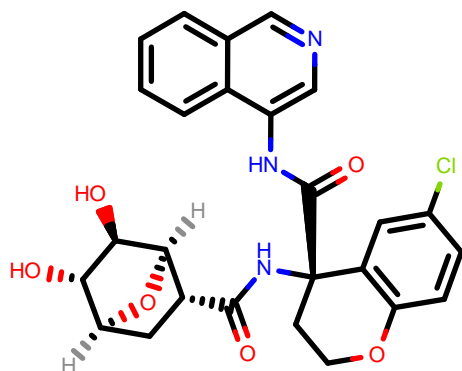
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)NC(=O)c5ccc6n[n-]1[n+]6c5

RUN: RUN3863

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.22

EN300-6764836_1_5_1



CID: EN300-6764836_1_5_1

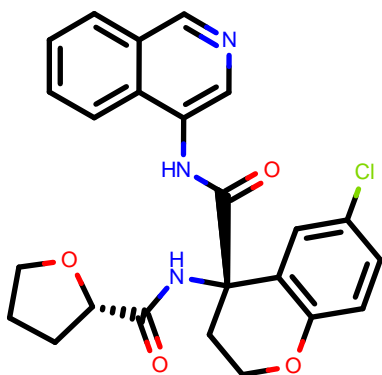
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@H]6[C@@H]([C@H]5)C6O

RUN: RUN2755

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.27

EN300-104395_1_1_1



CID: EN300-104395_1_1_1

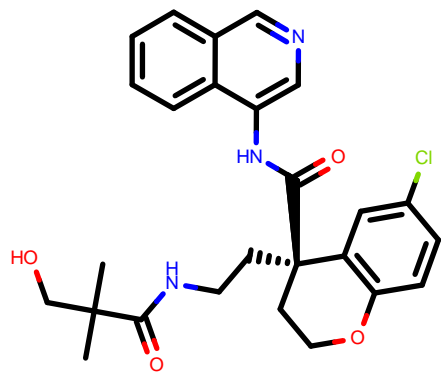
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCO5

RUN: RUN2897

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.22

EN300-65050_3_1_1



CID: EN300-65050_3_1_1

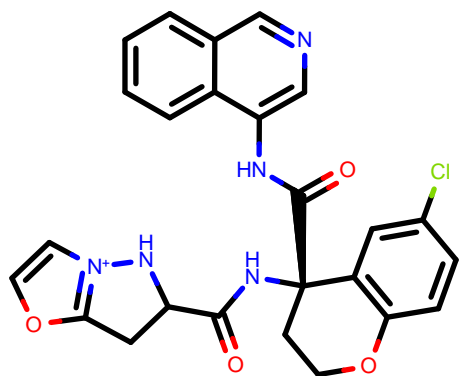
SMILES: CC(C)(CO)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN3707

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.26

EN300-181688_1_1_1



CID: EN300-181688_1_1_1

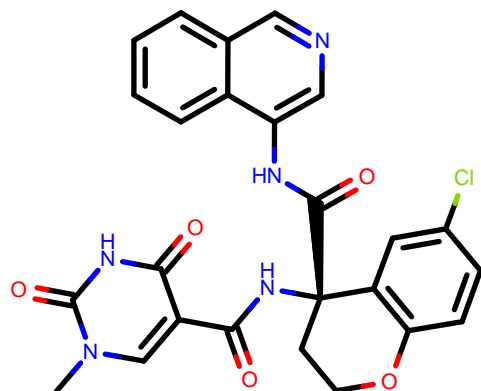
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6n(n5)CCO6

RUN: RUN2937

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.22

EN300-37123_1_1_1



CID: EN300-37123_1_1_1

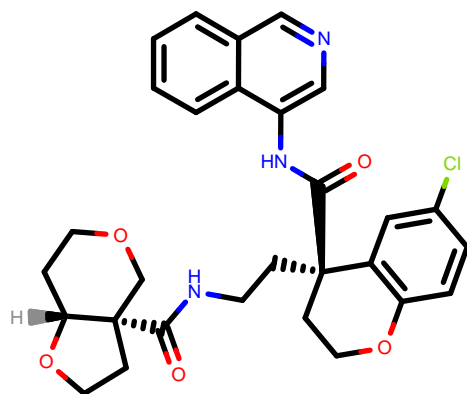
SMILES: Cn1cc(c(=O)[nH]c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN3579

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.30

EN300-341337_3_2_1



CID: EN300-341337_3_2_1

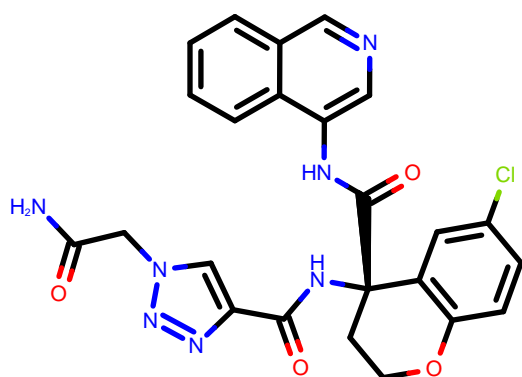
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]56CCO[C@@]5H56COO6

RUN: RUN4909

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.38

EN300-52380_1_1_1



CID: EN300-52380_1_1_1

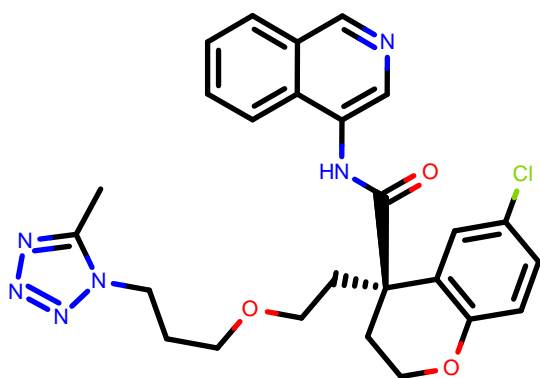
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn(nn5)CC(=O)N

RUN: RUN3402

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.26

EN300-197715_3_1_1



CID: EN300-197715_3_1_1

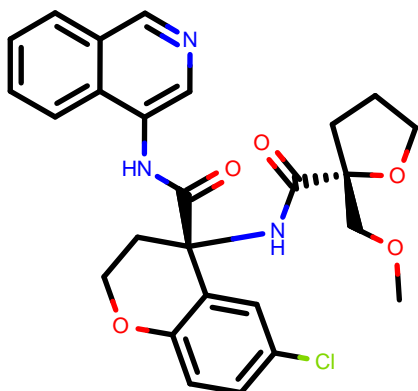
SMILES: Cc1nnnn1CCCOC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2860

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.33

EN300-1301381_1_2_1



CID: EN300-1301381_1_2_1

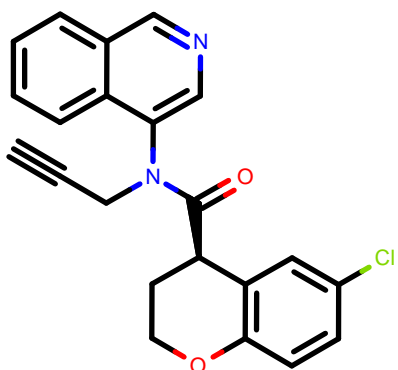
SMILES: COC[C@]1(CCCO1)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3062

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.27

DAR-DIA-5ff57136-13_1_1



CID: DAR-DIA-5ff57136-13_1_1

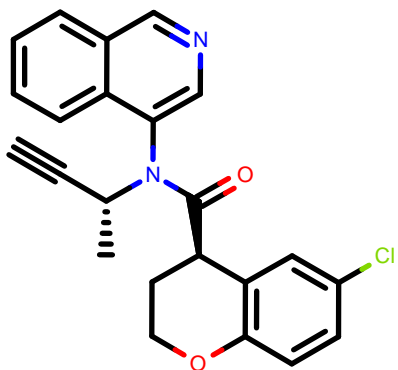
SMILES: C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2998

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.13

DAR-DIA-5ff57136-16_2_1



CID: DAR-DIA-5ff57136-16_2_1

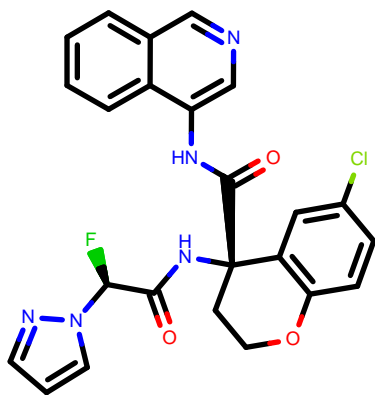
SMILES: C[C@H](C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN4314

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.14

EN300-1726277_1_1_1



CID: EN300-1726277_1_1_1

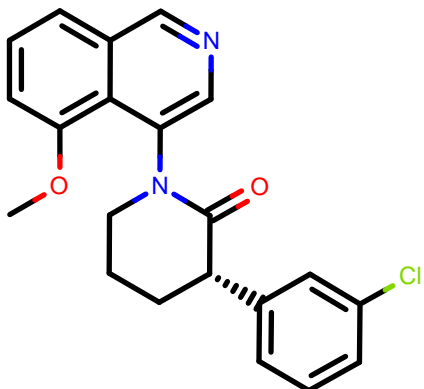
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](n5cccn5)F

RUN: RUN3606

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.20

MIC-UNK-50cce87d-12_2



CID: MIC-UNK-50cce87d-12_2

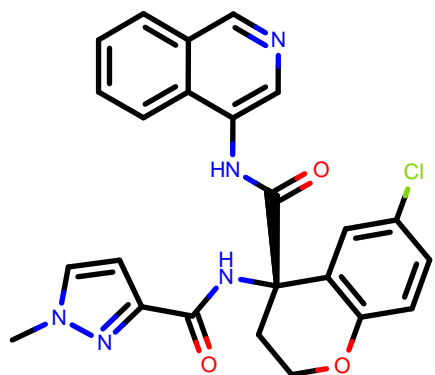
SMILES: COc1ccc2c1c(cnc2)N3CCCC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN556

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.32

EN300-66976_1_1_1



CID: EN300-66976_1_1_1

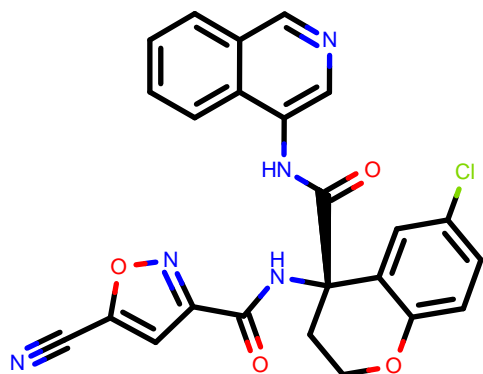
SMILES: Cn1ccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN2809

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.21

EN300-1178005_1_1_1



CID: EN300-1178005_1_1_1

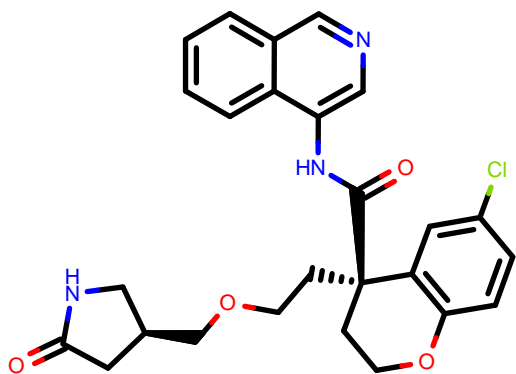
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(oc5)C#N

RUN: RUN3118

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.23

EN300-246747_3_2_1



CID: EN300-246747_3_2_1

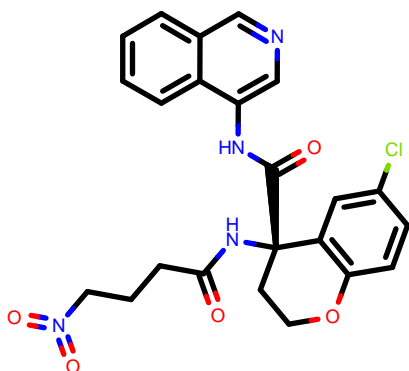
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5CC(=O)NCS

RUN: RUN3844

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.28

EN300-143449_1_1_1



CID: EN300-143449_1_1_1

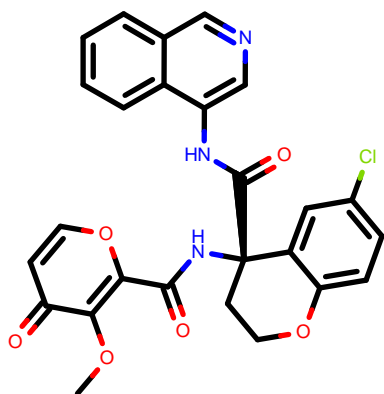
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCN(=O)=O

RUN: RUN3645

DDG (kcal/mol): -2.95

dDDG (kcal/mol): 0.21

EN300-7465954_1_1_1



CID: EN300-7465954_1_1_1

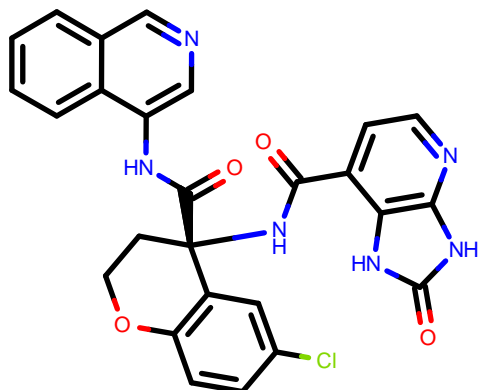
SMILES: COc1c(O)cccc1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3744

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.25

EN300-189901_1_1_1



CID: EN300-189901_1_1_1

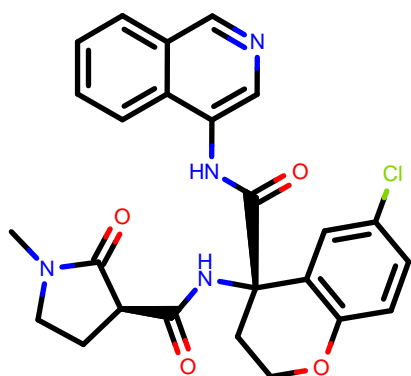
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc6c5[nH]c1=O[nH]6

RUN: RUN2758

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.24

EN300-141695_1_1_1



CID: EN300-141695_1_1_1

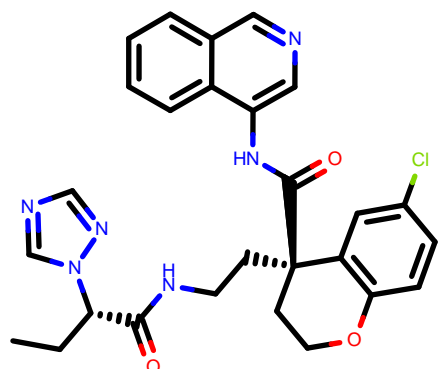
SMILES: CN1CC[C@@H](C1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2815

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.26

EN300-651307_3_1_1



CID: EN300-651307_3_1_1

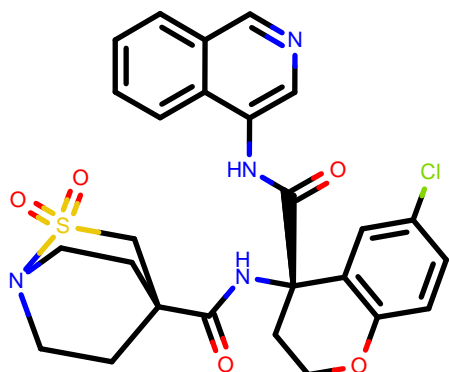
SMILES: CC[C@@H](C1=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncnc4c3ccoc4)n5cncn5

RUN: RUN3173

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.27

EN300-6731334_1_1_1



CID: EN300-6731334_1_1_1

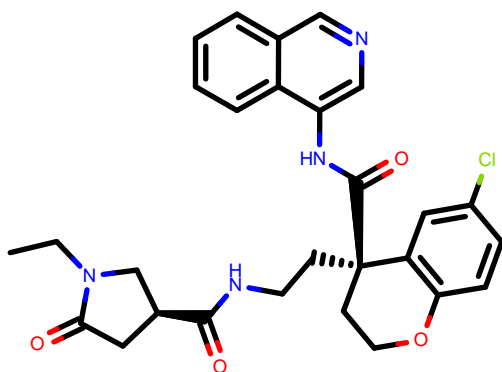
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C56CCN(CC5)S(=O)(=O)C6

RUN: RUN2780

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.36

EN300-33478_3_2_1



CID: EN300-33478_3_2_1

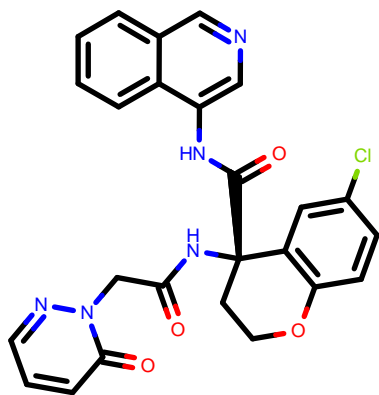
SMILES: CCN1C[C@@H](CC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4628

DDG (kcal/mol): -2.92

dDDG (kcal/mol): 0.44

EN300-237561_1_1_1



CID: EN300-237561_1_1_1

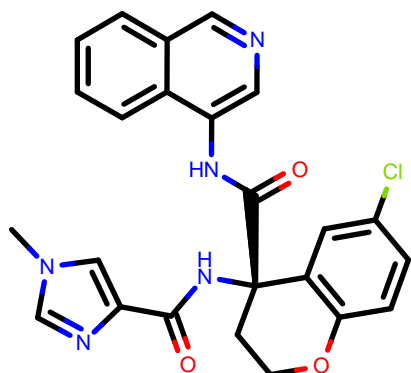
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c(=O)ccn5

RUN: RUN3129

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.33

EN300-97847_1_1_1



CID: EN300-97847_1_1_1

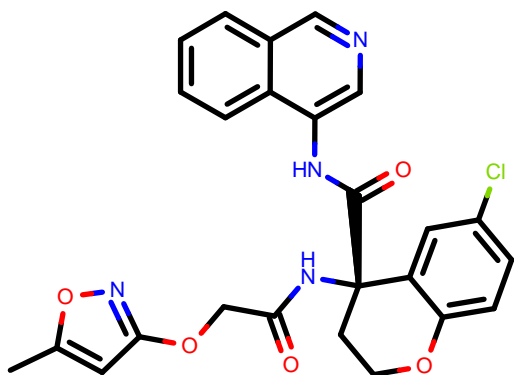
SMILES: Cn1cc(nc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc(=O)c5ccccc5

RUN: RUN3059

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.21

EN300-12929_1_1_1



CID: EN300-12929_1_1_1

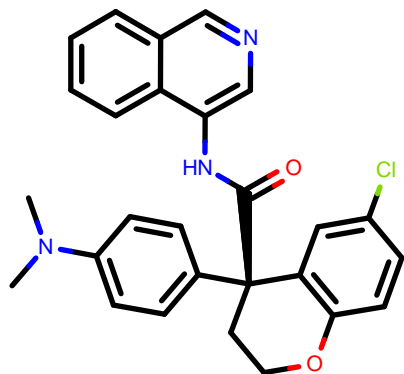
SMILES: Cc1cc(no1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc(=O)c5ccccc5

RUN: RUN3696

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.26

VLA-UCB-551c2366-1_1



CID: VLA-UCB-551c2366-1_1

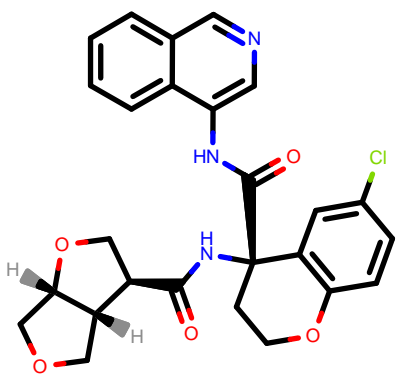
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc(=O)c5ccccc5

RUN: RUN995

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.20

EN300-6482296_1_5_1



CID: EN300-6482296_1_5_1

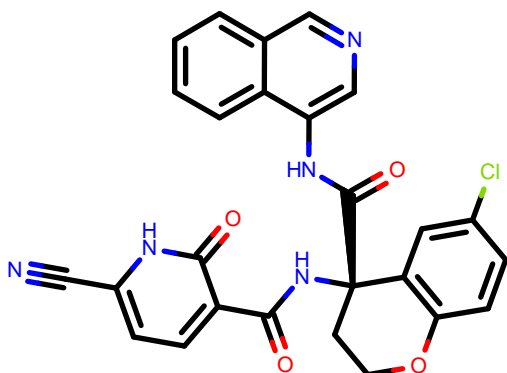
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)N(C=O)C@@H5CO[C@@H]5COC6

RUN: RUN3499

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.26

EN300-640698_1_1_1



CID: EN300-640698_1_1_1

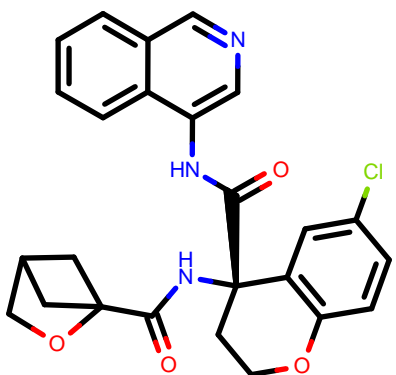
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)N(C=O)c5ccc([nH]c5=O)C#N

RUN: RUN2874

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.24

EN300-2007648_1_1_1



CID: EN300-2007648_1_1_1

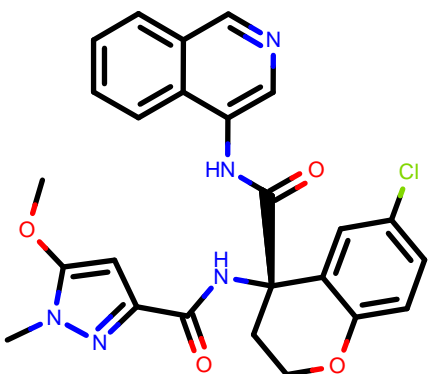
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)N(C=O)C56CC(C5)CO6

RUN: RUN2741

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.22

EN300-142240_1_1_1



CID: EN300-142240_1_1_1

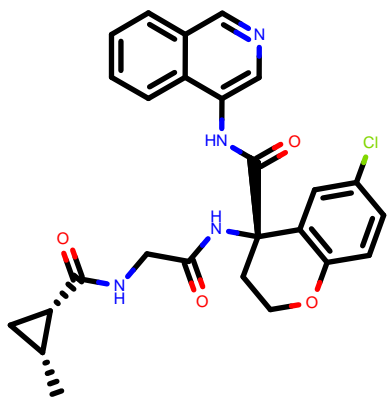
SMILES: Cn1c(cc(n1)C(=O)N)C@2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)OC

RUN: RUN2843

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.28

EN300-30768_1_1_1



CID: EN300-30768_1_1_1

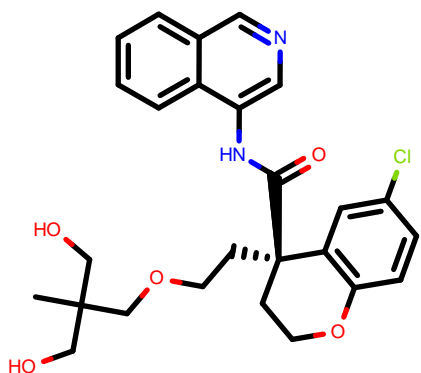
SMILES: C[C@@H]1C[C@@H]1C(=O)NCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3950

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.31

EN300-218116_3_1_1



CID: EN300-218116_3_1_1

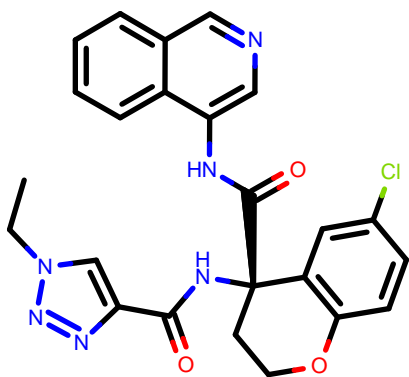
SMILES: CC(CO)(CO)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4937

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.42

EN300-262745_1_1_1



CID: EN300-262745_1_1_1

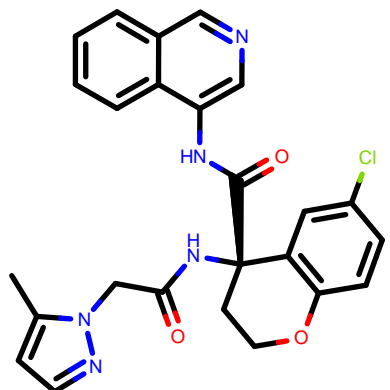
SMILES: CCn1cc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4404

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.22

EN300-83558_1_1_1



CID: EN300-83558_1_1_1

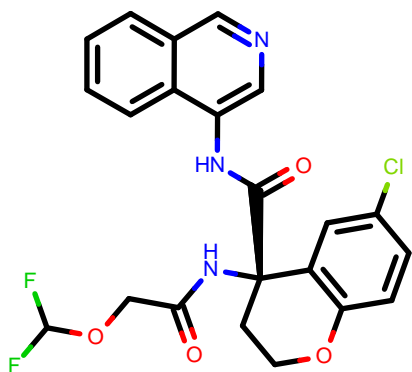
SMILES: Cc1ccnn1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3688

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.24

EN300-179091_1_1_1



CID: EN300-179091_1_1_1

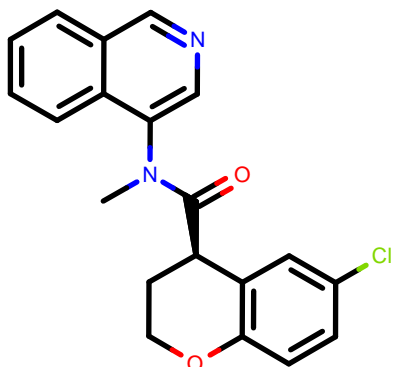
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F

RUN: RUN5288

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.18

MAK-UNK-3875bbc8-2_1_1



CID: MAK-UNK-3875bbc8-2_1_1

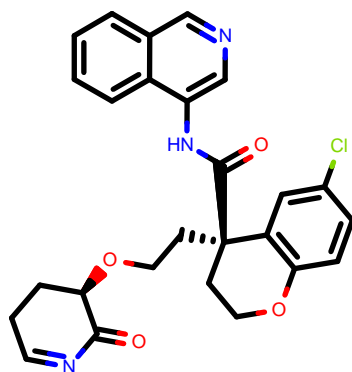
SMILES: CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN3363

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.09

EN300-107267_3_1_1



CID: EN300-107267_3_1_1

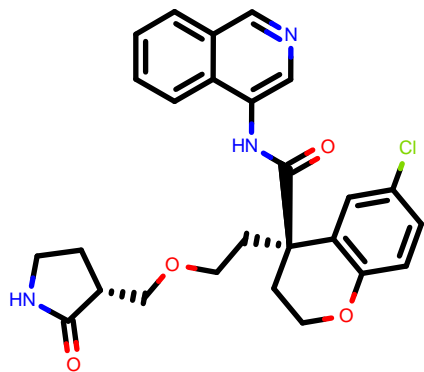
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCNC5=O

RUN: RUN3143

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.21

EN300-246248_3_2_1



CID: EN300-246248_3_2_1

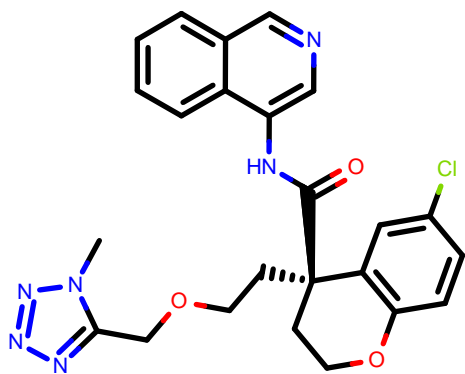
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN3788

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.27

EN300-62574_3_1_1



CID: EN300-62574_3_1_1

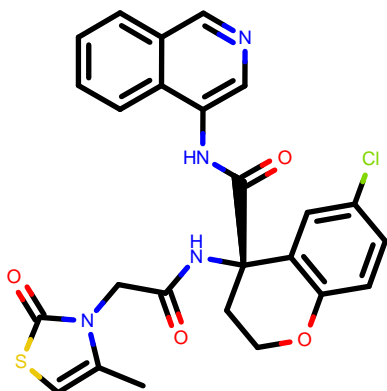
SMILES: Cn1c(nnn1)COCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3282

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.27

EN300-12067_1_1_1



CID: EN300-12067_1_1_1

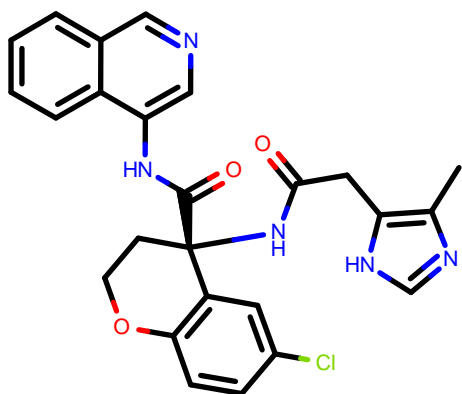
SMILES: Cc1csc(=O)n1CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2987

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.28

EN300-186929_1_1_1



CID: EN300-186929_1_1_1

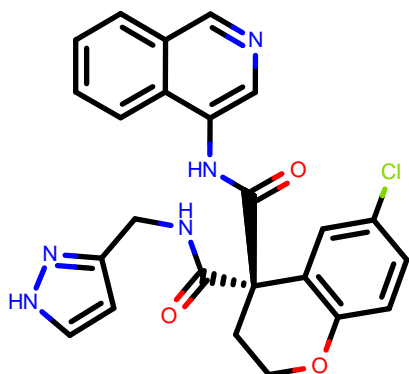
SMILES: Cc1c(nc[nH]1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2980

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.24

VLA-UCB-34f3ed0c-3_1_1



CID: VLA-UCB-34f3ed0c-3_1_1

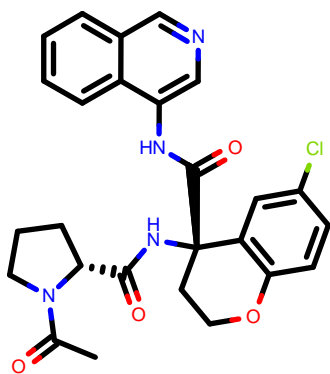
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)NC5ccn[nH]5

RUN: RUN2909

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.26

EN300-211777_1_1_1



CID: EN300-211777_1_1_1

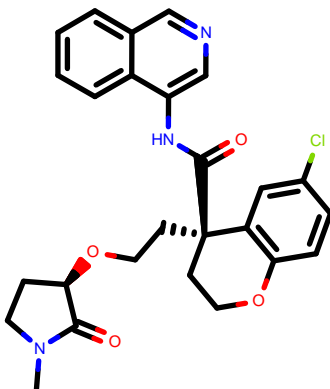
SMILES: CC(=O)N1CCC[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2810

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.33

EN300-98648_3_2_1



CID: EN300-98648_3_2_1

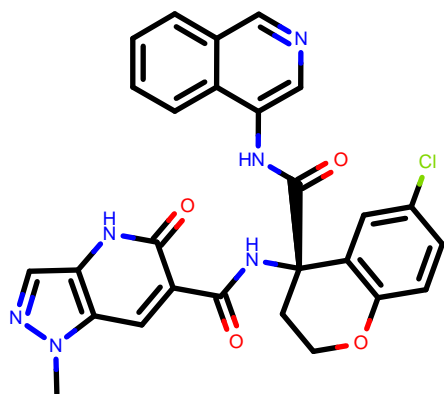
SMILES: CN1CC[C@H]1C(=O)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2936

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.28

EN300-805037_1_1_1



CID: EN300-805037_1_1_1

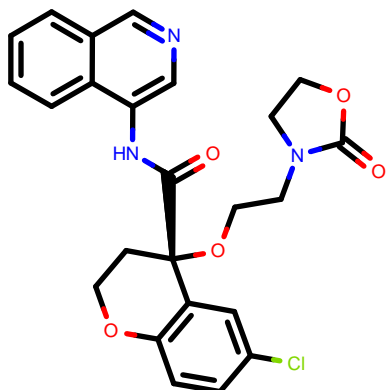
SMILES: Cn1c2cc(c(=O)[nH]c2cn1)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN3274

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.33

CHO-MSK-5891c1ff-3_1



CID: CHO-MSK-5891c1ff-3_1

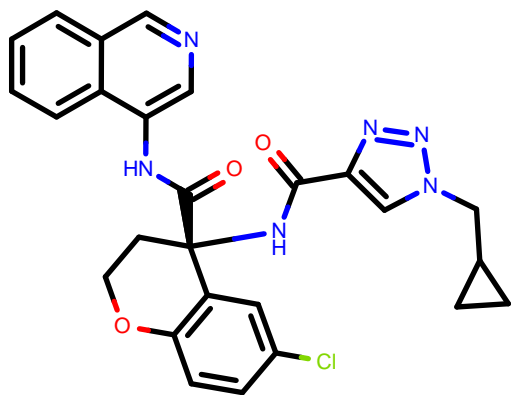
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCN5CCOC5=O

RUN: RUN1726

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.22

EN300-247428_1_1_1



CID: EN300-247428_1_1_1

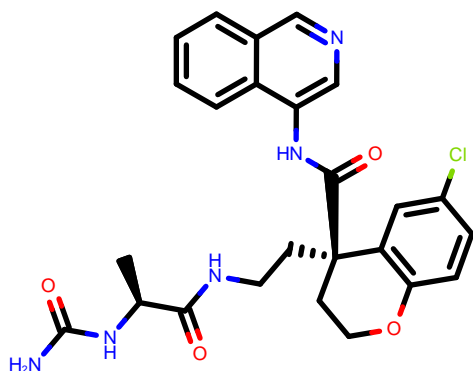
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)CC6CC6

RUN: RUN3302

DDG (kcal/mol): -2.82

dDDG (kcal/mol): 0.25

EN300-00271_3_1_1



CID: EN300-00271_3_1_1

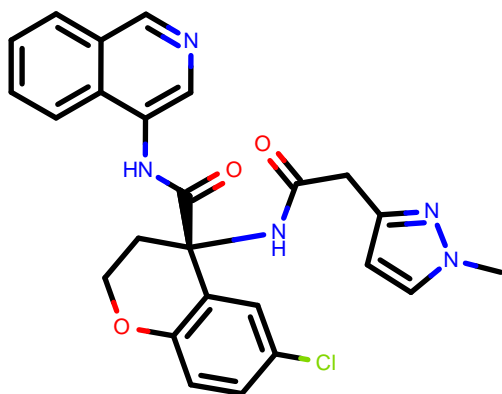
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4)NC(=O)N

RUN: RUN5617

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.33

EN300-258702_1_1_1



CID: EN300-258702_1_1_1

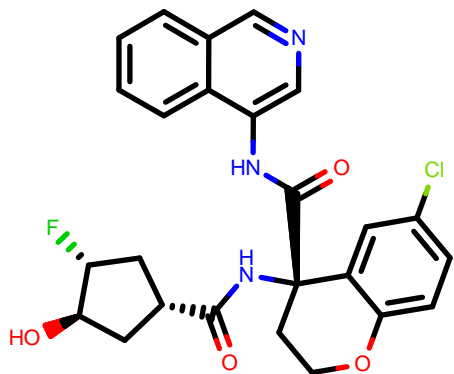
SMILES: Cn1ccc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncnc5c4ccc5

RUN: RUN3103

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.23

EN300-7461217_1_1_1



CID: EN300-7461217_1_1_1

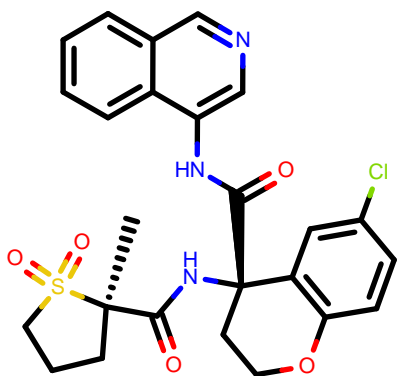
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H](C)F5O

RUN: RUN3199

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.25

EN300-373476_1_1_1



CID: EN300-373476_1_1_1

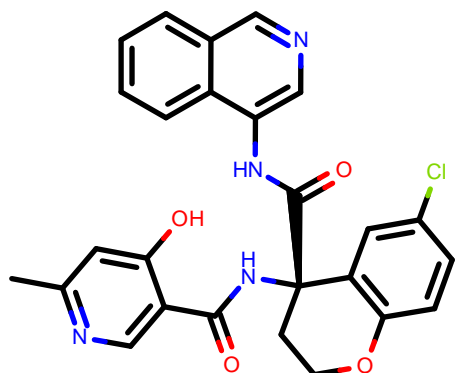
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2818

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.32

EN300-85853_1_1_1



CID: EN300-85853_1_1_1

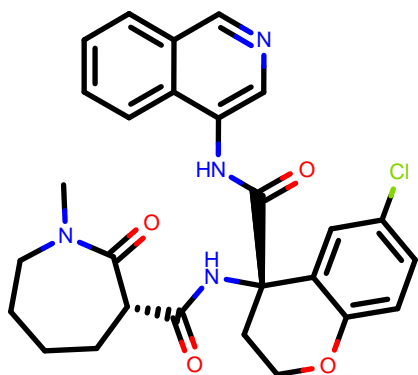
SMILES: Cc1cc(=O)c(c[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3700

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.30

EN300-304695_1_2_1



CID: EN300-304695_1_2_1

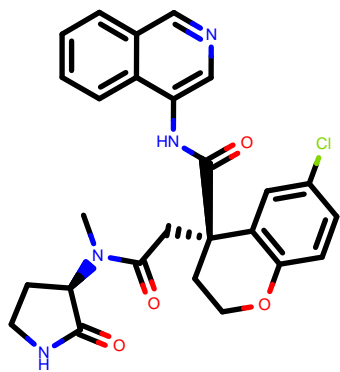
SMILES: CN1CCCC[C@@H](C1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3374

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.27

EN300-120119_1_1_1



CID: EN300-120119_1_1_1

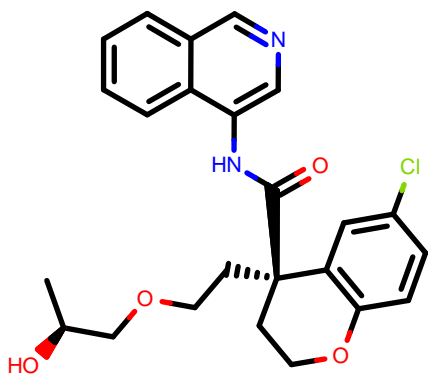
SMILES: CN1C[C@@H](C1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2824

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.24

EN300-185378_3_1_1



CID: EN300-185378_3_1_1

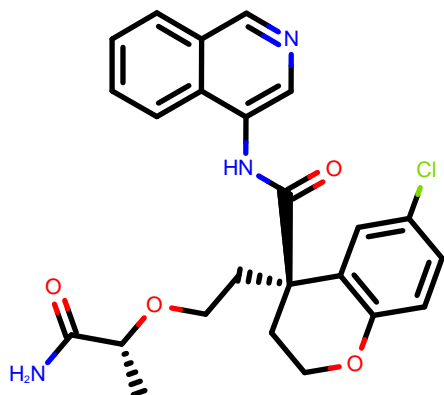
SMILES: C[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3277

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.30

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

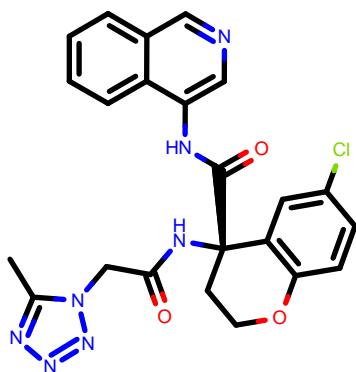
SMILES: C[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2992

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.22

EN300-1244816_1_1_1



CID: EN300-1244816_1_1_1

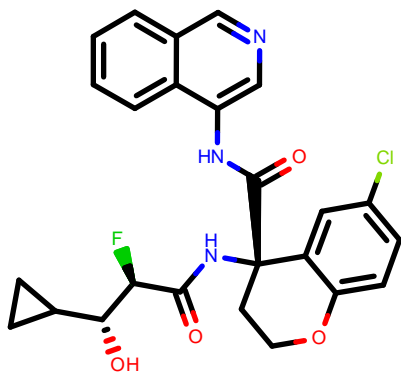
SMILES: Cc1nnnn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3046

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.25

EDG-MED-90036822-78_1



CID: EDG-MED-90036822-78_1

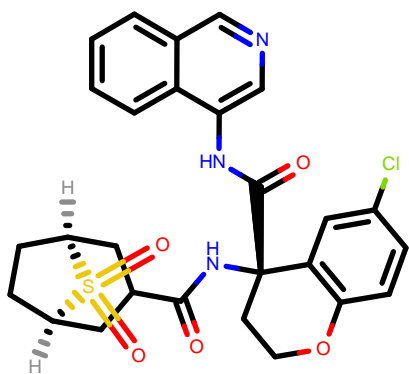
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H(C5CC5)O[F]

RUN: RUN1672

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.21

EN300-373435_1_1_1



CID: EN300-373435_1_1_1

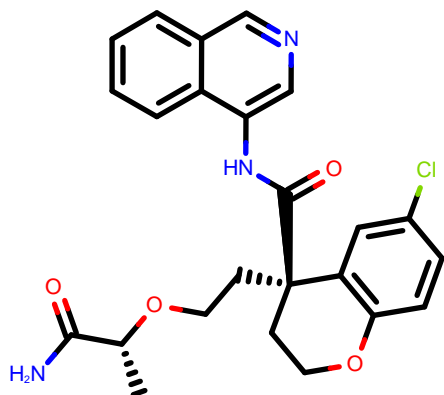
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3CC(=O)C(C)C(=O)C5C(C@H)NCC(C@H)C5S6(=O)=O

RUN: RUN6704

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.30

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

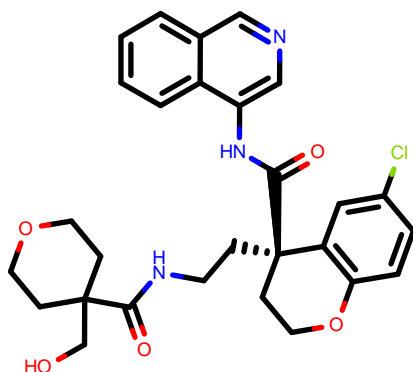
SMILES: C[C@H](C(=O)N)OCC[C@@]1(C)CCOC2C1CC(C(=O)N)C3CNC4C3CCCC4

RUN: RUN2896

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.24

EN300-244909_3_1_1



CID: EN300-244909_3_1_1

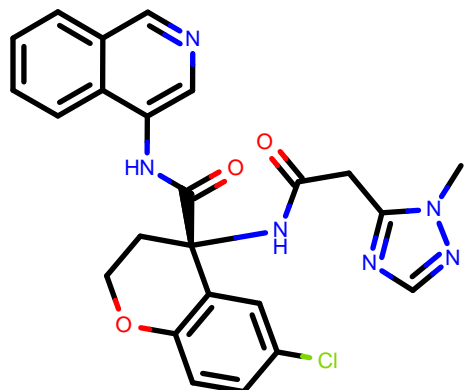
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3CC(=O)C(C)C(=O)C5(C)CCOC5CO

RUN: RUN2854

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.33

EN300-209316_1_1_1



CID: EN300-209316_1_1_1

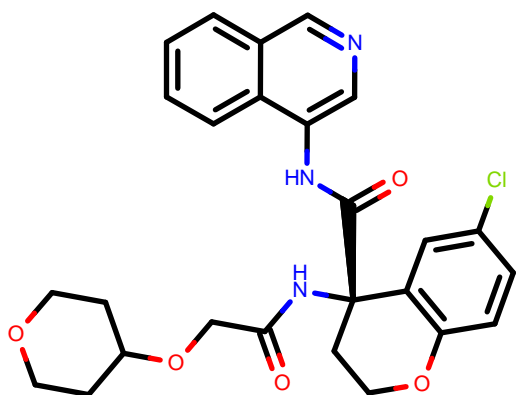
SMILES: Cn1c(ncn1)CC(=O)N[C@@]2(C)CCOC3C2CC(C)C(=O)Nc4cncc5c4cccc5

RUN: RUN2979

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.21

EN300-77520_1_1_1



CID: EN300-77520_1_1_1

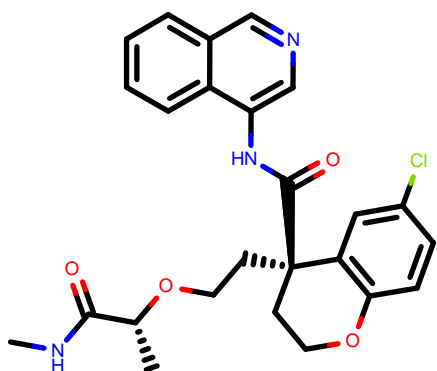
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COC5CCOCC5

RUN: RUN2786

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.21

EN300-211482_3_2_1



CID: EN300-211482_3_2_1

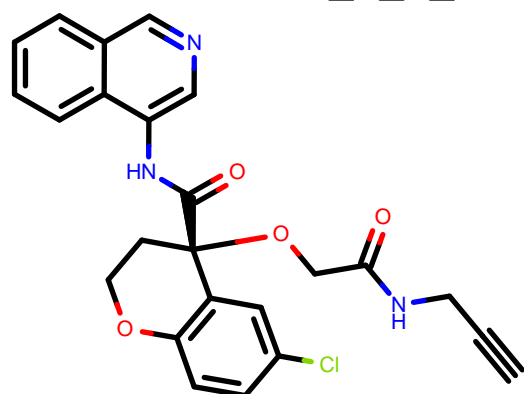
SMILES: C[C@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN2964

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.32

EN300-1659582_1_1_1



CID: EN300-1659582_1_1_1

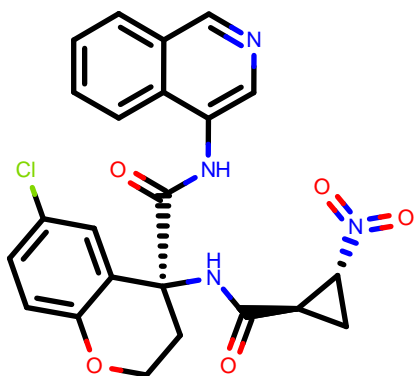
SMILES: C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN5419

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.21

EN300-254854_1_1_1



CID: EN300-254854_1_1_1

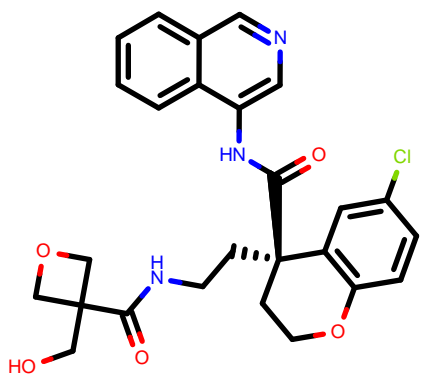
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(C)C(C)C5N(=O)=O

RUN: RUN2805

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.18

EN300-105693_3_1_1



CID: EN300-105693_3_1_1

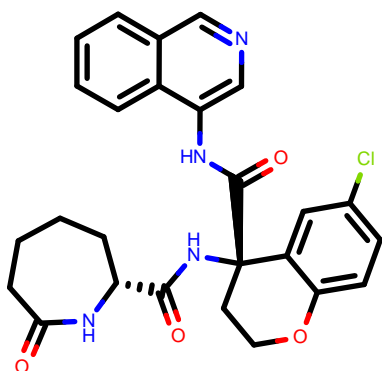
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C)CNC(=O)C5(COC5)CO

RUN: RUN3459

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.31

EN300-80083_1_2_1



CID: EN300-80083_1_2_1

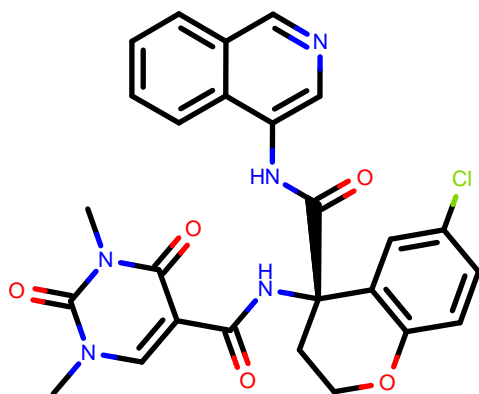
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C)NC(=O)[C@H]5CCCC(=O)N5

RUN: RUN3529

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.26

EN300-79497_1_1_1



CID: EN300-79497_1_1_1

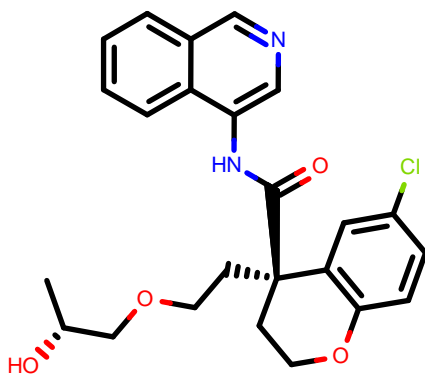
SMILES: Cn1cc(c(=O)n(c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3O)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4734

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.37

EN300-185378_3_2_1



CID: EN300-185378_3_2_1

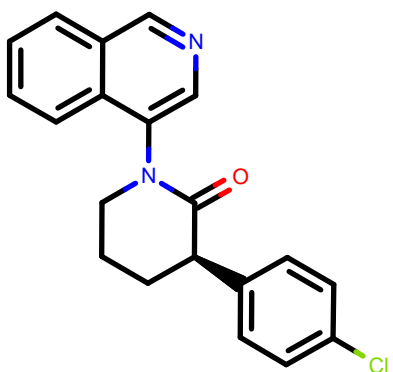
SMILES: C[C@H](COCC[C@@]1(CCOc2c1cc(cc2O)C)C(=O)Nc3cnc4c3cc4O

RUN: RUN4676

DDG (kcal/mol): -2.76

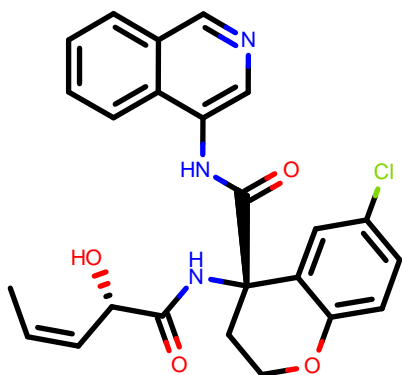
dDDG (kcal/mol): 0.31

ALP-POS-ce760d3f-8_1



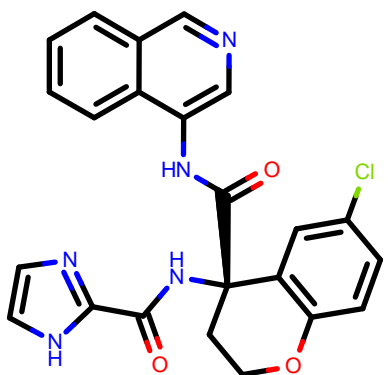
CID:	ALP-POS-ce760d3f-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3CCCC[C@@H](C3=O)c4ccc(cc4)Cl</chem>
RUN:	RUN1278
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.23

EN300-300217_1_1_1



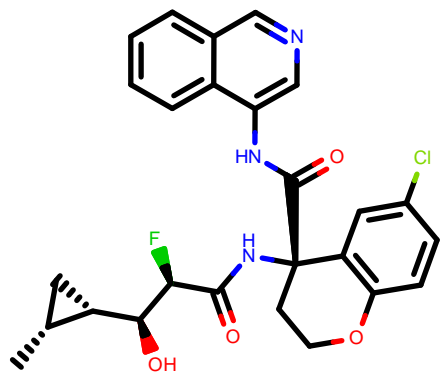
CID:	EN300-300217_1_1_1
SMILES:	<chem>C/C=C/[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O</chem>
RUN:	RUN3409
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.30

EN300-315836_1_1_1



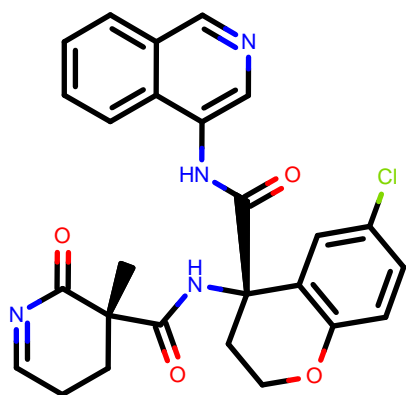
CID:	EN300-315836_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]cnc5</chem>
RUN:	RUN3201
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.19

EDG-MED-90036822-94_9



CID:	EDG-MED-90036822-94_9
SMILES:	<chem>C[C@@H](CC@@H(C@H)Cl)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5)F</chem>
RUN:	RUN1696
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.23

EN300-178876_1_2_1



CID: EN300-178876_1_2_1

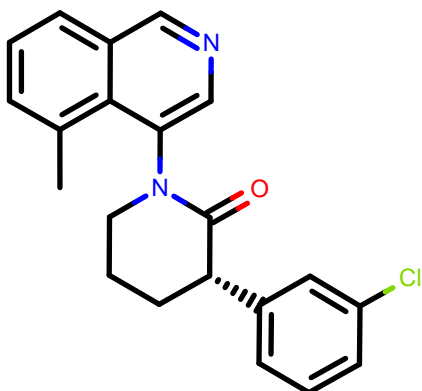
SMILES: C[C@]1(CCCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN7412

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.36

MIC-UNK-50cce87d-11_2



CID: MIC-UNK-50cce87d-11_2

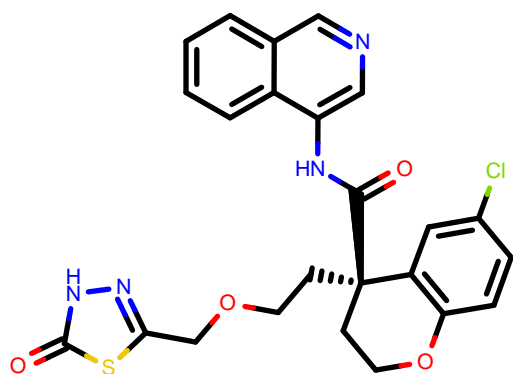
SMILES: Cc1cccc2c1c(cnc2)N3CCC[C@H](C3=O)c4cccc(c4)Cl

RUN: RUN550

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.27

EN300-171766_3_1_1



CID: EN300-171766_3_1_1

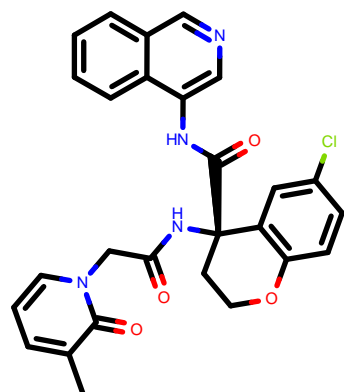
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(CCOc4c3cc(cc4)C)COCOC5N[nH]c5=O

RUN: RUN3186

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.22

EN300-126104_1_1_1



CID: EN300-126104_1_1_1

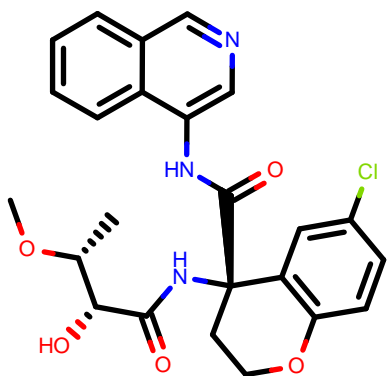
SMILES: Cc1cccn(c1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN3219

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.29

EN300-220194_1_4_1



CID: EN300-220194_1_4_1

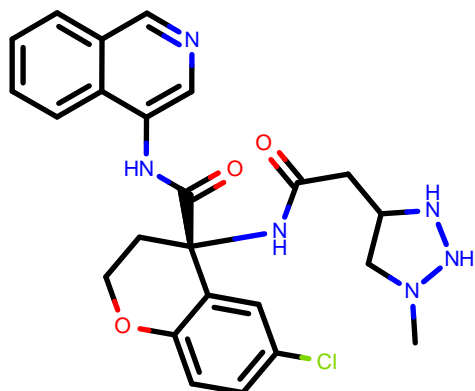
SMILES: C[C@H]([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4O)OC

RUN: RUN3131

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.26

EN300-1073264_1_1_1



CID: EN300-1073264_1_1_1

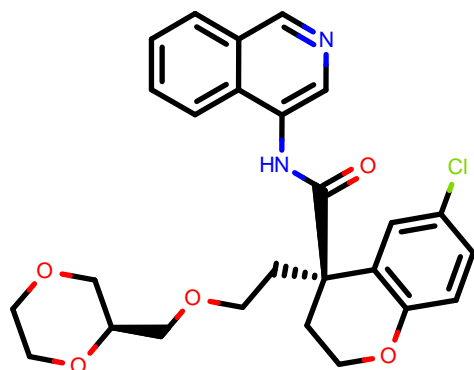
SMILES: Cn1cc(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN3347

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.23

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

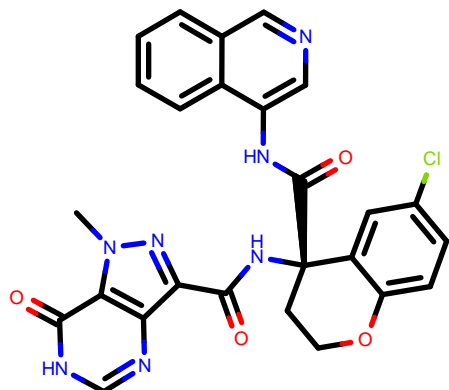
SMILES: c1ccc2c(c1)ncnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5OCOC5

RUN: RUN4110

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.27

EN300-7355981_1_1_1



CID: EN300-7355981_1_1_1

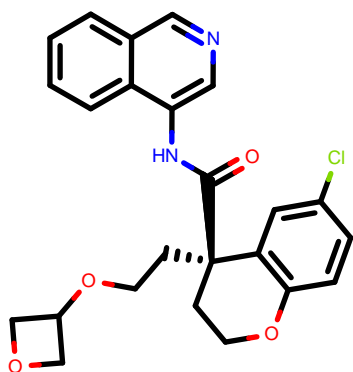
SMILES: Cn1c2c(c(n1)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncnc6c5cccc6)nc[nH]c2=O

RUN: RUN3625

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.30

EN300-317082_3_1_1



CID: EN300-317082_3_1_1

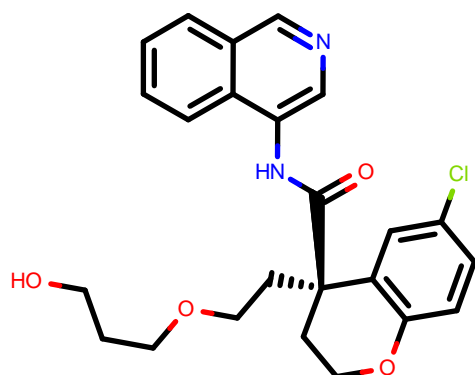
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5COC5

RUN: RUN2907

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.21

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

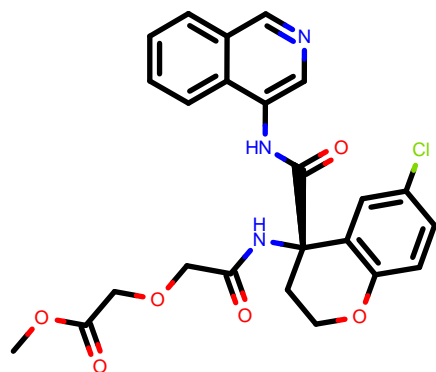
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN3306

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.25

EN300-205635_1_1_1



CID: EN300-205635_1_1_1

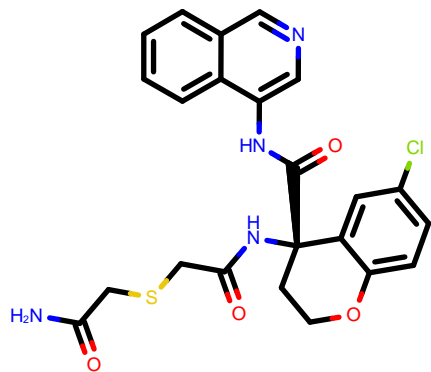
SMILES: COC(=O)COCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3334

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.23

EN300-33513_1_1_1



CID: EN300-33513_1_1_1

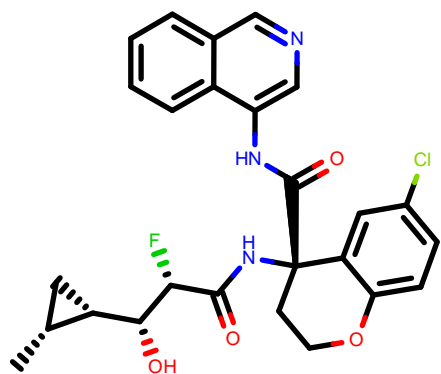
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CSCC(=O)N

RUN: RUN3871

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.22

EDG-MED-90036822-94_5



CID: EDG-MED-90036822-94_5

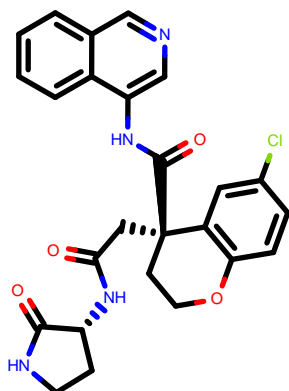
SMILES: C[C@@H]1[C@@H]2[C@@H]3[C@@H]4[C@@H]5[C@@H]6[C@@H]7[C@@H]8[C@@H]9[C@@H]10[C@@H]11[C@@H]12[C@@H]13[C@@H]14[C@@H]15[C@@H]16[C@@H]17[C@@H]18[C@@H]19[C@@H]20[C@@H]21[C@@H]22[C@@H]23[C@@H]24[C@@H]25[C@@H]26[C@@H]27[C@@H]28[C@@H]29[C@@H]30[C@@H]31[C@@H]32[C@@H]33[C@@H]34[C@@H]35[C@@H]36[C@@H]37[C@@H]38[C@@H]39[C@@H]40[C@@H]41[C@@H]42[C@@H]43[C@@H]44[C@@H]45[C@@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: RUN1663

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.28

EDJ-MED-d203f206-29_1



CID: EDJ-MED-d203f206-29_1

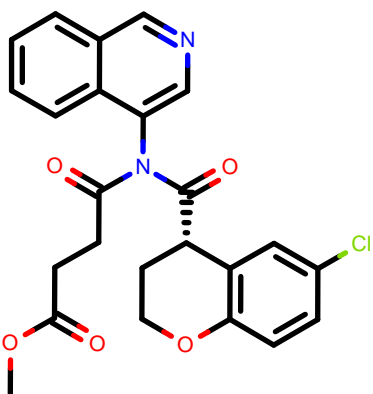
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)CC(=O)N[C@@]5H5CCNC5=O

RUN: RUN2405

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.32

MAT-POS-9db1e783-3_1



CID: MAT-POS-9db1e783-3_1

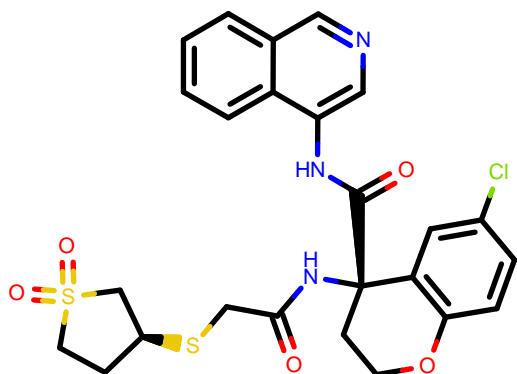
SMILES: COC(=O)C=C/C(=O)N(c1ccc2c1cccc2)C(=O)[C@@H]3CCOC4C3cc(cc4)Cl

RUN: RUN2639

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.38

EN300-13890_1_2_1



CID: EN300-13890_1_2_1

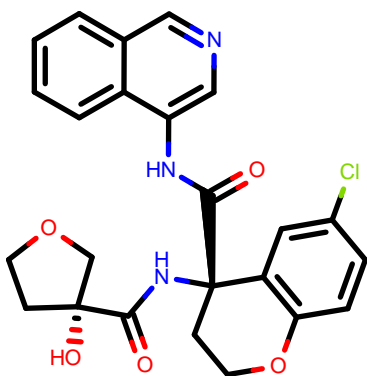
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)C)NC(=O)CS[C@@H]5SCCS(=O)(=O)C5

RUN: RUN4216

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.32

EN300-148421_1_2_1



CID: EN300-148421_1_2_1

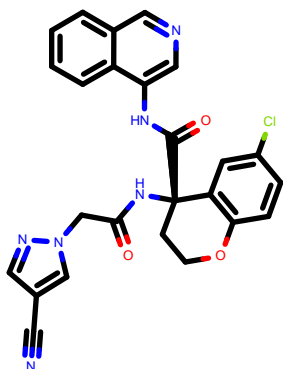
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@]5(CCOC5)O

RUN: RUN3115

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.36

EN300-1590388_1_1_1



CID: EN300-1590388_1_1_1

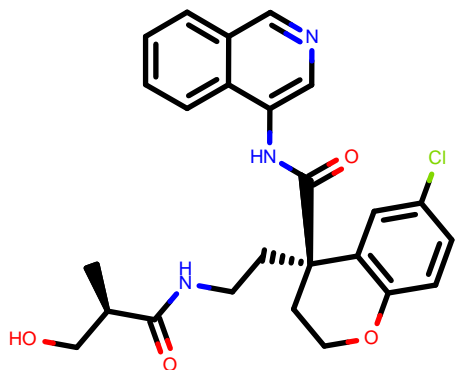
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ccn(cn5)C#N

RUN: RUN3506

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.24

EN300-55072_3_2_1



CID: EN300-55072_3_2_1

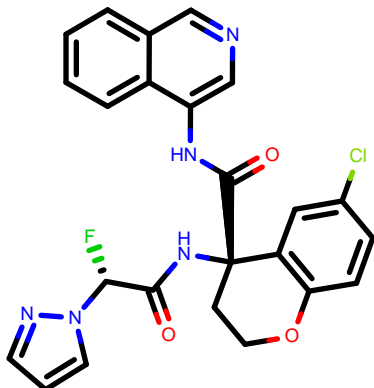
SMILES: C[C@H](CO)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN4429

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.26

EN300-1726277_1_2_1



CID: EN300-1726277_1_2_1

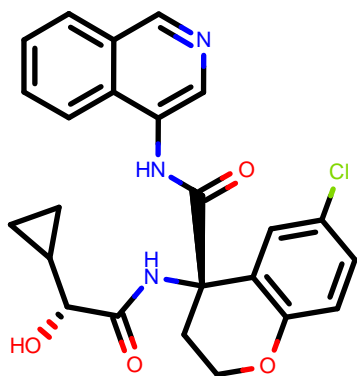
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](n5cccn5)F

RUN: RUN3178

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.21

EN300-72211_1_1_1



CID: EN300-72211_1_1_1

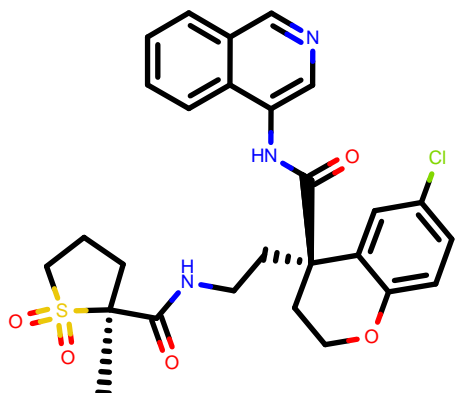
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](C5CC5)O

RUN: RUN3030

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.25

EN300-373476_3_2_1



CID: EN300-373476_3_2_1

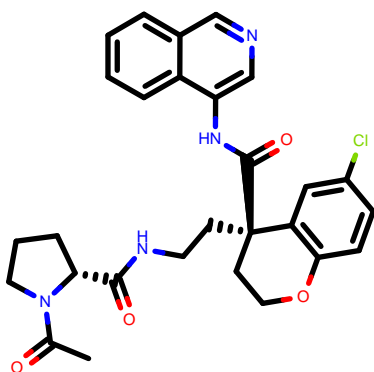
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5971

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.35

EN300-211777_3_1_1



CID: EN300-211777_3_1_1

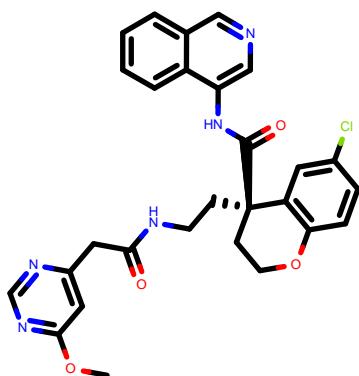
SMILES: CC(=O)N1CCC[C@@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7271

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.35

EN300-7444950_3_1_1



CID: EN300-7444950_3_1_1

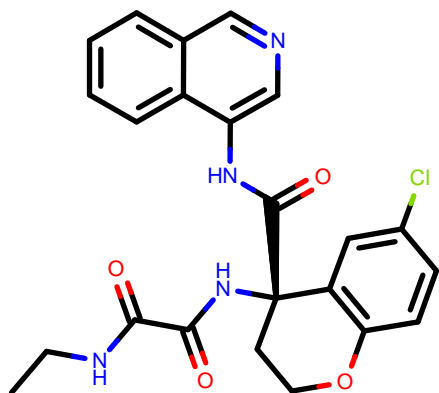
SMILES: COc1cc(ncn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3232

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.32

EN300-1262608_1_1_1



CID: EN300-1262608_1_1_1

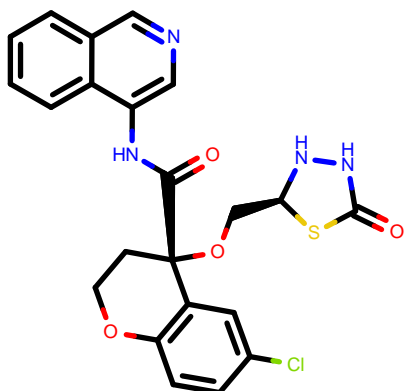
SMILES: CCNC(=O)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2871

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.24

EN300-171766_1_1_2



CID: EN300-171766_1_1_2

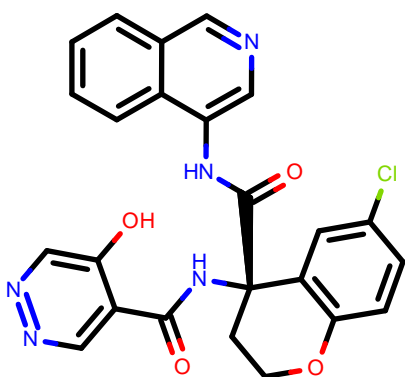
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5NNC(=O)S5

RUN: RUN3570

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.21

EN300-243828_1_1_1



CID: EN300-243828_1_1_1

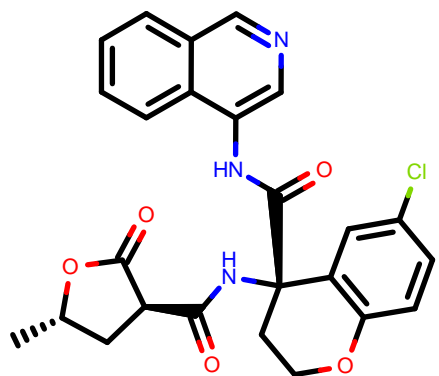
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]nc5=O

RUN: RUN2852

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.26

EN300-7444533_1_2_1



CID: EN300-7444533_1_2_1

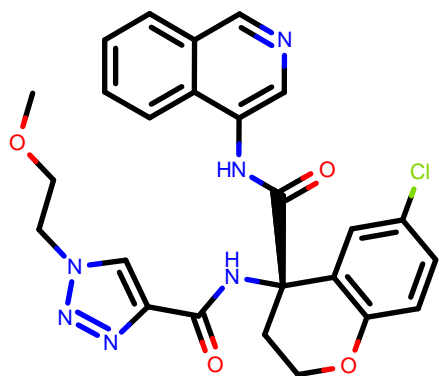
SMILES: C[C@H]1C[C@@H](C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c5c4cccc5

RUN: RUN2924

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.25

EN300-251867_1_1_1



CID: EN300-251867_1_1_1

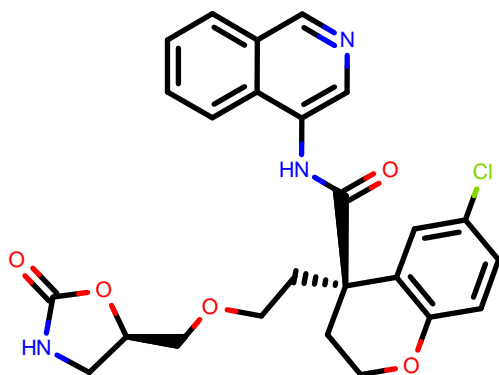
SMILES: COCc1cc(nn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3780

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.24

EN300-203293_3_2_1



CID: EN300-203293_3_2_1

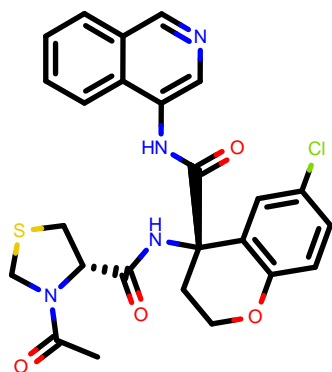
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)Cl)CCOC[C@H]5CNC(=O)O5

RUN: RUN2850

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.31

EN300-761220_1_1_1



CID: EN300-761220_1_1_1

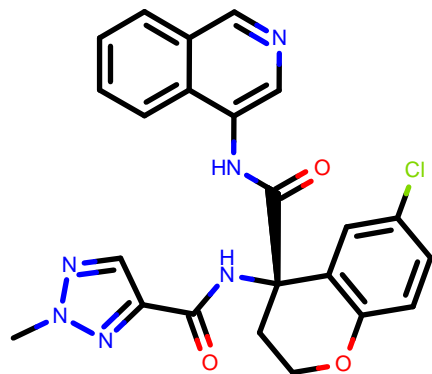
SMILES: CC(=O)N1CSC[C@@H]1C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2840

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.27

EN300-61694_1_1_1



CID: EN300-61694_1_1_1

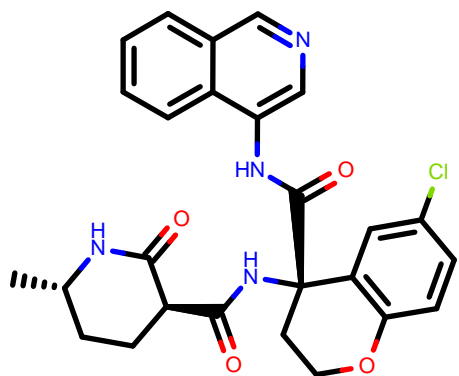
SMILES: Cn1ncc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3532

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.17

EN300-6505003_1_2_1



CID: EN300-6505003_1_2_1

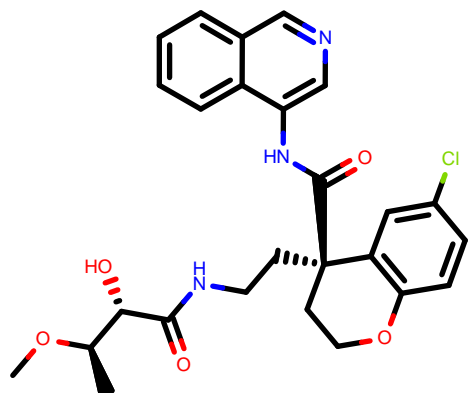
SMILES: C[C@H]1CC[C@@H](C(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3066

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.33

EN300-220194_3_2_1



CID: EN300-220194_3_2_1

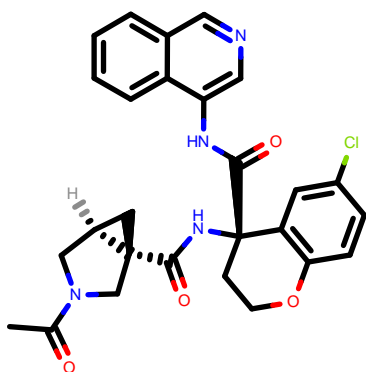
SMILES: C[C@H](C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O)OC

RUN: RUN6435

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.28

EN300-313062_1_4_1



CID: EN300-313062_1_4_1

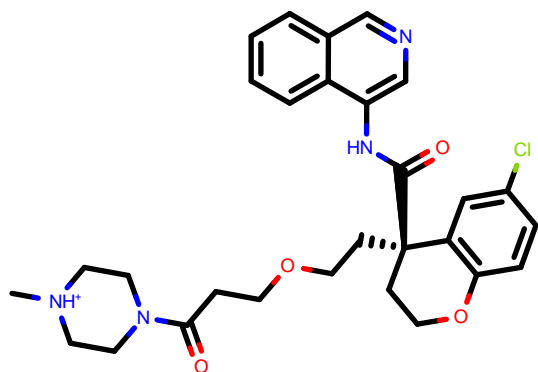
SMILES: CC(=O)N1C[C@@H]2C[C@@]2(C1)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN3009

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.29

EN300-178293_3_1_1



CID: EN300-178293_3_1_1

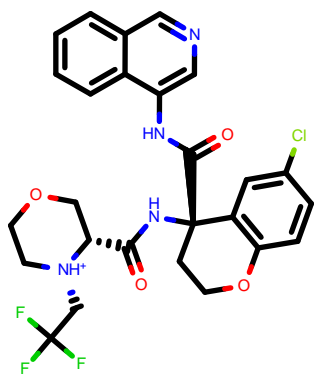
SMILES: C[NH+]1CCN(CC1)C(=O)CCOCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5145

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.38

EN300-201551_1_2_1



CID: EN300-201551_1_2_1

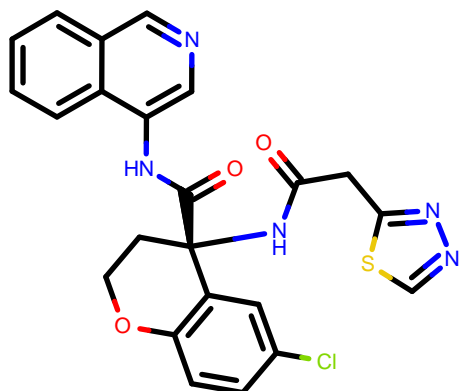
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5COCQ[N@@]5C(F)(F)F

RUN: RUN3098

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.28

EN300-6488240_1_1_1



CID: EN300-6488240_1_1_1

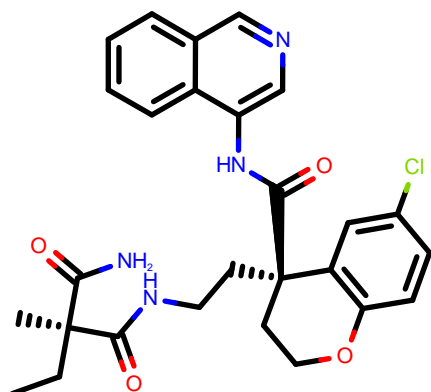
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nncs5

RUN: RUN2831

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.24

EN300-2908024_3_1_1



CID: EN300-2908024_3_1_1

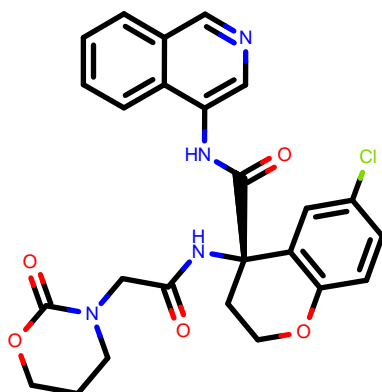
SMILES: CC(C@@)1(C)C(=O)N(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN3633

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.28

EN300-103638_1_1_1



CID: EN300-103638_1_1_1

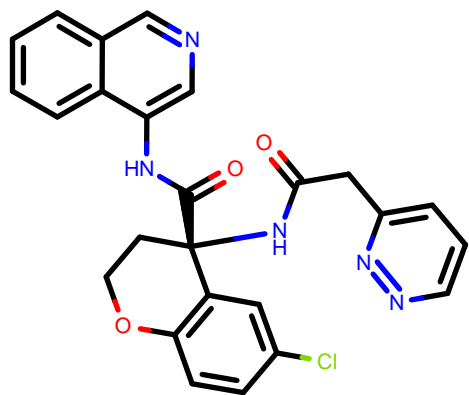
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O

RUN: RUN3712

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.32

EN300-7456948_1_1_1



CID: EN300-7456948_1_1_1

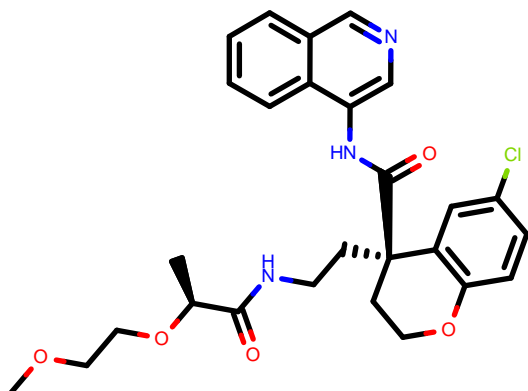
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cccn5

RUN: RUN3029

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.22

EN300-77359_3_1_1



CID: EN300-77359_3_1_1

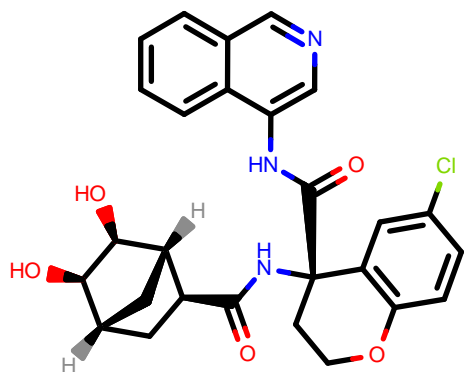
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)OCCOC

RUN: RUN5465

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.30

EN300-6744028_1_2_1



CID: EN300-6744028_1_2_1

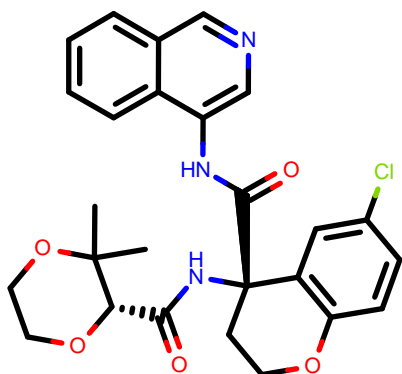
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)Nc5c6c7c8c9c10c5c6c7c8c9c10

RUN: RUN3395

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.29

EN300-1601684_1_1_1



CID: EN300-1601684_1_1_1

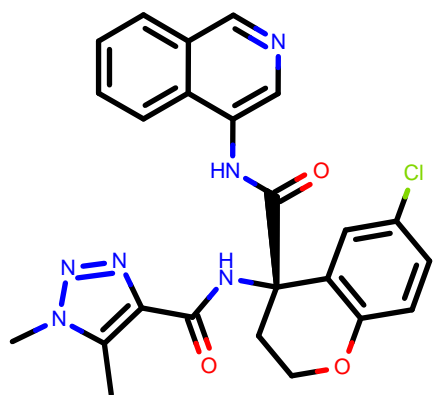
SMILES: CC1([C@@H](OCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN2971

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.28

EN300-85473_1_1_1



CID: EN300-85473_1_1_1

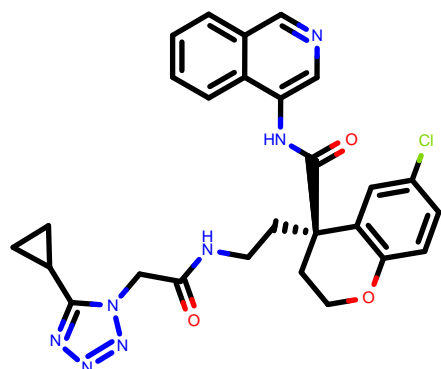
SMILES: Cc1c(nnn1C)C(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN6014

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.23

EN300-872798_3_1_1



CID: EN300-872798_3_1_1

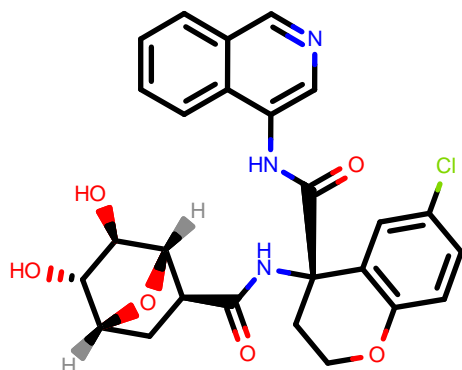
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C)CCNC(=O)Cn5c(nnn5)C6CC6

RUN: RUN3775

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.31

EN300-6764836_1_6_1



CID: EN300-6764836_1_6_1

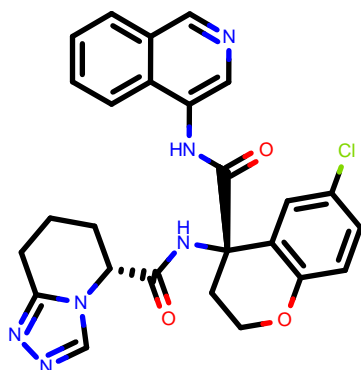
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C)N(C)C(=O)C@H5C[C@@]H6[C@@]H7[C@@]H8[C@@]H9[C@@]H10

RUN: RUN3369

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.27

EN300-6478631_1_2_1



CID: EN300-6478631_1_2_1

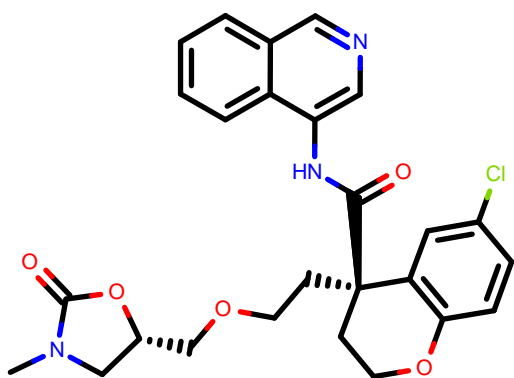
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4)C)N(C)C(=O)C@H5CCC6c6n5cnn6

RUN: RUN2947

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.24

EN300-222969_3_2_1



CID: EN300-222969_3_2_1

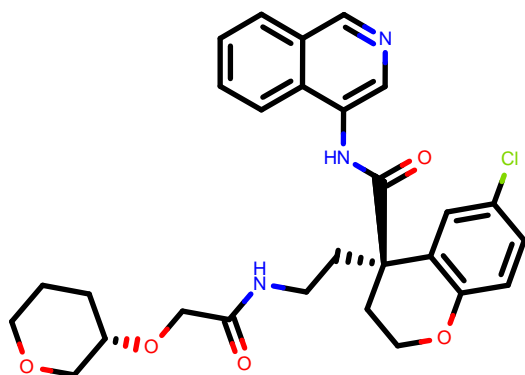
SMILES: CN1C[C@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccoc5

RUN: RUN2898

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.30

EN300-1627945_3_2_1



CID: EN300-1627945_3_2_1

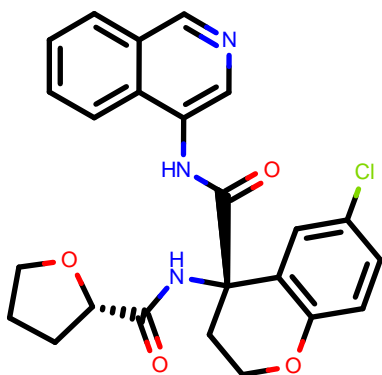
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@H]5CCOC5

RUN: RUN5777

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.23

EN300-21009_1_1_1



CID: EN300-21009_1_1_1

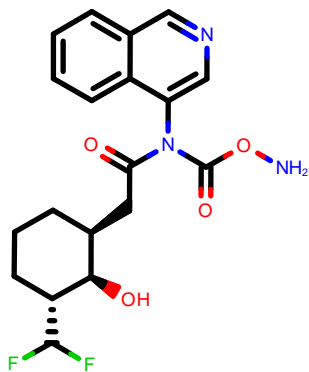
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC5

RUN: RUN3225

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.24

MAK-UNK-c749d764-29_3



CID: MAK-UNK-c749d764-29_3

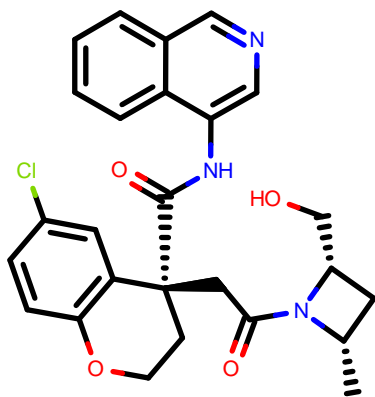
SMILES: c1ccc2c(c1)ncnc2N(C(=O)C[C@@H]3CCCC[C@H](C)[C@H]3O)C(F)F)C(=O)ON

RUN: RUN1085

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.37

EN300-1709410_1_4_1



CID: EN300-1709410_1_4_1

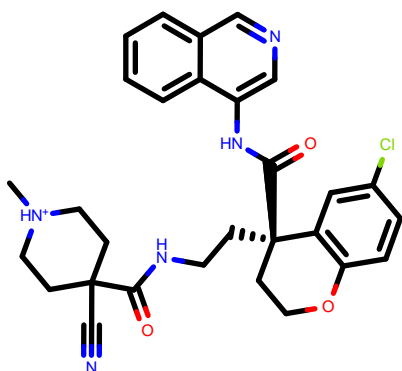
SMILES: C[C@H]1C[C@H](N1C(=O)C[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)CO

RUN: RUN4112

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.28

EN300-7473378_3_1_1



CID: EN300-7473378_3_1_1

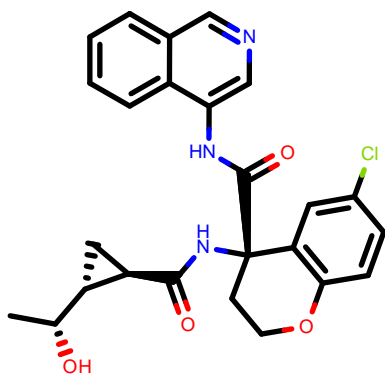
SMILES: C[NH+]1CCC(CC1)(C#N)C(=O)NCC[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4066

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.41

EN300-6729572_1_6_1



CID: EN300-6729572_1_6_1

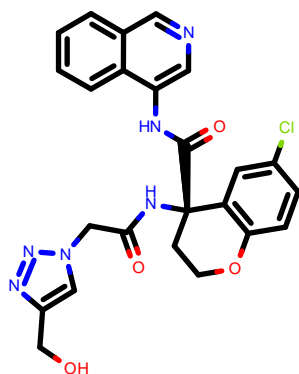
SMILES: C[C@H]([C@@H]1C[C@H]1C(=O)N[C@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3177

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.24

EN300-108236_1_1_1



CID: EN300-108236_1_1_1

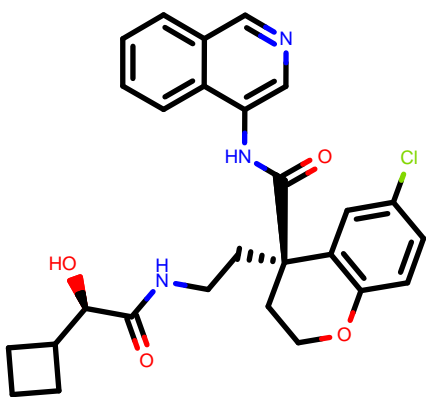
SMILES: c1ccc2c(c1)ccc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)Cn5ccn5)CO

RUN: RUN3500

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.28

EN300-249764_3_1_1



CID: EN300-249764_3_1_1

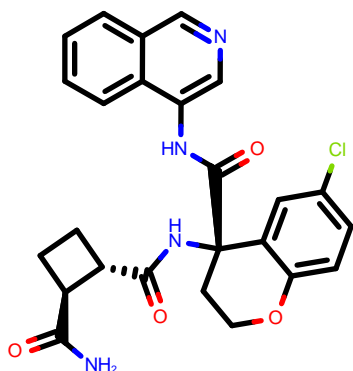
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C5CC5)O

RUN: RUN4223

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.23

EN300-217107_1_2_1



CID: EN300-217107_1_2_1

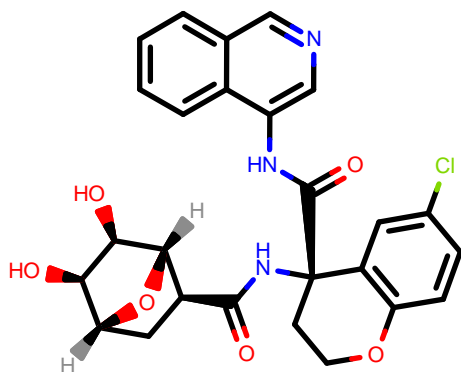
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C)N(C(=O)N)[C@@H](C5CC5)C(=O)N

RUN: RUN2806

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.26

EN300-6764836_1_8_1



CID: EN300-6764836_1_8_1

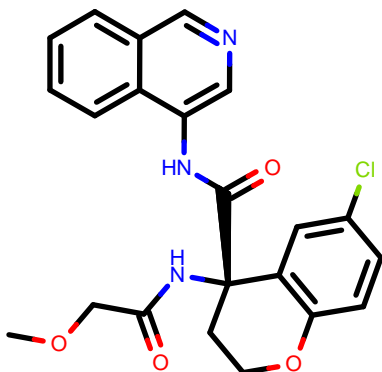
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C)N(C(=O)N)[C@@H](C5CC5)C(=O)N

RUN: RUN3412

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.27

EDG-MED-90036822-34_1



CID: EDG-MED-90036822-34_1

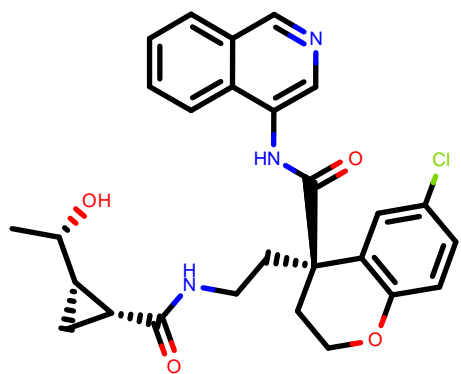
SMILES: COCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3cccc4

RUN: RUN1534

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.18

EN300-6729572_3_7_1



CID: EN300-6729572_3_7_1

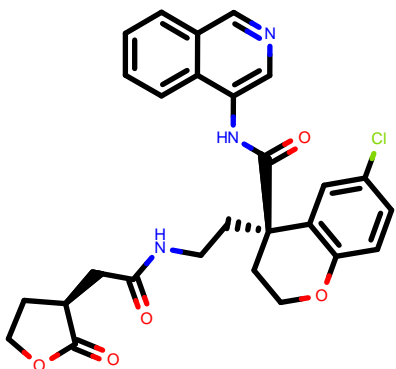
SMILES: C[C@@H][C@H]1C[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5O

RUN: RUN3648

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.28

EN300-1072972_3_1_1



CID: EN300-1072972_3_1_1

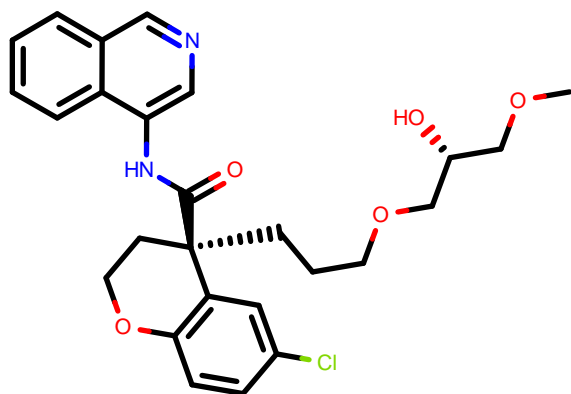
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@@H]5CCOC5=O

RUN: RUN4553

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.38

EN300-1915260_4_2_1



CID: EN300-1915260_4_2_1

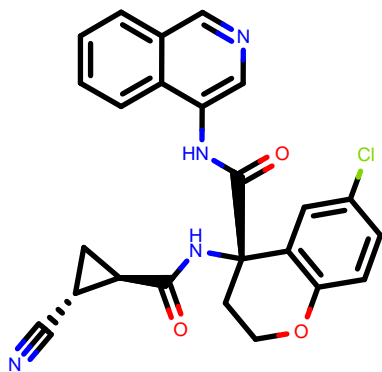
SMILES: COC[C@H](COC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4)O

RUN: RUN6041

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.45

EN300-1600363_1_1_1



CID: EN300-1600363_1_1_1

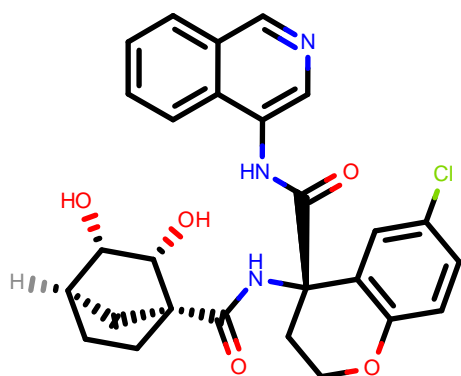
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@H]5C#N

RUN: RUN3654

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.20

EN300-7432302_1_1_1



CID: EN300-7432302_1_1_1

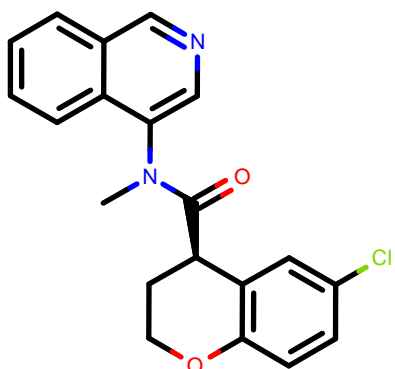
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(c4)C)N(C=O)[C@@H]5[C@@H](C)C=C[C@@H]5O

RUN: RUN2759

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.34

MAK-UNK-3875bbc8-2_1



CID: MAK-UNK-3875bbc8-2_1

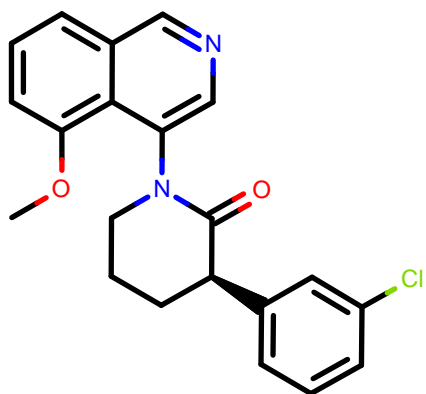
SMILES: CN(c1cnc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN718

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.09

MIC-UNK-50cce87d-12_1



CID: MIC-UNK-50cce87d-12_1

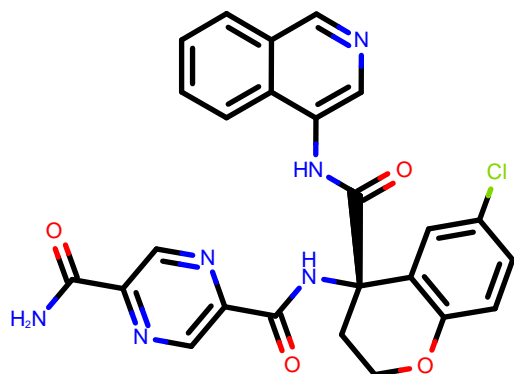
SMILES: COc1cccc2c1c(cnc2)N3CCCC[C@@H]3(C3=O)c4ccccc4Cl

RUN: RUN567

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.21

EN300-1273172_1_1_1



CID: EN300-1273172_1_1_1

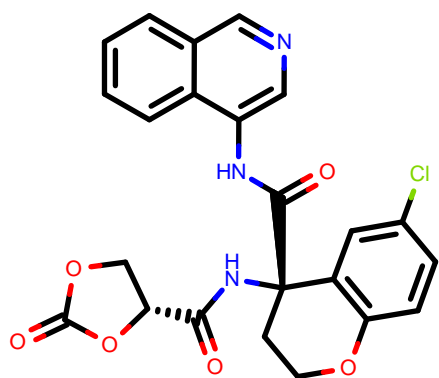
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(c4)C)N(C(=O)c5ncc(nc5)C(=O)N

RUN: RUN3820

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.26

EN300-5253939_1_2_1



CID: EN300-5253939_1_2_1

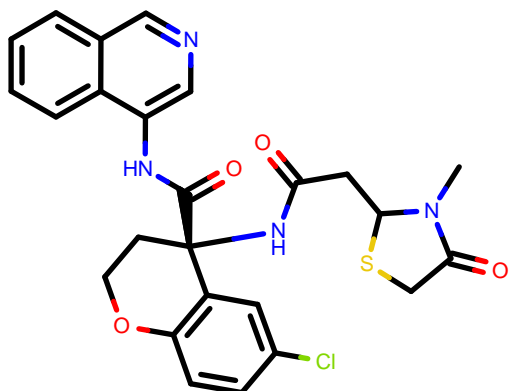
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@H5COC(=O)O5

RUN: RUN3790

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.22

EN300-143564_1_1_1



CID: EN300-143564_1_1_1

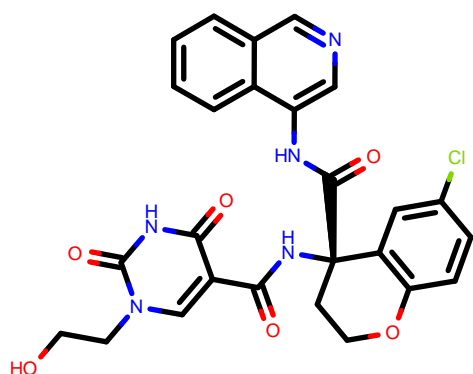
SMILES: CN1C(=O)CS/C1=C/C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5

RUN: RUN4048

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.22

EN300-101291_1_1_1



CID: EN300-101291_1_1_1

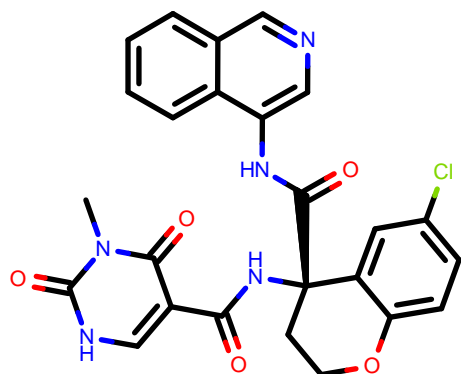
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)c5cn(c(=O)[nH]c5=O)CCO

RUN: RUN5631

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.39

EN300-102487_1_1_1



CID: EN300-102487_1_1_1

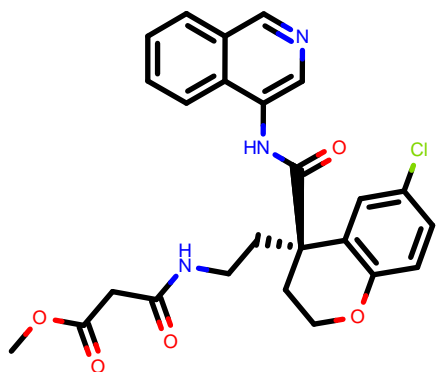
SMILES: Cn1c(=O)c(c[nH]c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4cccc5

RUN: RUN3427

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.31

EN300-20668_3_1_1



CID: EN300-20668_3_1_1

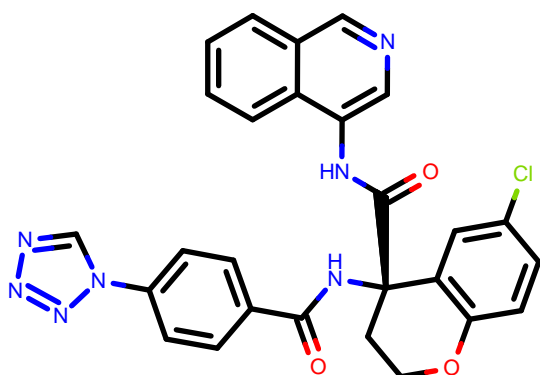
SMILES: COC(=O)CC(=O)NCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN5029

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.27

EN300-06030_1_1_1



CID: EN300-06030_1_1_1

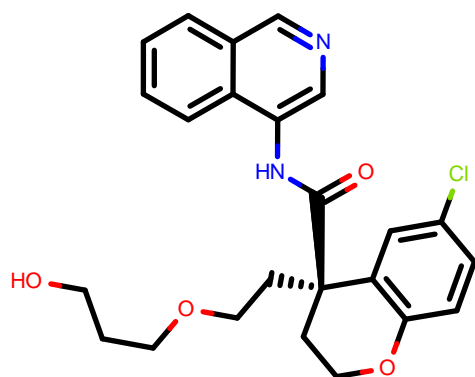
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)n6cnnn6

RUN: RUN4992

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.30

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

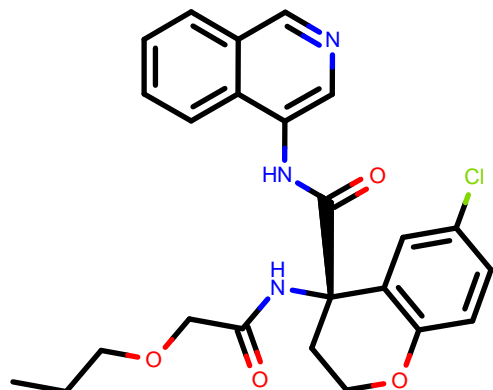
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN3784

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.25

EN300-44821_1_1_1



CID: EN300-44821_1_1_1

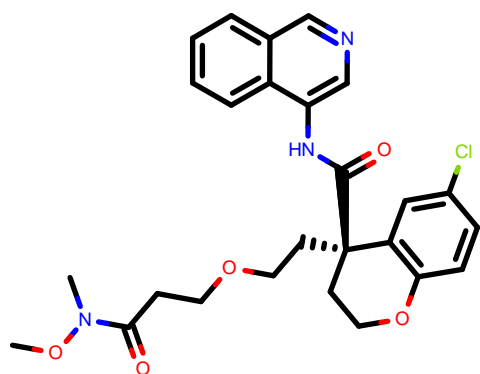
SMILES: C=CCOCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3405

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.18

EN300-174603_3_1_1



CID: EN300-174603_3_1_1

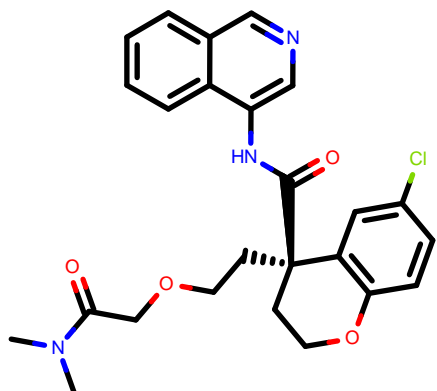
SMILES: CN(C(=O)CCOCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OC

RUN: RUN4409

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.31

EN300-216063_3_1_1



CID: EN300-216063_3_1_1

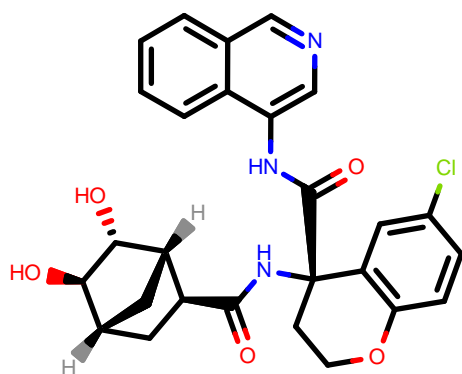
SMILES: CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3954

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.20

EN300-6744028_1_4_1



CID: EN300-6744028_1_4_1

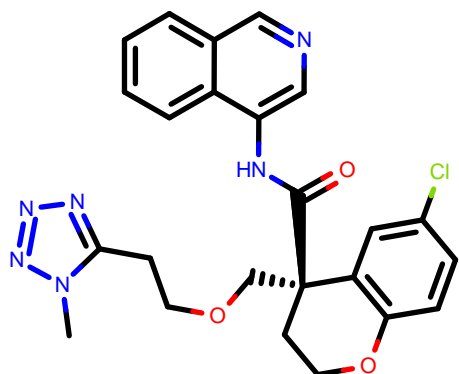
SMILES: c1ccc2c(c1)nccc2NCl+O[C@@]3(CCOc4c3ccc(cc4)C)N(C)C(=O)Nc5c6c7c8c9c10c6c7c8c9c10

RUN: RUN3548

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.29

EN300-365398_2_1_1



CID: EN300-365398_2_1_1

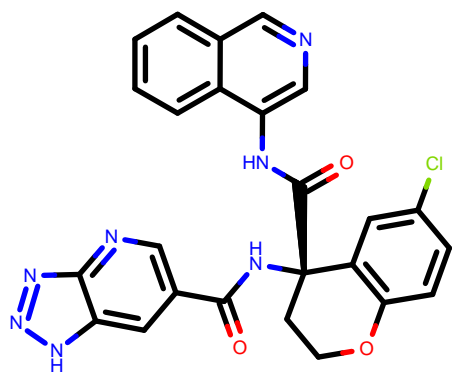
SMILES: Cn1c(nnn1)CCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3291

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.30

EDJ-MED-6864a934-7_1



CID: EDJ-MED-6864a934-7_1

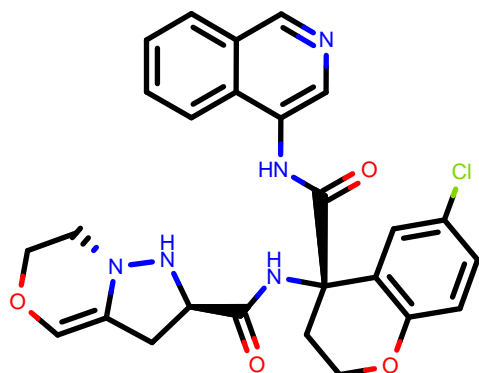
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(nc5)n[nH]6

RUN: RUN2435

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.22

EN300-244278_1_1_2



CID: EN300-244278_1_1_2

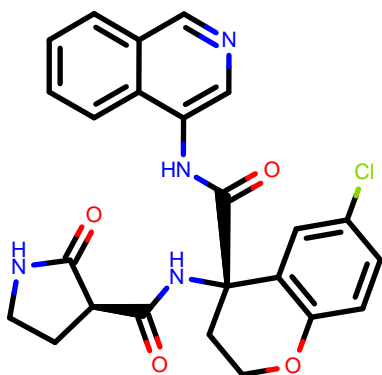
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C=C6COCOC[N@@]6N5

RUN: RUN2939

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.28

EN300-94945_1_2_1



CID: EN300-94945_1_2_1

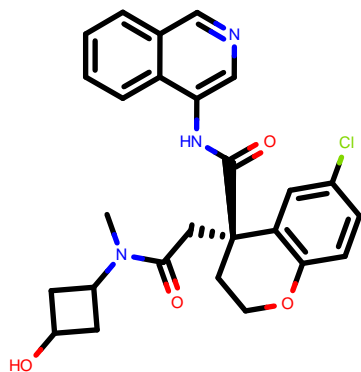
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCNC5=O

RUN: RUN3003

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.21

EN300-97697_1_1_1



CID: EN300-97697_1_1_1

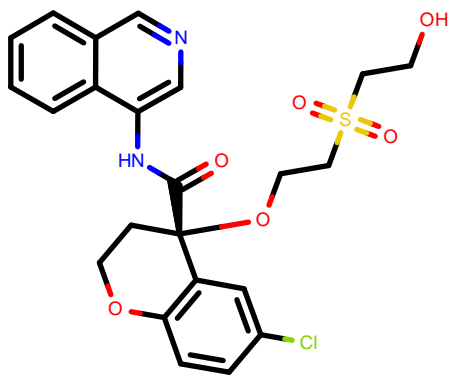
SMILES: CN(C1CC(C1)O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5=O

RUN: RUN3311

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.30

EN300-7463171_1_1_1



CID: EN300-7463171_1_1_1

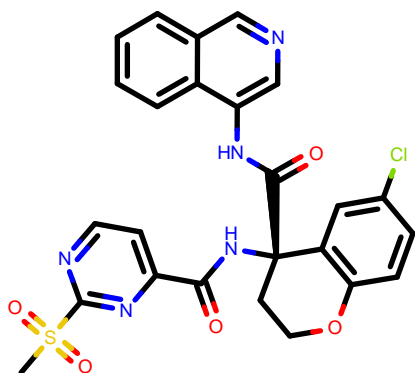
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCO

RUN: RUN3826

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.44

EN300-205622_1_1_1



CID: EN300-205622_1_1_1

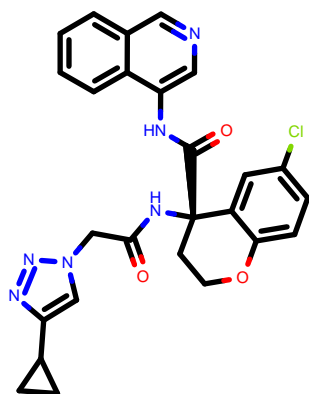
SMILES: CS(=O)(=O)c1nccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3236

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.28

EN300-107892_1_1_1



CID: EN300-107892_1_1_1

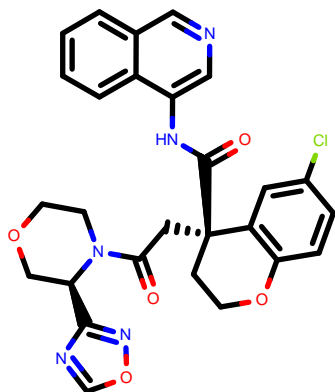
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccc(m5)C6C6

RUN: RUN3322

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.30

EDJ-MED-d203f206-3_1



CID: EDJ-MED-d203f206-3_1

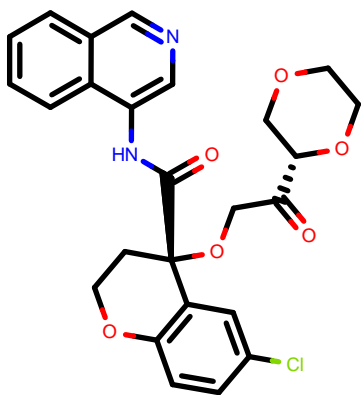
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@]H5c6ncon6

RUN: RUN2442

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.41

EN300-6238494_1_1_1



CID: EN300-6238494_1_1_1

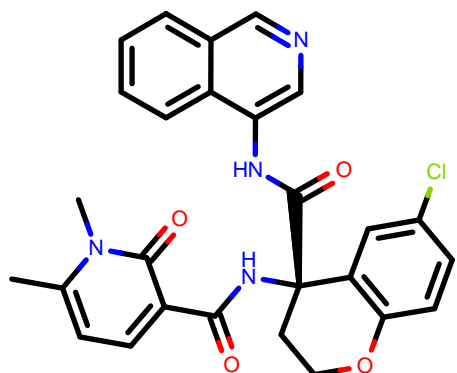
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COCOC5

RUN: RUN4186

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.28

EN300-41423_1_1_1



CID: EN300-41423_1_1_1

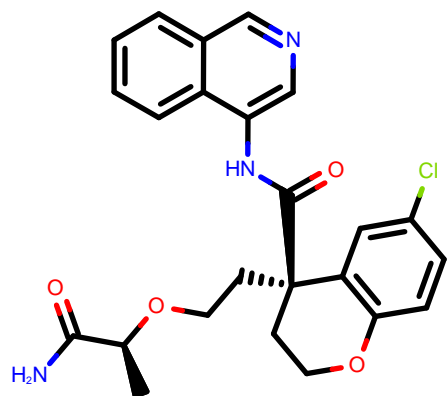
SMILES: Cc1ccc(c(=O)n1C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN3243

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.30

EN300-17381_3_1_1



CID: EN300-17381_3_1_1

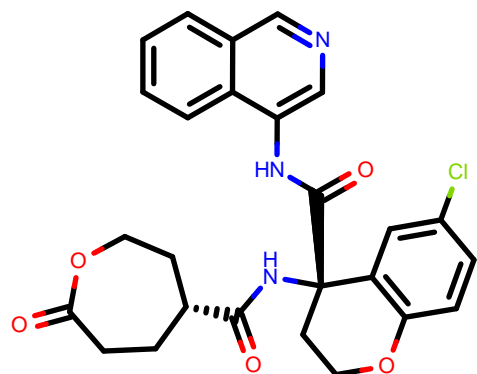
SMILES: C[C@@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN4638

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.25

EN300-2011083_1_1_1



CID: EN300-2011083_1_1_1

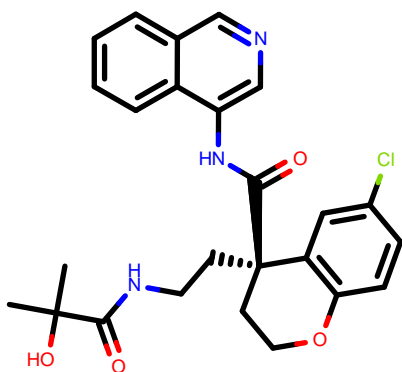
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)OCC5

RUN: RUN4483

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.29

EN300-59285_3_1_1



CID: EN300-59285_3_1_1

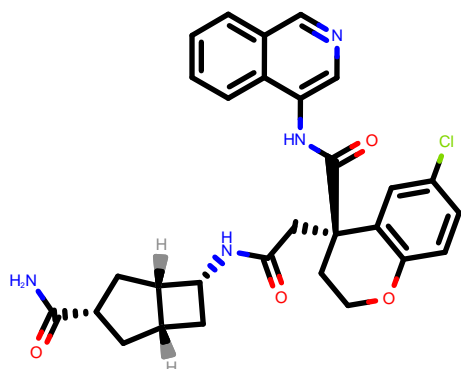
SMILES: CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN5564

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.27

EN300-1268016_1_11_1



CID: EN300-1268016_1_11_1

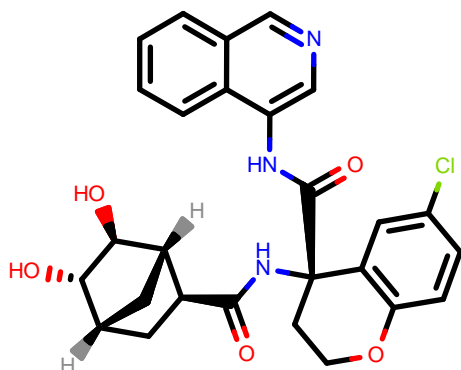
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)CC(=O)N[C@@]5H5C[C@@H]6[C@@H](C6)Cl=O

RUN: RUN4057

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.38

EN300-6744028_1_6_1



CID: EN300-6744028_1_6_1

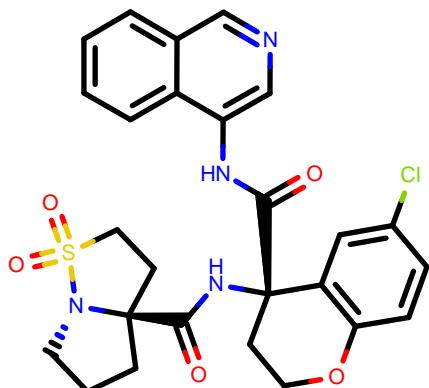
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)NC(=O)[C@@]5H5C[C@@H]6[C@@H](C6)O

RUN: RUN2931

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.23

EN300-6733459_1_1_1



CID: EN300-6733459_1_1_1

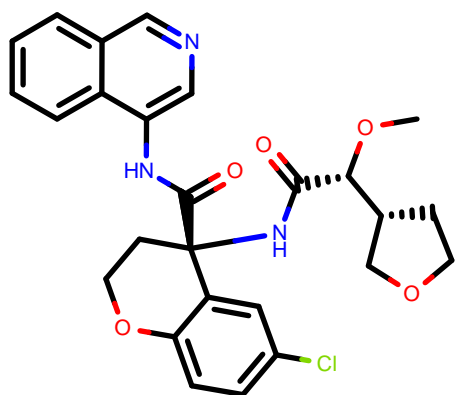
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)NC(=O)[C@@]5H5C[C@@H]6[C@@H](C6)OS(=O)(=O)N

RUN: RUN3185

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.53

EN300-298552_1_2_1



CID: EN300-298552_1_2_1

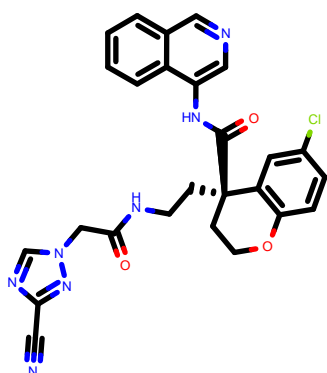
SMILES: CO[C@H]([C@@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3252

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.25

EN300-111863_3_1_1



CID: EN300-111863_3_1_1

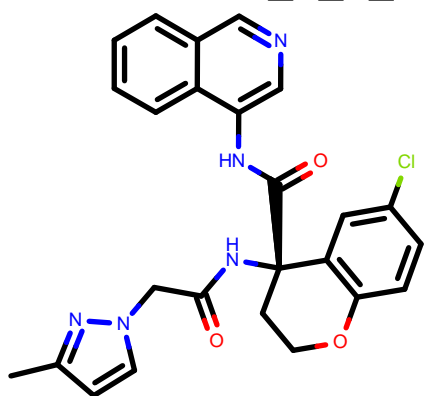
SMILES: c1ccc2c(c1)ncnc2N[C@@]([C@@]3[C@@]4COC4C3)C(=O)Nc5ccc6c5cnc6

RUN: RUN3386

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.30

EN300-226964_1_1_1



CID: EN300-226964_1_1_1

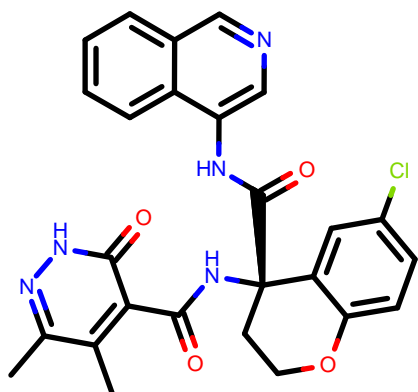
SMILES: Cc1ccn(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4851

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.21

EN300-29220_1_1_1



CID: EN300-29220_1_1_1

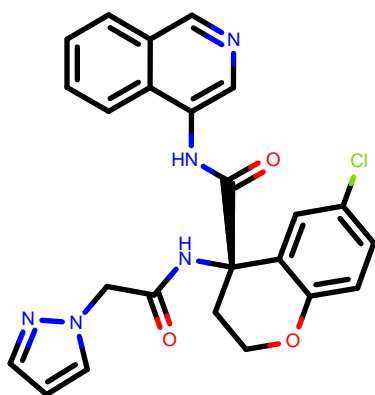
SMILES: Cc1c(n[nH]c1=O)c1c(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6549

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

EN300-23942_1_1_1



CID: EN300-23942_1_1_1

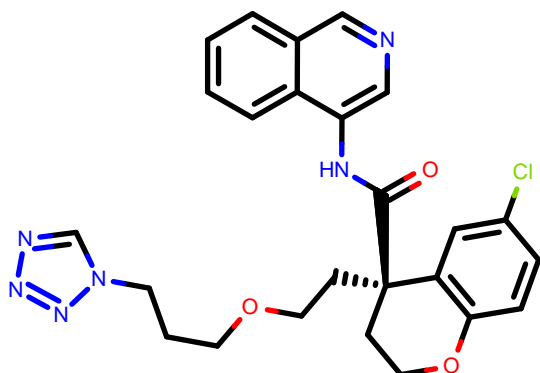
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cccn5

RUN: RUN3022

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.22

EN300-1696962_3_1_1



CID: EN300-1696962_3_1_1

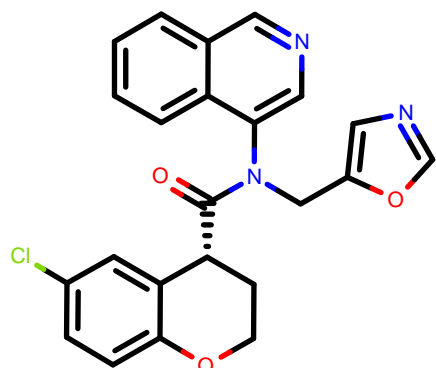
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5cnnn5

RUN: RUN3034

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

ALP-UNI-44c99a80-3_1



CID: ALP-UNI-44c99a80-3_1

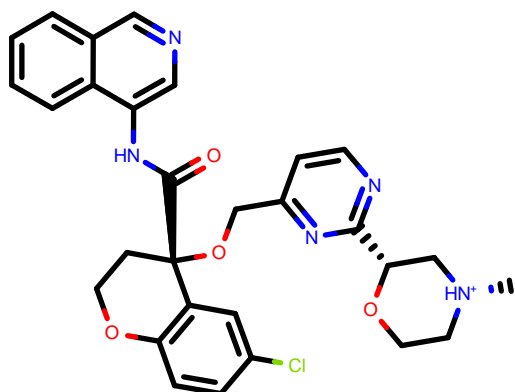
SMILES: c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN446

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.19

ED_-GRI-5b13fbe2-74_1



CID: ED_-GRI-5b13fbe2-74_1

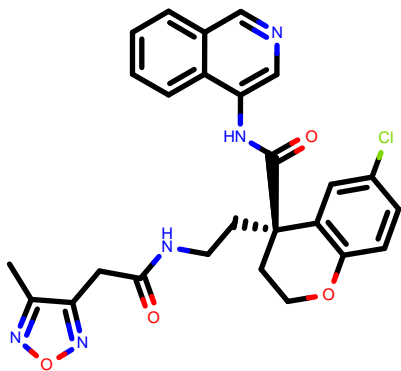
SMILES: CN([H])CCO[C@@H](C1=CN=CC=C1)C2=CC(=O)C(C)C(CO)C3=CC(=CC=C3)C(=O)N4CCCC4

RUN: RUN1538

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.33

EN300-254883_3_1_1



CID: EN300-254883_3_1_1

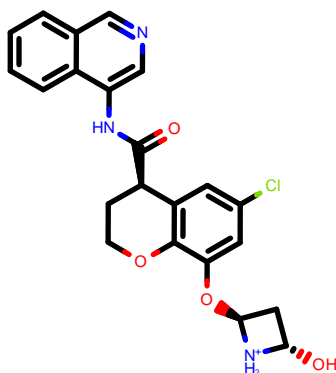
SMILES: Cc1c(non1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3642

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.26

VLA-UCB-50c39ae8-8_2_1



CID: VLA-UCB-50c39ae8-8_2_1

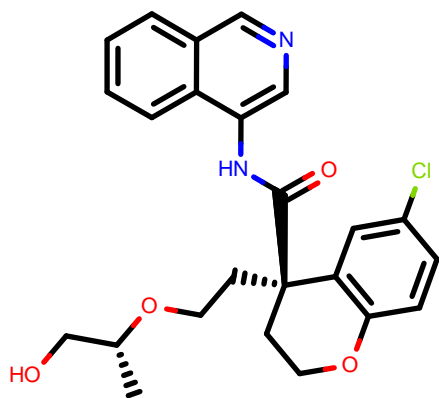
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl[C@H]5C[C@@H]([NH2+])OCl

RUN: RUN3384

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.33

EN300-175186_3_2_1



CID: EN300-175186_3_2_1

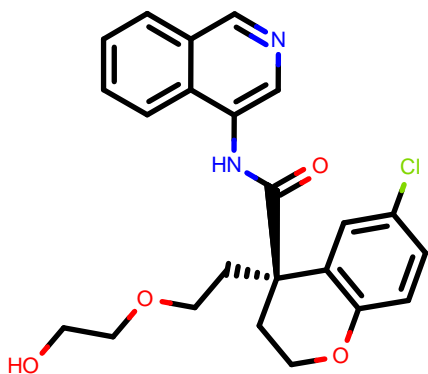
SMILES: C[C@H](CO)OCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN2885

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.28

EN300-21258_3_1_1



CID: EN300-21258_3_1_1

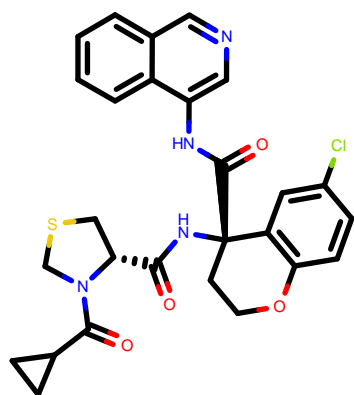
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOCCO

RUN: RUN3090

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.22

EN300-18928_1_2_1



CID: EN300-18928_1_2_1

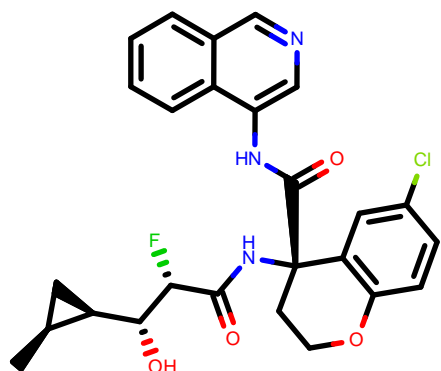
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CSCN5C(=O)C6CC6

RUN: RUN3392

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.35

EDG-MED-90036822-94_8



CID: EDG-MED-90036822-94_8

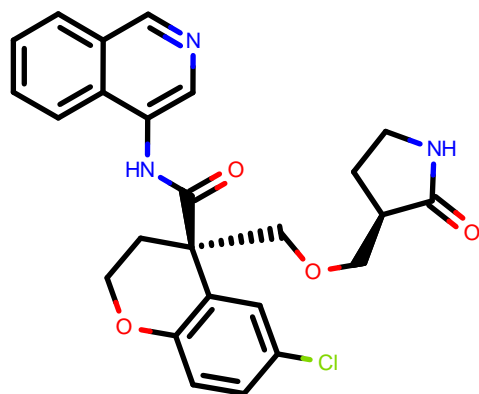
SMILES: C[C@@H]1C[C@@H]2[C@H](C[C@@H]1C(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N4c5ccc5c4ccccc5)F

RUN: RUN1670

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.26

EN300-246248_2_2_1



CID: EN300-246248_2_2_1

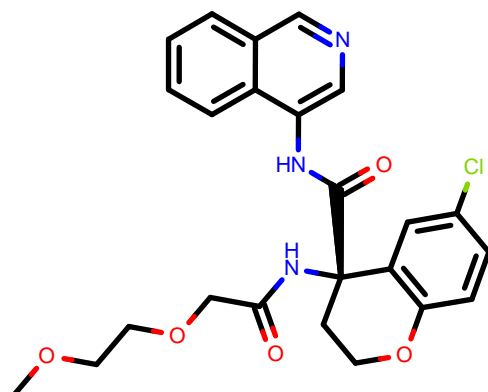
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCN5=O

RUN: RUN3590

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.23

EN300-20375_1_1_1



CID: EN300-20375_1_1_1

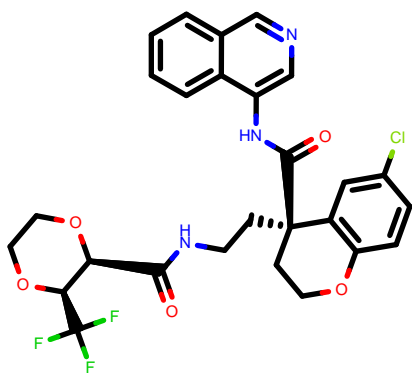
SMILES: COCOCOC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3224

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.23

EN300-322400_3_1_1



CID: EN300-322400_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOC4C3C(=O)C(CNC1=O)C@H5[C@@H](OCCO5)C(F)F

RUN:

RUN3082

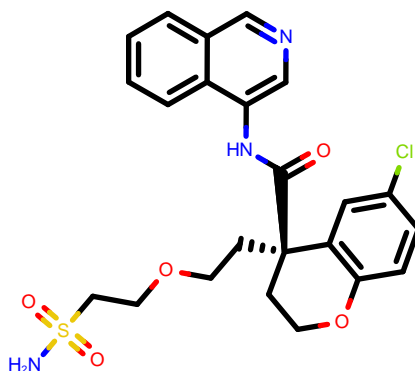
DDG (kcal/mol):

-2.41

dDDG (kcal/mol):

0.31

EN300-270710_3_1_1



CID: EN300-270710_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOC4C3C(=O)C(CNC(=O)N)C

RUN:

RUN3083

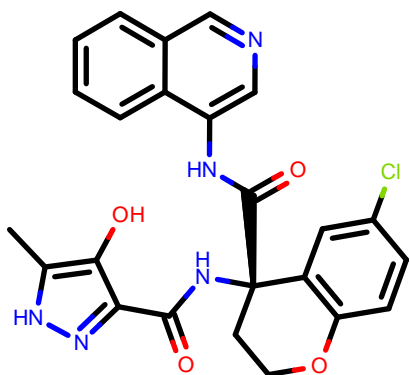
DDG (kcal/mol):

-2.40

dDDG (kcal/mol):

0.25

EN300-114526_1_1_1



CID: EN300-114526_1_1_1

SMILES:

Cc1c(c([nH]n1)C(=O)N)C@@2(C)CCOC3C2C(=O)C(C)C(=O)Nc4cncnc4O

RUN:

RUN2707

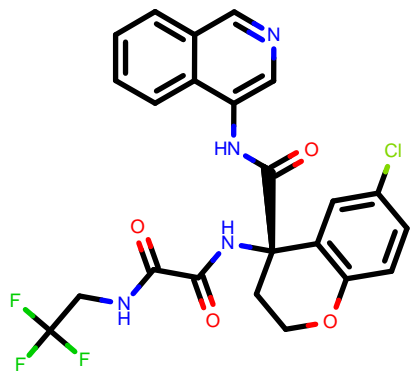
DDG (kcal/mol):

-2.40

dDDG (kcal/mol):

0.23

EN300-139268_1_1_1



CID: EN300-139268_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOC4C3C(=O)C(C)C(=O)N(C(F)F)F

RUN:

RUN5050

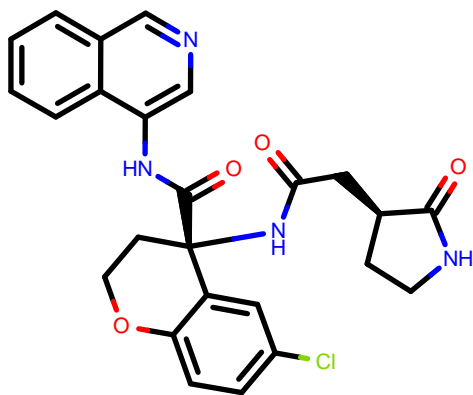
DDG (kcal/mol):

-2.40

dDDG (kcal/mol):

0.22

EN300-343474_1_1_1



CID: EN300-343474_1_1_1

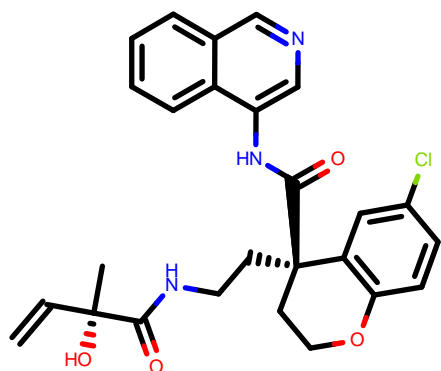
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)NC(=O)C[C@@H]5CCNC5=O

RUN: RUN3511

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.25

EN300-248888_3_2_1



CID: EN300-248888_3_2_1

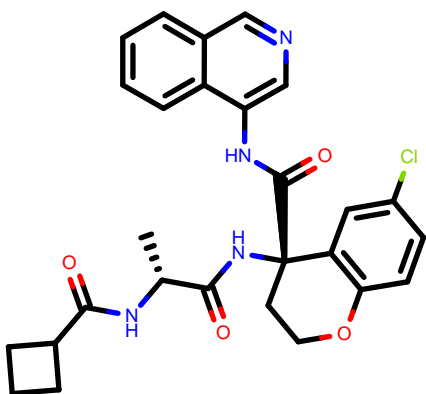
SMILES: C[C@H](C=C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2Cl)C)C(=O)Nc3nnc4c3cccc4)O

RUN: RUN6389

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.35

ALP-UNI-dbbfd3db-15_2



CID: ALP-UNI-dbbfd3db-15_2

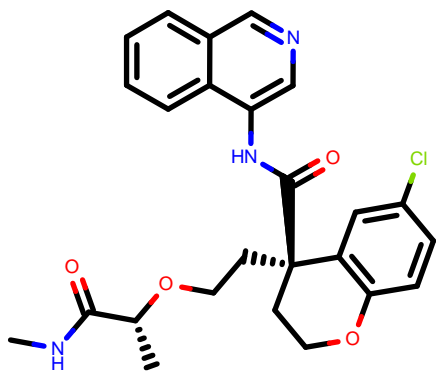
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C)C(=O)Nc3nnc4c3cccc4)NC(=O)C5CC5

RUN: RUN2652

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.32

EN300-211482_3_2_1



CID: EN300-211482_3_2_1

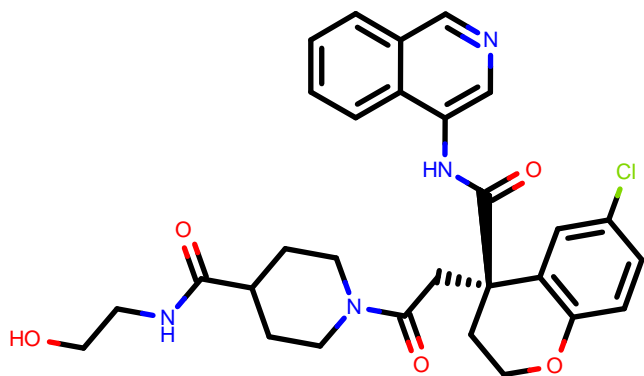
SMILES: C[C@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2Cl)C)C(=O)Nc3nnc4c3cccc4

RUN: RUN2995

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.33

EN300-344753_1_1_1



CID: EN300-344753_1_1_1

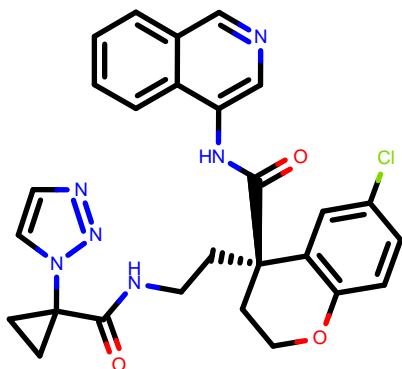
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(C5)C(=O)NCCO

RUN: RUN3993

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.48

EN300-658559_3_1_1



CID: EN300-658559_3_1_1

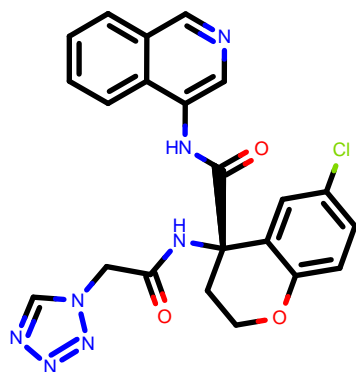
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(C5)n6ccnn6

RUN: RUN4391

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.35

EN300-20980_1_1_1



CID: EN300-20980_1_1_1

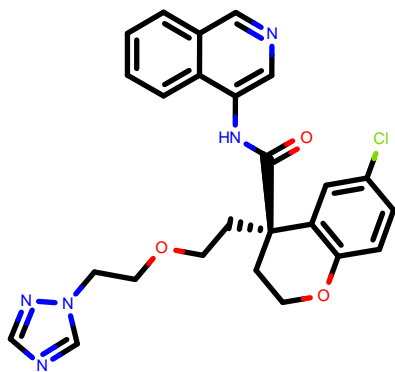
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnn5

RUN: RUN3116

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.24

EN300-6255179_3_1_1



CID: EN300-6255179_3_1_1

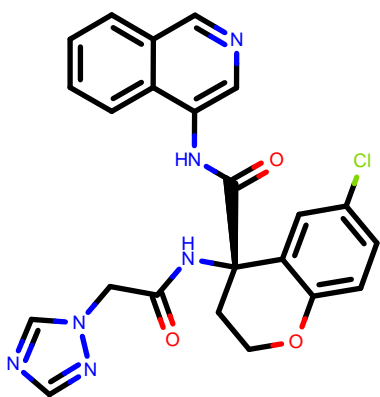
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnn5

RUN: RUN3624

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.31

EN300-06654_1_1_1



CID: EN300-06654_1_1_1

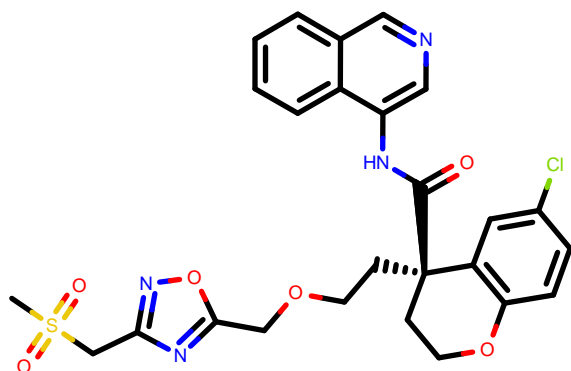
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncn5

RUN: RUN3582

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.22

EN300-94900_3_1_1



CID: EN300-94900_3_1_1

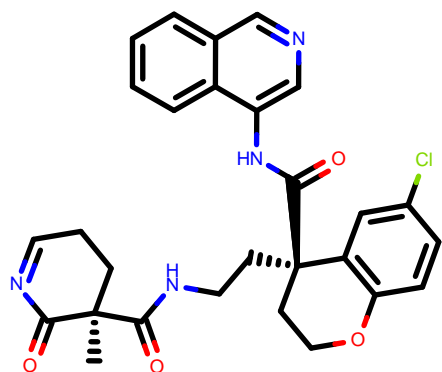
SMILES: CS(=O)(=O)Cc1nc(on1)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN: RUN3217

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.41

EN300-178876_3_2_1



CID: EN300-178876_3_2_1

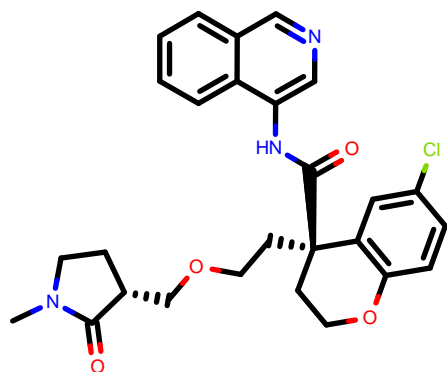
SMILES: C[C@@]1(CCCNC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN: RUN3787

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.47

EN300-260816_3_1_1



CID: EN300-260816_3_1_1

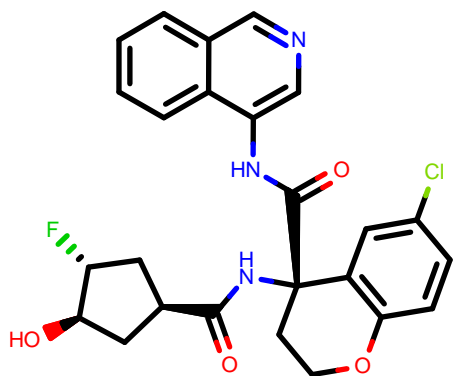
SMILES: CN1CC[C@@H](C1=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN: RUN3704

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.31

EN300-7461217_1_2_1



CID: EN300-7461217_1_2_1

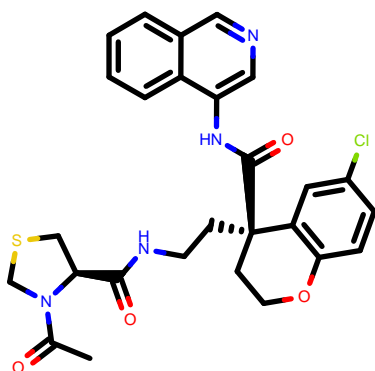
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C(=O)N[C@@H](C1=CC=C(C=C1)C(=O)N[C@@H](C)C(=O)N2)C(=O)N[C@@H](C)C(=O)N2

RUN: RUN5176

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.25

EN300-736749_3_1_1



CID: EN300-736749_3_1_1

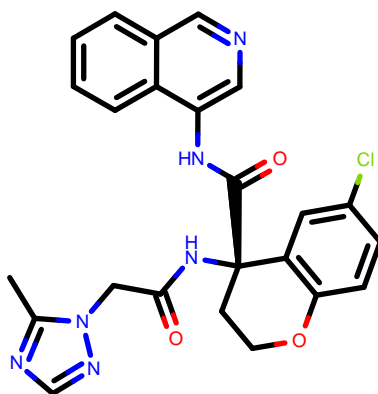
SMILES: CC(=O)N1CSC[C@H]1C(=O)N[C@@H](Cl)C(=O)N[C@@H](C1=CC=C(C=C1)C(=O)N[C@@H](C)C(=O)N2)C(=O)N[C@@H](C)C(=O)N2

RUN: RUN3321

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.32

EN300-7536177_1_1_1



CID: EN300-7536177_1_1_1

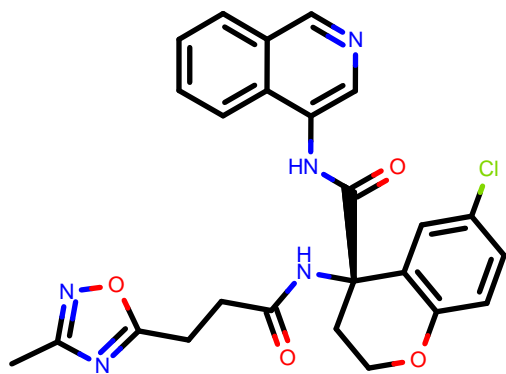
SMILES: Cc1nncn1CC(=O)N[C@@H](Cl)C(=O)N[C@@H](C1=CC=C(C=C1)C(=O)N[C@@H](C)C(=O)N2)C(=O)N[C@@H](C)C(=O)N2

RUN: RUN4299

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.24

EN300-27268_1_1_1



CID: EN300-27268_1_1_1

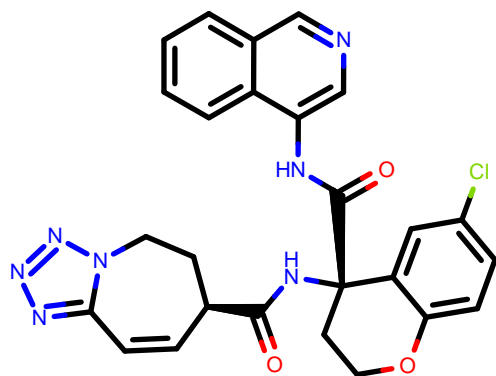
SMILES: Cc1nc(on1)CCC(=O)N[C@@H](Cl)C(=O)N[C@@H](C1=CC=C(C=C1)C(=O)N[C@@H](C)C(=O)N2)C(=O)N[C@@H](C)C(=O)N2

RUN: RUN3761

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.22

EN300-253571_1_2_1



CID: EN300-253571_1_2_1

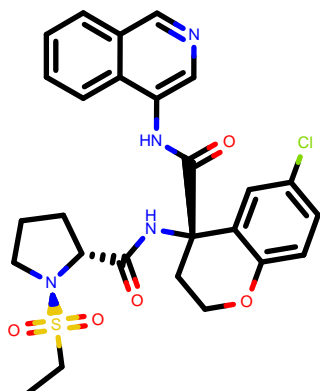
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC6nnc6CC5

RUN: RUN2976

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.31

EN300-16091_1_1_1



CID: EN300-16091_1_1_1

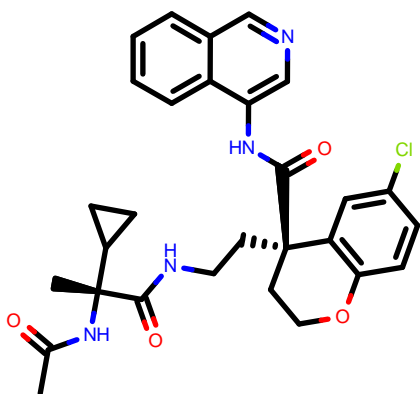
SMILES: CCS(=O)(=O)[N@@]1CCC[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5163

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.56

EN300-67073_3_2_1



CID: EN300-67073_3_2_1

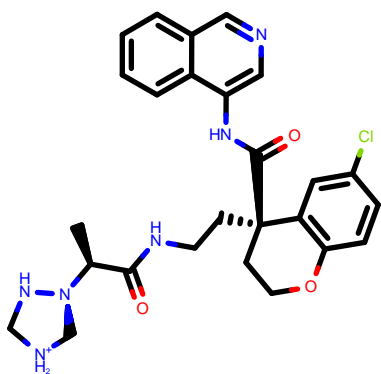
SMILES: CC(=O)N[C@@]1(C)C1CC1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6116

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.31

EN300-30397_3_1_1



CID: EN300-30397_3_1_1

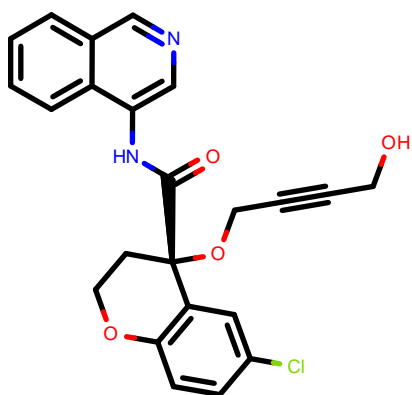
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)n5enon5

RUN: RUN4267

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.26

EN300-83766_1_1_1



CID: EN300-83766_1_1_1

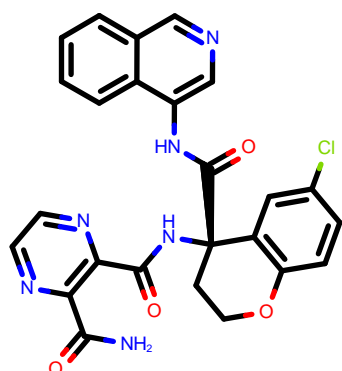
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC#CO

RUN: RUN3976

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.20

EN300-21200_1_1_1



CID: EN300-21200_1_1_1

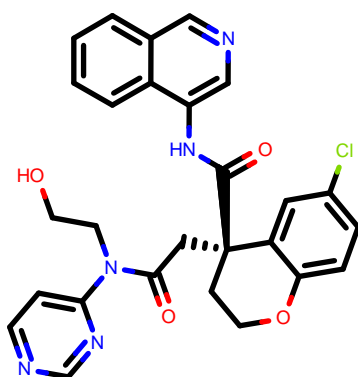
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ncn5)C(=O)N

RUN: RUN7136

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.25

EN300-256174_1_1_1



CID: EN300-256174_1_1_1

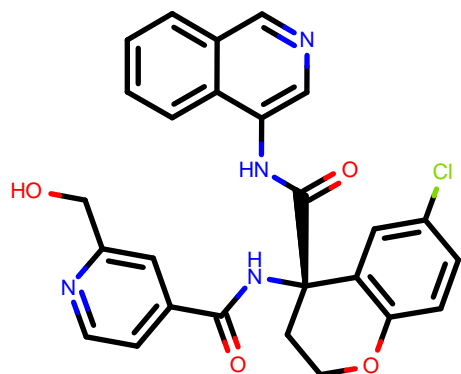
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5ccnnc5

RUN: RUN4593

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.40

EN300-396748_1_1_1



CID: EN300-396748_1_1_1

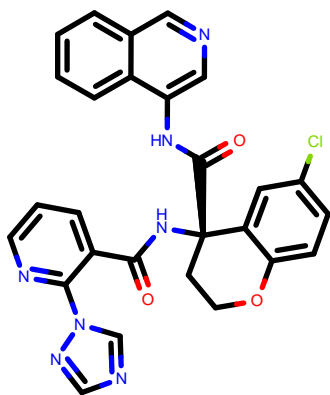
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccncc5CO

RUN: RUN3776

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.23

EN300-28571_1_1_1



CID: EN300-28571_1_1_1

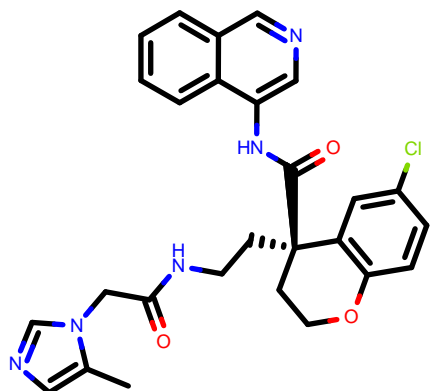
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cccn5n6cncn6

RUN: RUN3653

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.22

EN300-315453_3_1_1



CID: EN300-315453_3_1_1

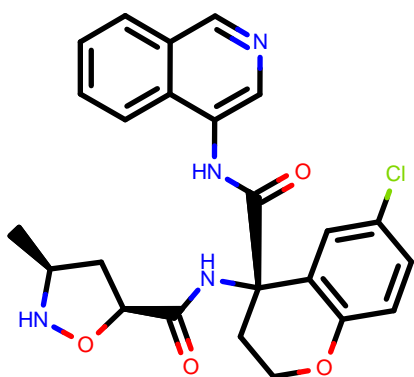
SMILES: Cc1cncn1CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4754

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.31

EN300-92447_1_1_2



CID: EN300-92447_1_1_2

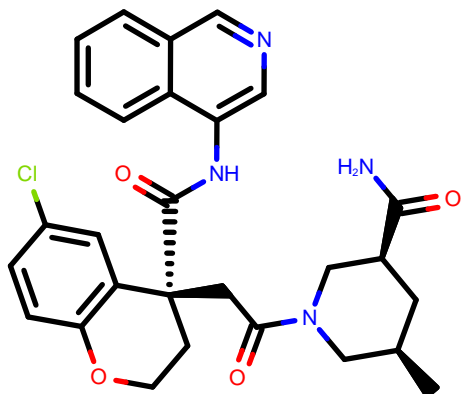
SMILES: C[C@@H]1C[C@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3437

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.30

EN300-1724086_1_1_1



CID: EN300-1724086_1_1_1

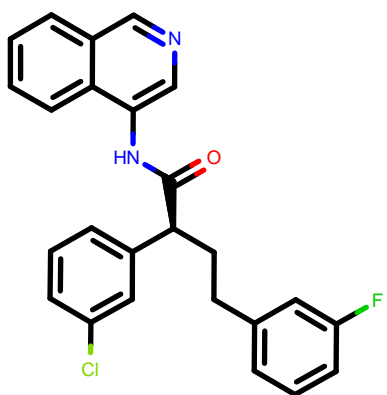
SMILES: C[C@@]1(C)[C@H](CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5)Cl=O

RUN: RUN3812

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.32

MIC-UNK-c66144cb-1_1



CID: MIC-UNK-c66144cb-1_1

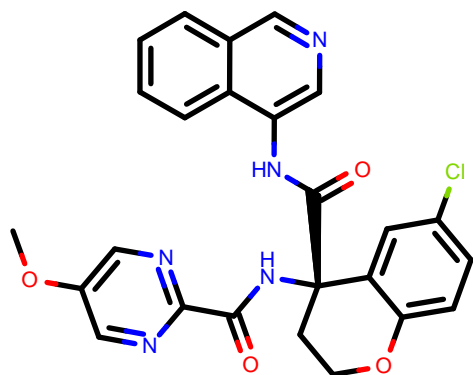
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](CCc3ccccc(c3)F)c4ccc(c4)Cl

RUN: RUN155

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.26

EN300-225053_1_1_1



CID: EN300-225053_1_1_1

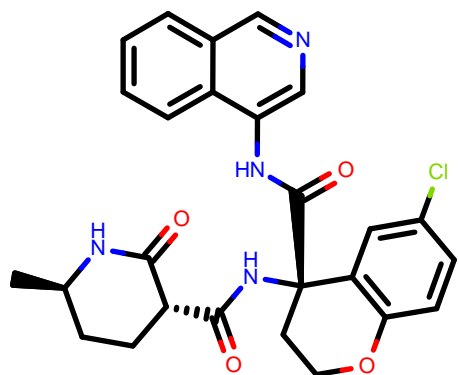
SMILES: COc1cnc(nc1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3641

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.19

EN300-6505003_1_3_1



CID: EN300-6505003_1_3_1

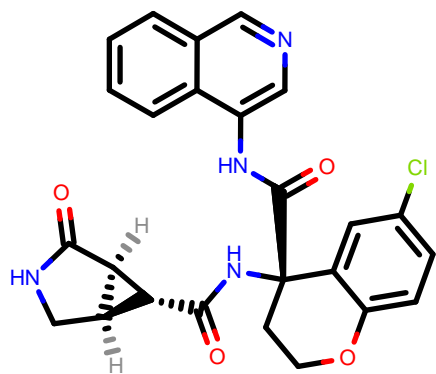
SMILES: C[C@@H]1CC[C@H](C(=O)N1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3440

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.24

EN300-7501017_1_1_1



CID: EN300-7501017_1_1_1

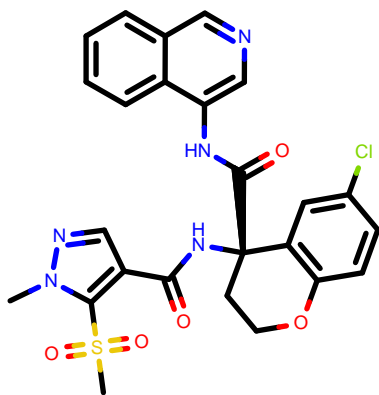
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(c4)NC(=O)[C@@H]5[C@@H]6[C@H]5[C@H]6

RUN: RUN3107

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.26

EN300-180069_1_1_1



CID: EN300-180069_1_1_1

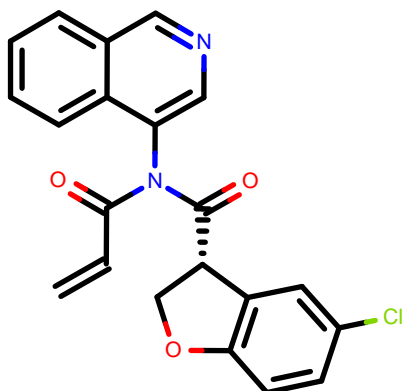
SMILES: Cn1c(c(en1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C

RUN: RUN3136

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.27

MAT-POS-e69ad64a-2_2



CID: MAT-POS-e69ad64a-2_2

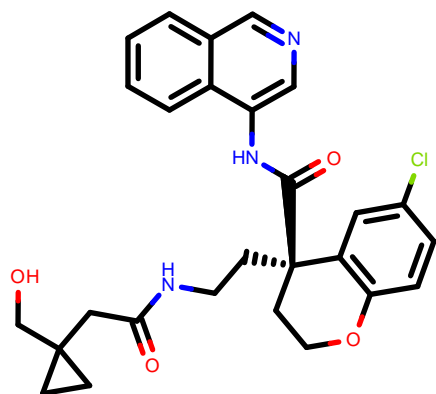
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl

RUN: RUN2150

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.28

EN300-107048_3_1_1



CID: EN300-107048_3_1_1

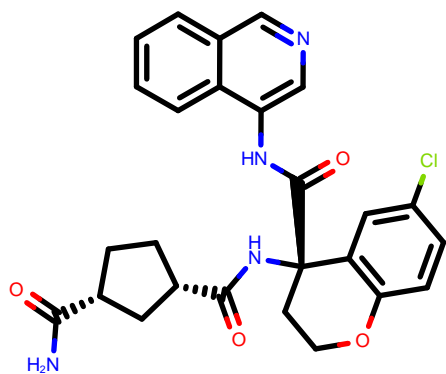
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)CC5(CC5)CO

RUN: RUN4779

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.31

EN300-370753_1_1_1



CID: EN300-370753_1_1_1

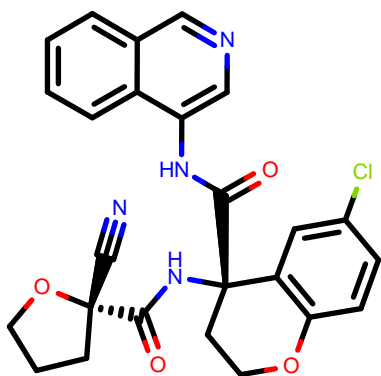
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](C5)C(=O)N

RUN: RUN3296

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.30

EN300-3710141_1_1_1



CID: EN300-3710141_1_1_1

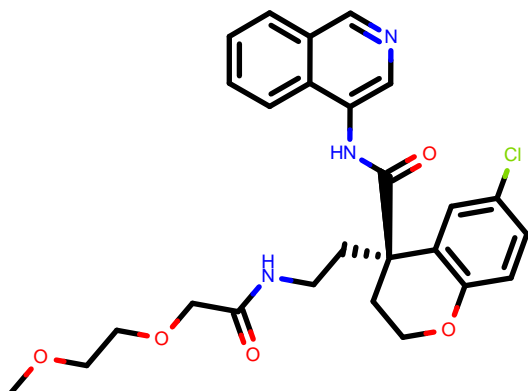
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCO5)C#N

RUN: RUN3287

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.29

EN300-20375_3_1_1



CID: EN300-20375_3_1_1

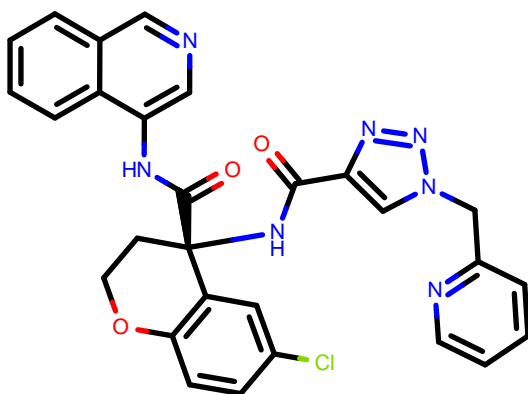
SMILES: COCCOCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cnc4c3ccccc4

RUN: RUN4126

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.32

EN300-91315_1_1_1



CID: EN300-91315_1_1_1

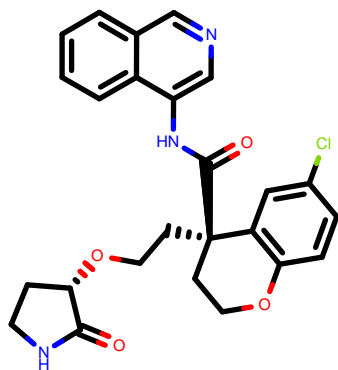
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nc5)Cc6ccccn6

RUN: RUN4837

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.31

EN300-6736413_3_2_1



CID: EN300-6736413_3_2_1

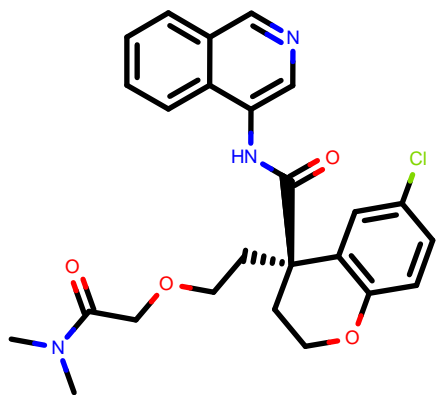
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@H]5CCNC5=O

RUN: RUN3530

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.27

EN300-216063_3_1_1



CID: EN300-216063_3_1_1

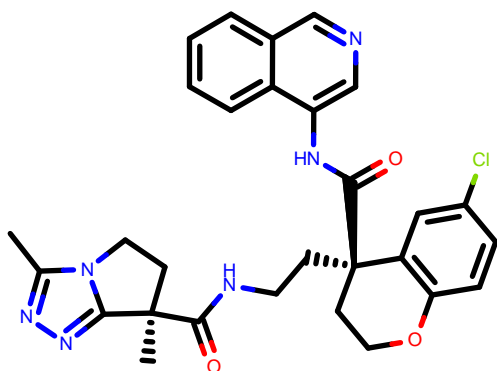
SMILES: CN(C)C(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4086

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.22

EN300-7431629_3_1_1



CID: EN300-7431629_3_1_1

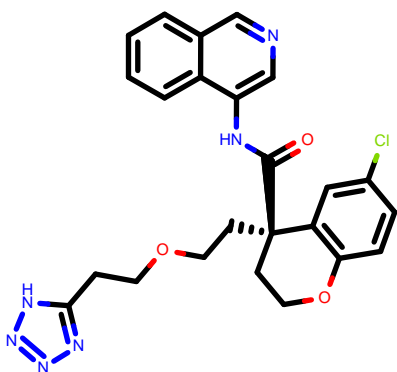
SMILES: Cc1nn2n1CC[C@@]2(C)C(=O)NCC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5cccc6

RUN: RUN2926

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.37

EN300-183231_3_1_1



CID: EN300-183231_3_1_1

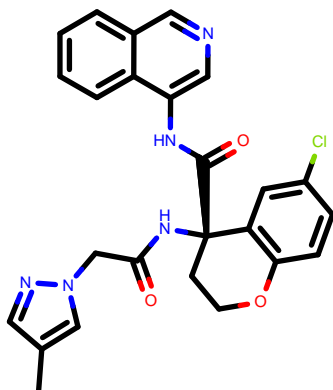
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5n[n-]nn5

RUN: RUN5369

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.39

EN300-51832_1_1_1



CID: EN300-51832_1_1_1

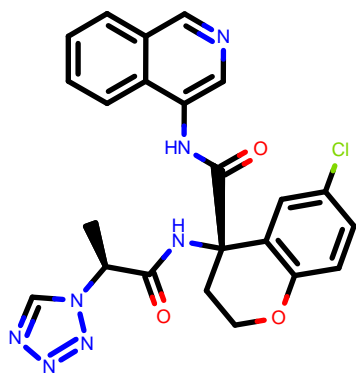
SMILES: Cc1cnn(c1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3324

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.23

EN300-191915_1_1_1



CID: EN300-191915_1_1_1

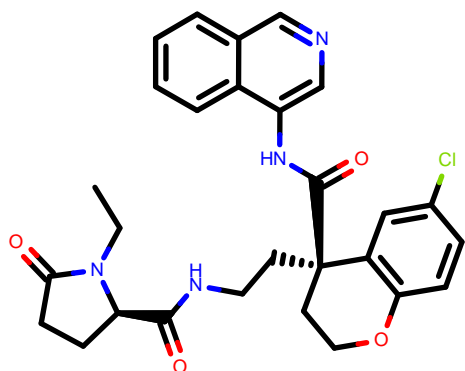
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4)n5ennn5

RUN: RUN2875

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.27

EN300-718785_3_2_1



CID: EN300-718785_3_2_1

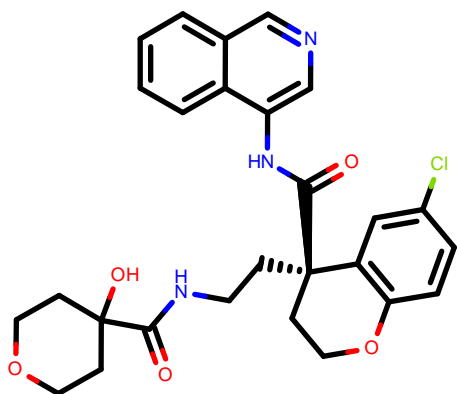
SMILES: CCN1[C@@H](CCC1=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN5531

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.36

EN300-69368_3_1_1



CID: EN300-69368_3_1_1

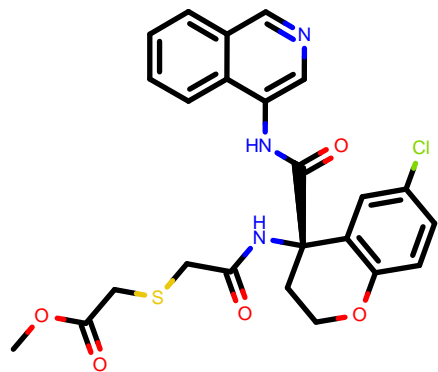
SMILES: c1ccc2c(c1)ncnc2N[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COCC5)O

RUN: RUN6910

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.34

EN300-135060_1_1_1



CID: EN300-135060_1_1_1

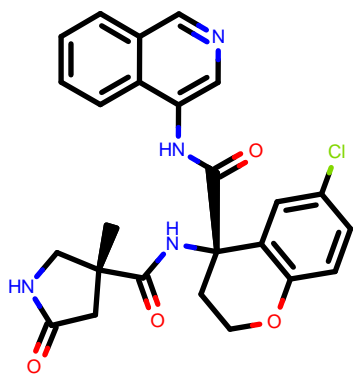
SMILES: COC(=O)CSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3ccc4

RUN: RUN3885

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.25

EN300-132157_1_2_1



CID: EN300-132157_1_2_1

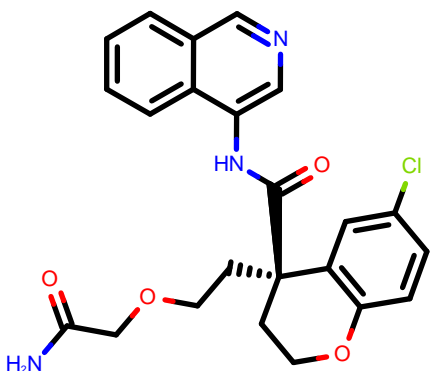
SMILES: C[C@]1(CC(=O)NC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN3237

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.27

EN300-18249_3_1_1



CID: EN300-18249_3_1_1

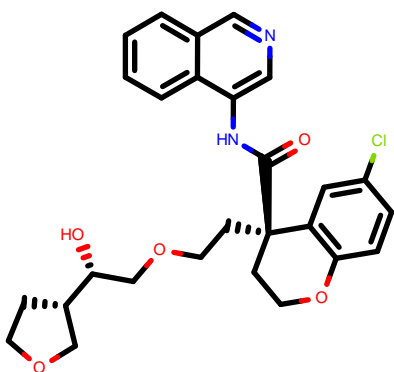
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N

RUN: RUN3071

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.20

EN300-1911992_3_4_1



CID: EN300-1911992_3_4_1

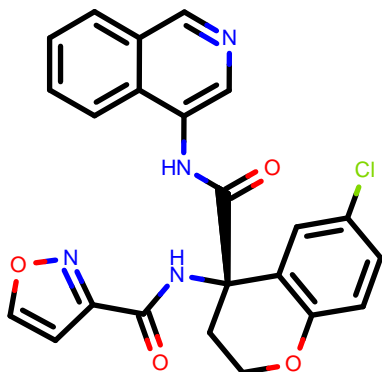
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]([C@@H]5CCOC(=O)5)O

RUN: RUN4858

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.45

EN300-22245_1_1_1



CID: EN300-22245_1_1_1

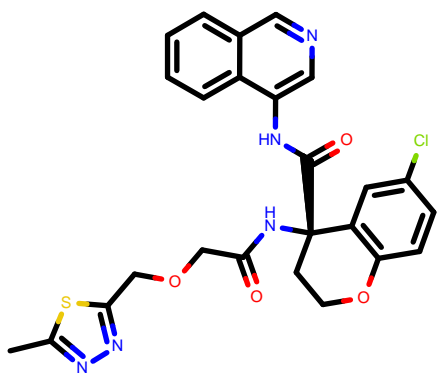
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccon5

RUN: RUN3190

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.19

EN300-206870_1_1_1



CID: EN300-206870_1_1_1

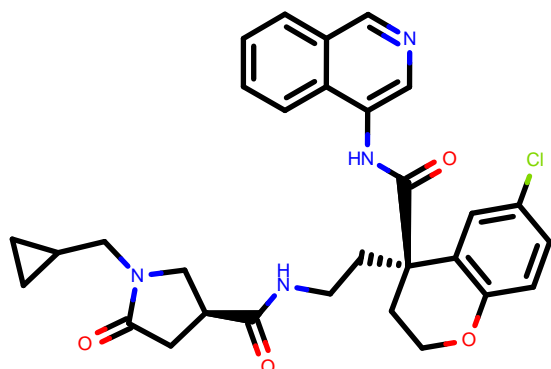
SMILES: Cc1nn(s1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3974

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.34

EN300-31969_3_2_1



CID: EN300-31969_3_2_1

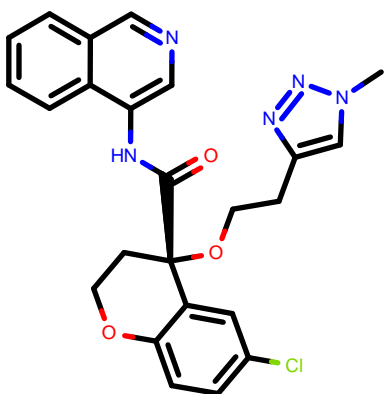
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)N[C@@H]5C(=O)N(C5)COC6C6

RUN: RUN6906

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.38

EN300-1600786_1_1_1



CID: EN300-1600786_1_1_1

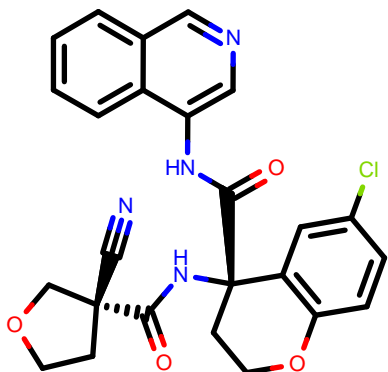
SMILES: Cn1cc(nn1)CCO[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4970

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.22

EN300-261210_1_1_1



CID: EN300-261210_1_1_1

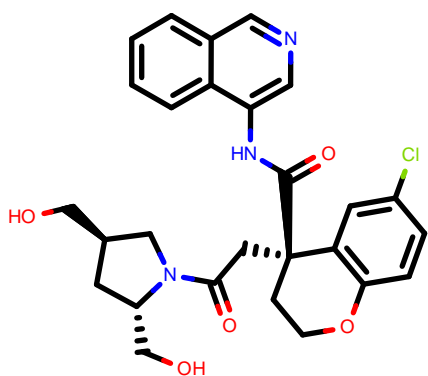
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)N[C@@]5(CCOCC5)C#N

RUN: RUN3323

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-1212400_1_3_1



CID: EN300-1212400_1_3_1

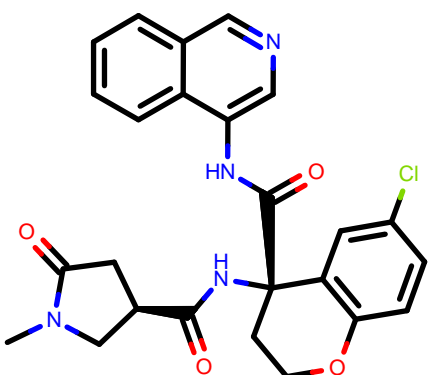
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H]5CO)CO

RUN: RUN4005

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.39

EN300-33601_1_1_1



CID: EN300-33601_1_1_1

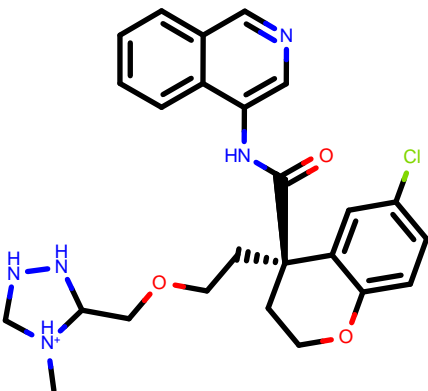
SMILES: CN1C[C@@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3899

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-113112_3_1_1



CID: EN300-113112_3_1_1

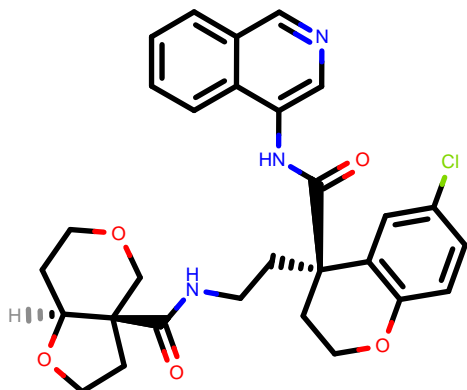
SMILES: Cn1cnc1COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3821

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-341337_3_3_1



CID: EN300-341337_3_3_1

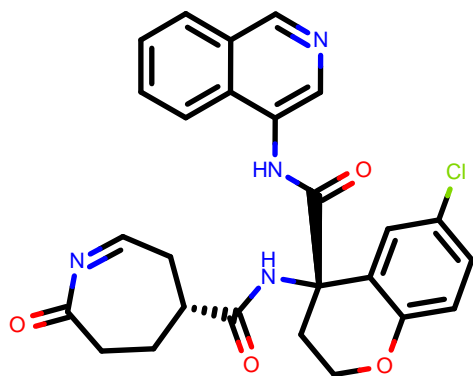
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]56CC[C@@H]5COO6

RUN: RUN3182

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.46

EN300-152337_1_1_1



CID: EN300-152337_1_1_1

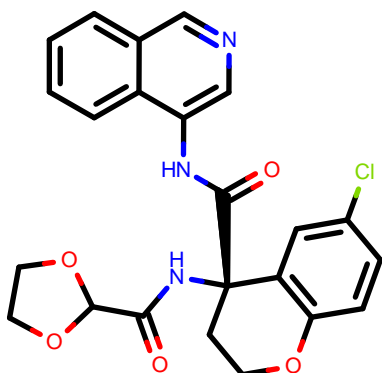
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CCC(=O)NC55

RUN: RUN3288

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.30

EN300-154942_1_1_1



CID: EN300-154942_1_1_1

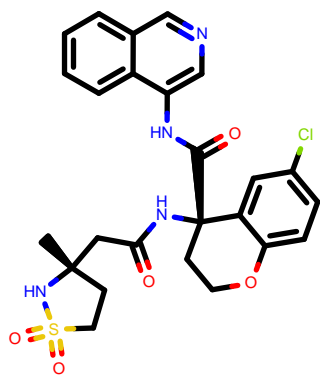
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCO5

RUN: RUN3394

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.19

EN300-385235_1_2_1



CID: EN300-385235_1_2_1

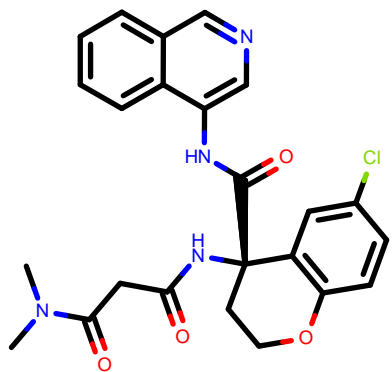
SMILES: C[C@]1(CCS(=O)(=O)N1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc4c3ccccc5

RUN: RUN3368

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.33

EN300-93573_1_1_1



CID: EN300-93573_1_1_1

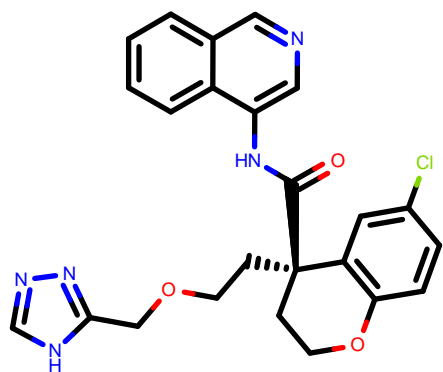
SMILES: CN(C)C(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4

RUN: RUN3120

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.27

EN300-306316_3_1_1



CID: EN300-306316_3_1_1

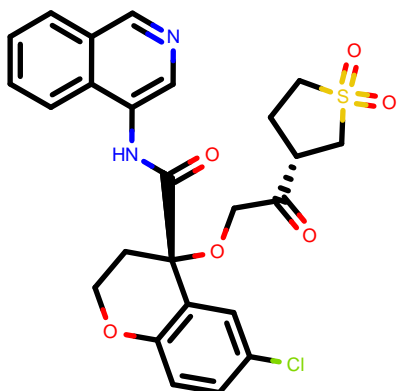
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]nnc5

RUN: RUN3105

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.22

EN300-226314_1_1_1



CID: EN300-226314_1_1_1

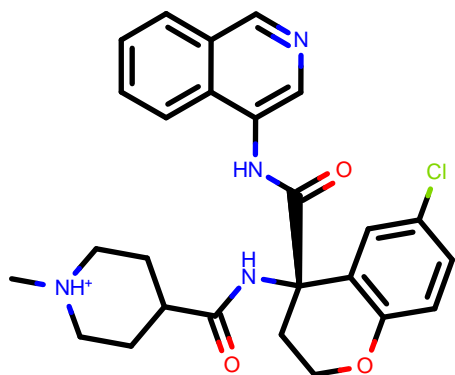
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5CCS(=O)(=O)C5

RUN: RUN5418

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.29

EN300-51886_1_1_1



CID: EN300-51886_1_1_1

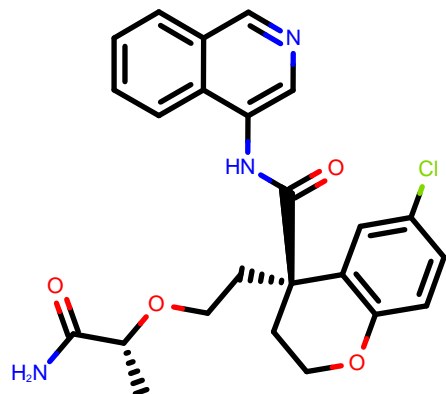
SMILES: C[NH+]1CCC(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4905

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.36

EN300-17381_3_2_1



CID: EN300-17381_3_2_1

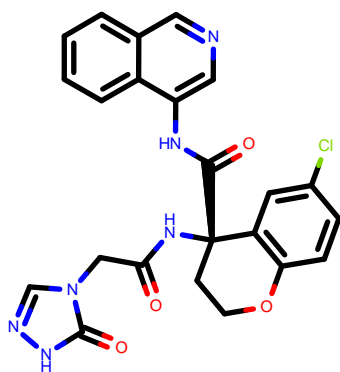
SMILES: C[C@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2986

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.24

EN300-120820_1_1_1



CID: EN300-120820_1_1_1

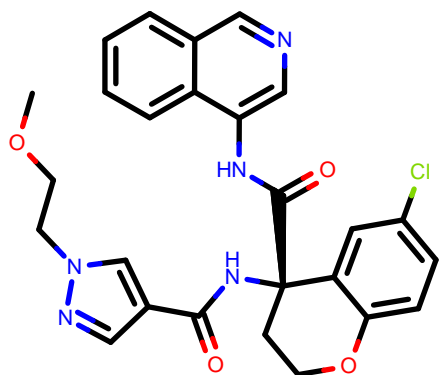
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)N)C(=O)Cn5cn[nH]c5=O

RUN: RUN3152

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.24

EN300-194199_1_1_1



CID: EN300-194199_1_1_1

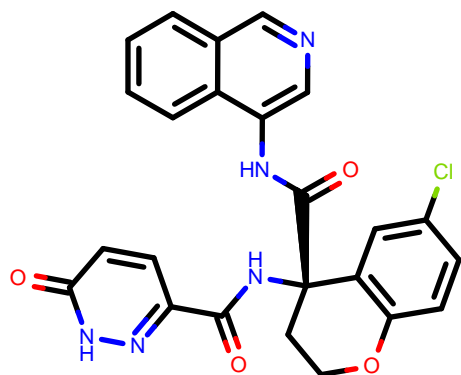
SMILES: COCc1cc(cn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3921

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.32

EN300-04614_1_1_1



CID: EN300-04614_1_1_1

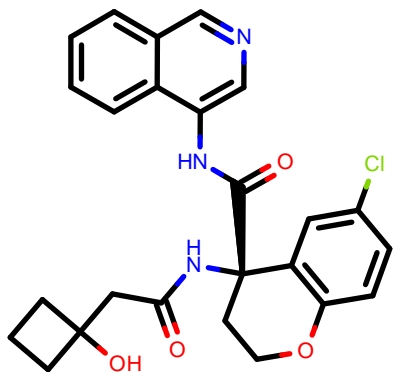
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)N)C(=O)c5ccc(=O)[nH]n5

RUN: RUN4428

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.19

EN300-246423_1_1_1



CID: EN300-246423_1_1_1

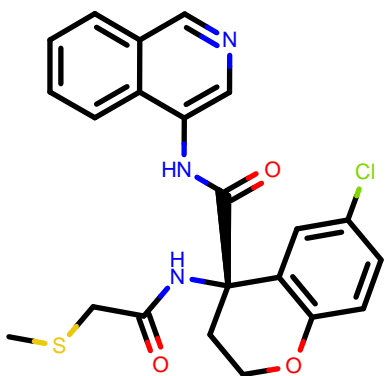
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)N)C(=O)CC5(CCC5)O

RUN: RUN3326

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.24

EN300-07879_1_1_1



CID: EN300-07879_1_1_1

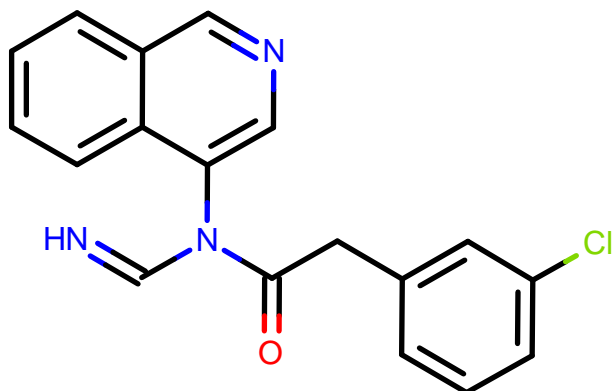
SMILES: CSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN2978

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.20

PET-UNK-5ecb6237-1_1



CID: PET-UNK-5ecb6237-1_1

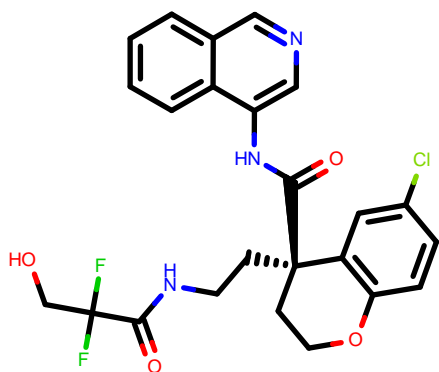
SMILES: c1ccc2c(c1)cnc2N(C#N)C(=O)Cc3cccc(c3)Cl

RUN: RUN443

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.31

EN300-123489_3_1_1



CID: EN300-123489_3_1_1

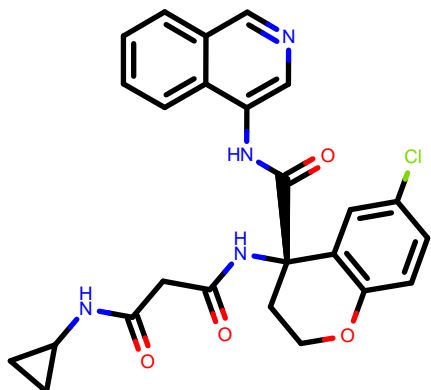
SMILES: c1ccc2c(c1)cnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(CO)(F)F

RUN: RUN3533

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.21

EN300-128464_1_1_1



CID: EN300-128464_1_1_1

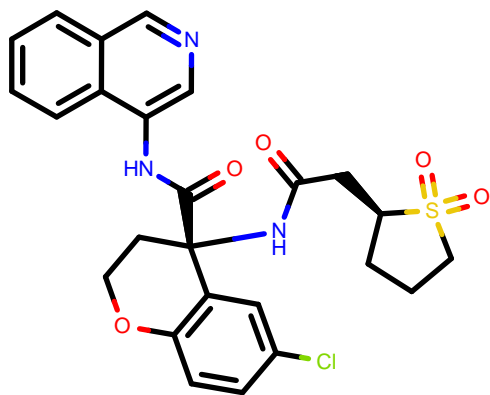
SMILES: c1ccc2c(c1)cnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)NC5CC5

RUN: RUN5263

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.28

EN300-155176_1_1_1



CID: EN300-155176_1_1_1

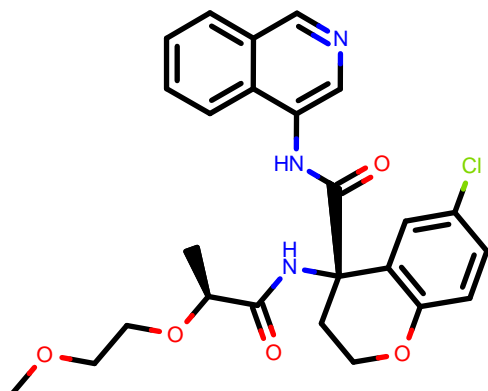
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCS5(=O)=O

RUN: RUN4124

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.34

EN300-77359_1_1_1



CID: EN300-77359_1_1_1

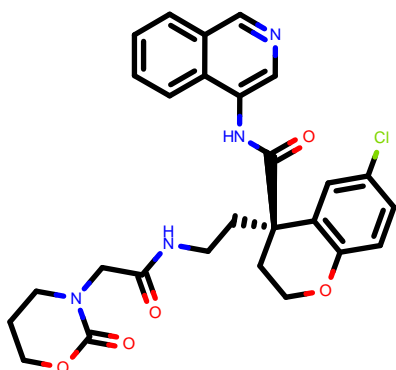
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)OCCOC

RUN: RUN3862

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.27

EN300-103638_3_1_1



CID: EN300-103638_3_1_1

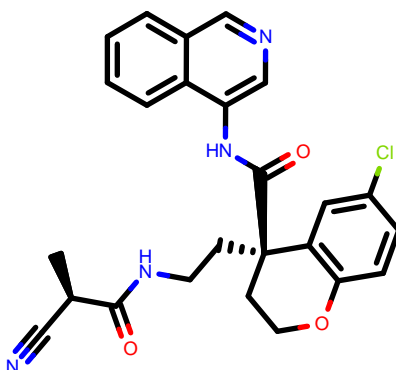
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5CCOC5=O

RUN: RUN3683

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.30

EN300-72730_3_2_1



CID: EN300-72730_3_2_1

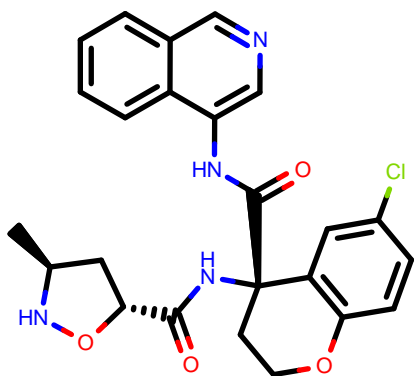
SMILES: C[C@@H](C#N)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5726

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.23

EN300-92447_1_2_2



CID: EN300-92447_1_2_2

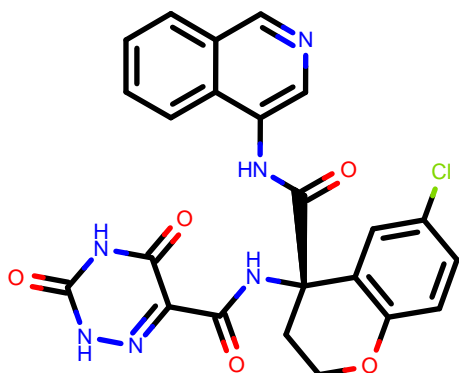
SMILES: C[C@H]1C[C@@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3494

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.28

EN300-122319_1_1_1



CID: EN300-122319_1_1_1

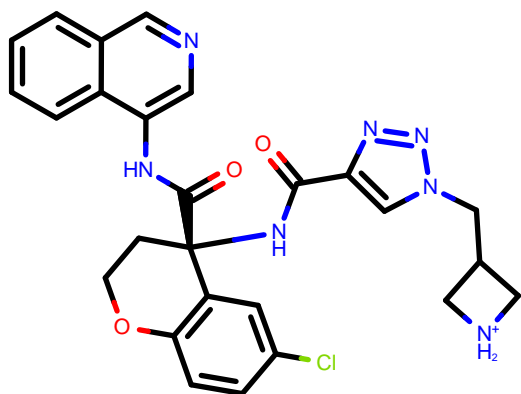
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5c(=O)[nH]c(=O)[nH]n5

RUN: RUN3356

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EDG-MED-90036822-6_1



CID: EDG-MED-90036822-6_1

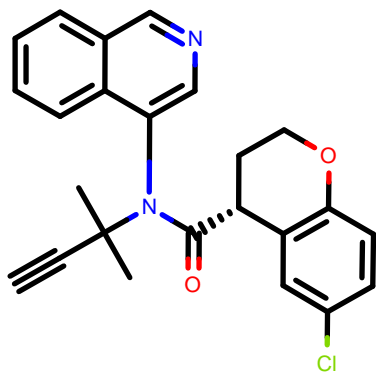
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cn(n5)CC6C[NH2+]C6

RUN: RUN1525

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.31

DAR-DIA-5ff57136-14_1



CID: DAR-DIA-5ff57136-14_1

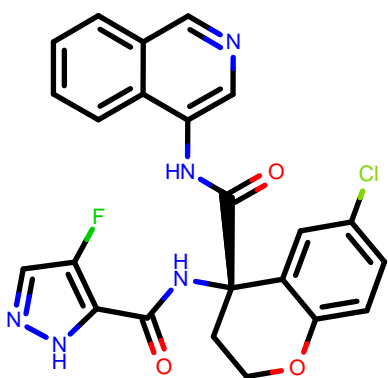
SMILES: CC(C)(C#C)N(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4Cl)C

RUN: RUN1258

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.18

EN300-98143_1_1_1



CID: EN300-98143_1_1_1

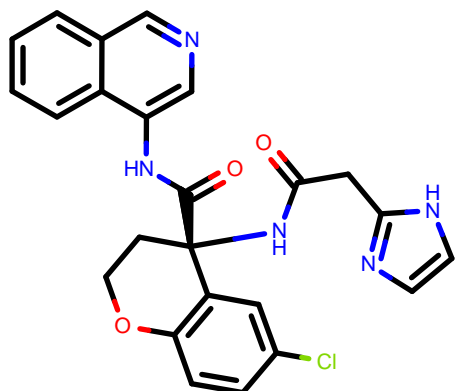
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]5F

RUN: RUN3605

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EN300-220527_1_1_1



CID: EN300-220527_1_1_1

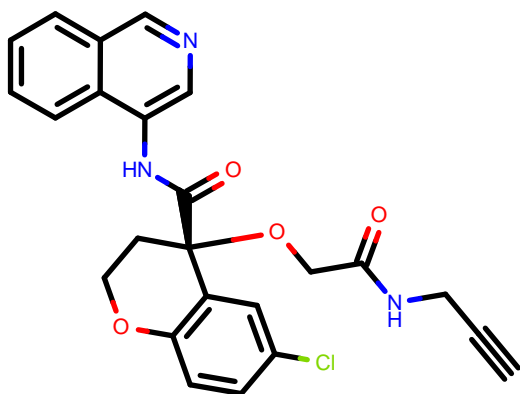
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C5[nH]5cn5

RUN: RUN3912

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.20

EN300-1659582_1_1_1



CID: EN300-1659582_1_1_1

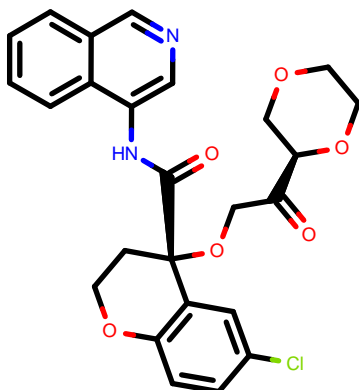
SMILES: C#CCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN4104

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.21

CHO-MSK-5891c1ff-2_1



CID: CHO-MSK-5891c1ff-2_1

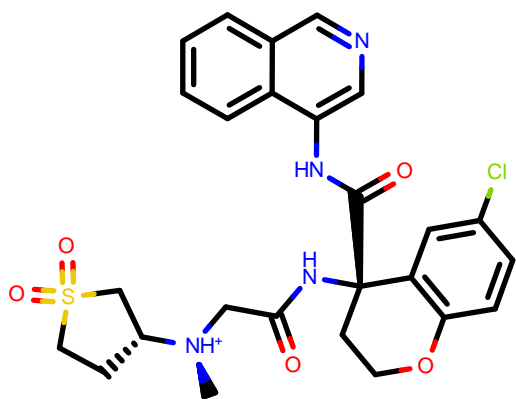
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)OCC(=O)[C@H]5COC5O5

RUN: RUN1774

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.29

EN300-14628_1_1_1



CID: EN300-14628_1_1_1

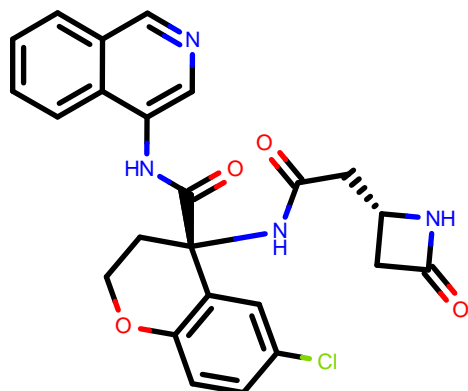
SMILES: C1Nc2cc3cc(C(=O)N[C@@H]4CSCC4)cc(C(=O)N[C@@H]5CC(=O)N5)c2c1

RUN: RUN5046

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.40

EN300-250593_1_2_1



CID: EN300-250593_1_2_1

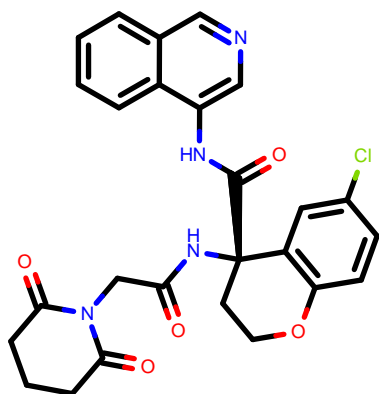
SMILES: C1c2cc3c(c1)nc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CC(=O)N5

RUN: RUN5544

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.23

EN300-54837_1_1_1



CID: EN300-54837_1_1_1

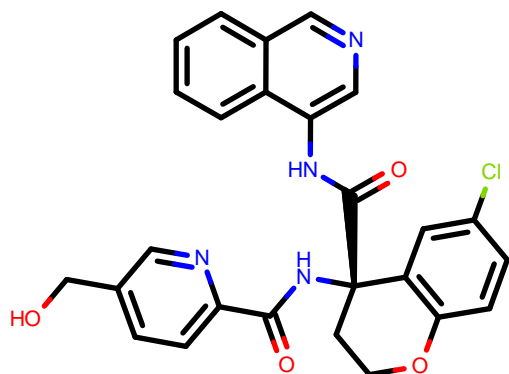
SMILES: C1c2cc3c(c1)nc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)C5CC(=O)CC5=O

RUN: RUN7331

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.27

EN300-1270299_1_1_1



CID: EN300-1270299_1_1_1

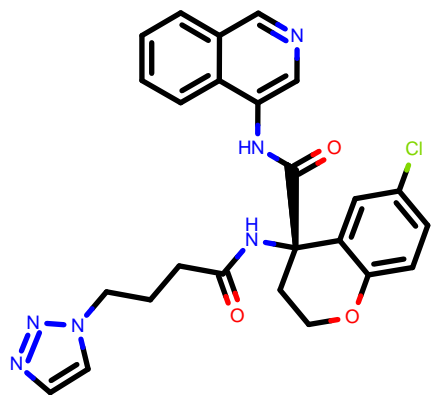
SMILES: C1c2cc3c(c1)nc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(cc5)CO

RUN: RUN5813

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.24

EN300-124301_1_1_1



CID: EN300-124301_1_1_1

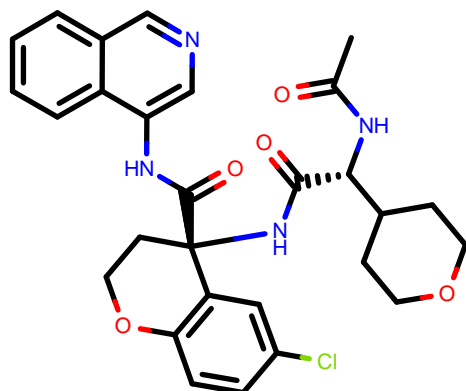
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5ccnn5

RUN: RUN3457

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.27

EN300-158292_1_2_1



CID: EN300-158292_1_2_1

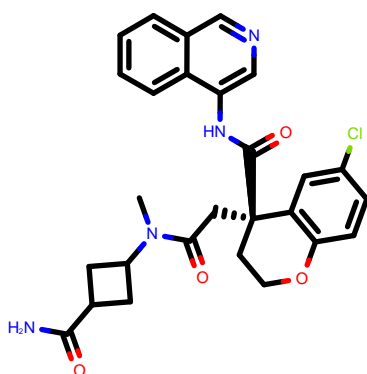
SMILES: CC(=O)N[C@@H](C1CCOCC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccoc5

RUN: RUN3767

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.27

EN300-321459_1_1_1



CID: EN300-321459_1_1_1

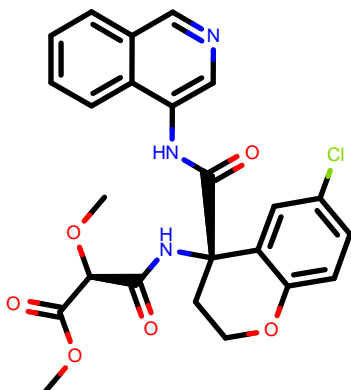
SMILES: CN(C1CC(C1)C(=O)N)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccoc5

RUN: RUN5309

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.23

EN300-1718194_1_1_1



CID: EN300-1718194_1_1_1

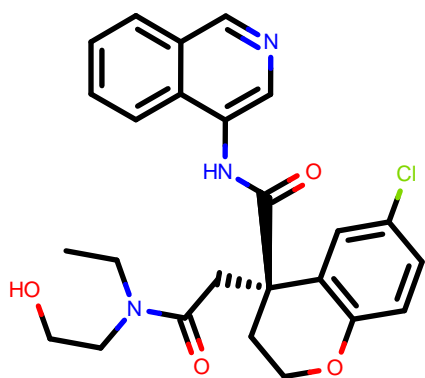
SMILES: CO[C@@]3(H)[C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3ccoc4)C(=O)OC

RUN: RUN3732

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.28

EN300-74448_1_1_1



CID: EN300-74448_1_1_1

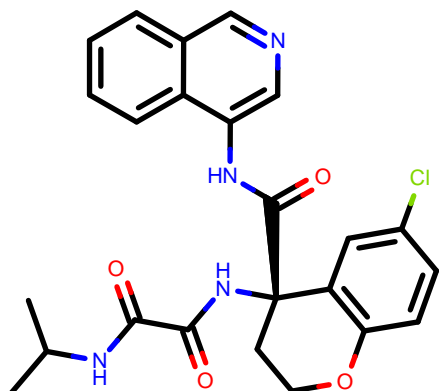
SMILES: CCN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3779

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.32

EN300-1262640_1_1_1



CID: EN300-1262640_1_1_1

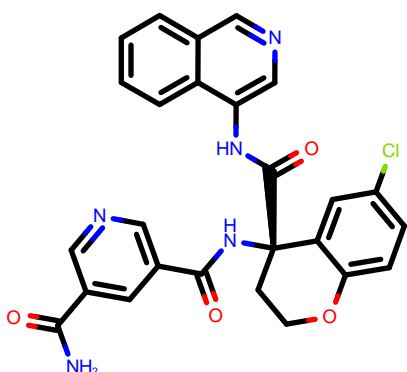
SMILES: CC(C)NC(=O)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3299

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.25

EN300-44993_1_1_1



CID: EN300-44993_1_1_1

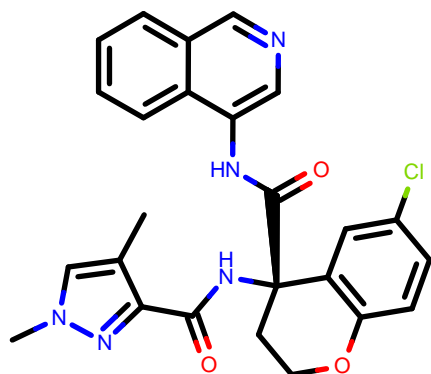
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(cnc5)C(=O)N

RUN: RUN6010

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.23

EN300-255422_1_1_1



CID: EN300-255422_1_1_1

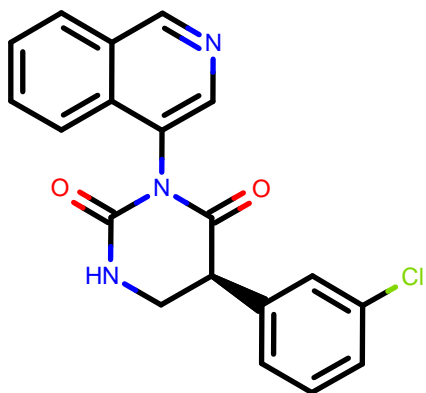
SMILES: Cc1cn(nc1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN3471

DDG (kcal/mol): -2.17

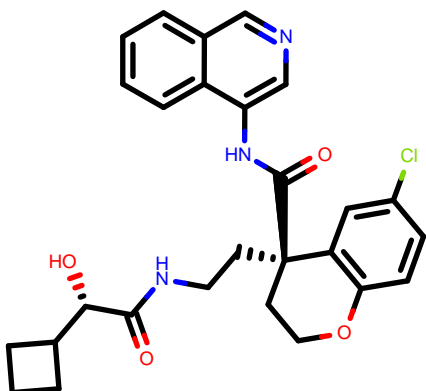
dDDG (kcal/mol): 0.25

VLA-UCB-1dbca3b4-18_2



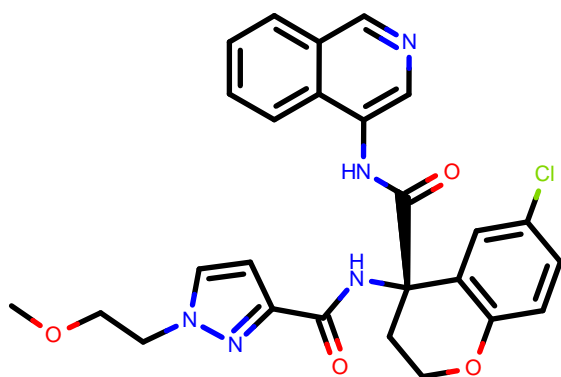
CID:	VLA-UCB-1dbca3b4-18_2
SMILES:	<chem>c1ccc2c(c1)cnc2N3C(=O)[C@H](CNC3=O)c4cccc(c4)Cl</chem>
RUN:	RUN111
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.21

EN300-249764_3_2_1



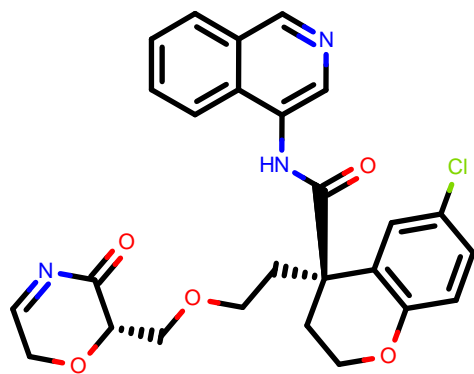
CID:	EN300-249764_3_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CCO5)O</chem>
RUN:	RUN3619
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.35

EN300-160277_1_1_1



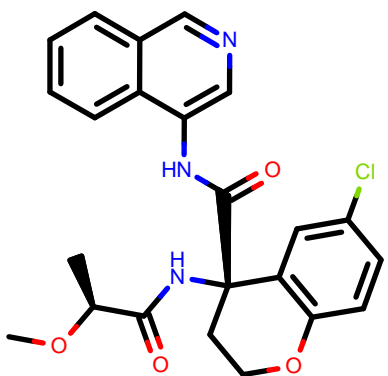
CID:	EN300-160277_1_1_1
SMILES:	<chem>COCc1ccc(n1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN2867
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.29

EN300-1706036_3_2_1



CID:	EN300-1706036_3_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C(=O)NCCO5</chem>
RUN:	RUN6796
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.33

EN300-258477_1_1_1



CID: EN300-258477_1_1_1

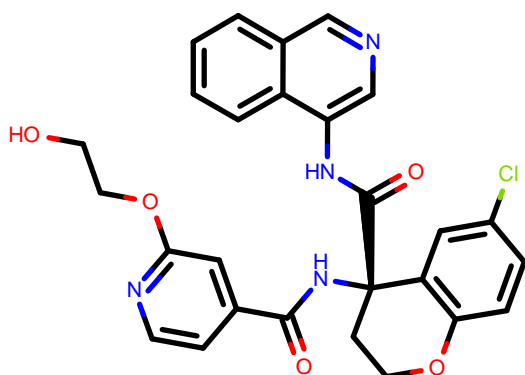
SMILES: C[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OC

RUN: RUN3932

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.25

EN300-101796_1_1_1



CID: EN300-101796_1_1_1

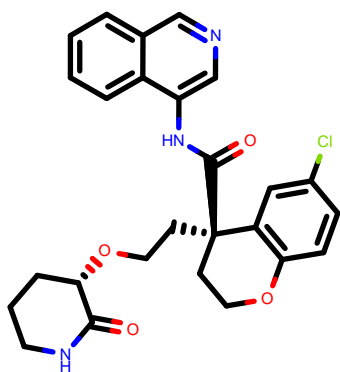
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)c5cnc(c5)OCCO

RUN: RUN4410

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.34

EN300-107267_3_2_1



CID: EN300-107267_3_2_1

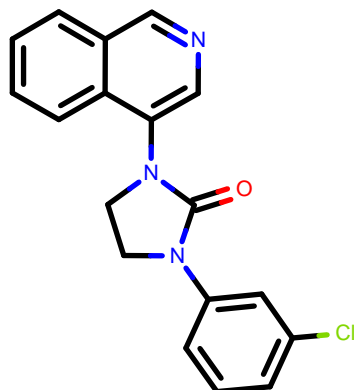
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCO[C@@H]5CCNCC5=O

RUN: RUN4293

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.26

PET-UNK-7be94445-2_1



CID: PET-UNK-7be94445-2_1

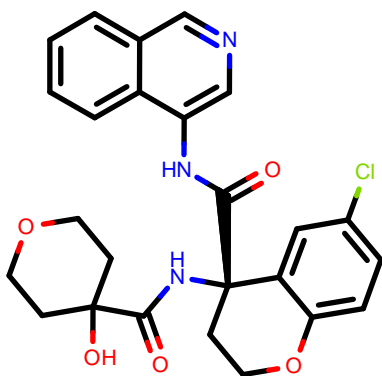
SMILES: c1ccc2c(c1)cncc2N3CCN(C3=O)c4cccc(c4)Cl

RUN: RUN42

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.35

EN300-69368_1_1_1



CID: EN300-69368_1_1_1

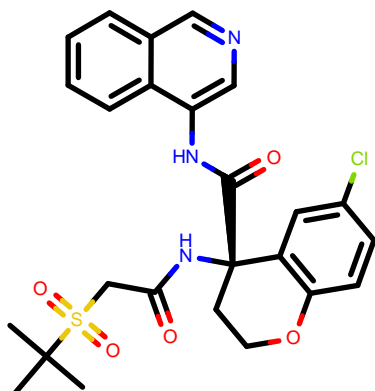
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCOCC5)O

RUN: RUN3244

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.27

EN300-123589_1_1_1



CID: EN300-123589_1_1_1

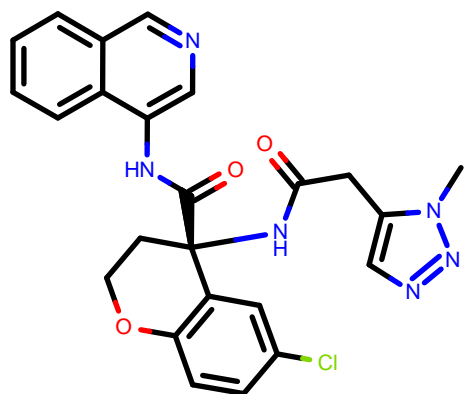
SMILES: CC(C)(C)S(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN3161

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.32

EN300-6486855_1_1_1



CID: EN300-6486855_1_1_1

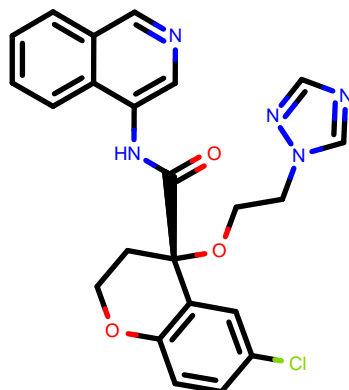
SMILES: Cn1c(cnn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN2984

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.23

EN300-6255179_1_1_1



CID: EN300-6255179_1_1_1

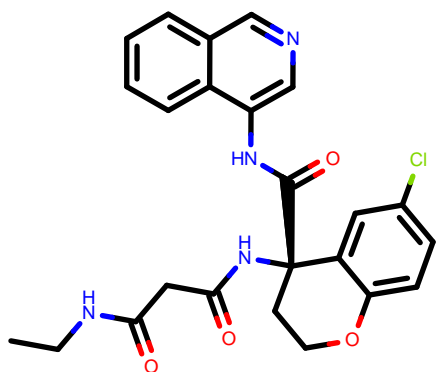
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCn5cncn5

RUN: RUN4412

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.25

EN300-129455_1_1_1



CID: EN300-129455_1_1_1

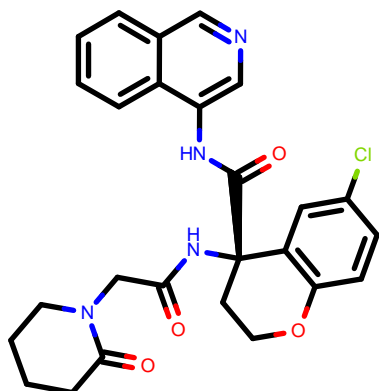
SMILES: CCNC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN3996

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.26

EN300-36111_1_1_1



CID: EN300-36111_1_1_1

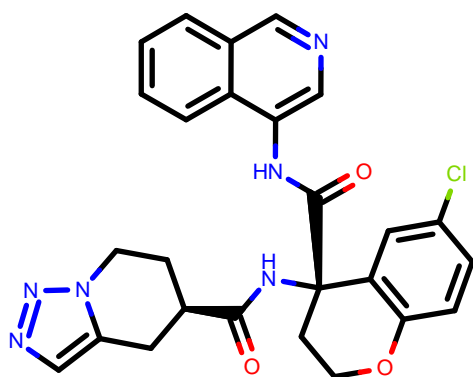
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCCC5=O

RUN: RUN4096

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.31

EN300-7430501_1_1_1



CID: EN300-7430501_1_1_1

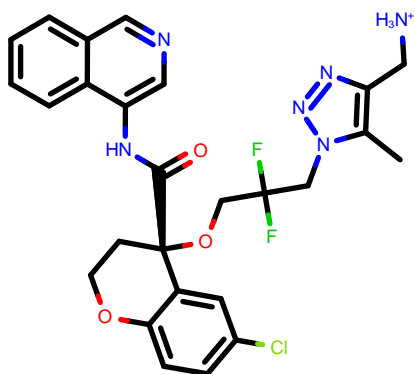
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNC6c(cnn6)C5

RUN: RUN2942

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-44_1



CID: ED_-GRI-5b13fbe2-44_1

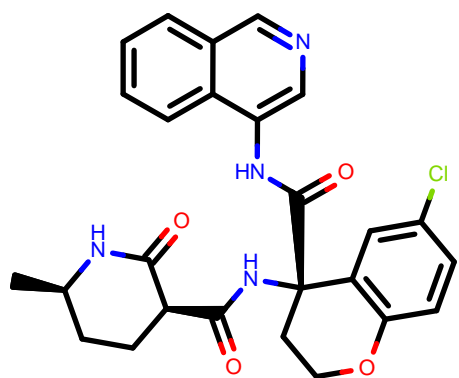
SMILES: Cc1c(nnn1CC(CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(F)F)C[NH3+]

RUN: RUN1484

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.33

EN300-6505003_1_1_1



CID: EN300-6505003_1_1_1

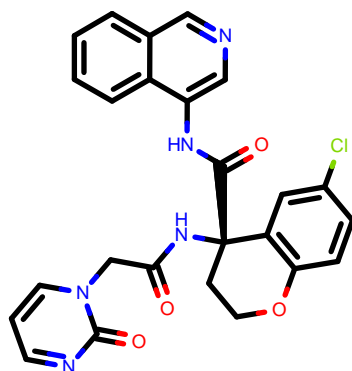
SMILES: C[C@@H]1CC[C@@H](C(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN2861

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.43

EN300-35789_1_1_1



CID: EN300-35789_1_1_1

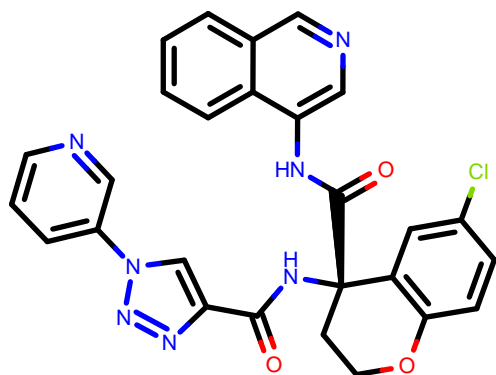
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Nc5ccncc5=O

RUN: RUN3892

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.28

EN300-151330_1_1_1



CID: EN300-151330_1_1_1

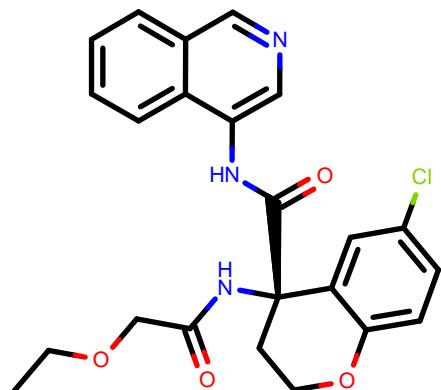
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn1n5c6ccncc6

RUN: RUN3312

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.20

EN300-21303_1_1_1



CID: EN300-21303_1_1_1

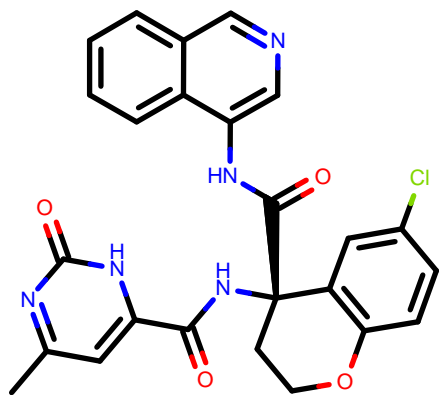
SMILES: CCOCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5019

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.20

EN300-42536_1_1_1



CID: EN300-42536_1_1_1

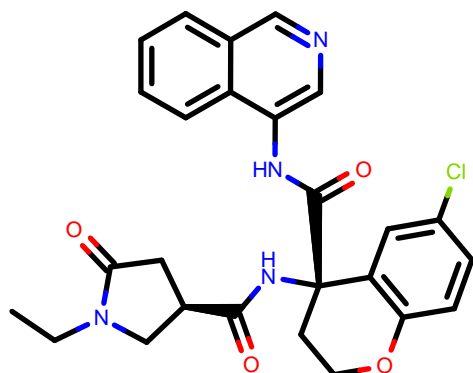
SMILES: Cc1cc(nc(=O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN4731

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.21

EN300-33478_1_1_1



CID: EN300-33478_1_1_1

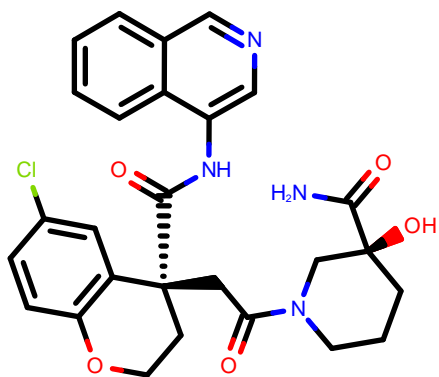
SMILES: CCN1C[C@@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN3770

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.26

EDJ-MED-d203f206-39_1



CID: EDJ-MED-d203f206-39_1

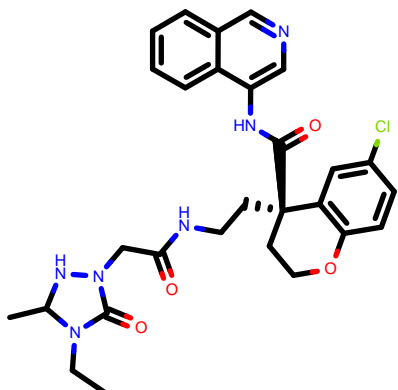
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@](C5)(C(=O)N)O

RUN: RUN2468

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.38

EN300-6478433_3_1_1



CID: EN300-6478433_3_1_1

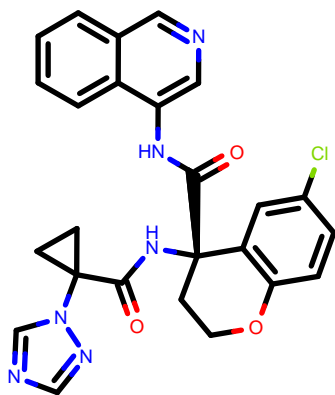
SMILES: CCn1c(nn(c1=O)CC(=O)N)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN7558

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.38

EN300-246440_1_1_1



CID: EN300-246440_1_1_1

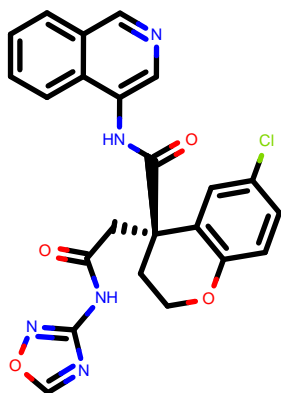
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)n6ncn6

RUN: RUN3088

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.28

CHO-MSK-a31cca77-4_1



CID: CHO-MSK-a31cca77-4_1

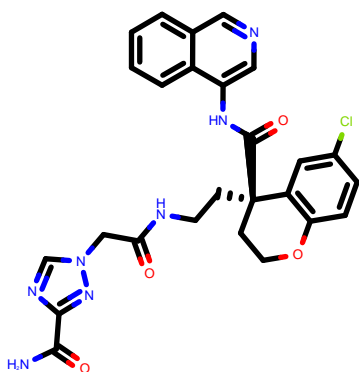
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncn5

RUN: RUN2050

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.22

EN300-262604_3_1_1



CID: EN300-262604_3_1_1

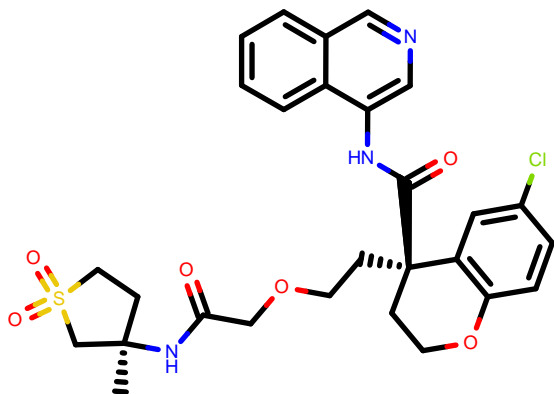
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ncnc(n5)C(=O)N

RUN: RUN4815

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.28

EN300-10414_3_2_1



CID: EN300-10414_3_2_1

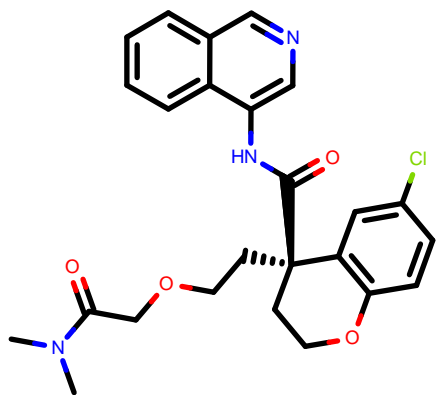
SMILES: C[C@@]1(CCS(=O)(=O)C1)NC(=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN6404

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.42

EN300-216063_3_1_1



CID: EN300-216063_3_1_1

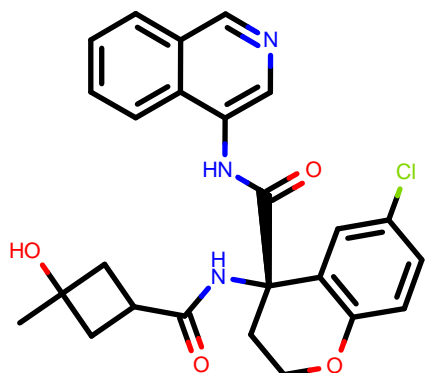
SMILES: CN(C)C(=O)COCC[C@]1(C)C(CO)C2C1CC(C2)C(=O)Nc3ccc4c3ccc4

RUN: RUN4149

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.23

EN300-247343_1_1_1



CID: EN300-247343_1_1_1

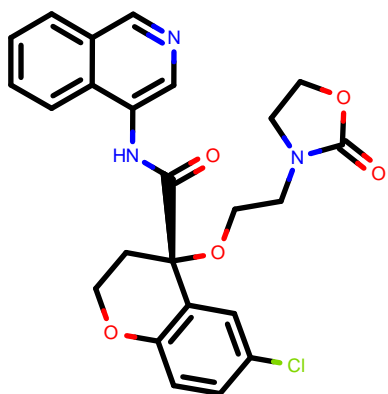
SMILES: CC1(CC(C1)C(=O)N[C@]2(C)C(CO)C3C2CC(C3)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN4948

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.22

EN300-370967_1_1_1



CID: EN300-370967_1_1_1

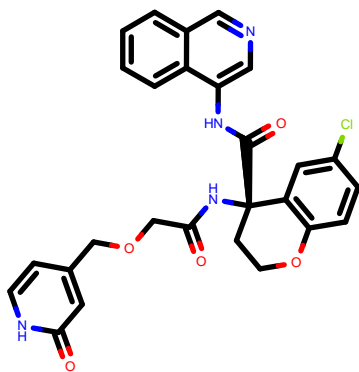
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4C3CC(C4)C(=O)NCC5CCOC5=O

RUN: RUN3449

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.27

EN300-316258_1_1_1



CID: EN300-316258_1_1_1

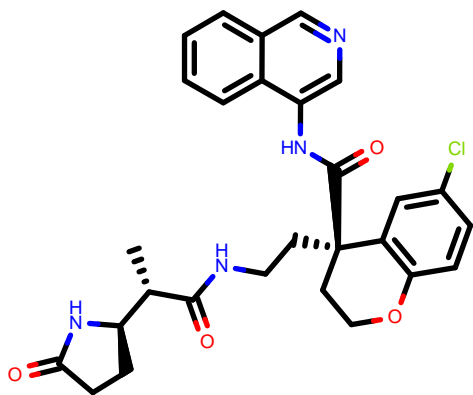
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4C3CC(C4)C(=O)NCC5C=CN=C5

RUN: RUN3524

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.25

EN300-249421_3_3_1



CID: EN300-249421_3_3_1

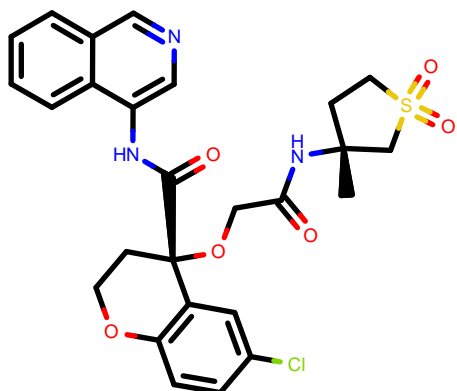
SMILES: C[C@@H]([C@H]1CCC(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3458

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.33

EN300-10414_1_2_1



CID: EN300-10414_1_2_1

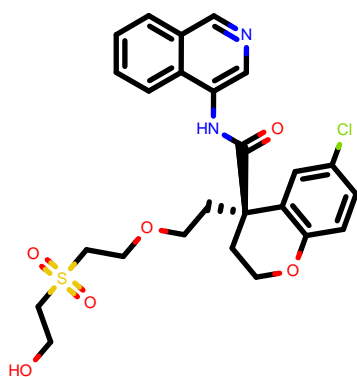
SMILES: C[C@]1(CCS(=O)(=O)C1)NC(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4472

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.43

EN300-7463171_3_1_1



CID: EN300-7463171_3_1_1

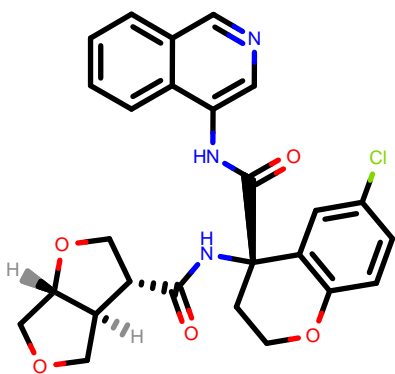
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)CO

RUN: RUN3231

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.55

EN300-6482296_1_2_1



CID: EN300-6482296_1_2_1

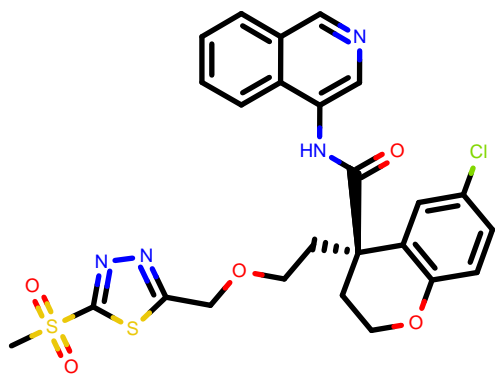
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CO[C@H]5COC6

RUN: RUN3417

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.26

EN300-160080_3_1_1



CID: EN300-160080_3_1_1

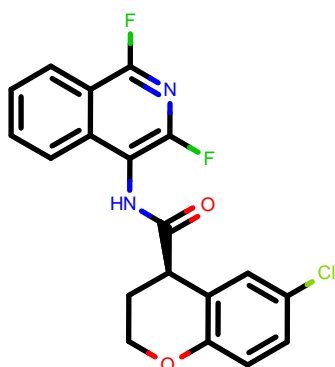
SMILES: CS(=O)(=O)c1nnc(s1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4442

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.32

JOH-SUS-a69c159d-6_1



CID: JOH-SUS-a69c159d-6_1

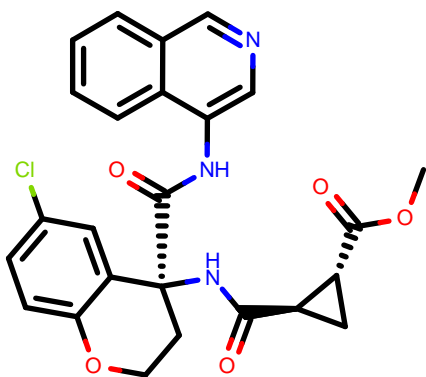
SMILES: c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN1060

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.06

EN300-66764_1_3_1



CID: EN300-66764_1_3_1

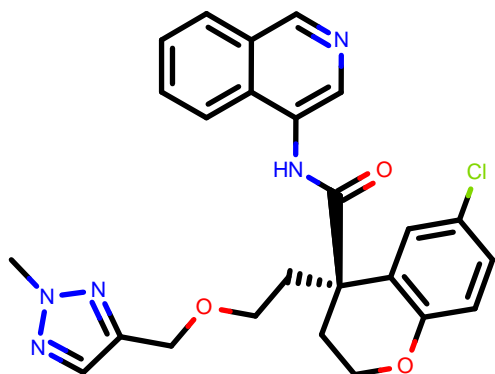
SMILES: COC(=O)[C@@H]1[C@@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3768

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-219020_3_1_1



CID: EN300-219020_3_1_1

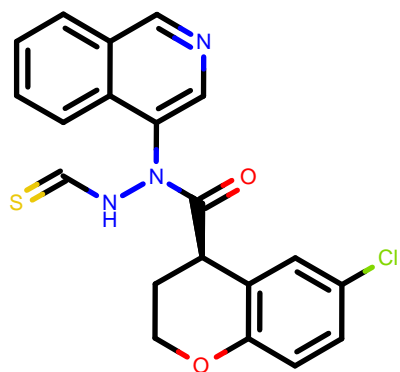
SMILES: Cn1ncc(n1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3431

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.27

DAR-DIA-5ff57136-18_1



CID: DAR-DIA-5ff57136-18_1

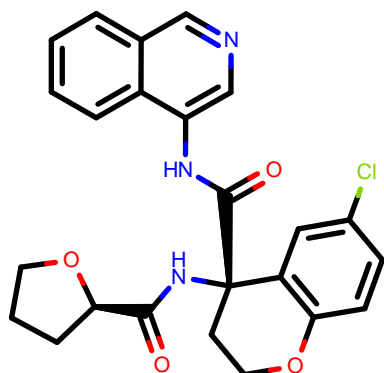
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)N=C=S

RUN: RUN1269

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.14

EN300-116234_1_1_1



CID: EN300-116234_1_1_1

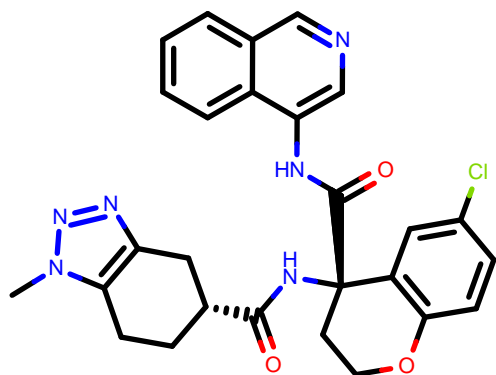
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@H]3[C@@H](CCOCc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCCO5

RUN: RUN2816

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-185727_1_1_1



CID: EN300-185727_1_1_1

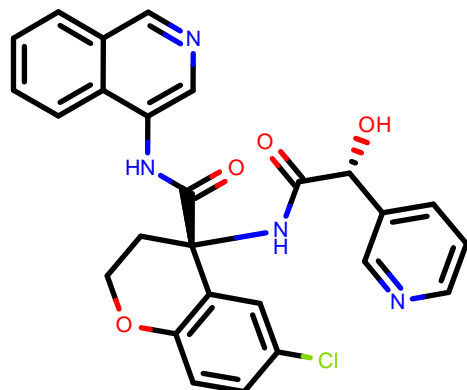
SMILES: Cn1c2c(m1)C[C@@H](CC2)C(=O)N[C@@H]3[C@@H](CCOCc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN4348

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.30

EN300-134855_1_1_1



CID: EN300-134855_1_1_1

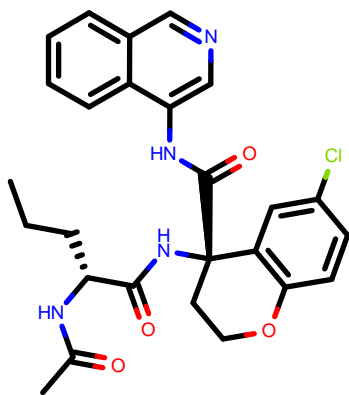
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOCc4c3cc(cc4)Cl)NC(=O)[C@@H]5c5ccn5O

RUN: RUN3806

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.24

EN300-51801_1_2_1



CID: EN300-51801_1_2_1

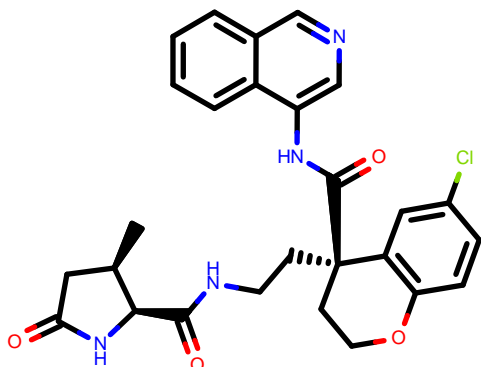
SMILES: CCC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)C

RUN: RUN3307

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.32

EN300-155362_3_1_1



CID: EN300-155362_3_1_1

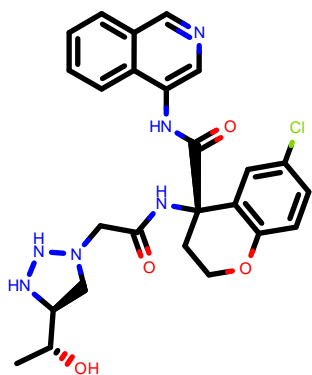
SMILES: C[C@@H]1CC(=O)N[C@@]2(CO)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4232

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.29

EN300-109540_1_2_1



CID: EN300-109540_1_2_1

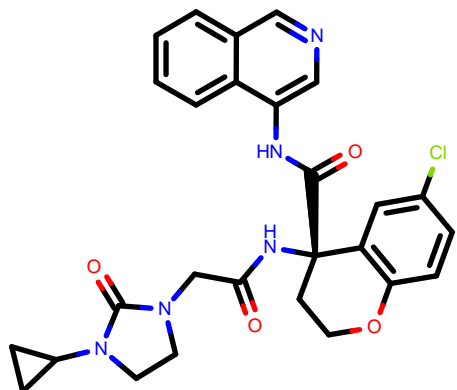
SMILES: C[C@H](c1cn(n1)CC(=O)N[C@@]2(CO)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN5391

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.35

KAD-UNI-8a629cb0-13_1



CID: KAD-UNI-8a629cb0-13_1

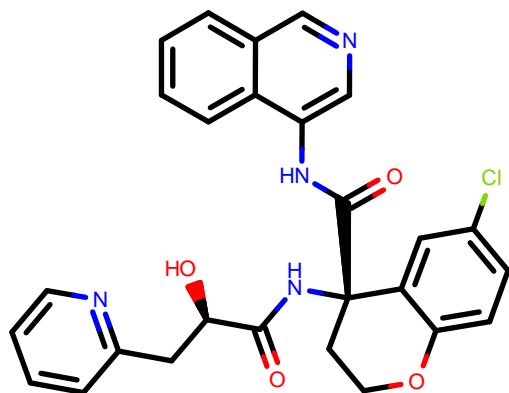
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCN(C5=O)C6CC6

RUN: RUN2010

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.33

EN300-6762327_1_1_1



CID: EN300-6762327_1_1_1

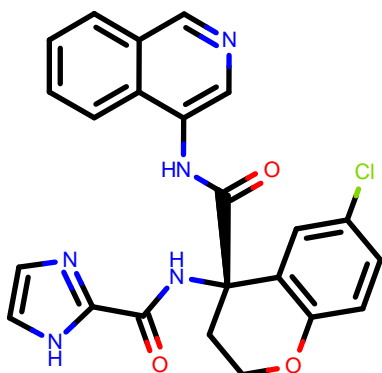
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]3[C@@]3(C5ccccc5)O

RUN: RUN4997

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.29

EN300-315836_1_1_1



CID: EN300-315836_1_1_1

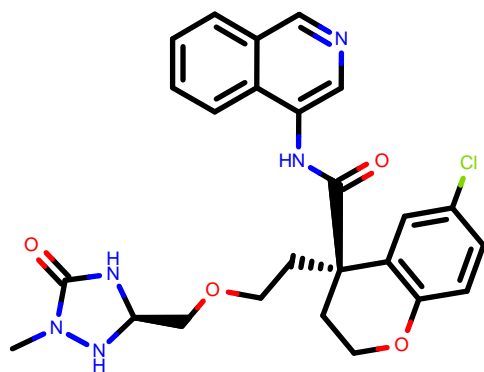
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]cnc5

RUN: RUN2838

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.22

EN300-124918_3_1_2



CID: EN300-124918_3_1_2

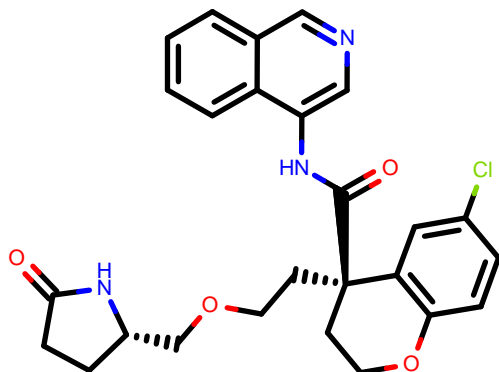
SMILES: CN1C(=O)N[C@@H]([NH2+])COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccccc5

RUN: RUN4443

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.36

EN300-195756_3_1_1



CID: EN300-195756_3_1_1

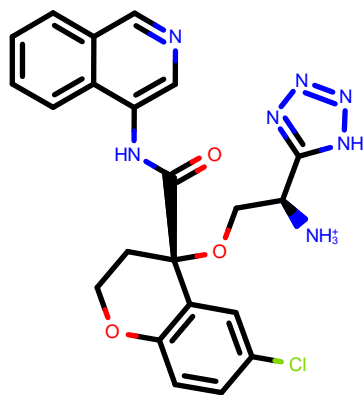
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]3[C@@]3(C5CC(=O)N5)

RUN: RUN3332

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.26

ED_-GRI-5b13fbe2-5_1



CID: ED_-GRI-5b13fbe2-5_1

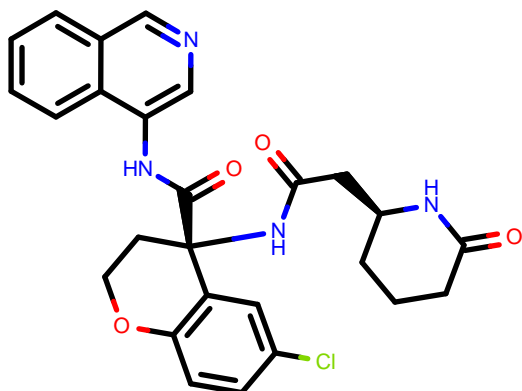
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)OC[C@@H](c5[n-]m5)[NH3+]

RUN: RUN1401

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.31

EN300-210084_1_1_1



CID: EN300-210084_1_1_1

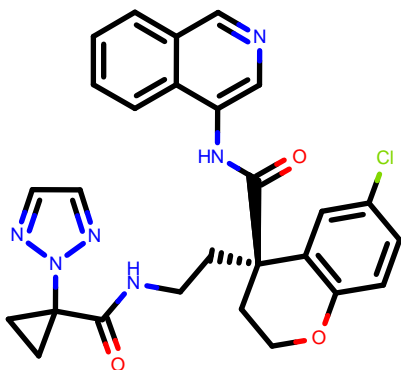
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCC(=O)N5

RUN: RUN3247

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.20

EN300-1722017_3_1_1



CID: EN300-1722017_3_1_1

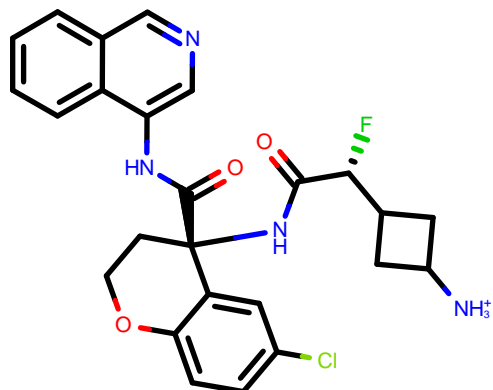
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CC5)n6ncn6

RUN: RUN2965

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.30

EDG-MED-90036822-35_2



CID: EDG-MED-90036822-35_2

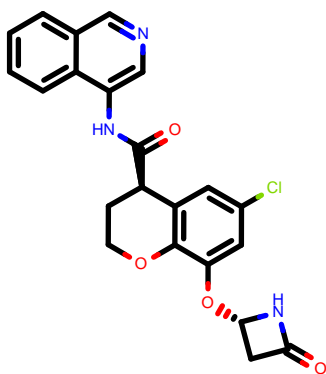
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)C[C@@H](F)C5(C5)N5[NH3+]

RUN: RUN1559

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.33

VLA-UCB-50c39ae8-8_2



CID: VLA-UCB-50c39ae8-8_2

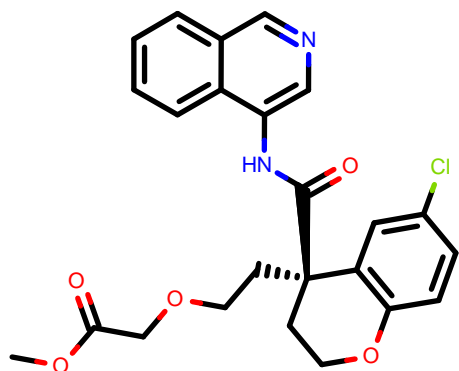
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC(=O)N5)Cl

RUN: RUN320

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.20

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

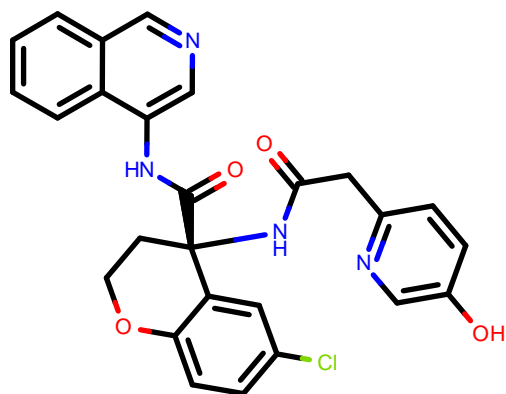
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3638

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.22

EN300-188341_1_1_1



CID: EN300-188341_1_1_1

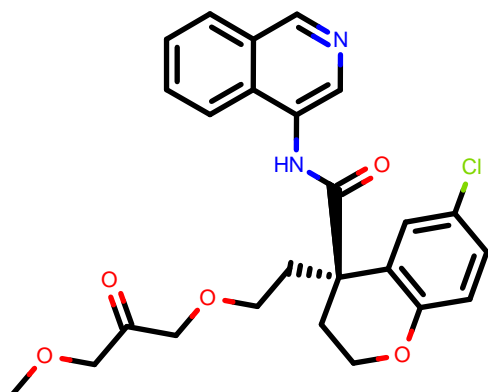
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(O)5O

RUN: RUN3637

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.21

EN300-125140_3_1_1



CID: EN300-125140_3_1_1

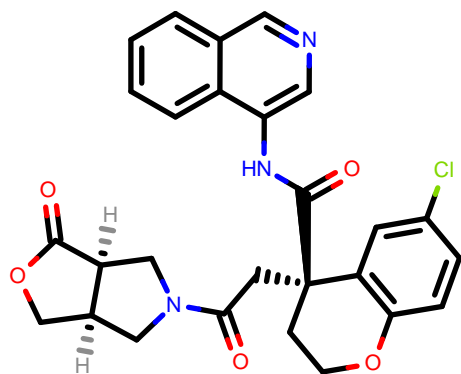
SMILES: COCC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3333

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.28

EN300-316193_1_1_1



CID: EN300-316193_1_1_1

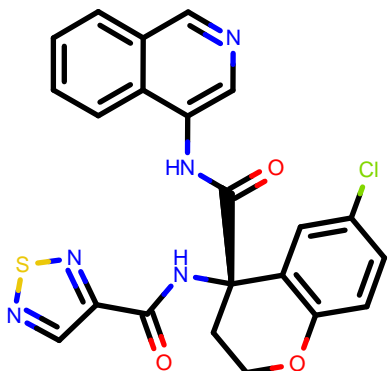
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)C(=O)N5C[C@H]6COC1=O[C@H]6C5

RUN: RUN4365

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.34

EN300-42270_1_1_1



CID: EN300-42270_1_1_1

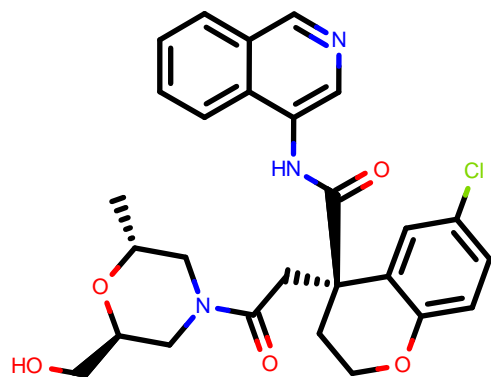
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)NC(=O)c5cnsn5

RUN: RUN2830

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.17

EN300-157776_1_3_1



CID: EN300-157776_1_3_1

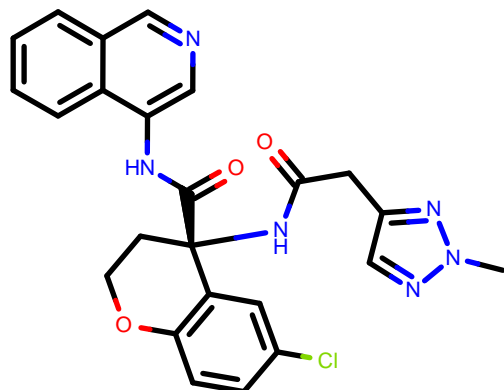
SMILES: C[C@@H]1CN(C[C@H](O1)CO)C(=O)C[C@@]2(CCOc3ccc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3555

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.38

EN300-755161_1_1_1



CID: EN300-755161_1_1_1

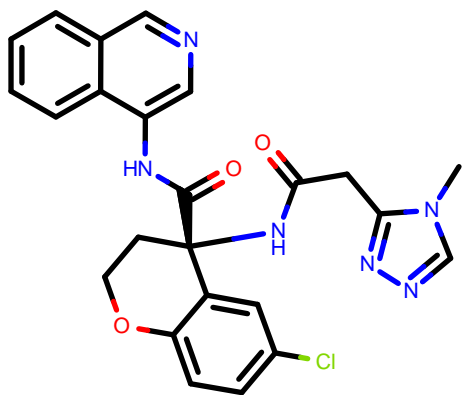
SMILES: Cn1ncc(n1)CC(=O)N[C@@]2(CCOc3ccc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3665

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.24

EN300-6494474_1_1_1



CID: EN300-6494474_1_1_1

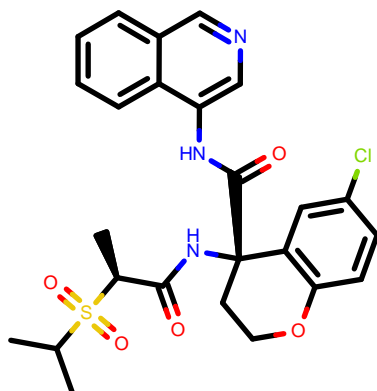
SMILES: Cn1cnc1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3198

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.25

EN300-40947_1_1_1



CID: EN300-40947_1_1_1

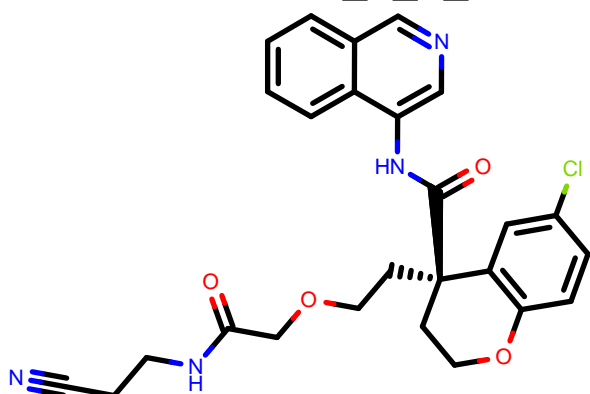
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)S(=O)(=O)C(C)C

RUN: RUN3491

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.35

EN300-10895_3_1_1



CID: EN300-10895_3_1_1

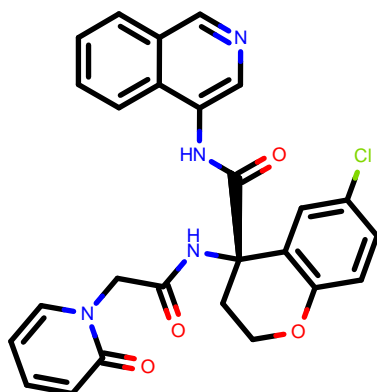
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCCC#N

RUN: RUN3623

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.26

EN300-11714_1_1_1



CID: EN300-11714_1_1_1

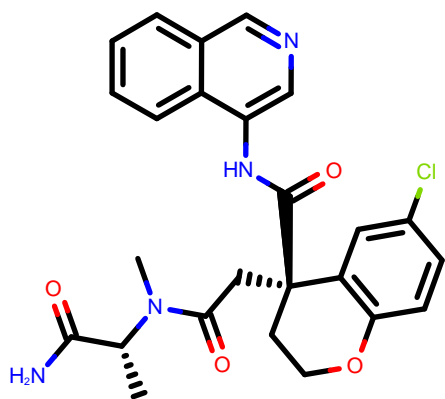
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cccc5=O

RUN: RUN3041

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.29

EN300-125409_1_2_1



CID: EN300-125409_1_2_1

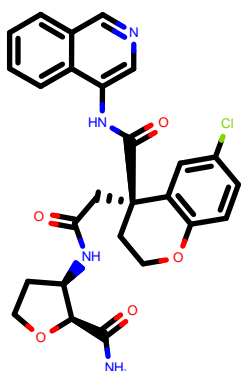
SMILES: C[C@H](C(=O)N)N(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3794

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.33

EN300-7435545_1_1_1



CID: EN300-7435545_1_1_1

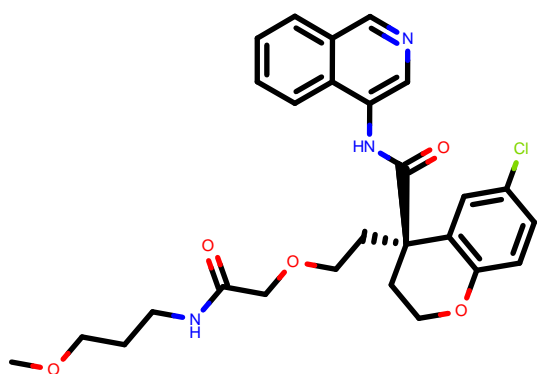
SMILES: c1cc2c(e1)nc2N(C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC@@H5CCO[C@@H]5Cl=O)N

RUN: RUN3695

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.32

EN300-04492_3_1_1



CID: EN300-04492_3_1_1

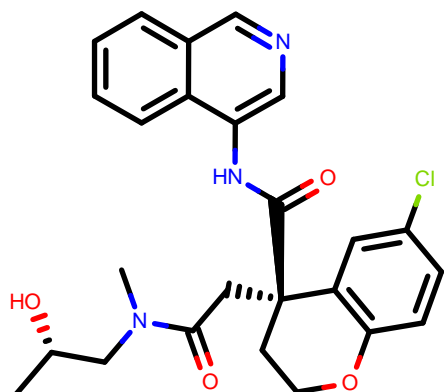
SMILES: COCCCN(C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7758

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.28

EN300-210254_1_1_1



CID: EN300-210254_1_1_1

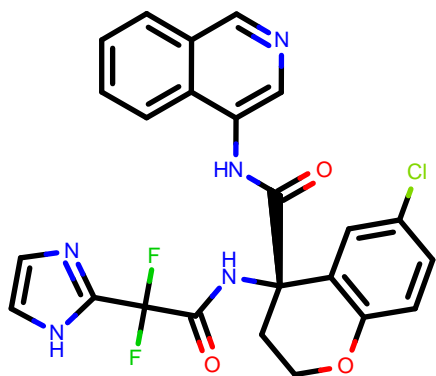
SMILES: C[C@@H](CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN4479

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.37

EDG-MED-90036822-45_1



CID: EDG-MED-90036822-45_1

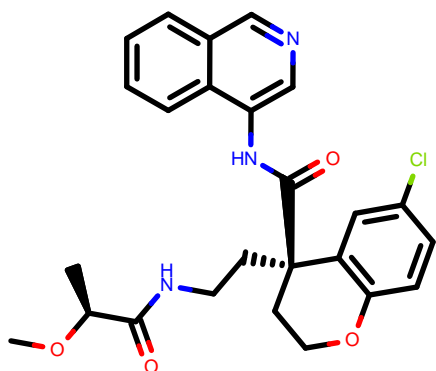
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(c5[nH]cnc5)F)F

RUN: RUN1579

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.22

EN300-51257_3_1_1



CID: EN300-51257_3_1_1

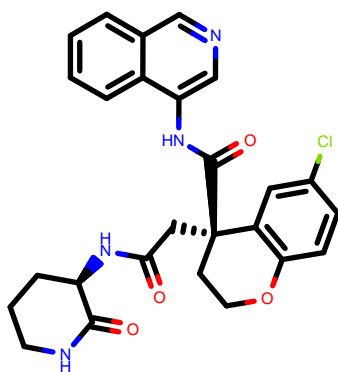
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)OC

RUN: RUN4424

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.24

EDJ-MED-d203f206-23_1



CID: EDJ-MED-d203f206-23_1

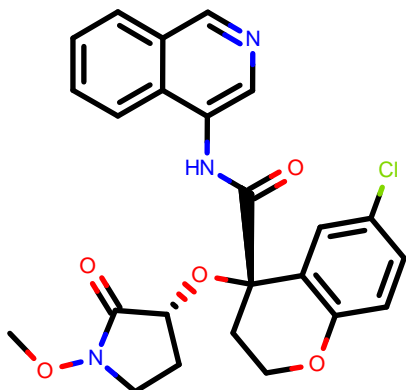
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCNC5=O

RUN: RUN2418

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.25

EN300-302058_1_2_1



CID: EN300-302058_1_2_1

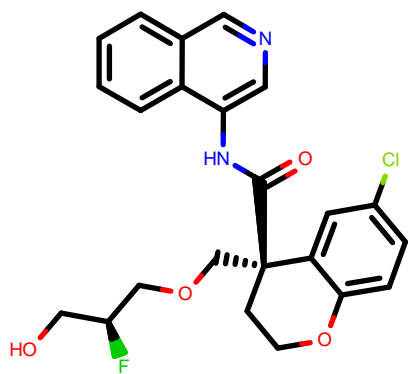
SMILES: CON1CC[C@@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN7115

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.24

EN300-1600517_2_2_1



CID: EN300-1600517_2_2_1

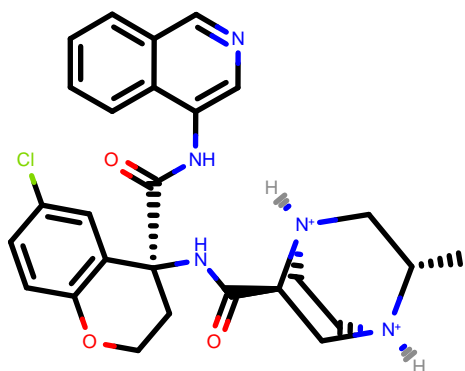
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F

RUN: RUN3797

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.29

EN300-120414_1_4_1



CID: EN300-120414_1_4_1

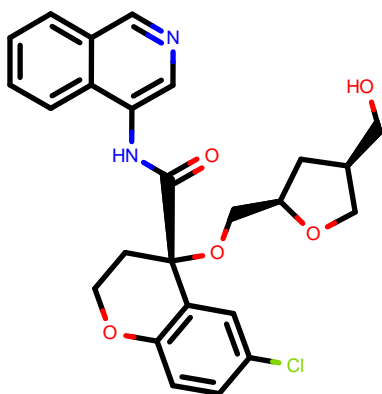
SMILES: C[C@H]1CN[C@@]2CCN[C@@H]1C[C@@H]2C(=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C[C@H]5C[C@@H](CO)N5

RUN: RUN5420

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.37

EN300-6494158_1_4_1



CID: EN300-6494158_1_4_1

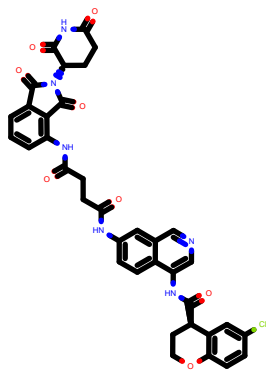
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@@H](CO)C5

RUN: RUN3175

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.32

DAR-DIA-9e4459de-15_8



CID: DAR-DIA-9e4459de-15_8

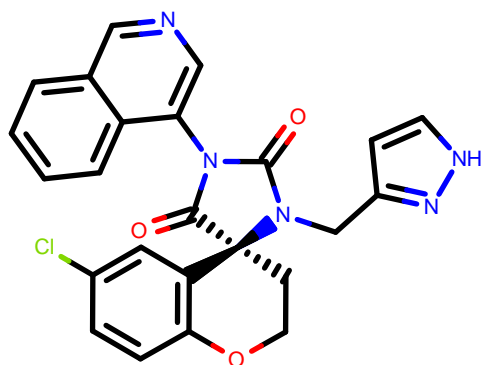
SMILES: c1cc2c(c1)NC(=O)CC[C@@]3(O)Nc3ccc4c(c3)cncc4NC(=O)[C@@]5(CCOc6c5cc(cc6)Cl)C[C@H]7C[C@@H](CO)N7=O

RUN: RUN1380

DDG (kcal/mol): -2.02

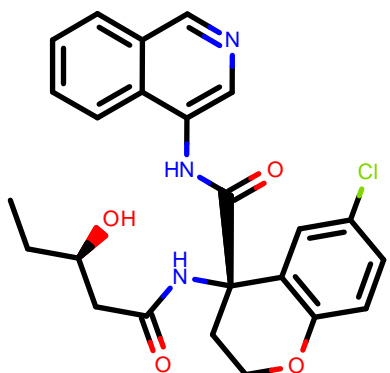
dDDG (kcal/mol): 0.25

VLA-UNK-f702bf1c-2_1



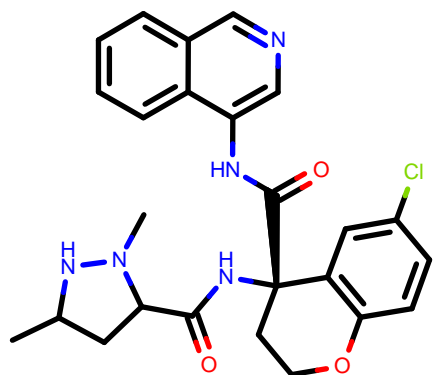
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCCOc5c4cc(cc5)Cl)N(C3=O)C6ccn[nH]6</chem>
RUN:	RUN2113
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.29

EN300-224741_1_2_1



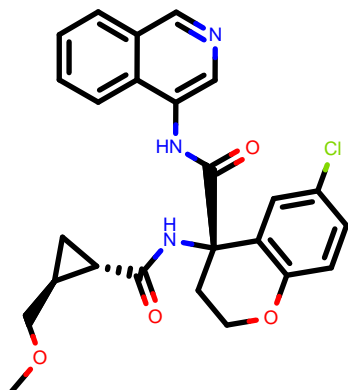
CID:	EN300-224741_1_2_1
SMILES:	<chem>CC[C@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)O</chem>
RUN:	RUN5030
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.22

EN300-51244_1_1_1



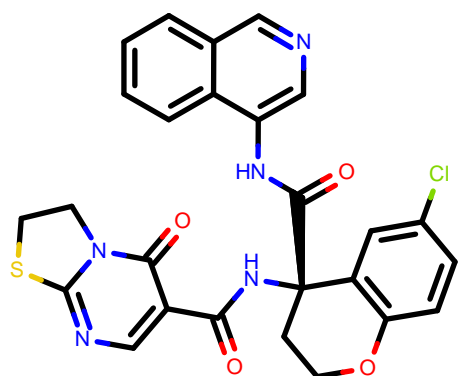
CID:	EN300-51244_1_1_1
SMILES:	<chem>Cc1cc(n(n1)C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5</chem>
RUN:	RUN3824
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.18

EN300-7352438_1_1_1



CID:	EN300-7352438_1_1_1
SMILES:	<chem>COC[C@H]1C[C@@]H1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5</chem>
RUN:	RUN3272
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.28

EN300-14405_1_1_1



CID: EN300-14405_1_1_1

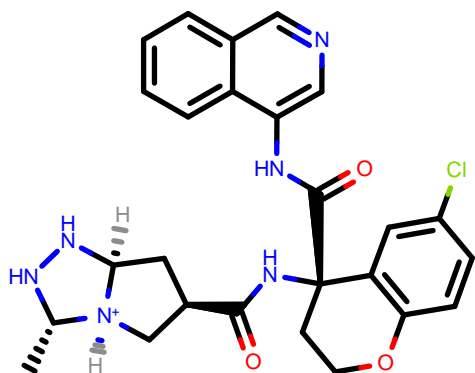
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)C)NC(=O)c5cnc6n(c5=O)CCS6

RUN: RUN4229

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.31

EN300-6729747_1_1_1



CID: EN300-6729747_1_1_1

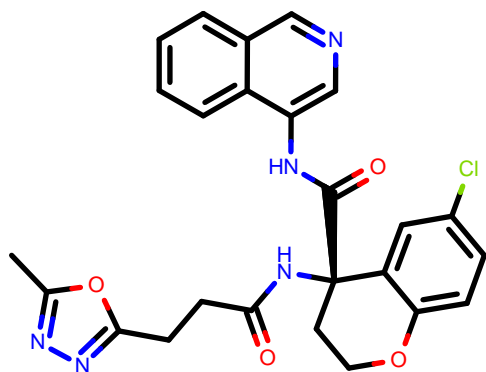
SMILES: C[C@@]1N[C@@]2N[C@@H]1C[C@@]3[C@@](C(=O)N[C@@]3(CCO4c3cc(cc4)C)C(=O)N5cnc6c5ccccc6

RUN: RUN3155

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.47

EN300-304662_1_1_1



CID: EN300-304662_1_1_1

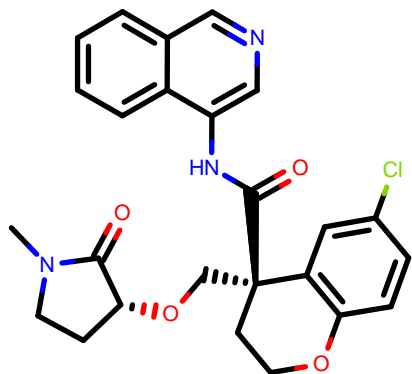
SMILES: Cc1nnc(o1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)N4cnc5c4cccc5

RUN: RUN4811

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.28

EN300-98648_2_2_1



CID: EN300-98648_2_2_1

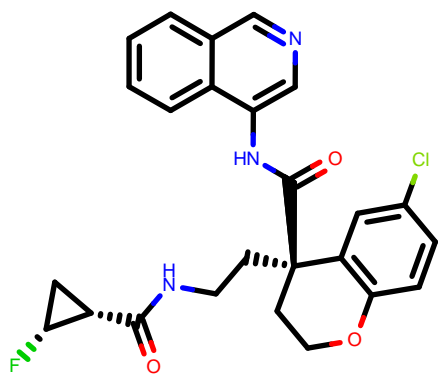
SMILES: CN1CC[C@@H](C1=O)OC[C@@]2(CCOc3c2cc(cc3)C)C(=O)N4cnc5c4cccc5

RUN: RUN4012

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.25

EN300-97300_3_4_1



CID: EN300-97300_3_4_1

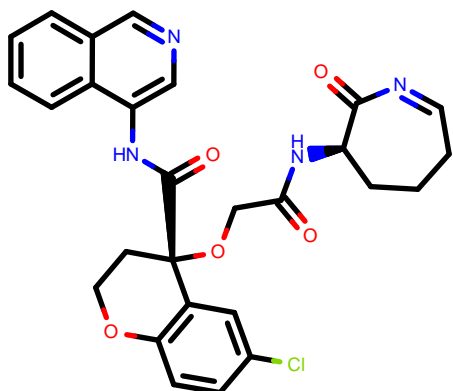
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C[C@H]5F

RUN: RUN3221

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.21

EN300-37195_1_1_1



CID: EN300-37195_1_1_1

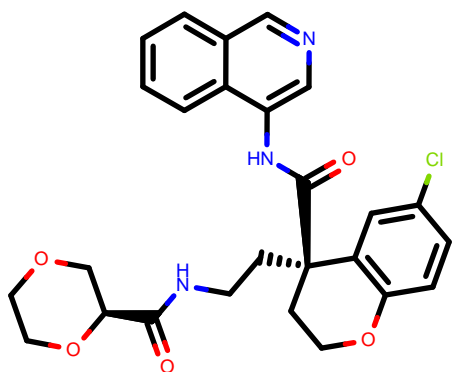
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N[C@@]5CCCCNC5=O

RUN: RUN7710

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.29

EN300-36158_3_1_1



CID: EN300-36158_3_1_1

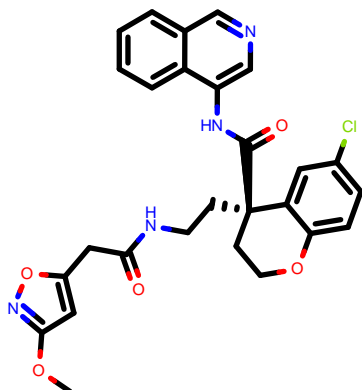
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5COCCO5

RUN: RUN5247

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.23

EN300-127197_3_1_1



CID: EN300-127197_3_1_1

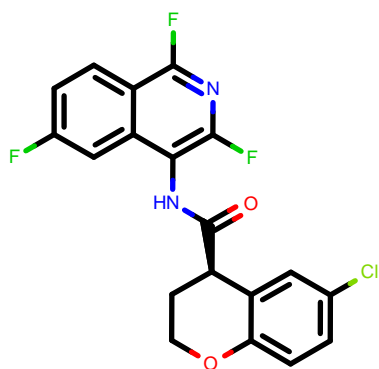
SMILES: COc1cc(oc1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3220

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

JOH-SUS-a69c159d-7_1



CID: JOH-SUS-a69c159d-7_1

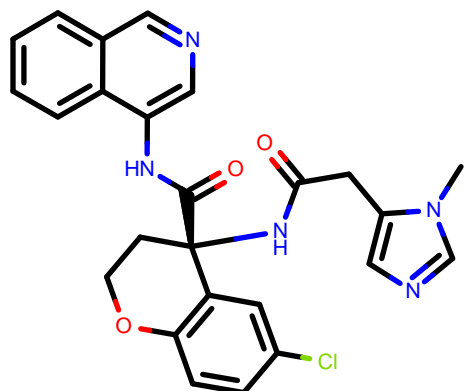
SMILES: c1cc2c(cc1F)c(nc2F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1045

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.06

EN300-152418_1_1_1



CID: EN300-152418_1_1_1

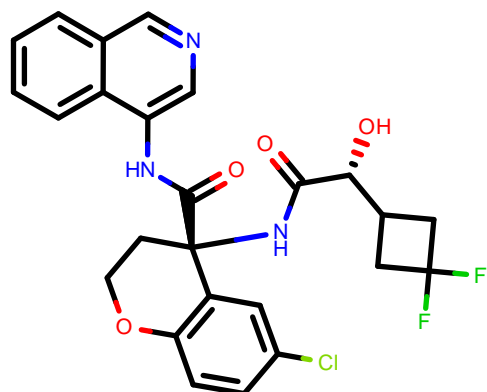
SMILES: Cn1cncc1CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3558

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.25

EDG-MED-90036822-101_1



CID: EDG-MED-90036822-101_1

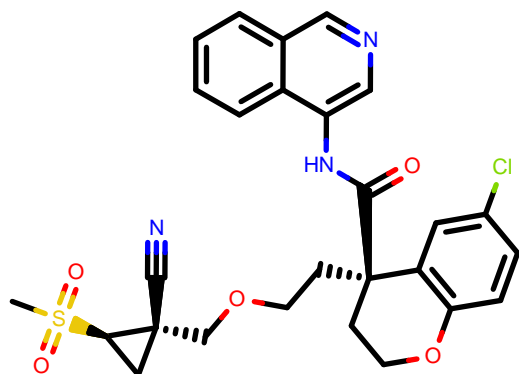
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)[C@@H](C5CC(C5)(F)F)O

RUN: RUN1709

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.31

EN300-633533_3_1_1



CID: EN300-633533_3_1_1

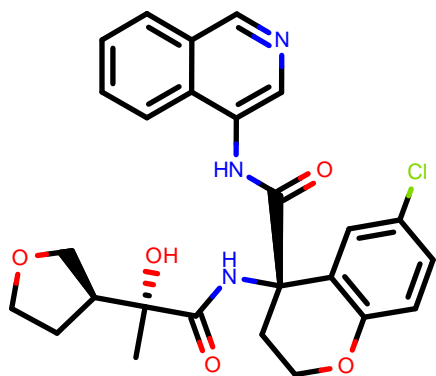
SMILES: CS(=O)(=O)[C@@H]1C[C@@]1(COCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N

RUN: RUN3849

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-217494_1_3_1



CID: EN300-217494_1_3_1

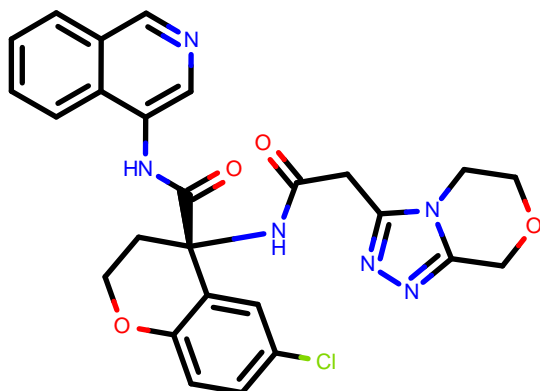
SMILES: C[C@@H](C[C@@H]1CCOC1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccccc5)O

RUN: RUN6883

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-1718836_1_1_1



CID: EN300-1718836_1_1_1

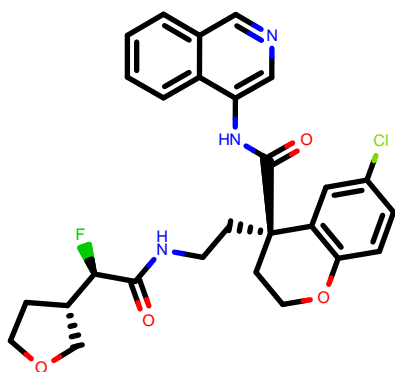
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5nnc6n5CCOC6

RUN: RUN3109

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.28

EN300-783124_3_3_1



CID: EN300-783124_3_3_1

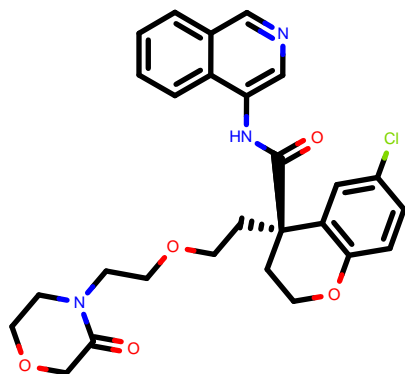
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C)[C@@H]5CCOC5F

RUN: RUN5208

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.27

EN300-219330_3_1_1



CID: EN300-219330_3_1_1

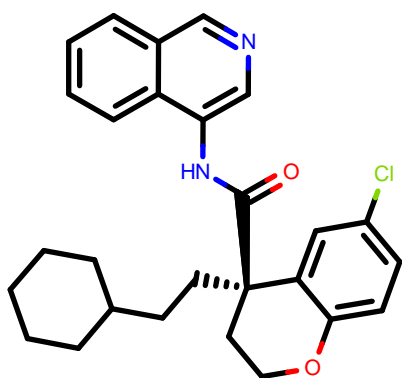
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCN5CCOCC5=O

RUN: RUN3869

DDG (kcal/mol): -1.98

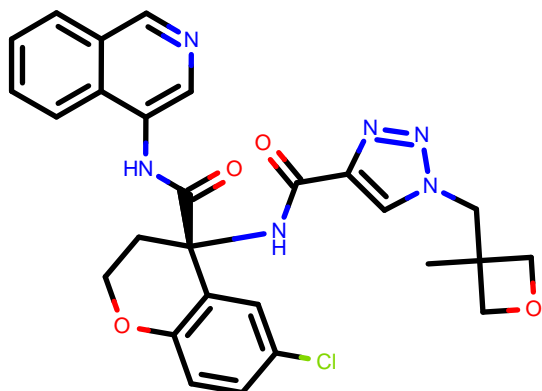
dDDG (kcal/mol): 0.30

VLA-UCB-50c39ae8-10_1_1



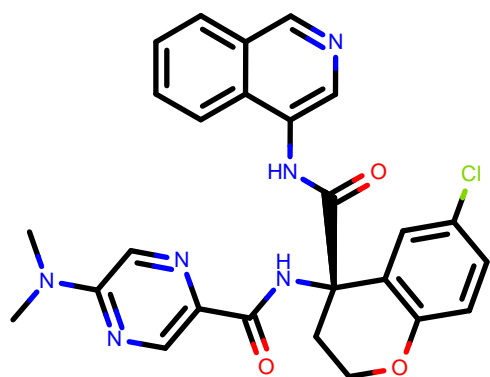
CID:	VLA-UCB-50c39ae8-10_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCC5CCCC5</chem>
RUN:	RUN3517
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.26

EN300-135660_1_1_1



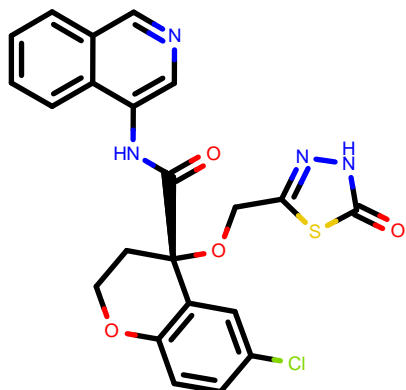
CID:	EN300-135660_1_1_1
SMILES:	<chem>CC1(COC1)Cn2cc(m2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccc6</chem>
RUN:	RUN4073
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.25

EN300-123916_1_1_1



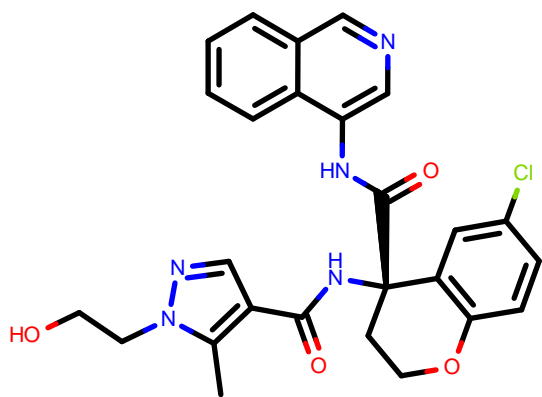
CID:	EN300-123916_1_1_1
SMILES:	<chem>CN(C)c1cnc(en1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5</chem>
RUN:	RUN4739
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.25

CHO-MSK-5891c1ff-7_1



CID:	CHO-MSK-5891c1ff-7_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5n[nH]c(=O)s5</chem>
RUN:	RUN1722
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.20

EN300-40225_1_1_1



CID: EN300-40225_1_1_1

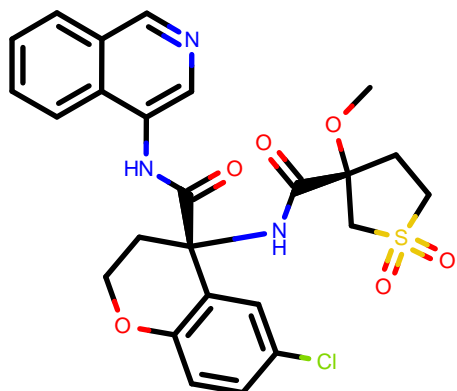
SMILES: Cc1c(cnn1CCO)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3578

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.26

EN300-385267_1_1_1



CID: EN300-385267_1_1_1

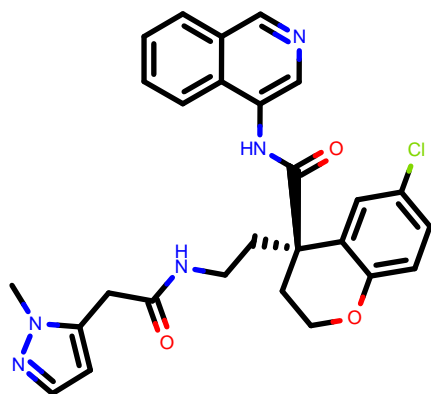
SMILES: CO[C@@]1(CCS(=O)(=O)C1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN7409

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.39

EN300-114805_3_1_1



CID: EN300-114805_3_1_1

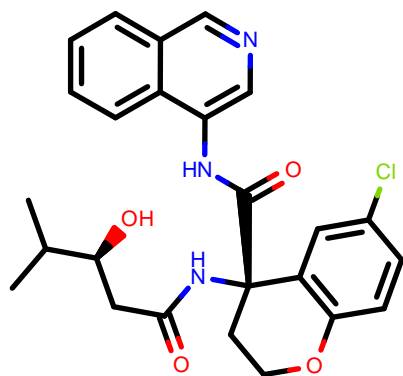
SMILES: Cn1c(ccn1)CC(=O)NCC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5179

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.32

EN300-155498_1_1_2



CID: EN300-155498_1_1_2

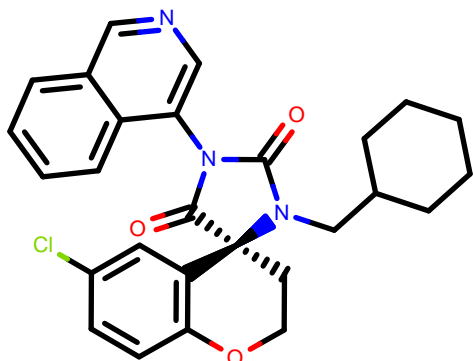
SMILES: CC(C)[C@H](CC(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O

RUN: RUN6531

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.30

VLA-UNK-f702bf1c-6_1



CID: VLA-UNK-f702bf1c-6_1

SMILES:

c1ccc2c(c1)cnc2N3C(=O)[C@@]4(CCOc5c4cc(c5)C)N(C3=O)CC6CCCC6

RUN:

RUN2134

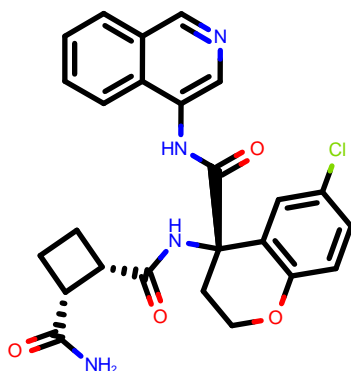
DDG (kcal/mol):

-1.97

dDDG (kcal/mol):

0.31

EN300-217107_1_4_1



CID: EN300-217107_1_4_1

SMILES:

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

RUN:

RUN3032

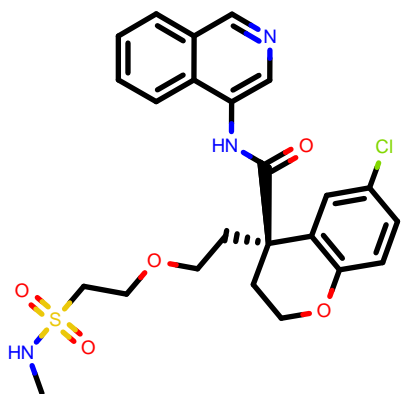
DDG (kcal/mol):

-1.97

dDDG (kcal/mol):

0.23

EN300-6482967_3_1_1



CID: EN300-6482967_3_1_1

SMILES:

CNS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)C)N(C(=O)Nc3ncc4c3cccc4

RUN:

RUN3883

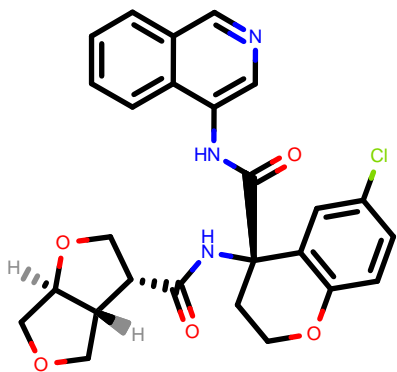
DDG (kcal/mol):

-1.97

dDDG (kcal/mol):

0.33

EN300-6482296_1_8_1



CID: EN300-6482296_1_8_1

SMILES:

c1ccc2c(c1)cnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)[C@H]5C[C@H]5C(=O)O

RUN:

RUN3139

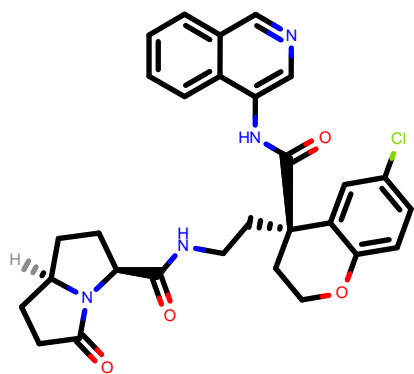
DDG (kcal/mol):

-1.97

dDDG (kcal/mol):

0.22

EN300-6479181_3_3_1



CID: EN300-6479181_3_3_1

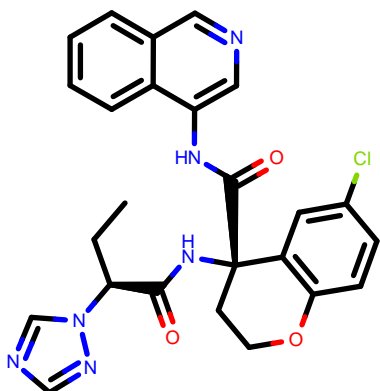
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H](CCOc4c3ccc(cc4)C)CCNC(=O)C[C@@H](NSC)C(=O)CC6

RUN: RUN4248

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.34

EN300-651307_1_1_1



CID: EN300-651307_1_1_1

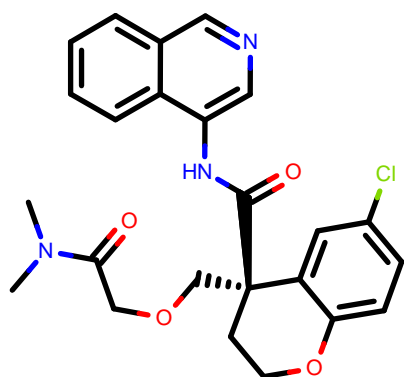
SMILES: CC[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)n5cncn5

RUN: RUN2858

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.27

EN300-216063_2_1_1



CID: EN300-216063_2_1_1

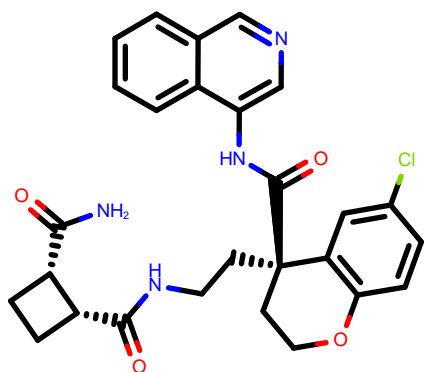
SMILES: CN(C)C(=O)COC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5100

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.21

EN300-217107_3_1_1



CID: EN300-217107_3_1_1

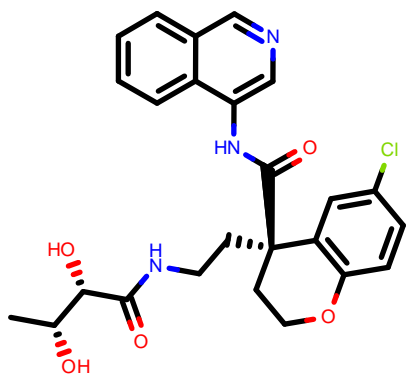
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H](CCOc4c3ccc(cc4)C)CCNC(=O)C[C@@H](SC)C[C@@H](Cl)O=N

RUN: RUN4239

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.33

EN300-6974806_3_1_1



CID: EN300-6974806_3_1_1

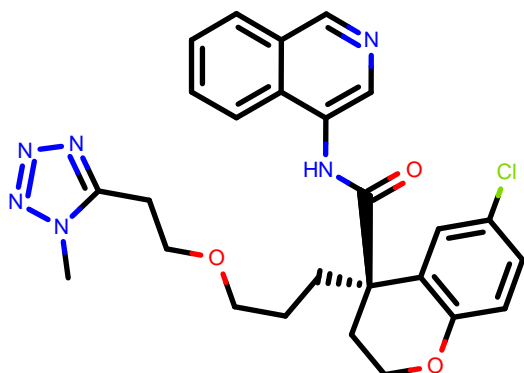
SMILES: C[C@@H]([C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)O)O

RUN: RUN4292

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.35

EN300-365398_4_1_1



CID: EN300-365398_4_1_1

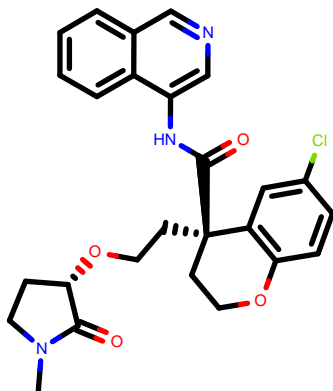
SMILES: Cn1c(nnn1)CCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3352

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.37

EN300-98648_3_1_1



CID: EN300-98648_3_1_1

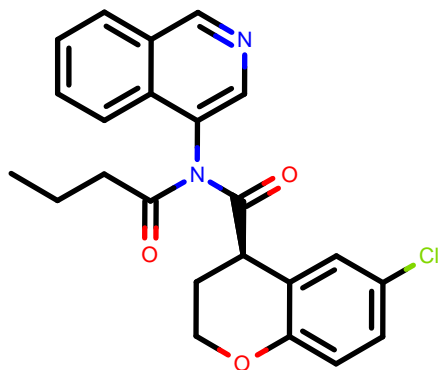
SMILES: CN1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4906

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.24

DAR-DIA-5ff57136-11_1



CID: DAR-DIA-5ff57136-11_1

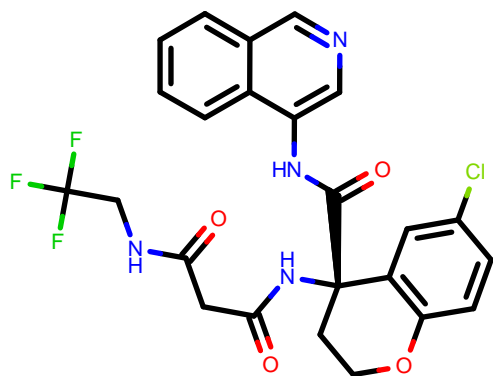
SMILES: C=CC(=O)N(c1cnc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN1277

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.21

EN300-128715_1_1_1



CID: EN300-128715_1_1_1

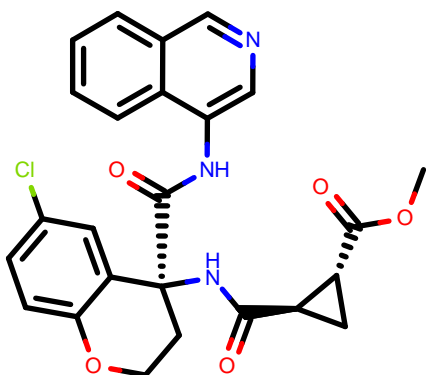
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC(=O)NCC(F)(F)F

RUN: RUN3736

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.24

EN300-765003_1_1_1



CID: EN300-765003_1_1_1

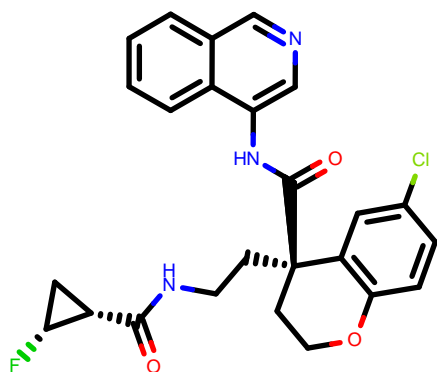
SMILES: COC(=O)[C@@H]1[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4227

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.25

EN300-6953121_3_1_1



CID: EN300-6953121_3_1_1

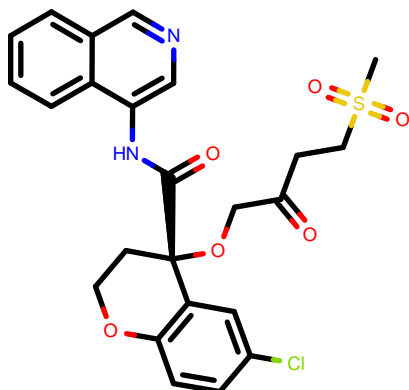
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5[C@@H]5F

RUN: RUN5746

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.23

EN300-1988306_1_1_1



CID: EN300-1988306_1_1_1

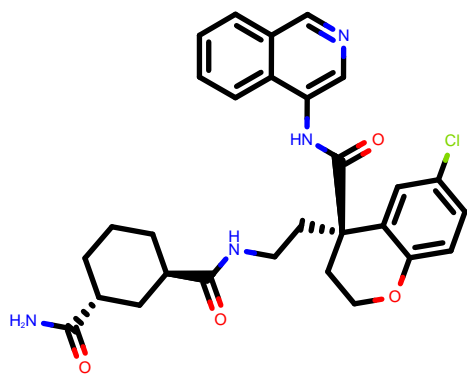
SMILES: CS(=O)(=O)CCC(=O)CO[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN7032

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.33

EN300-90142_3_3_1



CID: EN300-90142_3_3_1

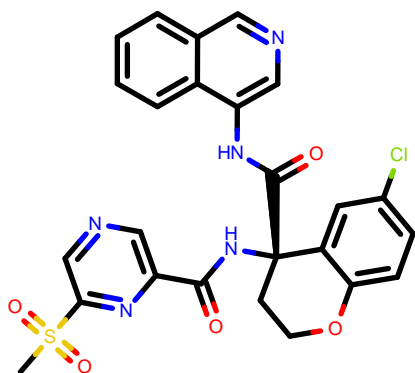
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)CCNC(=O)[C@@H]5CC[C@H](C5)Cl=O

RUN: RUN4684

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.29

EN300-206646_1_1_1



CID: EN300-206646_1_1_1

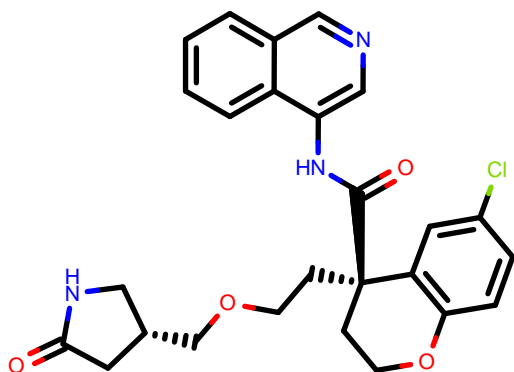
SMILES: CS(=O)(=O)c1nccc(n1)C(=O)N[C@@]2(C)CCOc3c2cc(cc3)C(=O)Nc4nccc5c4cccc5

RUN: RUN3673

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.31

EN300-246747_3_1_1



CID: EN300-246747_3_1_1

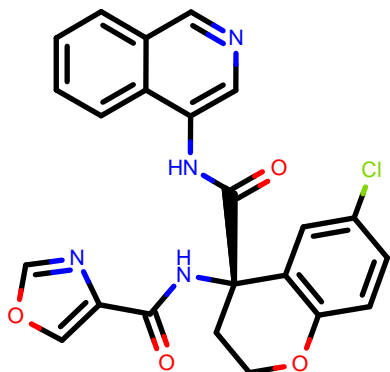
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(=O)Nc5cnc(=O)c5

RUN: RUN3753

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.28

EN300-68618_1_1_1



CID: EN300-68618_1_1_1

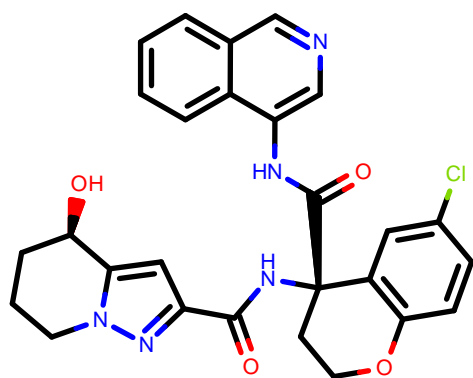
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(=O)Nc5cnc(=O)c5

RUN: RUN3520

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.18

EN300-399606_1_2_1



CID: EN300-399606_1_2_1

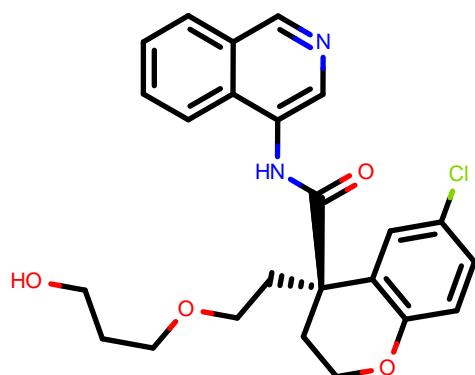
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCC[C@H]6O

RUN: RUN4832

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.33

EN300-221518_3_1_1



CID: EN300-221518_3_1_1

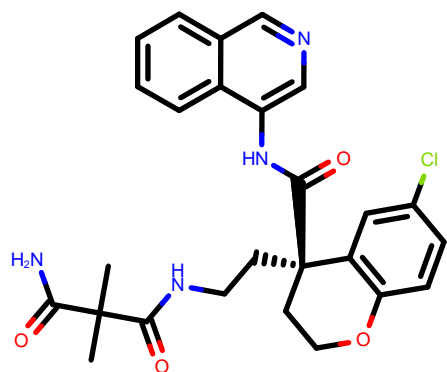
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN3959

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.21

EN300-182913_3_1_1



CID: EN300-182913_3_1_1

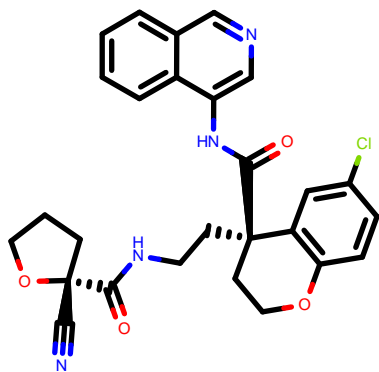
SMILES: CC(C)(C(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN6176

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.27

EN300-3710141_3_2_1



CID: EN300-3710141_3_2_1

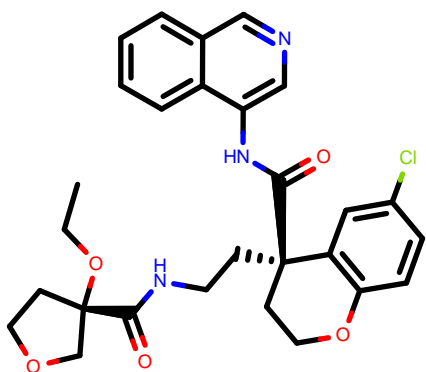
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCCO5)C#N

RUN: RUN3733

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.25

EN300-259694_3_2_1



CID: EN300-259694_3_2_1

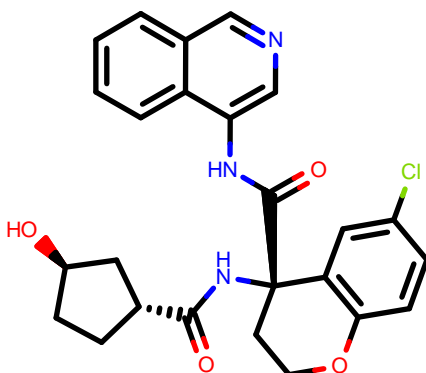
SMILES: CCOC[C@]1(CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc5

RUN: RUN4682

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.45

EN300-321597_1_1_1



CID: EN300-321597_1_1_1

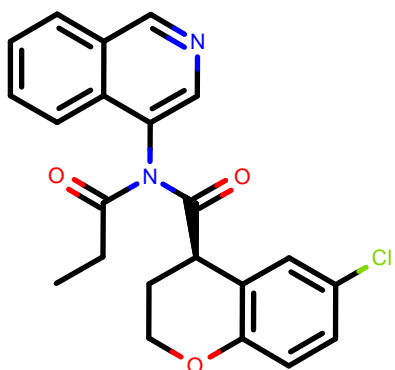
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CC[C@H](C5)O

RUN: RUN3346

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.25

VLA-UCB-50c39ae8-7_1_1



CID: VLA-UCB-50c39ae8-7_1_1

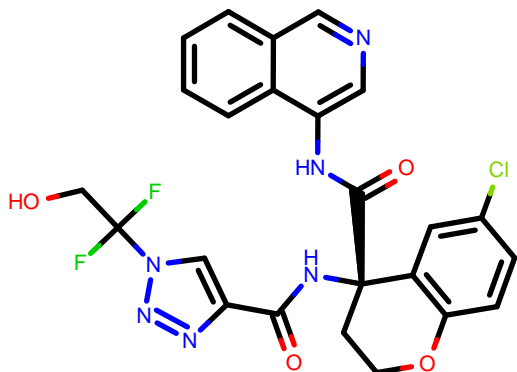
SMILES: C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN5545

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.17

EN300-716207_1_1_1



CID: EN300-716207_1_1_1

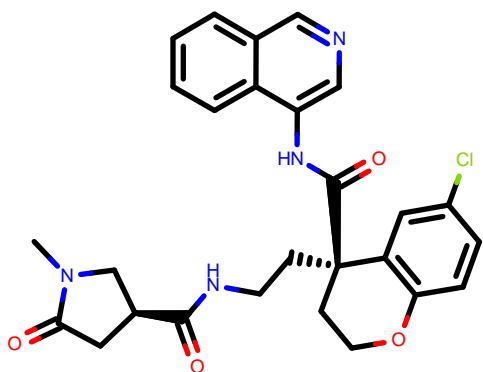
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(n5)C(CO)(F)F

RUN: RUN6475

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.26

EN300-33601_3_2_1



CID: EN300-33601_3_2_1

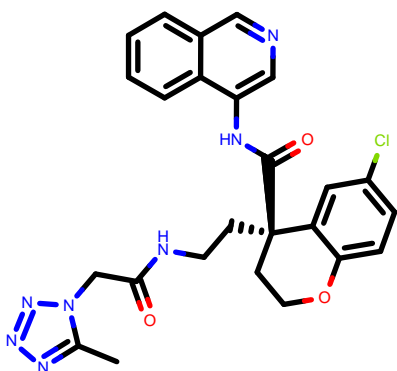
SMILES: CN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4316

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.29

EN300-1244816_3_1_1



CID: EN300-1244816_3_1_1

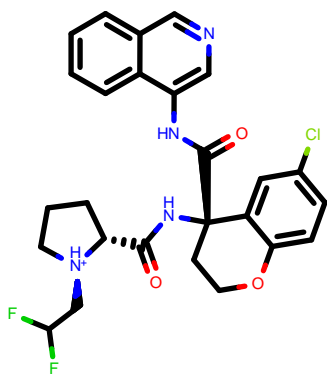
SMILES: Cc1nnnn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN2901

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.31

EDG-MED-90036822-98_4



CID: EDG-MED-90036822-98_4

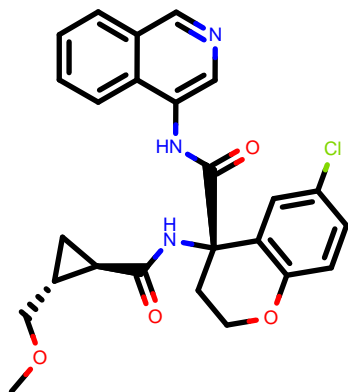
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCCN5[C@@](F)F

RUN: RUN1684

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.25

EN300-705386_1_1_1



CID: EN300-705386_1_1_1

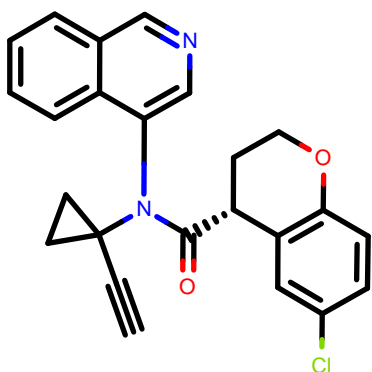
SMILES: COC[C@@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3344

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.22

DAR-DIA-5ff57136-15_1



CID: DAR-DIA-5ff57136-15_1

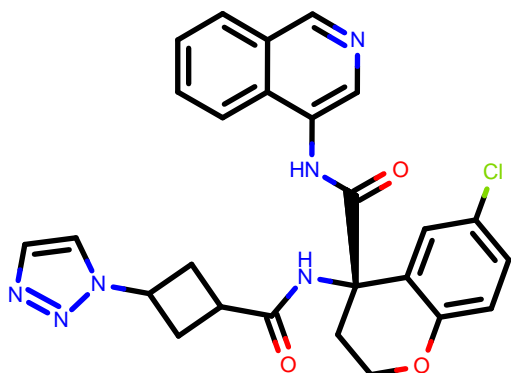
SMILES: C#CC1(CC1)N(c2nccc3c2cccc3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN1263

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.18

EN300-2008240_1_1_1



CID: EN300-2008240_1_1_1

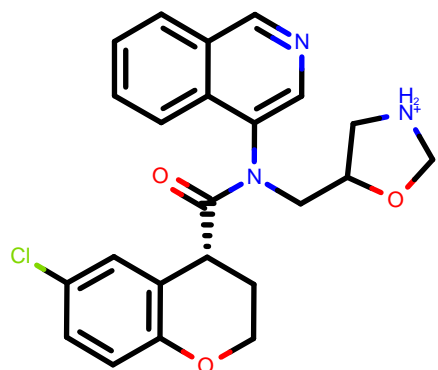
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(C5)n6cnm6

RUN: RUN5388

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.30

ALP-UNI-44c99a80-3_1_1



CID: ALP-UNI-44c99a80-3_1_1

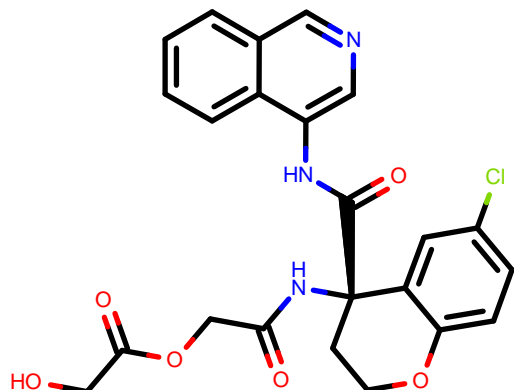
SMILES: c1ccc2c(c1)nccc2N(Cc3nccc3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN4050

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.17

EN300-7459916_1_1_1



CID: EN300-7459916_1_1_1

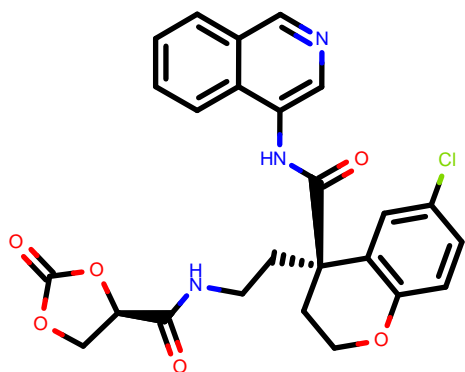
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(=O)CO

RUN: RUN4031

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.23

EN300-5253939_3_2_1



CID: EN300-5253939_3_2_1

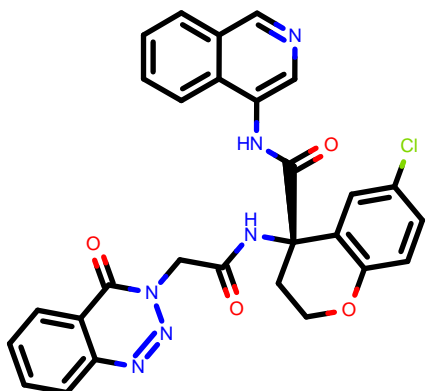
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5COC(=O)O5

RUN: RUN5154

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.26

EN300-21813_1_1_1



CID: EN300-21813_1_1_1

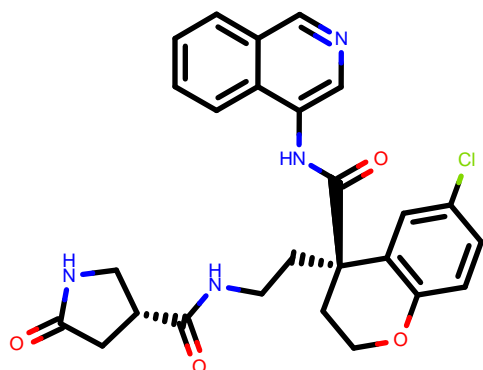
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c(=O)c6ccccc6n5

RUN: RUN6071

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.40

EN300-59487_3_1_1



CID: EN300-59487_3_1_1

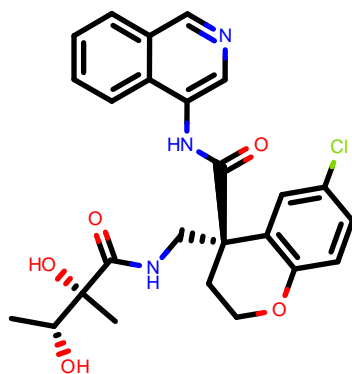
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CC(=O)N5

RUN: RUN3658

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.29

EN300-202922_2_4_1



CID: EN300-202922_2_4_1

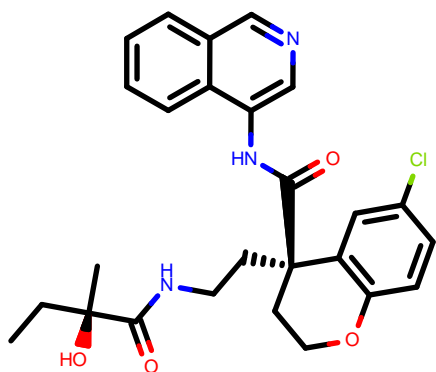
SMILES: C[C@@H]([C@@](C)(C(=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)O)O

RUN: RUN5336

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.30

EN300-104746_3_2_1



CID: EN300-104746_3_2_1

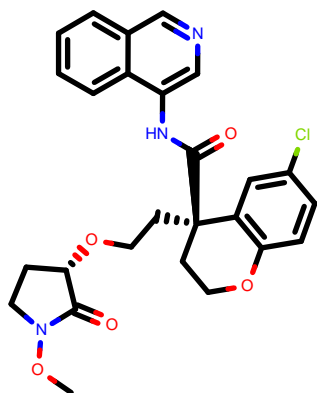
SMILES: CC[C@](C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN4518

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-302058_3_1_1



CID: EN300-302058_3_1_1

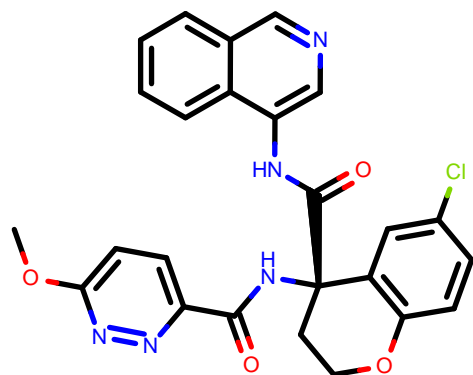
SMILES: CON1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6295

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.26

EN300-82553_1_1_1



CID: EN300-82553_1_1_1

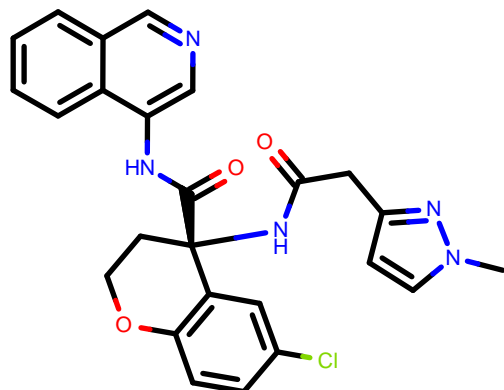
SMILES: COc1ccc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4173

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-258702_1_1_1



CID: EN300-258702_1_1_1

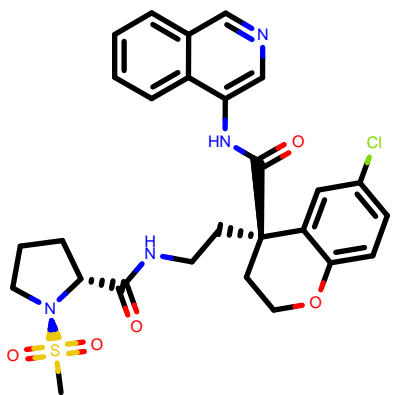
SMILES: Cn1ccc(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3354

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-10402_3_1_1



CID: EN300-10402_3_1_1

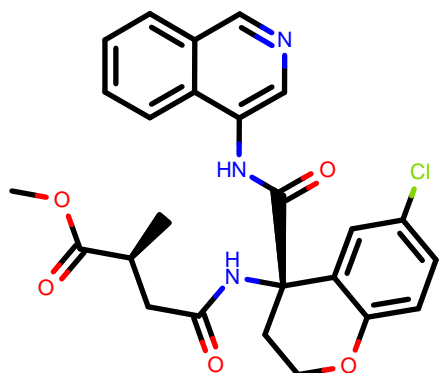
SMILES: CS(=O)(=O)N[C@@H]1CC[C@@H]1C(=O)NC[C@@H]2(COC3C2cc3)C[C@@H]2N4nc5c4ccccc5

RUN: RUN4295

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-108413_1_1_1



CID: EN300-108413_1_1_1

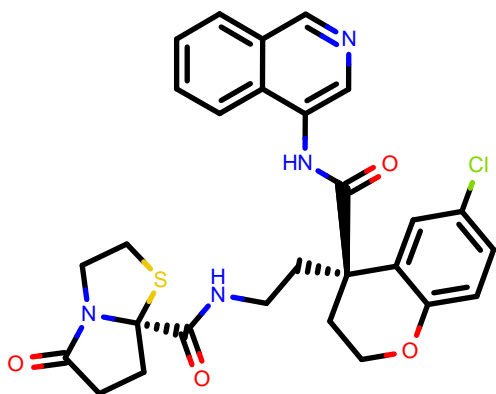
SMILES: C[C@@H](CC(=O)N[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)C(=O)OC

RUN: RUN5185

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.27

EN300-10334_3_2_1



CID: EN300-10334_3_2_1

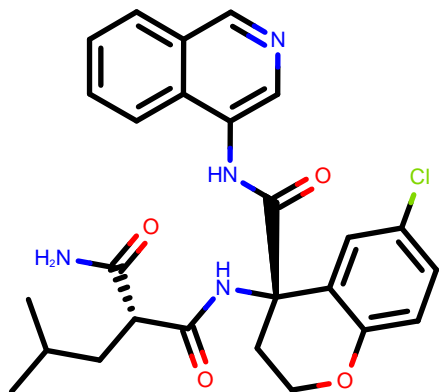
SMILES: c1ccc2c(c1)ncoc2N[C@@H](C@@)3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]56CCC(=O)N5CCS6

RUN: RUN5880

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.34

EN300-250126_1_2_1



CID: EN300-250126_1_2_1

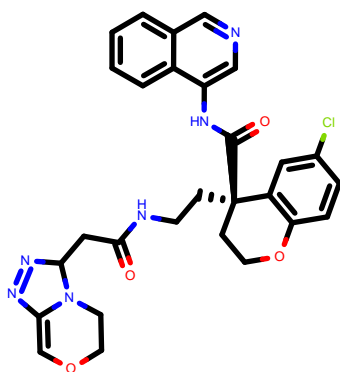
SMILES: CC(C)C[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5140

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.25

EN300-1718836_3_1_1



CID: EN300-1718836_3_1_1

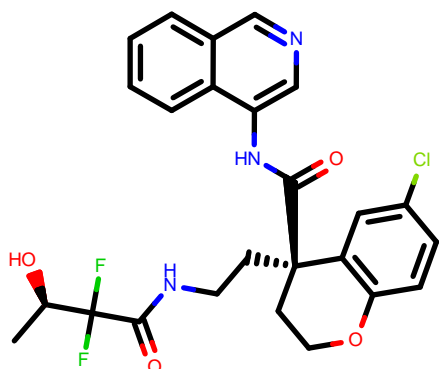
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5nnc6n5CCOC6

RUN: RUN4688

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.31

EN300-185398_3_2_1



CID: EN300-185398_3_2_1

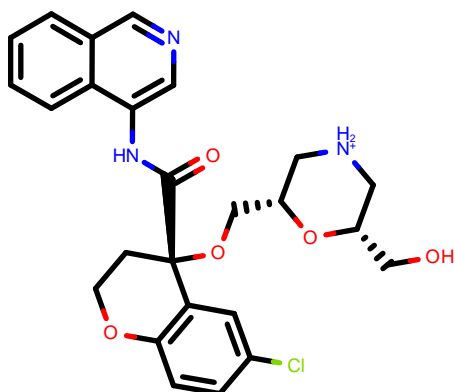
SMILES: C[C@H](C(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)(F)F)O

RUN: RUN4618

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-21_1



CID: ED_-GRI-5b13fbe2-21_1

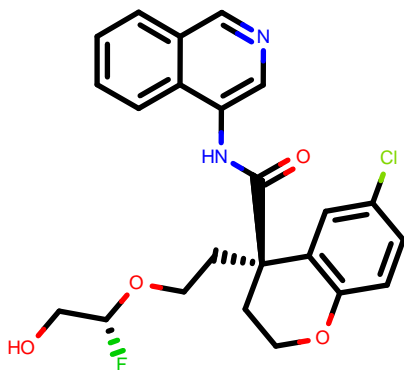
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC[C@@]4(N)CCO[C@H]4O

RUN: RUN1432

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.35

EN300-861925_3_1_1



CID: EN300-861925_3_1_1

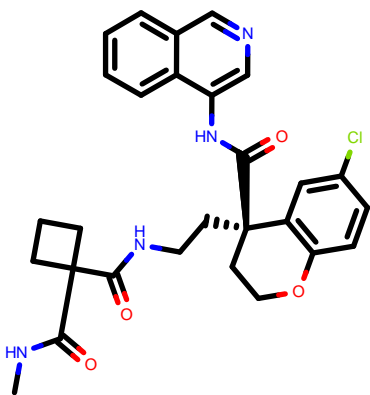
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H](CO)F

RUN: RUN4555

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.26

EN300-70064_3_1_1



CID: EN300-70064_3_1_1

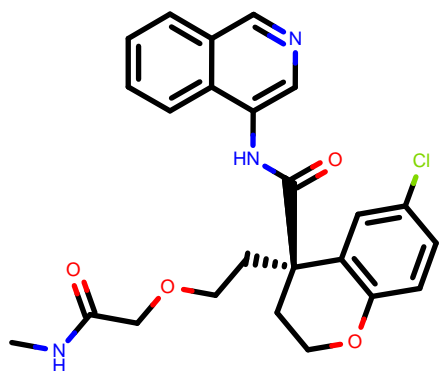
SMILES: CNC(=O)C1(CCC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5266

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.44

EN300-2977549_3_1_1



CID: EN300-2977549_3_1_1

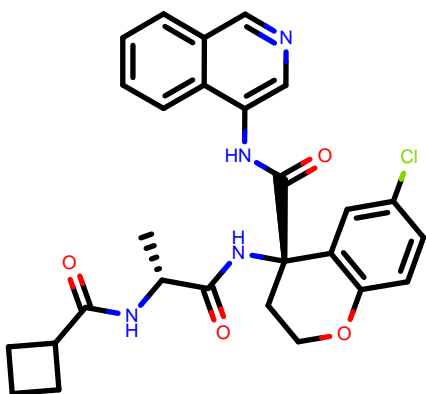
SMILES: CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4156

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.20

EN300-66082_1_2_1



CID: EN300-66082_1_2_1

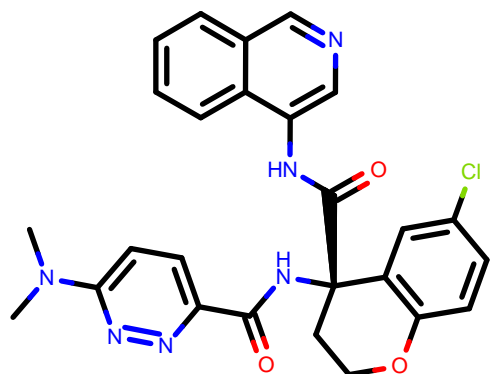
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)NC(=O)C5CC5

RUN: RUN4191

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.33

EN300-7535922_1_1_1



CID: EN300-7535922_1_1_1

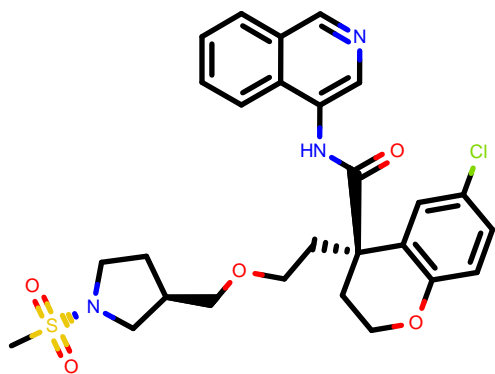
SMILES: CN(C)c1ccc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7727

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.22

KAD-UNI-8a629cb0-1_2



CID: KAD-UNI-8a629cb0-1_2

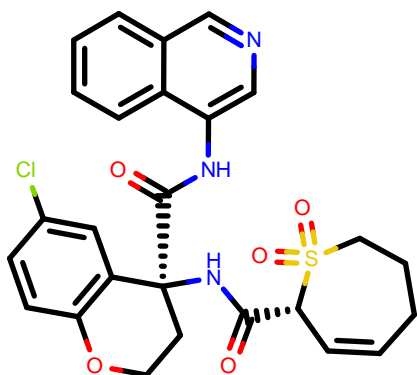
SMILES: CS(=O)(=O)N@1CC[C@H](C1)COC[C@2](CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN1976

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.48

EN300-6499531_1_2_1



CID: EN300-6499531_1_2_1

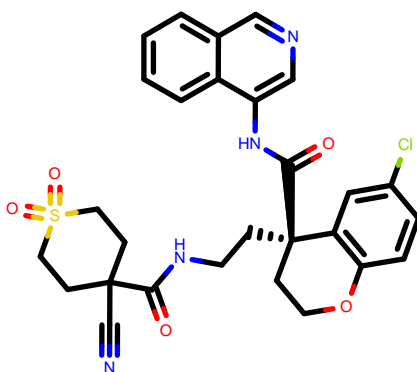
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCCC5S(=O)(=O)

RUN: RUN2881

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.27

EN300-73967_3_1_1



CID: EN300-73967_3_1_1

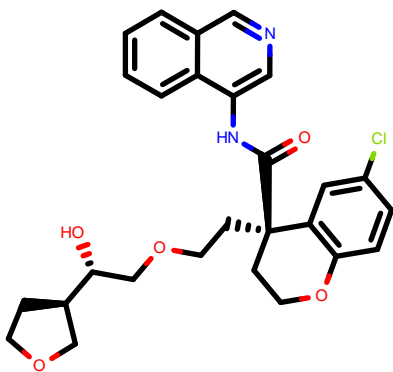
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCS(=O)(=O)CC5)C#N

RUN: RUN3870

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.38

EN300-1911992_3_2_1



CID: EN300-1911992_3_2_1

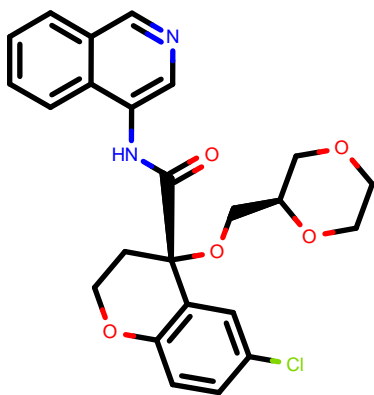
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)CCOCC@H5CCOC5O

RUN: RUN6759

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.36

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

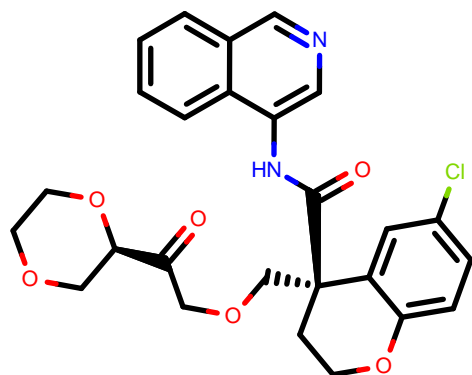
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5COCCO5

RUN: RUN3851

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.26

EN300-6238494_2_2_1



CID: EN300-6238494_2_2_1

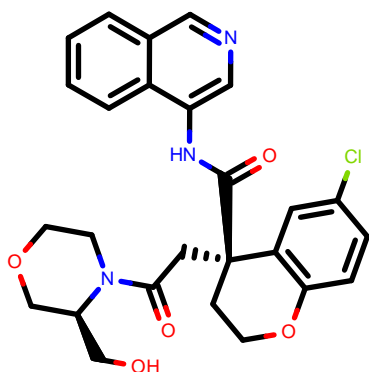
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)[C@H]5COCCO5

RUN: RUN3308

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.40

EN300-154201_1_1_1



CID: EN300-154201_1_1_1

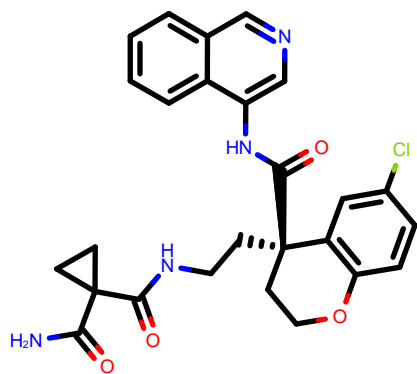
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCOC[C@H]5CO

RUN: RUN3838

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.34

EN300-69070_3_1_1



CID: EN300-69070_3_1_1

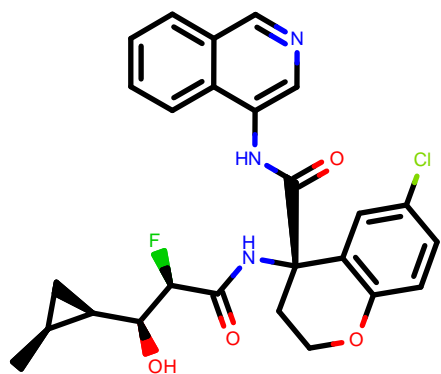
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CC5)C(=O)N

RUN: RUN3454

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.37

EDG-MED-90036822-94_12



CID: EDG-MED-90036822-94_12

SMILES:

C[C@@H]1C[C@@H]1[C@@H]2[C@@H]3[C@@H]2[C@@H]3C(=O)NC(=O)C1(C)C(=O)Nc3ccc4c3ccc5F1O

RUN:

RUN1682

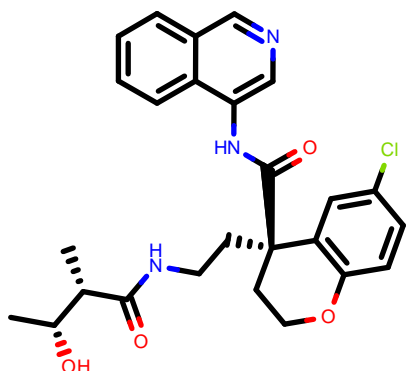
DDG (kcal/mol):

-1.87

dDDG (kcal/mol):

0.25

EN300-7089802_3_1_1



CID: EN300-7089802_3_1_1

SMILES:

C[C@@H]1[C@@H]1[C@@H]2[C@@H]3[C@@H]2[C@@H]3C(=O)NC(=O)C1(C)C(=O)Nc3ccc4c3ccc4O

RUN:

RUN3632

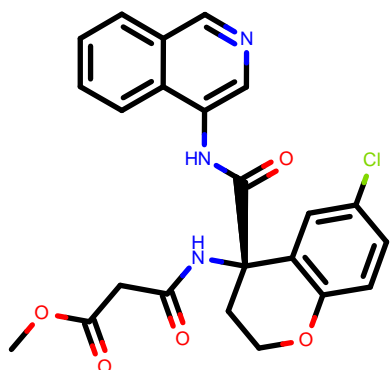
DDG (kcal/mol):

-1.87

dDDG (kcal/mol):

0.30

EN300-20668_1_1_1



CID: EN300-20668_1_1_1

SMILES:

COC(=O)CC(=O)N[C@@H]1(C)C(=O)Nc3ccc4c3ccc4O

RUN:

RUN3927

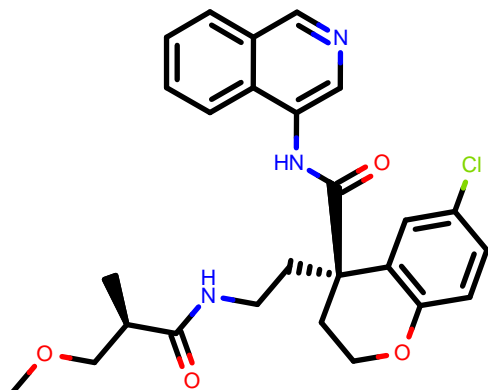
DDG (kcal/mol):

-1.87

dDDG (kcal/mol):

0.21

EN300-69162_3_2_1



CID: EN300-69162_3_2_1

SMILES:

C[C@@H]1(C)C(=O)Nc3ccc4c3ccc4O

RUN:

RUN7813

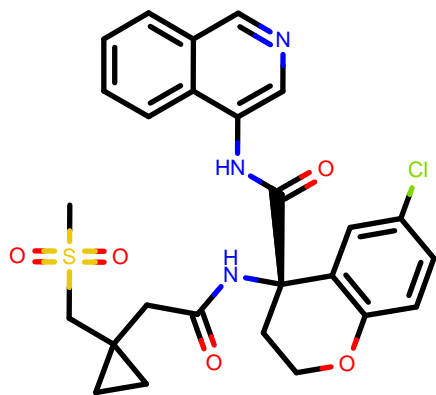
DDG (kcal/mol):

-1.87

dDDG (kcal/mol):

0.34

EN300-97904_1_1_1



CID: EN300-97904_1_1_1

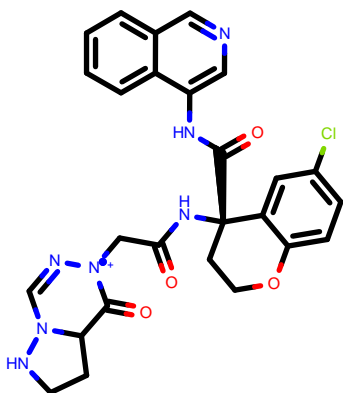
SMILES: CS(=O)(=O)CC1(CC1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN4422

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.35

KAD-UNI-8a629cb0-37_1



CID: KAD-UNI-8a629cb0-37_1

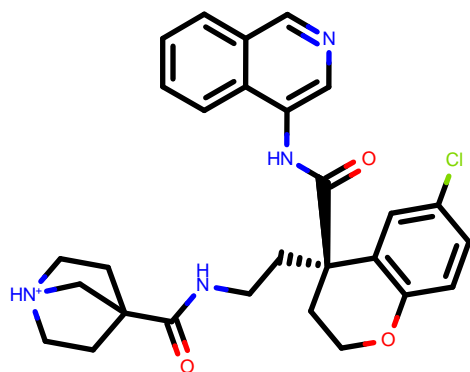
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5c(c1)c6ccnn6cn5

RUN: RUN1955

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.33

EN300-313366_3_1_1



CID: EN300-313366_3_1_1

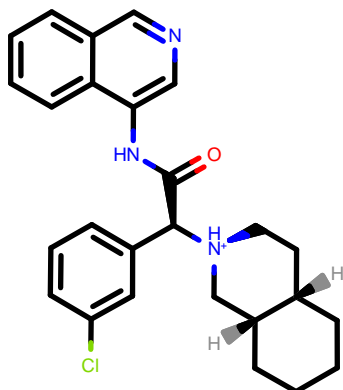
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CC[NH+]1(C5)CC6

RUN: RUN7566

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.29

MIC-UNK-5a93dd5f-3_4



CID: MIC-UNK-5a93dd5f-3_4

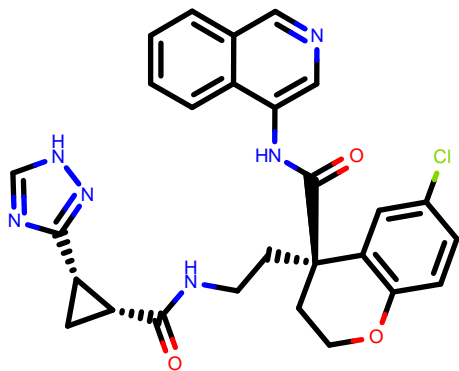
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccccc3)Cl)[N@H+]4CC[C@@]5H5CCCC[C@@]5H5C4

RUN: RUN640

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.34

EN300-6477724_3_1_1



CID: EN300-6477724_3_1_1

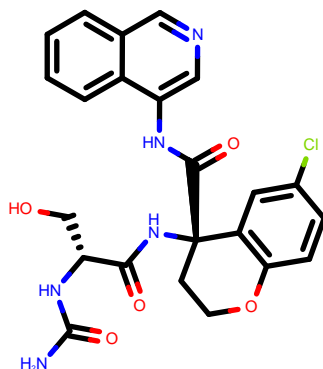
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4cc3cc4C)CCNC(=O)C@@H5C[C@@H]5c6c[nH]n6

RUN: RUN3102

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.40

EN300-10170_1_1_1



CID: EN300-10170_1_1_1

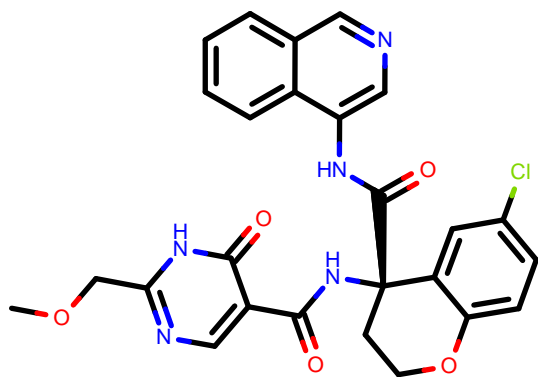
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4cc3cc4C)NC(=O)C@@H5C(CO)NC(=O)N

RUN: RUN4055

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.27

EN300-685492_1_1_1



CID: EN300-685492_1_1_1

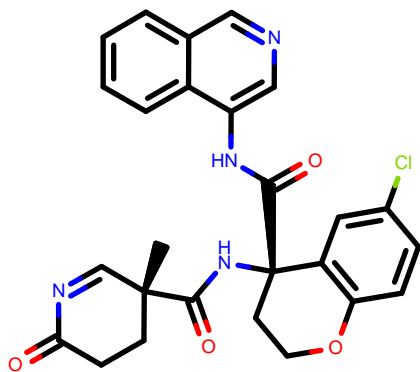
SMILES: COCc1[nH]c2c(=O)c(c[n1])C(=O)N[C@@2](COCc3cc2cc3C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN6686

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.29

EN300-195924_1_2_1



CID: EN300-195924_1_2_1

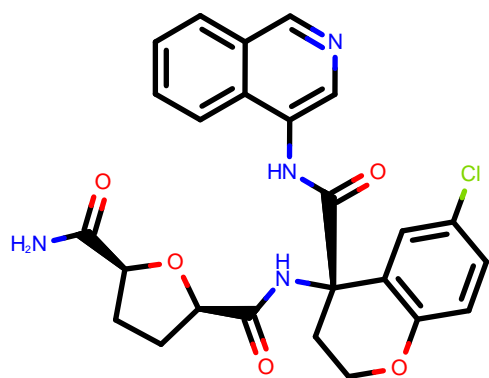
SMILES: C[C@@1](CCC(=O)NC1)C(=O)N[C@@2](COCc3cc2cc3C)C(=O)Nc4cnc5c4ccccc5

RUN: RUN5347

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.23

EN300-315238_1_1_1



CID: EN300-315238_1_1_1

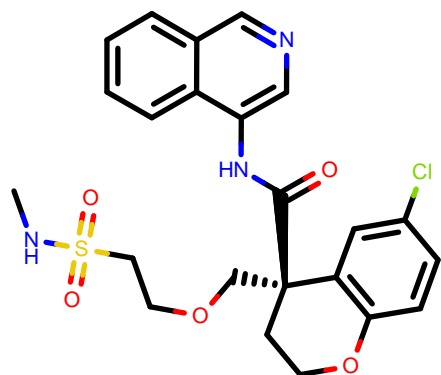
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](O5)C(=O)N

RUN: RUN2859

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.30

EN300-6482967_2_1_1



CID: EN300-6482967_2_1_1

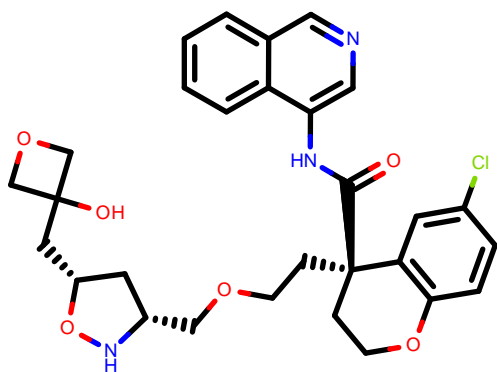
SMILES: CNS(=O)(=O)CCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3286

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.27

EN300-7457160_3_1_2



CID: EN300-7457160_3_1_2

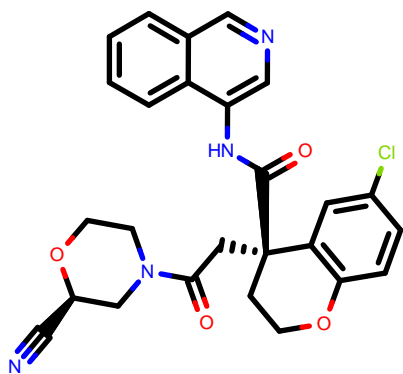
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)[C@H]5C[C@H](O)N5COC6COCC6O

RUN: RUN4017

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.35

EN300-70489_1_1_1



CID: EN300-70489_1_1_1

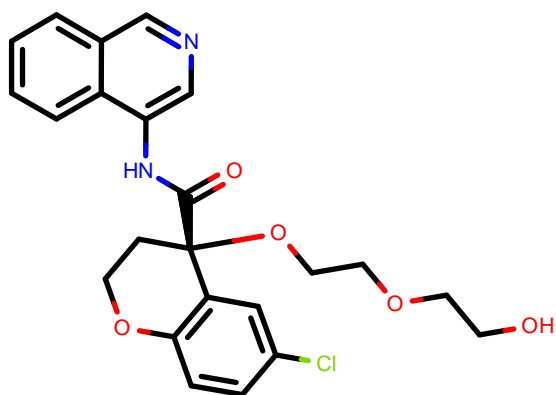
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@]6(H)(C5)C#N

RUN: RUN3553

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.24

EN300-52467_1_1_1



CID: EN300-52467_1_1_1

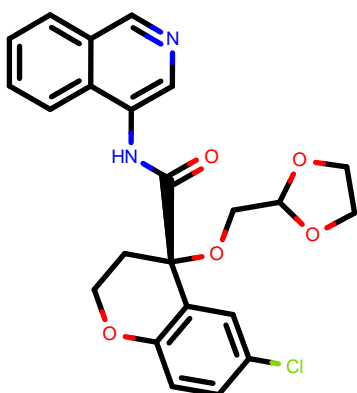
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN4787

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.23

EN300-77092_1_1_1



CID: EN300-77092_1_1_1

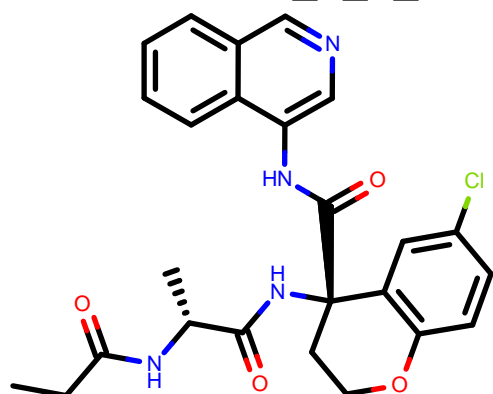
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5OCCO5

RUN: RUN5517

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.26

EN300-31148_1_2_1



CID: EN300-31148_1_2_1

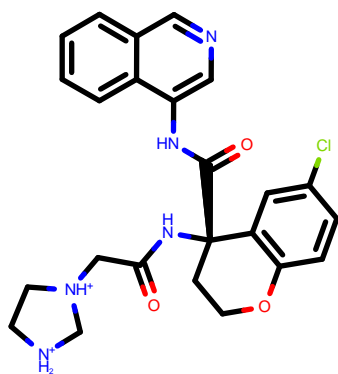
SMILES: CCC(=O)N[C@@H](C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN4193

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.24

EDG-MED-90036822-18_1



CID: EDG-MED-90036822-18_1

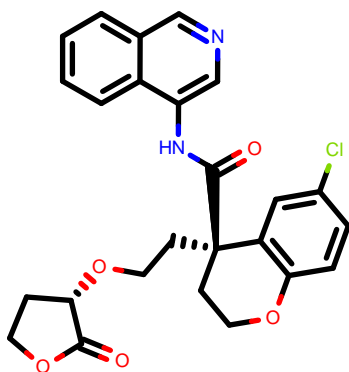
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc5

RUN: RUN1553

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.22

EN300-20496_3_2_1



CID: EN300-20496_3_2_1

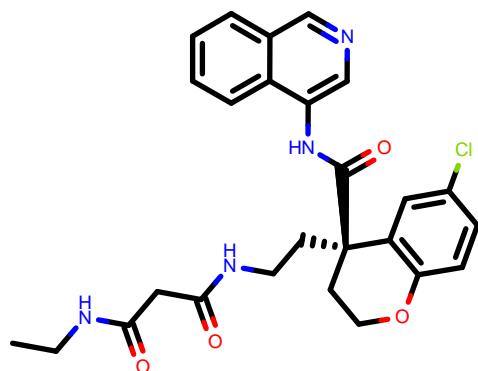
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCOC5=O

RUN: RUN3049

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.26

EN300-129455_3_1_1



CID: EN300-129455_3_1_1

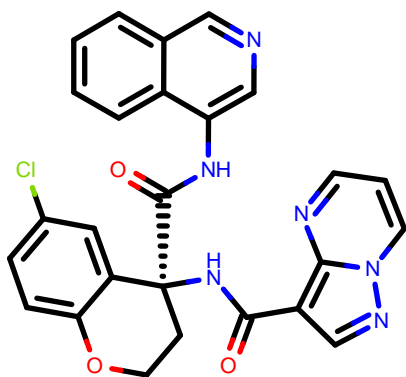
SMILES: CCNC(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3853

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.33

EN300-29520_1_1_1



CID: EN300-29520_1_1_1

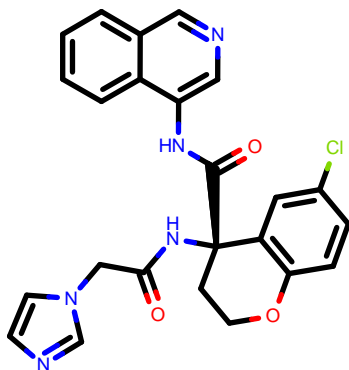
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5ncc6

RUN: RUN3639

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.24

EN300-38979_1_1_1



CID: EN300-38979_1_1_1

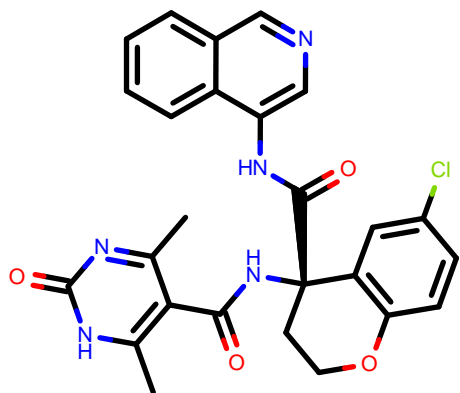
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc5

RUN: RUN3447

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.20

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)Nc4ncoc5c4ccoc5

RUN:

RUN3741

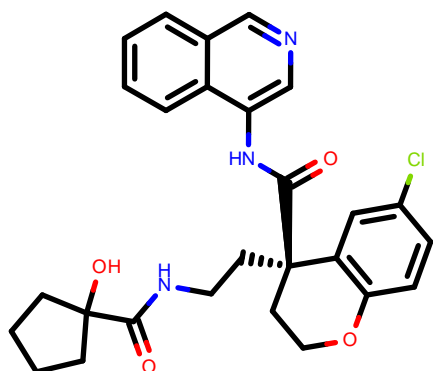
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.28

EN300-25960_3_1_1



CID: EN300-25960_3_1_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCC5)O

RUN:

RUN4867

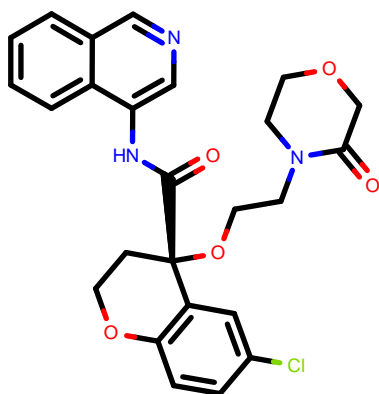
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.34

CHO-MSK-5891c1ff-6_1



CID: CHO-MSK-5891c1ff-6_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5C(=O)CCO5=O

RUN:

RUN1701

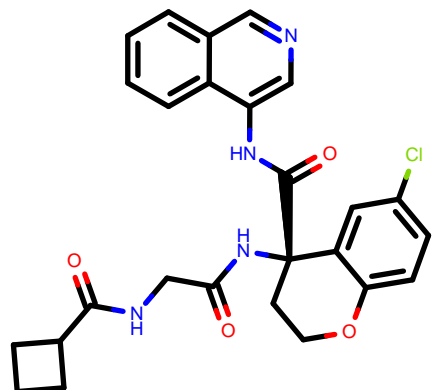
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.25

EN300-62448_1_1_1



CID: EN300-62448_1_1_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)C5C(=O)C5

RUN:

RUN4625

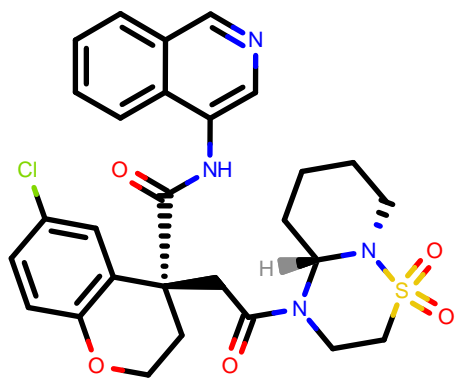
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.25

ALP-UNI-3496895b-1_2



CID: ALP-UNI-3496895b-1_2

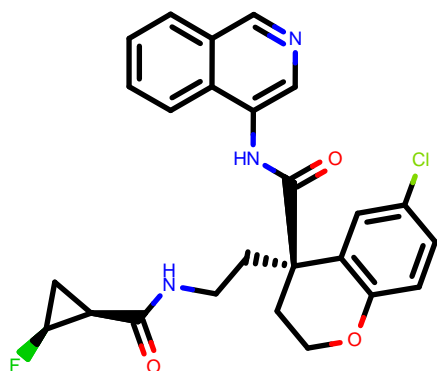
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSCCS(=O)(=O)N@H[C@@H]5CCCC5

RUN: RUN2352

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.48

EN300-1654606_3_1_1



CID: EN300-1654606_3_1_1

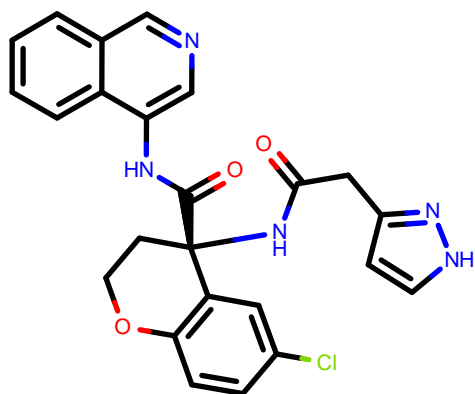
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN3426

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

VLA-UCB-34f3ed0c-4_1_1



CID: VLA-UCB-34f3ed0c-4_1_1

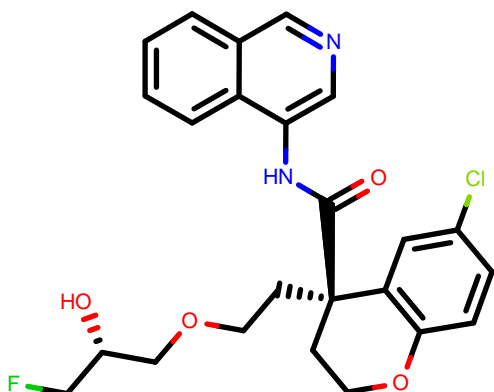
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5ccn[nH]5

RUN: RUN3934

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

EN300-1968342_3_2_1



CID: EN300-1968342_3_2_1

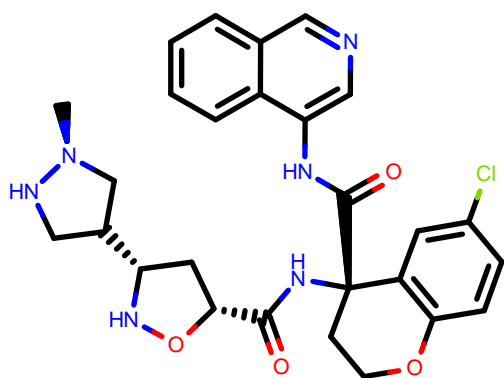
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN4030

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.34

EN300-92605_1_2_1



CID: EN300-92605_1_2_1

SMILES:

Cn1cccnc1[C@@H]2[C@@H](ON2)C(=O)NC@@3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc5ccc5

RUN:

RUN4280

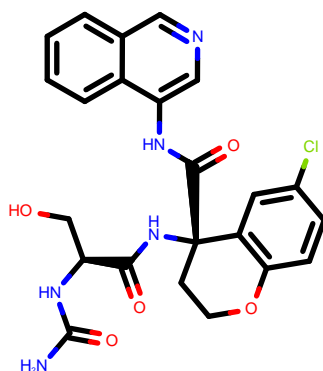
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.32

EN300-10170_1_2_1



CID: EN300-10170_1_2_1

SMILES:

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

RUN:

RUN6443

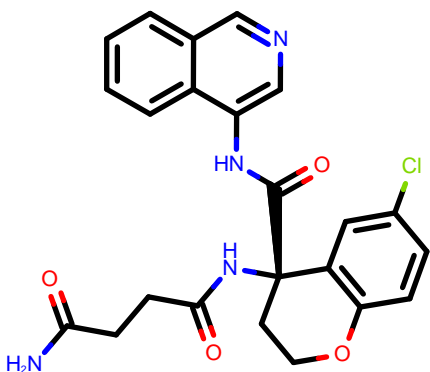
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.23

EN300-178515_1_1_1



CID: EN300-178515_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)CCC(=O)N

RUN:

RUN4801

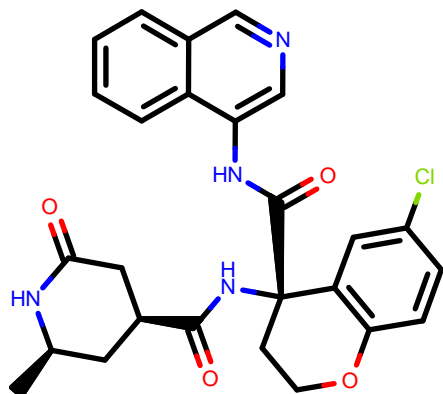
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.23

EN300-7435400_1_1_1



CID: EN300-7435400_1_1_1

SMILES:

C[C@@H]1[C@@H](C[C@@H](CC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN:

RUN3709

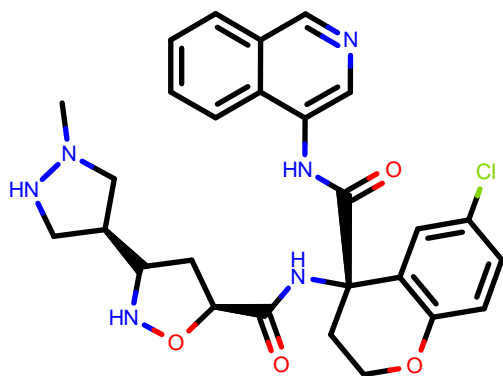
DDG (kcal/mol):

-1.82

dDDG (kcal/mol):

0.25

ALP-UNI-dbbfd3db-13_1



CID: ALP-UNI-dbbfd3db-13_1

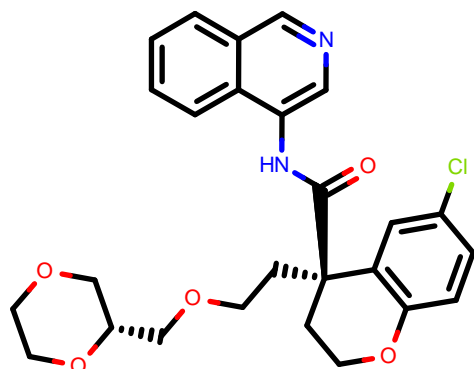
SMILES: Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN2629

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.24

EN300-139167_3_2_1



CID: EN300-139167_3_2_1

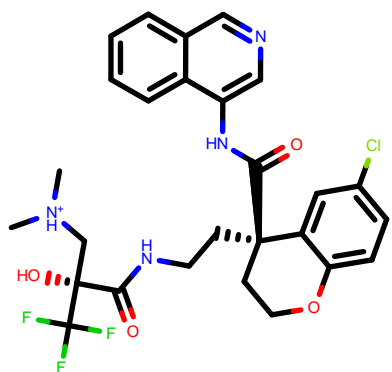
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COC5

RUN: RUN4100

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-7459545_3_1_1



CID: EN300-7459545_3_1_1

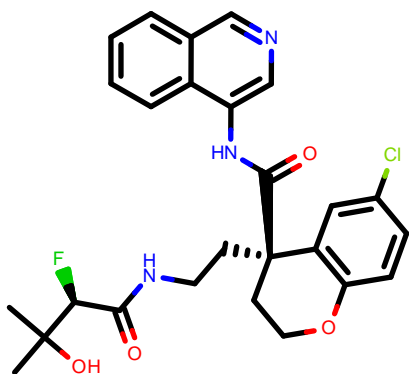
SMILES: CN(C)C[C@@](C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)(C(F)(F)F)O

RUN: RUN3276

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.62

EN300-264744_3_2_1



CID: EN300-264744_3_2_1

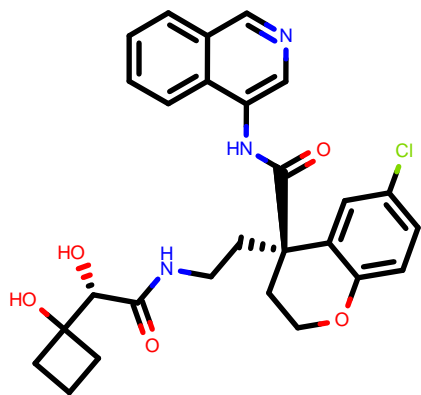
SMILES: CC(C)(C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)F)O

RUN: RUN3685

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-1073320_3_2_1



CID: EN300-1073320_3_2_1

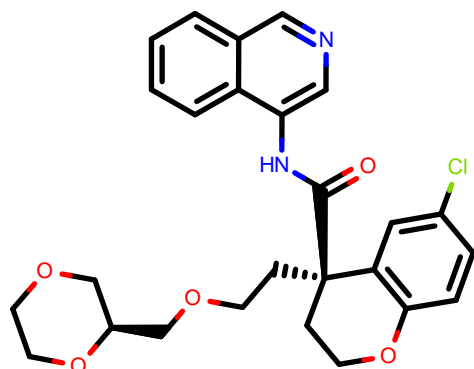
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COCc4cc3cc4)CNC(=O)[C@H](C5(CCC5)O)O

RUN: RUN7048

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.27

EN300-139167_3_1_1



CID: EN300-139167_3_1_1

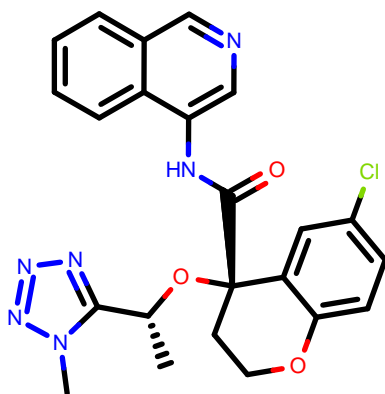
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COCc4cc3cc4)COC[C@@H]5OCOC5

RUN: RUN3113

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.32

EN300-173006_1_2_1



CID: EN300-173006_1_2_1

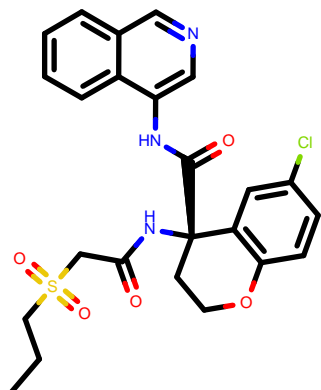
SMILES: C[C@H](c1nnnn1)C[C@@]2(CCOc3cc2cc3)C(=O)Nc4cnc5c4ccc5

RUN: RUN6136

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.23

EN300-52325_1_1_1



CID: EN300-52325_1_1_1

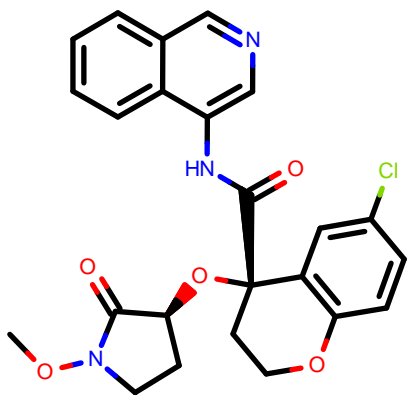
SMILES: CCCS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc2)C(=O)Nc3cnc4c3ccc4

RUN: RUN3904

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.33

EN300-302058_1_1_1



CID: EN300-302058_1_1_1

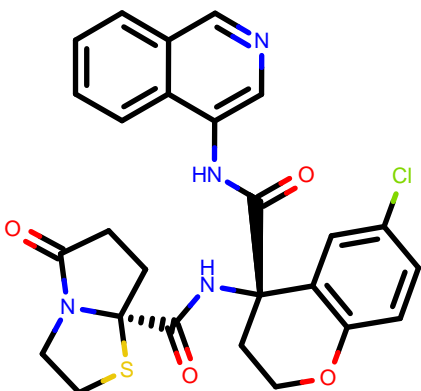
SMILES: CON1CC[C@@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4382

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.25

EN300-10334_1_1_1



CID: EN300-10334_1_1_1

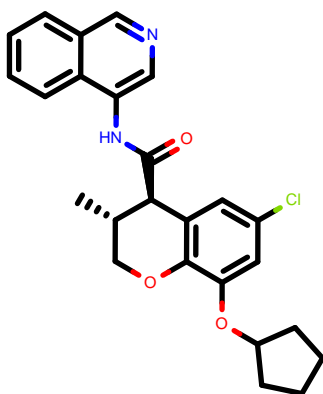
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCCC(=O)N5CCS6

RUN: RUN3914

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-4_1



CID: DAR-DIA-0d514e7d-4_1

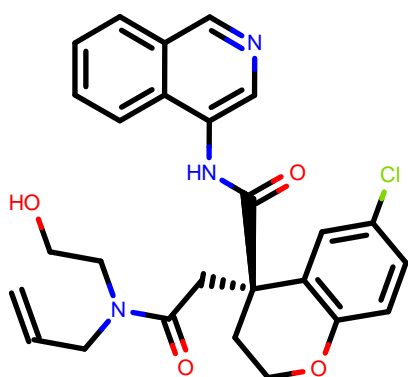
SMILES: C[C@@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@]3[H]1C(=O)Nc4ncc5c4cccc5

RUN: RUN793

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.21

EN300-79536_1_1_1



CID: EN300-79536_1_1_1

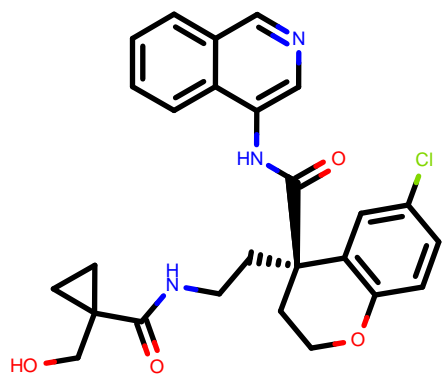
SMILES: C=CCN(CCO)C(=O)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4793

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.34

EN300-146174_3_1_1



CID: EN300-146174_3_1_1

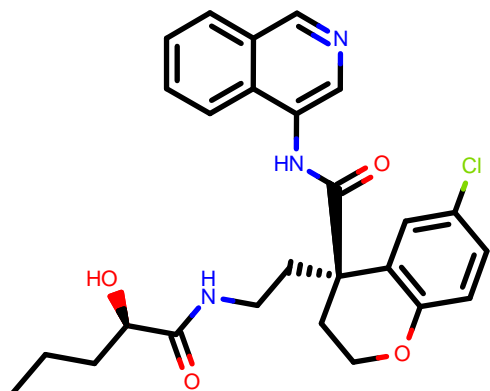
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)CO

RUN: RUN4260

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.27

EN300-300217_3_3_1



CID: EN300-300217_3_3_1

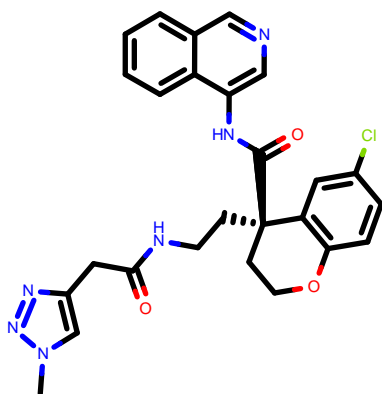
SMILES: C/C=C/[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6615

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.33

EN300-1073264_3_1_1



CID: EN300-1073264_3_1_1

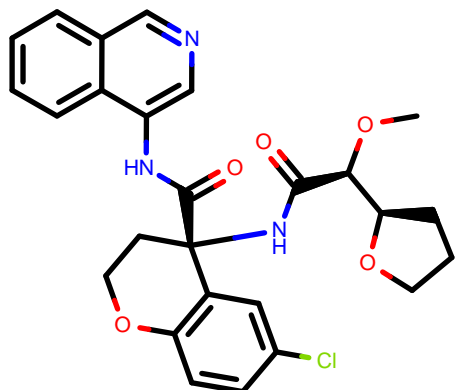
SMILES: Cn1cc(nn1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6865

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.29

EN300-6277108_1_3_1



CID: EN300-6277108_1_3_1

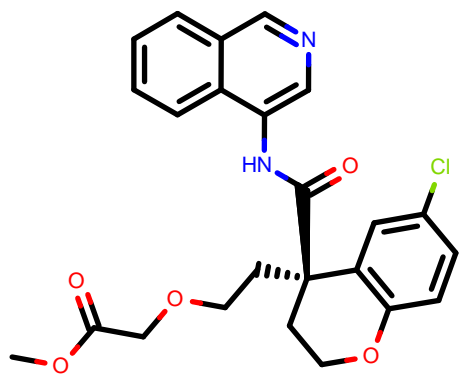
SMILES: CO[C@@H]([C@H]1CCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3669

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.28

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

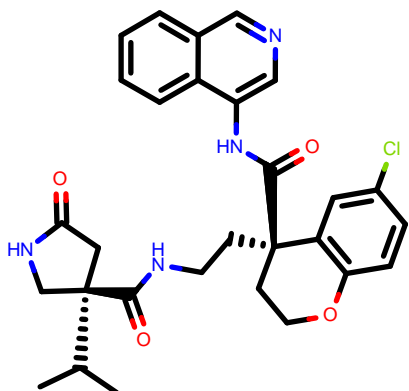
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4172

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.25

EN300-211203_3_2_1



CID: EN300-211203_3_2_1

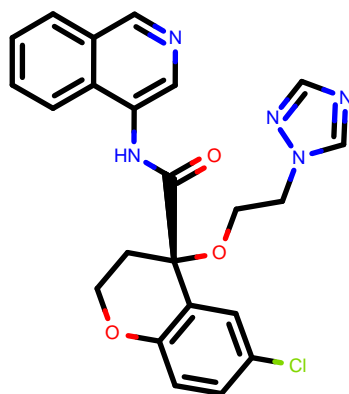
SMILES: CC(C)[C@@]1(C(=O)NC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3743

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.36

EN300-6255179_1_1_1



CID: EN300-6255179_1_1_1

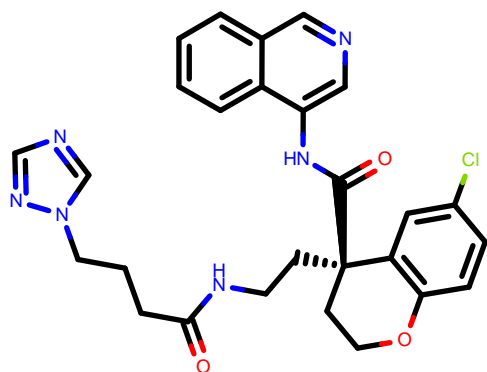
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cncn5

RUN: RUN4814

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.20

EN300-316216_3_1_1



CID: EN300-316216_3_1_1

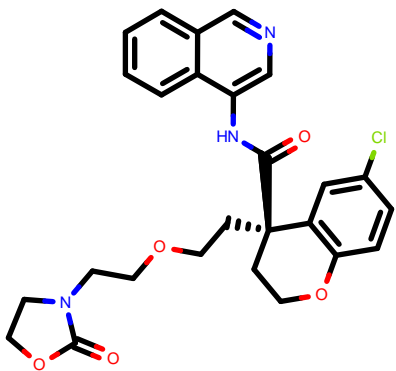
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cncn5

RUN: RUN3677

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.33

EN300-370967_3_1_1



CID: EN300-370967_3_1_1

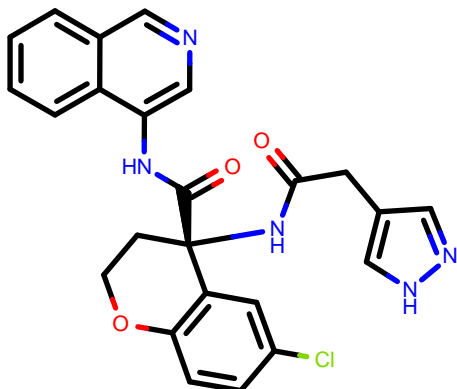
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOC5=O

RUN: RUN4033

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.26

EN300-1589101_1_1_1



CID: EN300-1589101_1_1_1

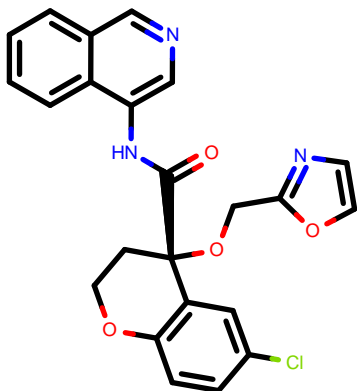
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]n5

RUN: RUN2981

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.21

EN300-317555_1_1_1



CID: EN300-317555_1_1_1

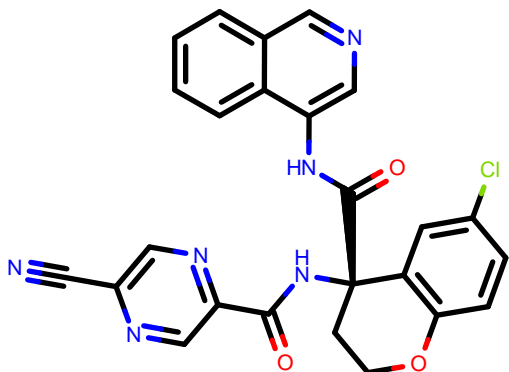
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5

RUN: RUN3804

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.22

EN300-149224_1_1_1



CID: EN300-149224_1_1_1

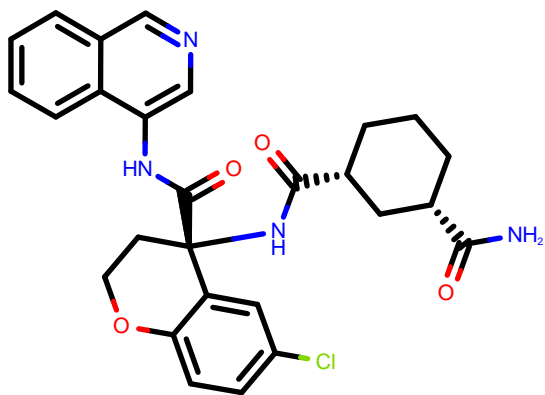
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncnc5C#N

RUN: RUN3245

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.24

EN300-90142_1_1_1



CID: EN300-90142_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(c4)C)N(C)C@H5(CCC)C@H1(C5)C1=O

RUN:

RUN3907

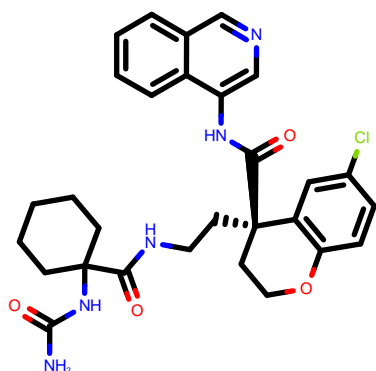
DDG (kcal/mol):

-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(c4)C)CNC(=O)C5(CCCC5)NC(=O)N

RUN:

RUN6344

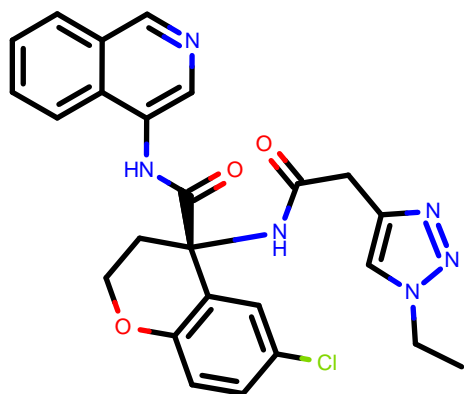
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.36

EN300-717276_1_1_1



CID: EN300-717276_1_1_1

SMILES:

CCn1cc(nn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN:

RUN4081

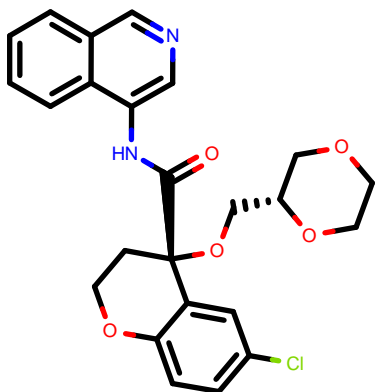
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.24

EN300-139167_1_1_1



CID: EN300-139167_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)C)OC[C@@H]5COC5

RUN:

RUN4402

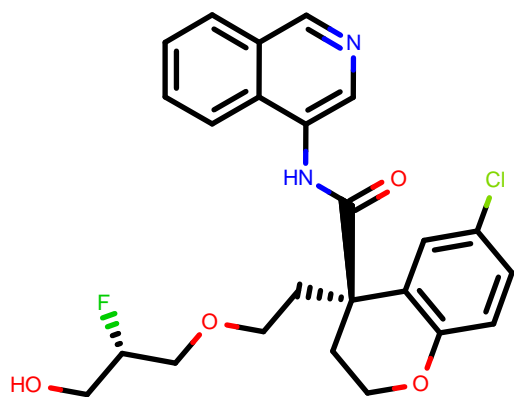
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.28

EN300-1600517_3_2_1



CID: EN300-1600517_3_2_1

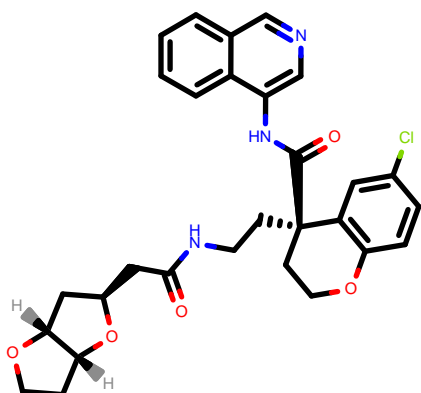
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)F

RUN: RUN3791

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.31

EN300-7355519_3_5_1



CID: EN300-7355519_3_5_1

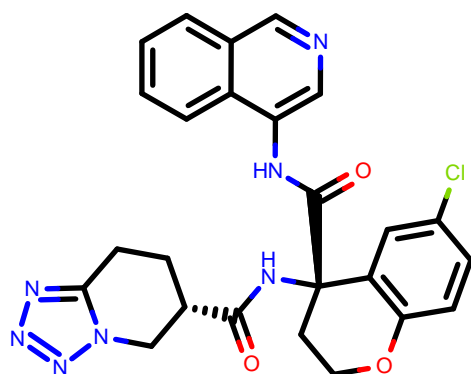
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](O)COC6

RUN: RUN5254

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.33

EN300-269453_1_2_1



CID: EN300-269453_1_2_1

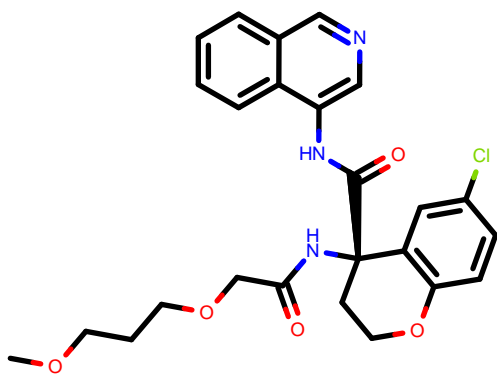
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCc6nnc6C5

RUN: RUN2938

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-125769_1_1_1



CID: EN300-125769_1_1_1

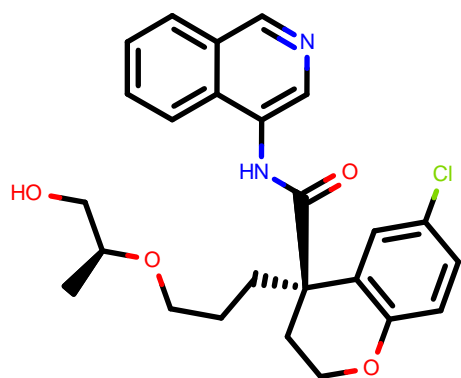
SMILES: COCCCCOC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3262

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.28

EN300-175186_4_1_1



CID: EN300-175186_4_1_1

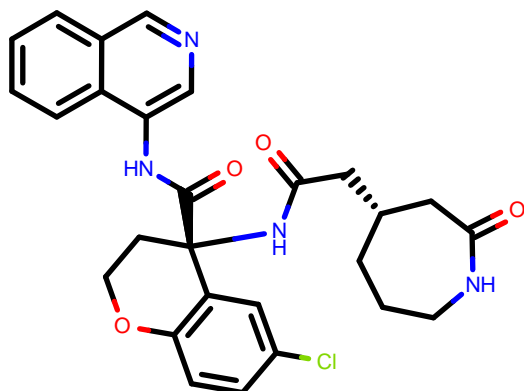
SMILES: C[C@@H](CO)OCCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3902

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.34

EN300-195590_1_2_1



CID: EN300-195590_1_2_1

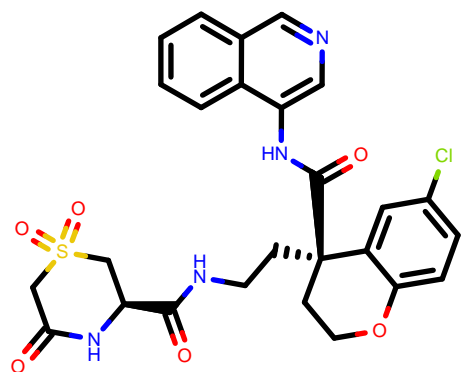
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]5CCNC(=O)C5

RUN: RUN4473

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.35

EN300-754584_3_1_1



CID: EN300-754584_3_1_1

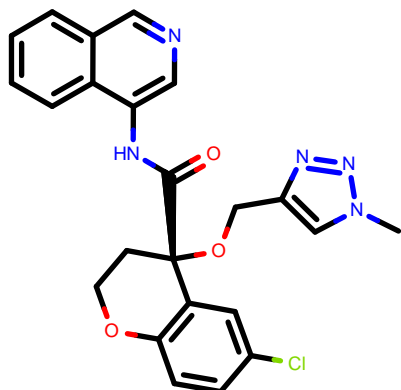
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H]5CS(=O)(=O)N5

RUN: RUN5226

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-120282_1_1_1



CID: EN300-120282_1_1_1

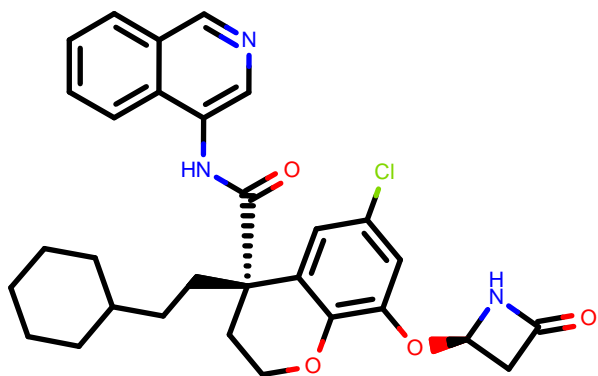
SMILES: Cn1cc(nn1)CO[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4786

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.19

VLA-UCB-05e51b3f-12_1



CID: VLA-UCB-05e51b3f-12_1

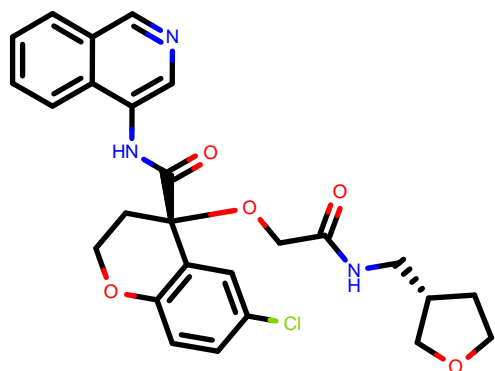
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)Cl)CCc6CCCC6

RUN: RUN311

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.54

EN300-46832_1_1_1



CID: EN300-46832_1_1_1

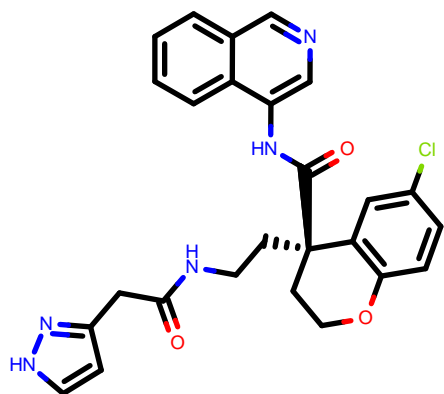
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCOC5

RUN: RUN4665

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.25

EN300-71405_3_1_1



CID: EN300-71405_3_1_1

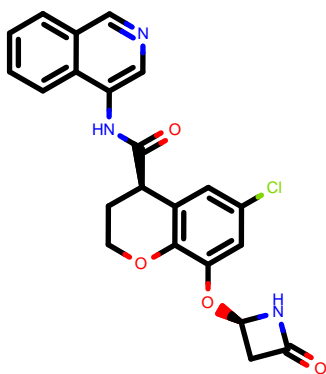
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5c[nH]5

RUN: RUN5277

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.28

VLA-UCB-50c39ae8-8_1



CID: VLA-UCB-50c39ae8-8_1

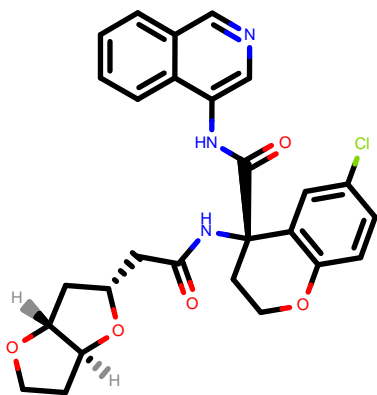
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)Cl

RUN: RUN342

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.23

EN300-7355519_1_2_1



CID: EN300-7355519_1_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4)Cl)NC(=O)C[C@@H]5C[C@@H](O5)CCO6

RUN:

RUN3737

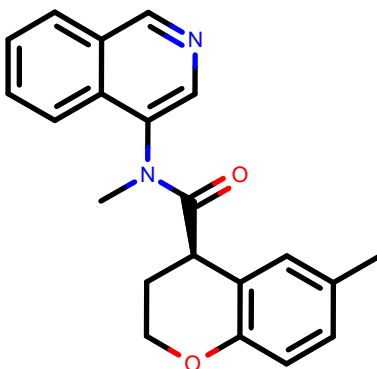
DDG (kcal/mol):

-1.77

dDDG (kcal/mol):

0.26

MAK-UNK-3875bbc8-1_1



CID: MAK-UNK-3875bbc8-1_1

SMILES:

Cc1ccc2c(c1)[C@@H](C(=O)N(C)C)C3cncnc4c3cccc4

RUN:

RUN703

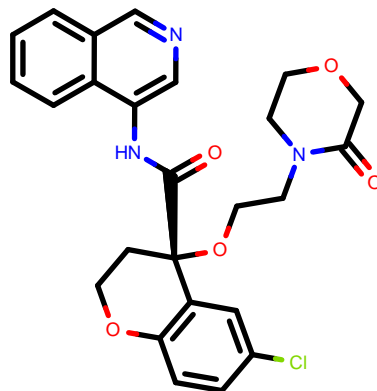
DDG (kcal/mol):

-1.77

dDDG (kcal/mol):

0.09

EN300-219330_1_1_1



CID: EN300-219330_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4)Cl)OCCN5CCOCC5=O

RUN:

RUN3242

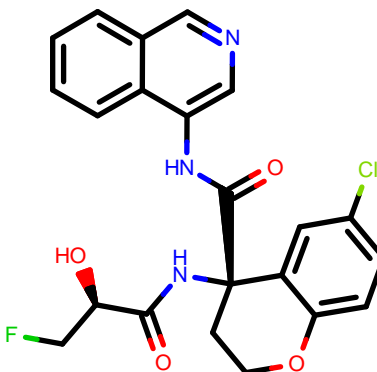
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

0.22

EDG-MED-90036822-17_1



CID: EDG-MED-90036822-17_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4)Cl)NC(=O)[C@@H](CF)O

RUN:

RUN1542

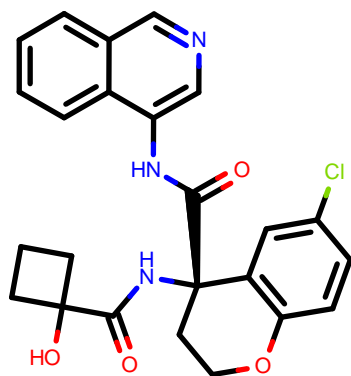
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

0.28

EN300-52009_1_1_1



CID: EN300-52009_1_1_1

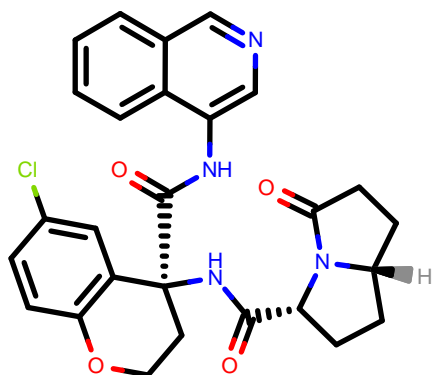
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)O

RUN: RUN3211

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.26

EN300-6479181_1_2_1



CID: EN300-6479181_1_2_1

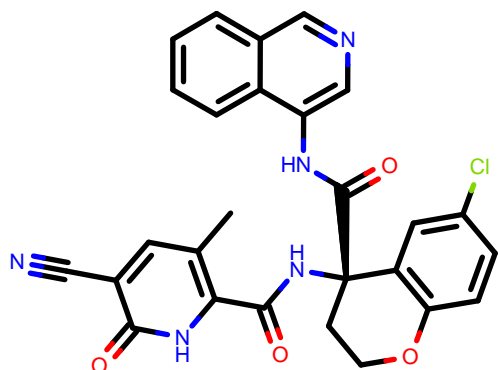
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)O

RUN: RUN3292

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.30

EN300-358956_1_1_1



CID: EN300-358956_1_1_1

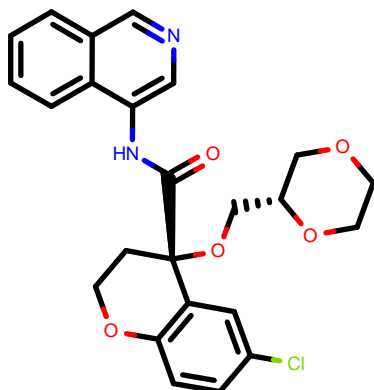
SMILES: Cc1cc(c(=O)[nH]c1C(=O)N)C@@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)C#N

RUN: RUN4347

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.36

EN300-139167_1_1_1



CID: EN300-139167_1_1_1

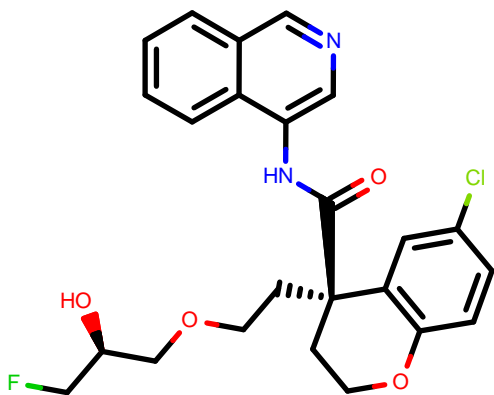
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COC5

RUN: RUN4349

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.27

EN300-1968342_3_1_1



CID: EN300-1968342_3_1_1

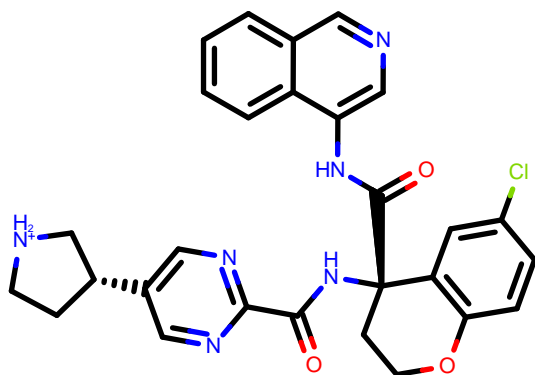
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3ccc(cc4)C)CCOC[C@@H](CF)O

RUN: RUN2958

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.31

EDG-MED-90036822-104_1



CID: EDG-MED-90036822-104_1

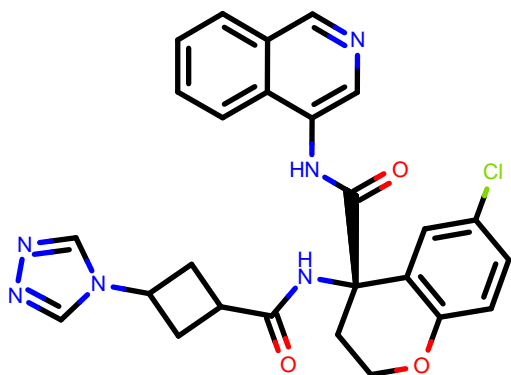
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3ccc(cc4)C)NC(=O)c5nccn5[C@@H]6CQ[NH2+]c6

RUN: RUN1693

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.33

EN300-1717596_1_1_1



CID: EN300-1717596_1_1_1

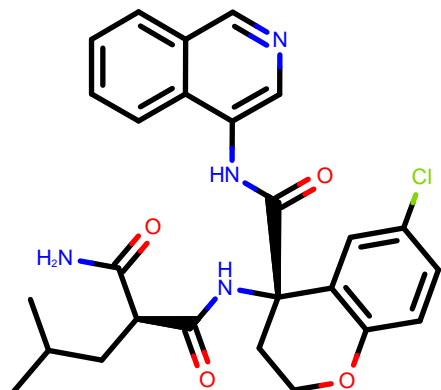
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3ccc(cc4)C)NC(=O)C5C[C@H]5n6nnn6

RUN: RUN4270

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.35

EN300-250126_1_1_1



CID: EN300-250126_1_1_1

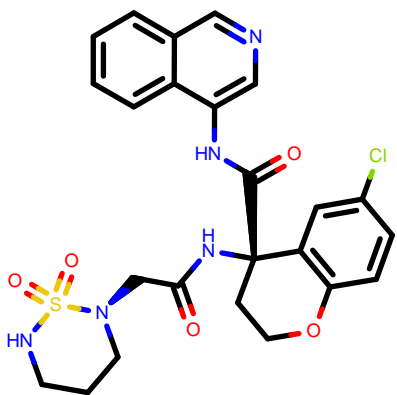
SMILES: CC(C)C[C@@H](C(=O)N)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4

RUN: RUN2769

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.26

EN300-4726186_1_1_1



CID: EN300-4726186_1_1_1

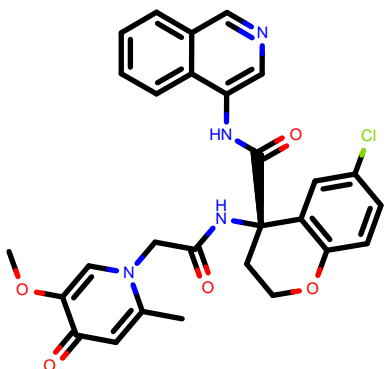
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[N@]5SCCN5S(=O)=O

RUN: RUN5310

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.43

EN300-1271924_1_1_1



CID: EN300-1271924_1_1_1

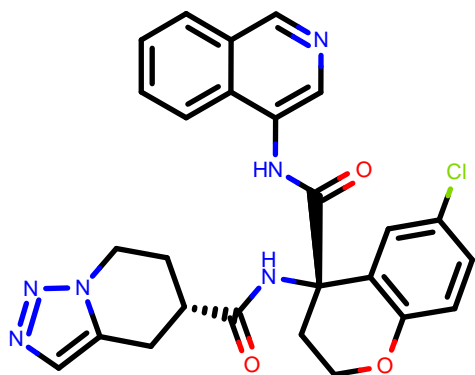
SMILES: Cc1cc(=O)c(n1CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)OC

RUN: RUN5058

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.30

EN300-7430501_1_2_1



CID: EN300-7430501_1_2_1

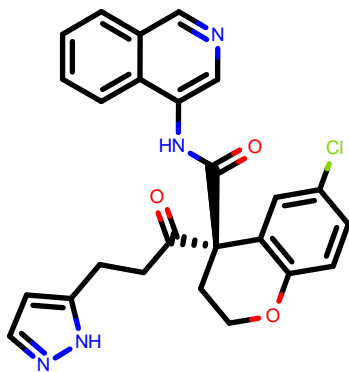
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]5CCn6c(cnn6)C5

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

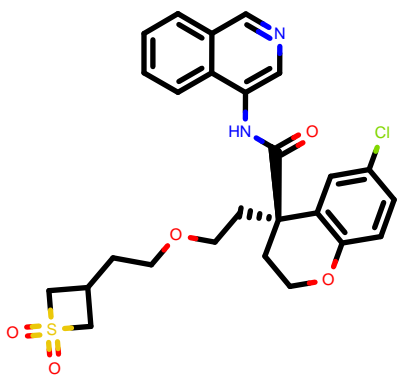
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]5

RUN: RUN3067

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.22

EN300-189563_3_1_1



CID: EN300-189563_3_1_1

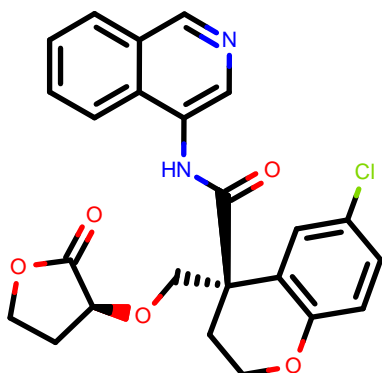
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCS(=O)(=O)CS

RUN: RUN3584

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.28

EDJ-MED-fcba3f31-8_1



CID: EDJ-MED-fcba3f31-8_1

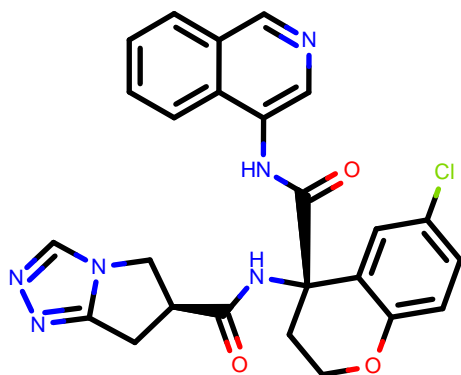
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCOC5=O

RUN: RUN2360

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.20

EN300-6745453_1_2_1



CID: EN300-6745453_1_2_1

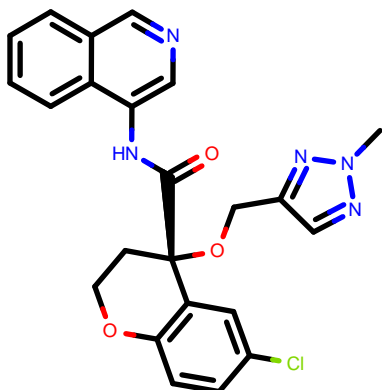
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C6nncn6CS

RUN: RUN4550

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.31

EN300-219020_1_1_1



CID: EN300-219020_1_1_1

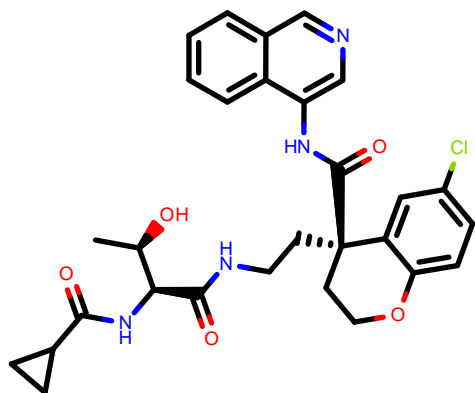
SMILES: Cn1nc(n1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4351

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.22

EN300-96362_3_2_1



CID: EN300-96362_3_2_1

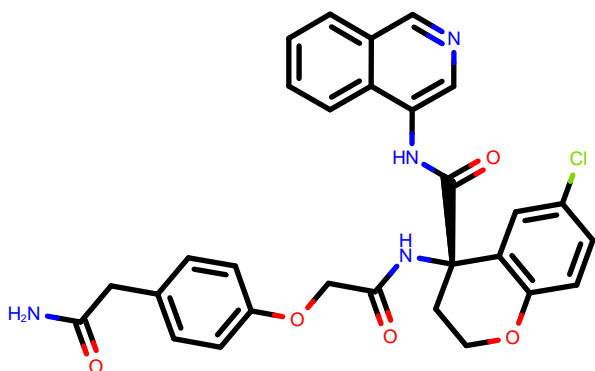
SMILES: C[C@H](C[C@H](C1=O)NC(C)C1)C(CO)N(C)C(=O)C2=CC=C(C)C=C2

RUN: RUN4255

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.43

EN300-50514_1_1_1



CID: EN300-50514_1_1_1

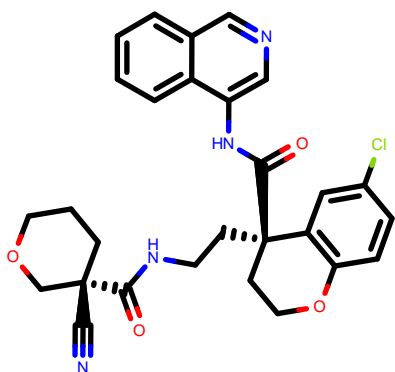
SMILES: C1=CC=C(C=C1)N(C)C(=O)C2=CC=C(C)C=C2C(=O)COC3=CC=C(N)C=C3

RUN: RUN3443

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.35

EN300-301925_3_2_1



CID: EN300-301925_3_2_1

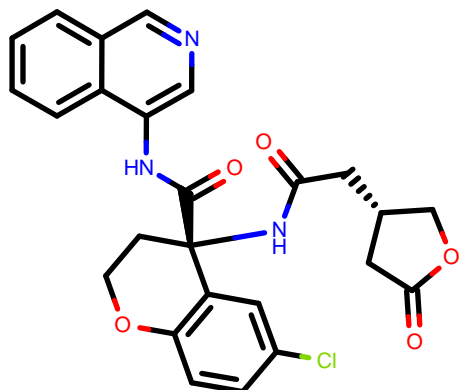
SMILES: C1=CC=C(C=C1)N(C)C(=O)C2=CC=C(C)C=C2C(=O)N(C)C3=CC=CC=C3C#N

RUN: RUN3125

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.25

EN300-109535_1_2_1



CID: EN300-109535_1_2_1

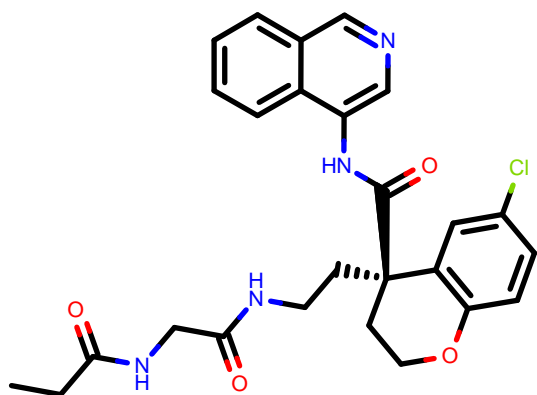
SMILES: C1=CC=C(C=C1)N(C)C(=O)C2=CC=C(C)C=C2C(=O)C3=CC=CC=C3C(=O)O

RUN: RUN3903

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.21

EN300-31099_3_1_1



CID: EN300-31099_3_1_1

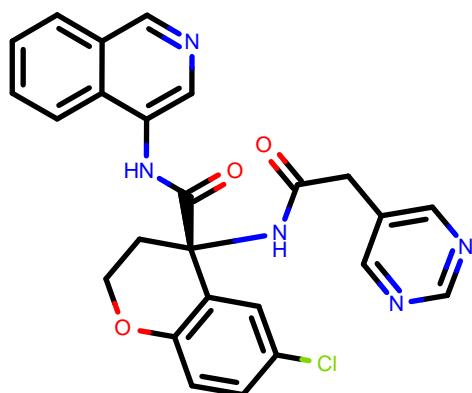
SMILES: CCC(=O)NCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5833

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-185751_1_1_1



CID: EN300-185751_1_1_1

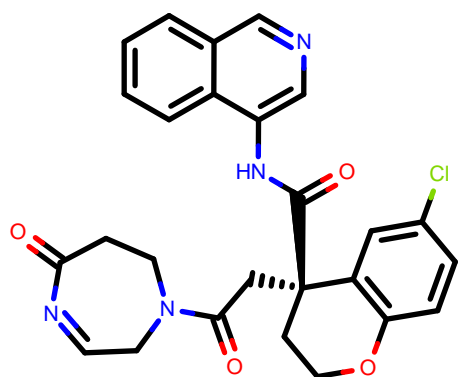
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnc5

RUN: RUN4780

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.21

EN300-69107_1_1_1



CID: EN300-69107_1_1_1

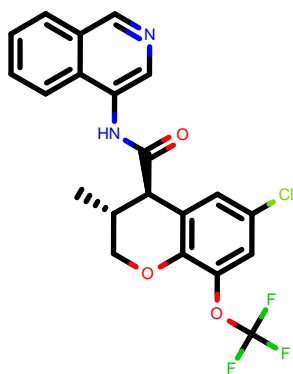
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN(=O)NCC5

RUN: RUN2902

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

DAR-DIA-0d514e7d-18_1_1



CID: DAR-DIA-0d514e7d-18_1_1

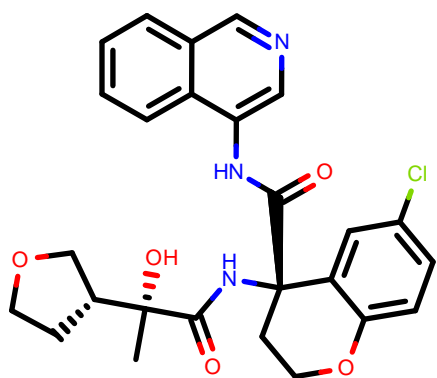
SMILES: C[C@H]1COc2c(cc(cc2OC(F)(F)F)Cl)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncc4c3cccc4

RUN: RUN4737

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.16

EN300-217494_1_1_1



CID: EN300-217494_1_1_1

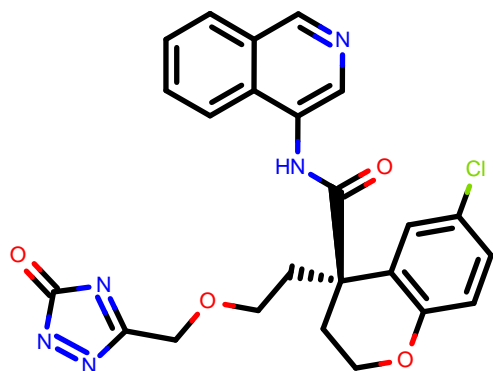
SMILES: C[C@@]([C@@H]1CCOC1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c5c4cc5)O

RUN: RUN3496

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-73772_3_1_1



CID: EN300-73772_3_1_1

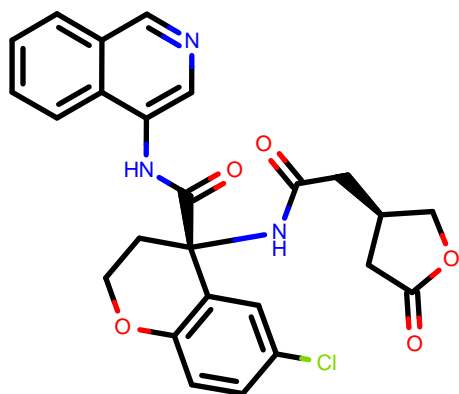
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]n5

RUN: RUN3358

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.23

EN300-109535_1_1_1



CID: EN300-109535_1_1_1

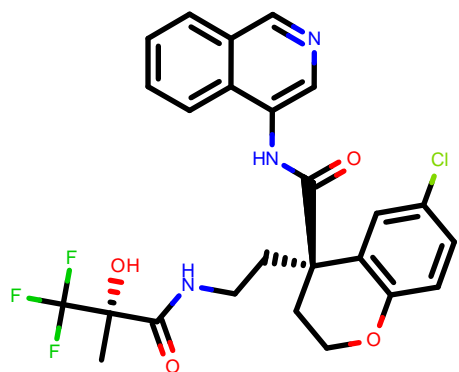
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(=O)OC5

RUN: RUN7166

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-159633_3_2_1



CID: EN300-159633_3_2_1

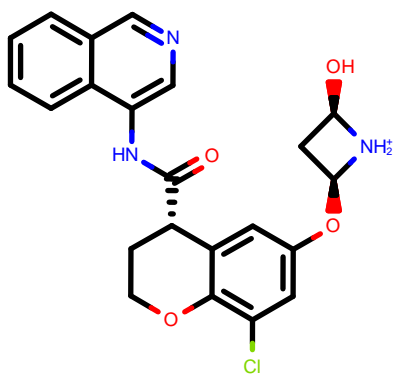
SMILES: C[C@@]([C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4)(C(F)(F)F)O

RUN: RUN4018

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.33

FRA-DIA-b66f7109-3_2_1



CID: FRA-DIA-b66f7109-3_2_1

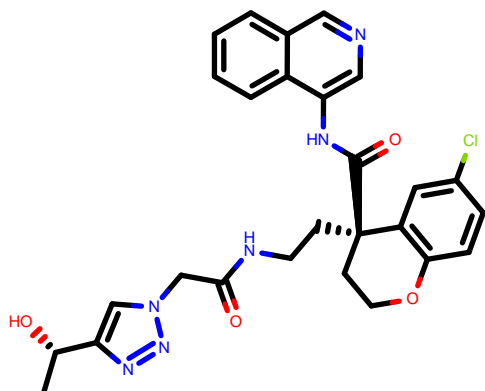
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3CCOCc4c3cc(cc4Cl)O[C@H]5C[C@H]([NH2+])O

RUN: RUN3341

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.52

EN300-109540_3_1_1



CID: EN300-109540_3_1_1

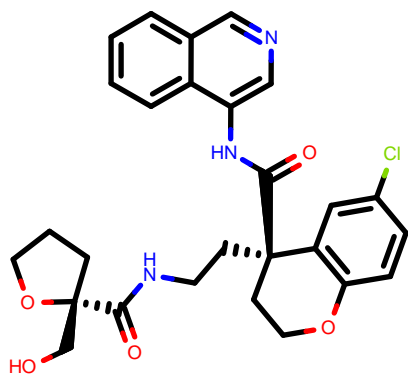
SMILES: C[C@@H]([C@H]1CN(CN1)CC(=O)NCC[C@]2(CCOc4c3cc(cc3Cl)C(=O)Nc4ncnc5c4ccc5)O

RUN: RUN3163

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.30

EN300-1425677_3_2_1



CID: EN300-1425677_3_2_1

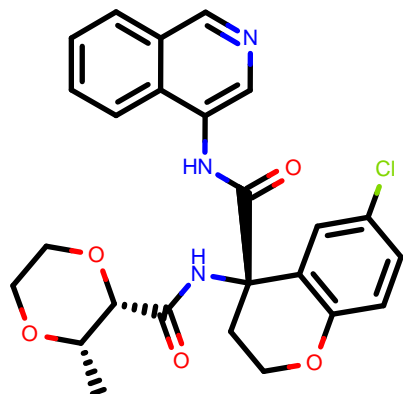
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@]5(CCCO5)CO

RUN: RUN4635

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.38

EN300-299215_1_1_1



CID: EN300-299215_1_1_1

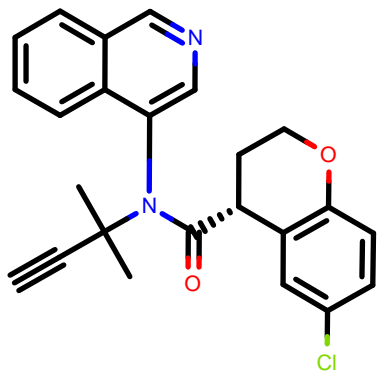
SMILES: C[C@H]1[C@H](OCCO1)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN2767

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.26

DAR-DIA-5ff57136-14_1_1



CID: DAR-DIA-5ff57136-14_1_1

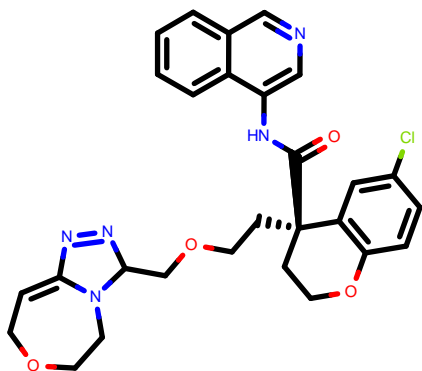
SMILES: CC(C)(C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN5433

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.19

EN300-310888_3_1_1



CID: EN300-310888_3_1_1

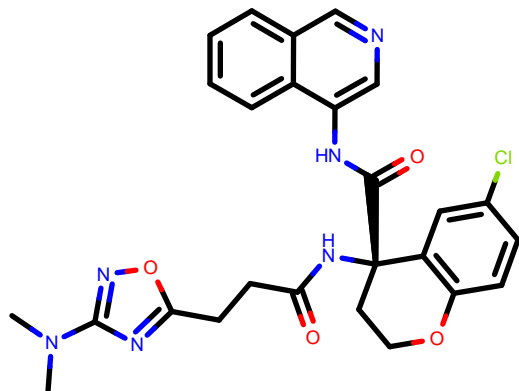
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5nnc6n5COCOC6

RUN: RUN4950

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.33

EN300-152913_1_1_1



CID: EN300-152913_1_1_1

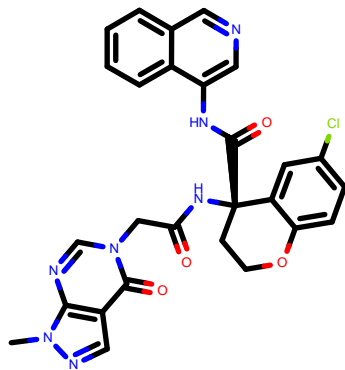
SMILES: CN(C)c1nc(on1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3711

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.30

ALP-UNI-dbbfd3db-16_1



CID: ALP-UNI-dbbfd3db-16_1

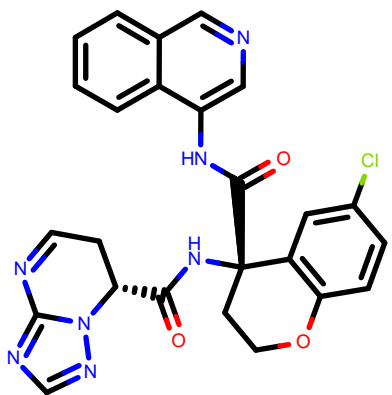
SMILES: Cn1c2c(en1)c(=O)n(en2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN2617

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EN300-28262_1_1_2



CID: EN300-28262_1_1_2

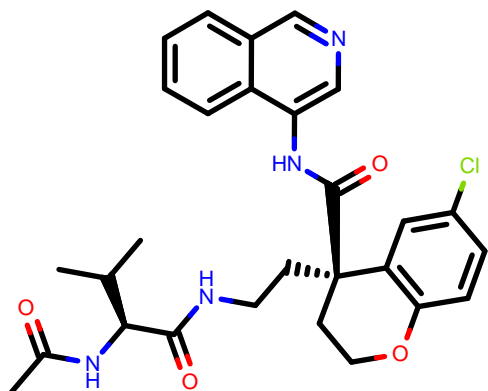
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC=Nc6n5ncn6

RUN: RUN6514

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.34

EN300-16582_3_1_1



CID: EN300-16582_3_1_1

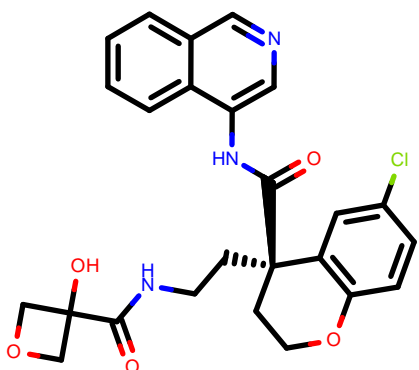
SMILES: CC(C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4)NC(=O)C

RUN: RUN5533

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.40

EN300-101443_3_1_1



CID: EN300-101443_3_1_1

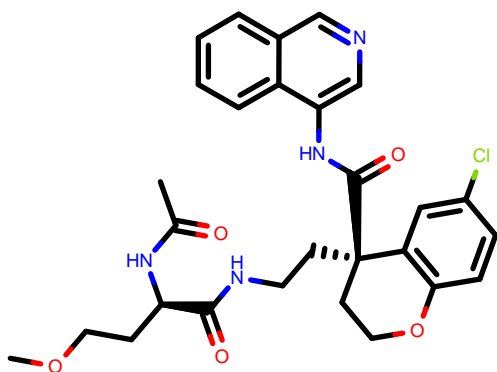
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(COC5)O

RUN: RUN6455

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EN300-62074_3_2_1



CID: EN300-62074_3_2_1

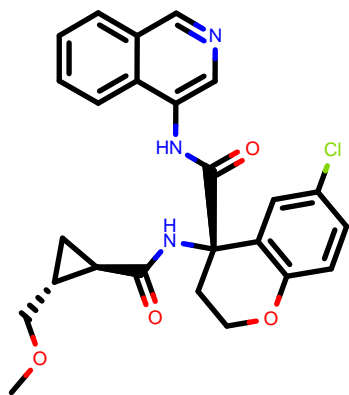
SMILES: CC(=O)N[C@@H](COC)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4

RUN: RUN6369

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.31

EN300-705386_1_1_1



CID: EN300-705386_1_1_1

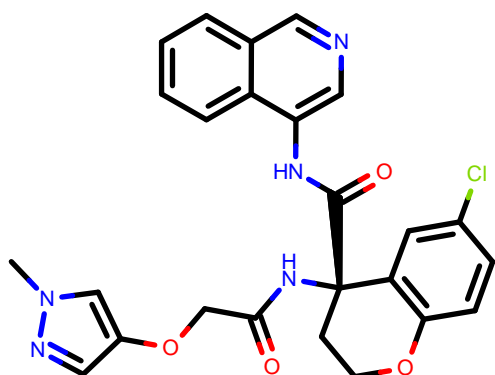
SMILES: COC[C@@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3429

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.23

EN300-201553_1_1_1



CID: EN300-201553_1_1_1

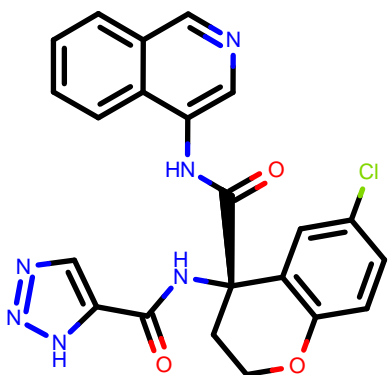
SMILES: C[n+1]cc(c[nH]1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5411

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.25

EN300-31998_1_1_1



CID: EN300-31998_1_1_1

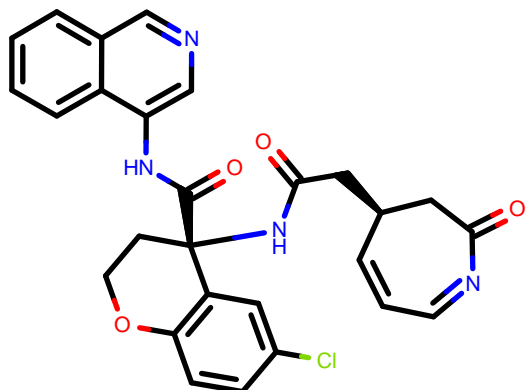
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]n5

RUN: RUN2787

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.20

EN300-195590_1_1_1



CID: EN300-195590_1_1_1

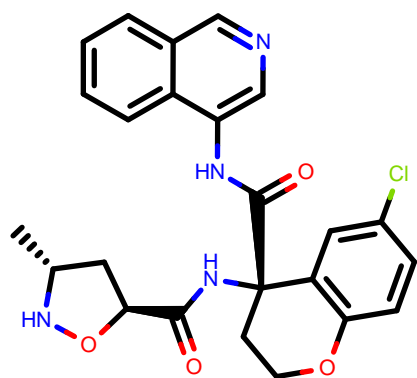
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5CNC(=O)C5

RUN: RUN5613

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.26

EN300-92447_1_1_1



CID: EN300-92447_1_1_1

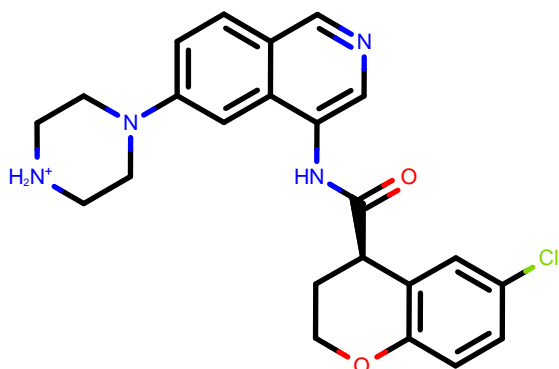
SMILES: C[C@@H]1[C@H](ON1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3430

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.30

MAK-UNK-8be7dca9-4_1



CID: MAK-UNK-8be7dca9-4_1

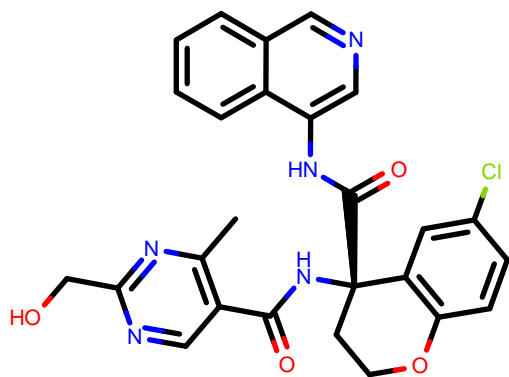
SMILES: c1cc2nccc(c2cc1N3CC[NH2+])CC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN440

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.09

EN300-6497975_1_1_1



CID: EN300-6497975_1_1_1

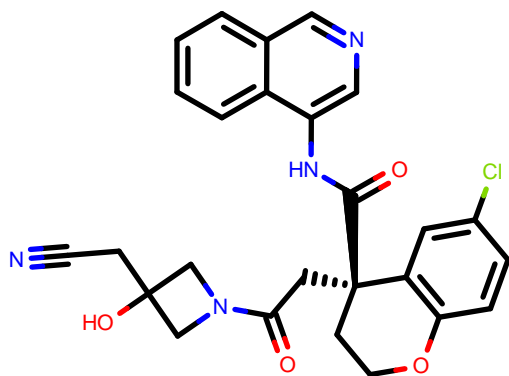
SMILES: Cc1c(nc(n1)CO)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4627

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.26

EN300-155823_1_1_1



CID: EN300-155823_1_1_1

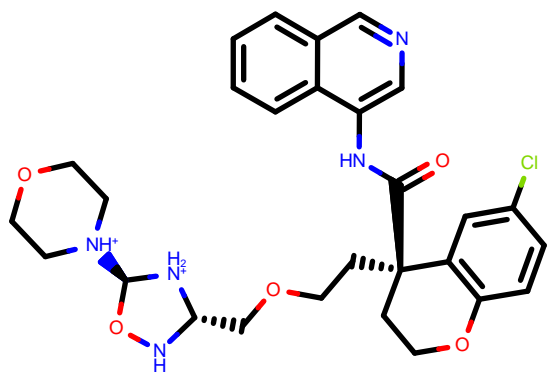
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CC#N)O

RUN: RUN4916

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.24

EN300-1608590_3_1_2



CID: EN300-1608590_3_1_2

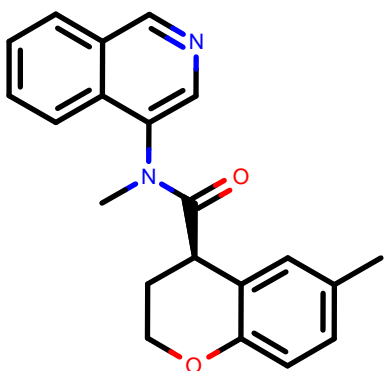
SMILES: c1ccc2c(c1)ncnc2Nc1cnc2c1O[C@@H](C(=O)Nc3cnc4c3ccccc4)[C@@H](N5CCOCC5)Nc6ccccc6

RUN: RUN4647

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.56

MAK-UNK-3875bbc8-1_1_1



CID: MAK-UNK-3875bbc8-1_1_1

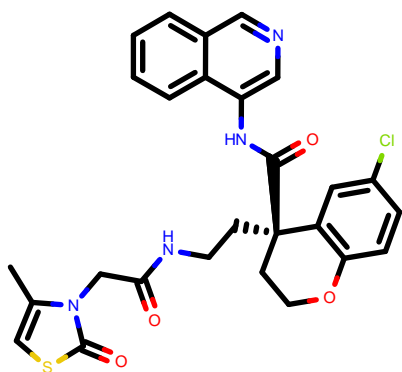
SMILES: Cc1ccc2c(c1)[C@@H](C(=O)Nc3cnc4c3ccccc4)N(C)C5CCOCC5

RUN: RUN4944

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.11

EN300-12067_3_1_1



CID: EN300-12067_3_1_1

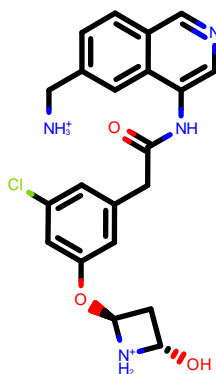
SMILES: Cc1csc(=O)n1CC(=O)NCC[C@@H](C(=O)Nc2cnc3c2ccccc3)C(=O)Nc4cnc5c4ccccc5

RUN: RUN3070

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.29

ALF-EVA-0b412456-5_2



CID: ALF-EVA-0b412456-5_2

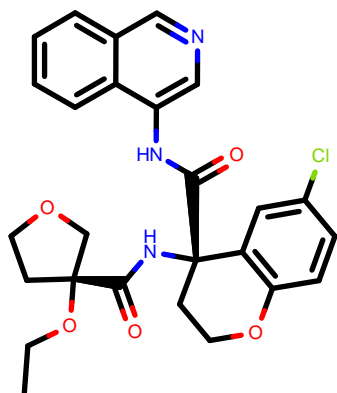
SMILES: c1cc2cnc(c2cc1C[NH3+])NC(=O)Cc3cc(ccc3)ClO[C@@H](N4CC(=O)N4)N

RUN: RUN2571

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.48

EN300-259694_1_1_1



CID: EN300-259694_1_1_1

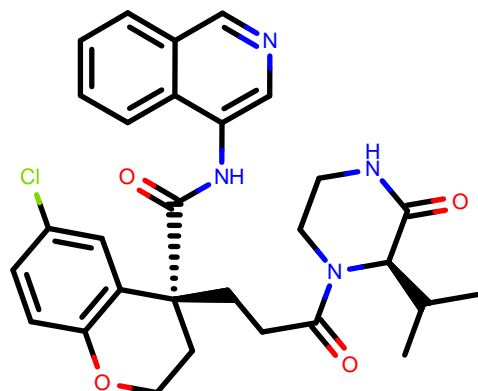
SMILES: CC[C@@H]1(CCOC1C(=O)N)C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN7493

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.32

EN300-67791_2_1_1



CID: EN300-67791_2_1_1

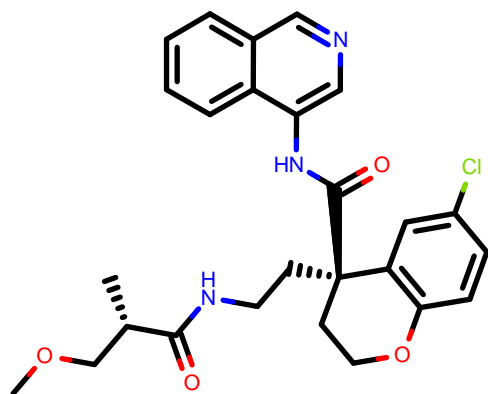
SMILES: CC(C)[C@@H]1C(=O)NCCN1C(=O)CC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN7790

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.40

EN300-69162_3_1_1



CID: EN300-69162_3_1_1

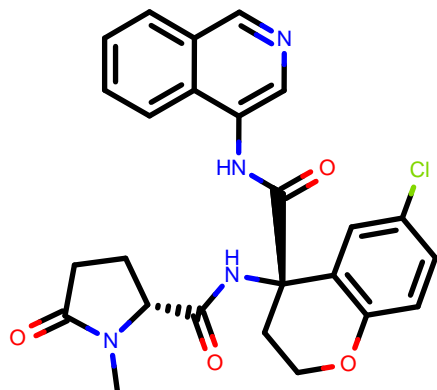
SMILES: C[C@@H](COC)C(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4

RUN: RUN3622

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

EN300-343787_1_1_1



CID: EN300-343787_1_1_1

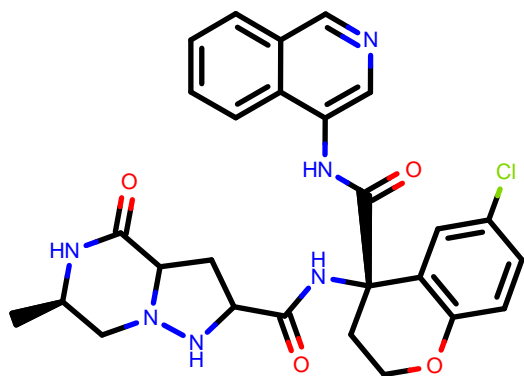
SMILES: CN1[C@@H](CCC1=O)C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN3489

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-265285_1_1_1



CID: EN300-265285_1_1_1

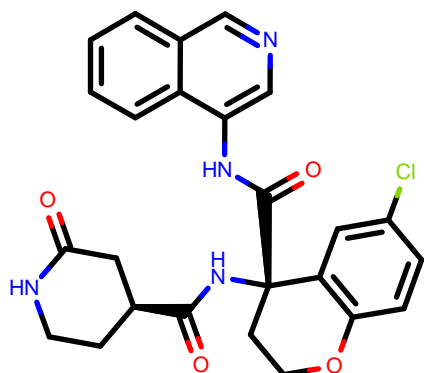
SMILES: C[C@@H]1Cn2c(cc(n2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)C(=O)N1

RUN: RUN4775

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

EN300-107493_1_2_1



CID: EN300-107493_1_2_1

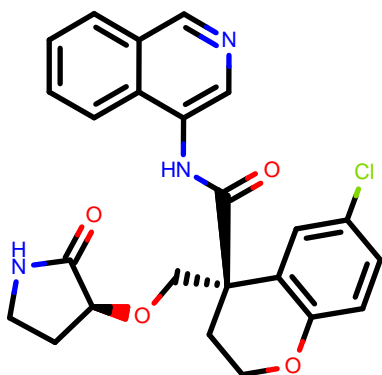
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCNC(=O)C5

RUN: RUN3628

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.25

EDJ-MED-fcba3f31-7_1



CID: EDJ-MED-fcba3f31-7_1

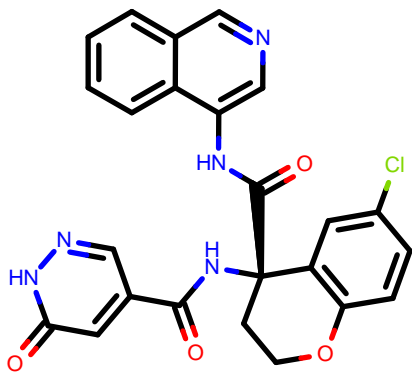
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCNC(=O)5

RUN: RUN2339

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.20

EN300-159634_1_1_1



CID: EN300-159634_1_1_1

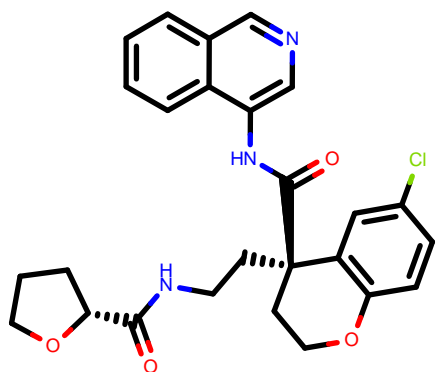
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]jnc5

RUN: RUN4994

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-116234_3_1_1



CID: EN300-116234_3_1_1

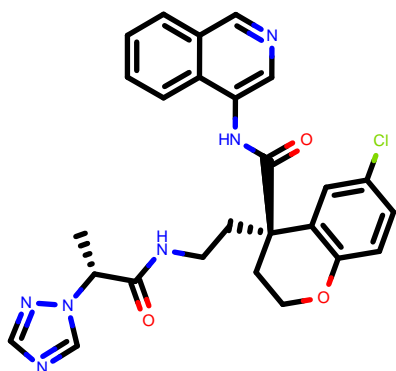
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CCNC(=O)[C@H]5CCOC5

RUN: RUN4928

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-30397_3_2_1



CID: EN300-30397_3_2_1

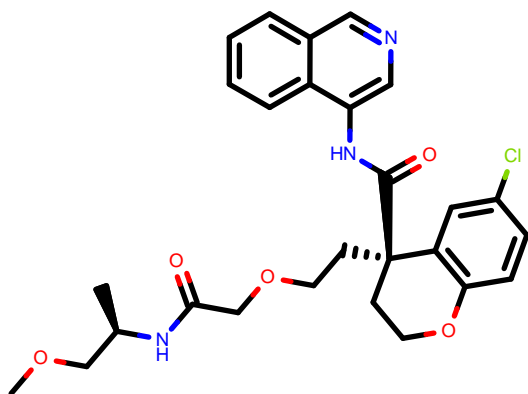
SMILES: C[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)n5cnnc5

RUN: RUN3692

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.41

EN300-02067_3_2_1



CID: EN300-02067_3_2_1

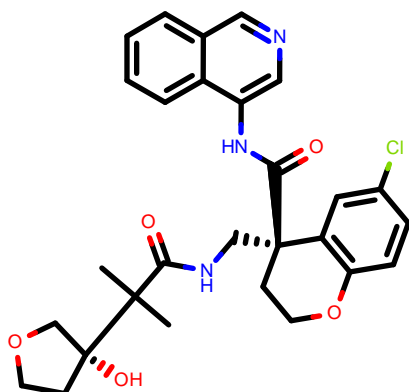
SMILES: C[C@H](COC)NC(=O)COC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN6976

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-1630093_2_2_1



CID: EN300-1630093_2_2_1

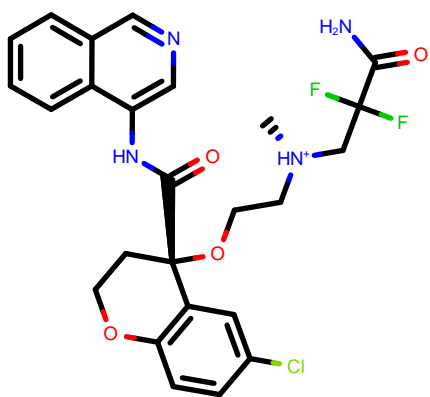
SMILES: CC(C)(C(=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccoc4)[C@]5(CCOCS)O

RUN: RUN7325

DDG (kcal/mol): -1.68

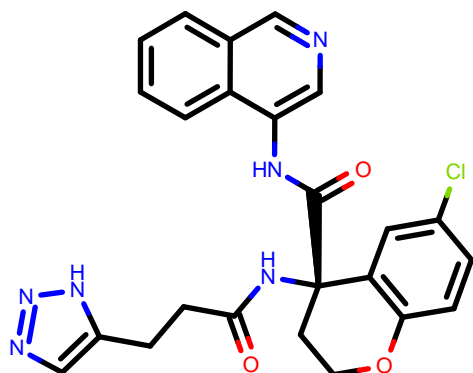
dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-34_1



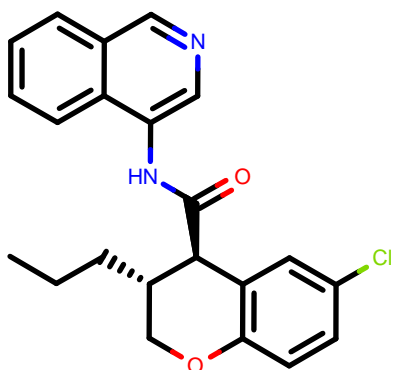
CID:	ED_-GRI-5b13fbe2-34_1
SMILES:	<chem>CN@]([C@@]1(CO)C(=O)C(=O)Nc3ccc4c3ccc4)C(C(=O)N)F)F</chem>
RUN:	RUN1446
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.33

EN300-244947_1_1_1



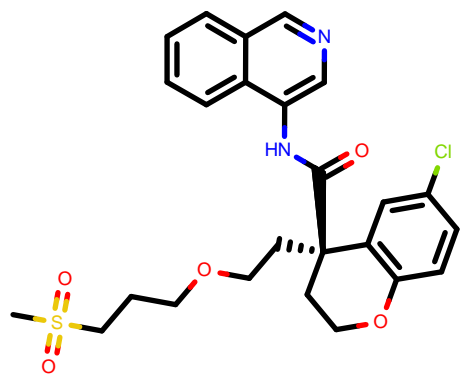
CID:	EN300-244947_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CO)C(=O)C(=O)Nc4ccc4)C(C(=O)N)F)F</chem>
RUN:	RUN3864
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.24

EDJ-MED-e4b030d8-6_1



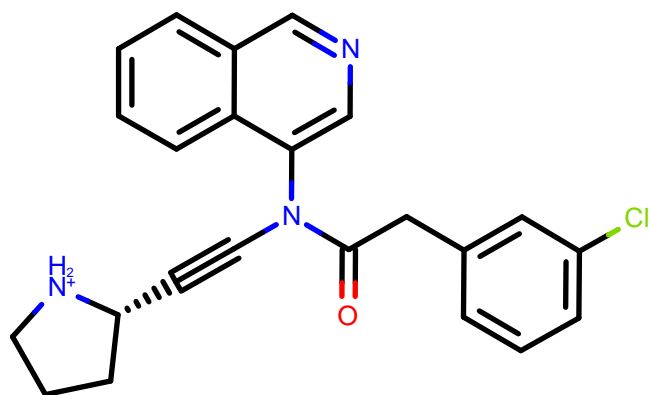
CID:	EDJ-MED-e4b030d8-6_1
SMILES:	<chem>CCC[C@@H]1COC2ccc(cc2)C(=O)Nc3ccc4c3ccc4)C(C(=O)N)F)F</chem>
RUN:	RUN254
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.10

EN300-68794_3_1_1



CID:	EN300-68794_3_1_1
SMILES:	<chem>CS(=O)(=O)CCCOC[C@@]1(CO)C(=O)C(=O)Nc3ccc4c3ccc4)C(C(=O)N)F)F</chem>
RUN:	RUN6094
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.30

DAR-DIA-076fb6ea-9_1



CID: DAR-DIA-076fb6ea-9_1

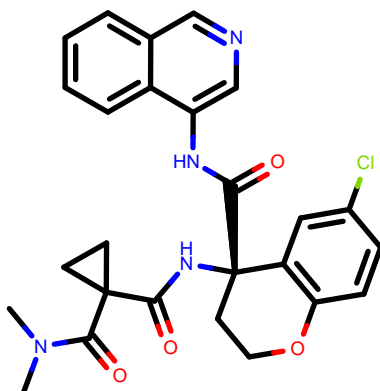
SMILES: c1ccc2c(c1)cnc2N(C#C[C@H]3CCCC[NH2+](3)C(=O)Cc4cccc(c4)Cl

RUN: RUN1273

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.35

EN300-180875_1_1_1



CID: EN300-180875_1_1_1

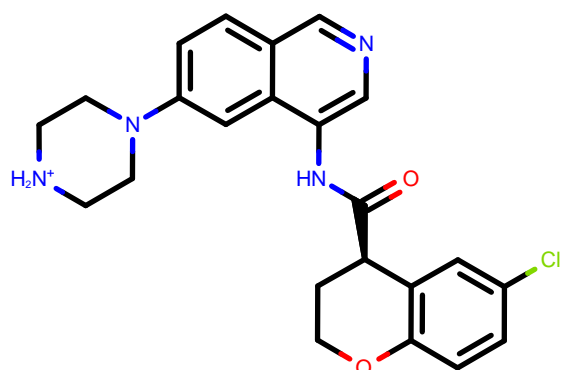
SMILES: CN(C)C(=O)C1(CC1)C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN4535

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.31

MAK-UNK-8be7dca9-4_1_1



CID: MAK-UNK-8be7dca9-4_1_1

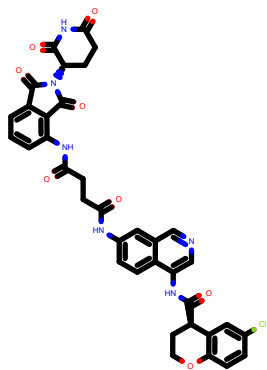
SMILES: c1cc2cnc(c2cc1N3CC[NH2+](CC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN5625

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.09

DAR-DIA-9e4459de-15_6



CID: DAR-DIA-9e4459de-15_6

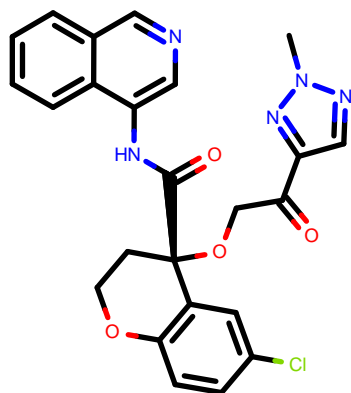
SMILES: c1cc2c(c1)NC(=O)C(C(=O)Nc3cccc4c3)nc4NC(=O)[C@@H]5COCc6c5cc(cc6)Cl)N(C(=O)C(=O)C(=O)Nc7cccc8c7cccc8)Cl

RUN: RUN1318

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.33

EN300-204935_1_1_1



CID: EN300-204935_1_1_1

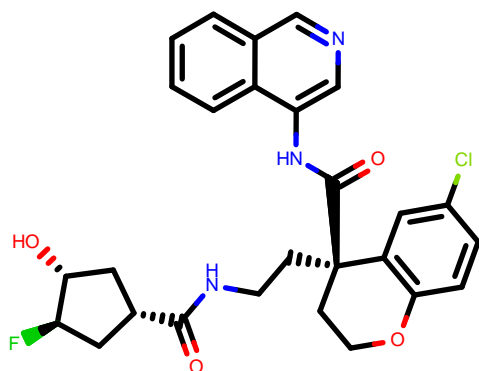
SMILES: Cn1ncc(n1)C(=O)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6060

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.29

EN300-7461217_3_2_1



CID: EN300-7461217_3_2_1

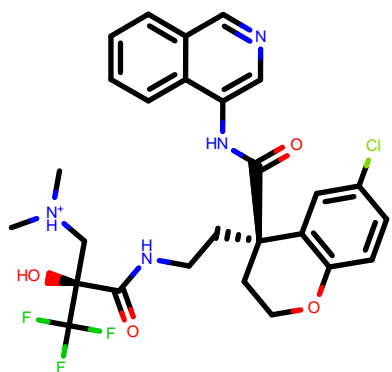
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCOC4c3cc(cc4)Cl)CN(C1=O)[C@@H]5C[C@@H](C1)[C@@H](C5)F)O

RUN: RUN5038

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.28

EN300-7459545_3_2_1



CID: EN300-7459545_3_2_1

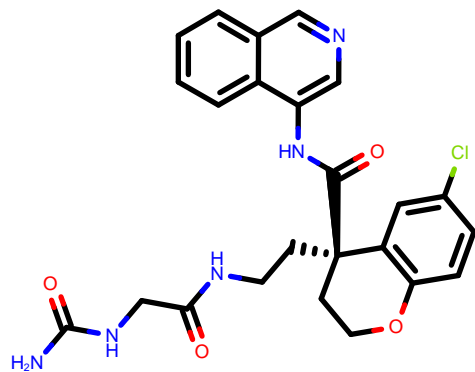
SMILES: CN(C)C[C@@](C(=O)NCC[C@@]1(COCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O

RUN: RUN3651

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.52

EN300-10397_3_1_1



CID: EN300-10397_3_1_1

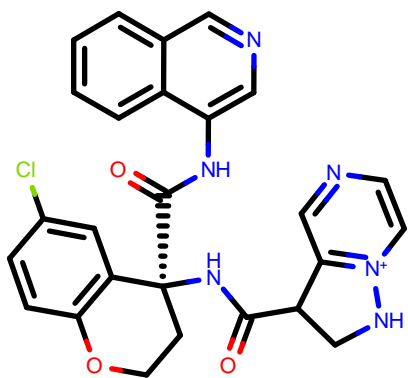
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCOC4c3cc(cc4)Cl)CN(C1=O)CNC(=O)N

RUN: RUN5461

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.26

EN300-131572_1_1_1



CID: EN300-131572_1_1_1

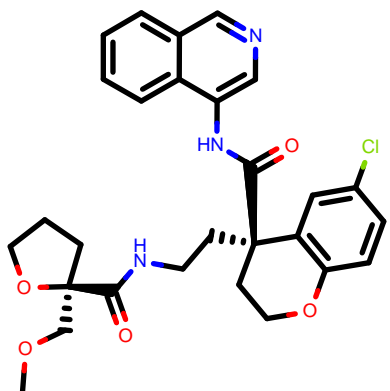
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn6c5cnc6

RUN: RUN4322

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.22

EN300-1301381_3_2_1



CID: EN300-1301381_3_2_1

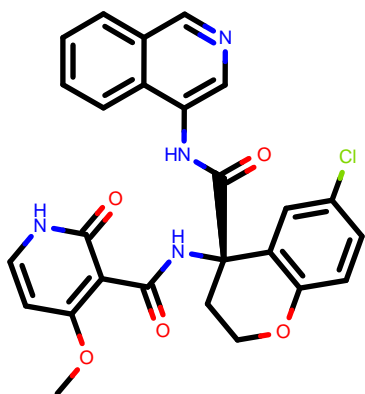
SMILES: COC[C@@]1(CCCO1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN4969

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.29

EN300-156318_1_1_1



CID: EN300-156318_1_1_1

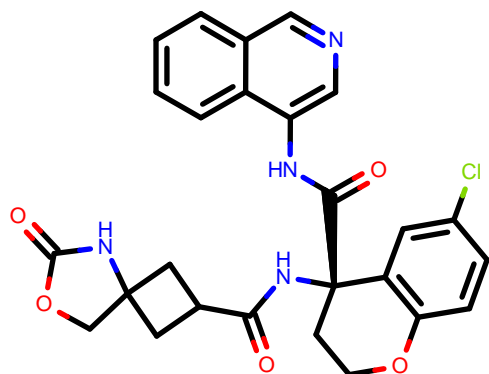
SMILES: COc1cc[nH]c(=O)c1C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN3484

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.27

EN300-7447185_1_1_1



CID: EN300-7447185_1_1_1

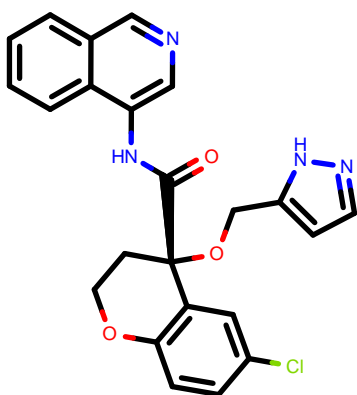
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC6(C5)COC(=O)N6

RUN: RUN3415

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-57_1



CID: ED_-GRI-5b13fbe2-57_1

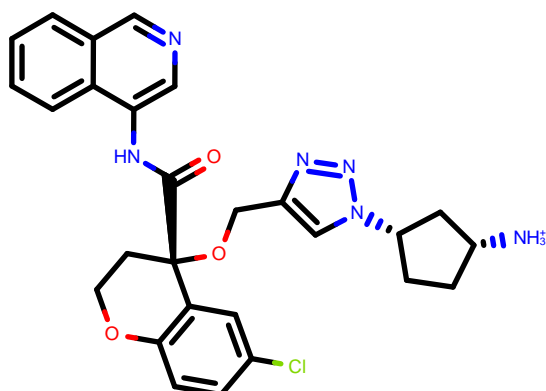
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)OCc5cn[nH]5

RUN: RUN1428

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.17

ED_-GRI-5b13fbe2-64_1



CID: ED_-GRI-5b13fbe2-64_1

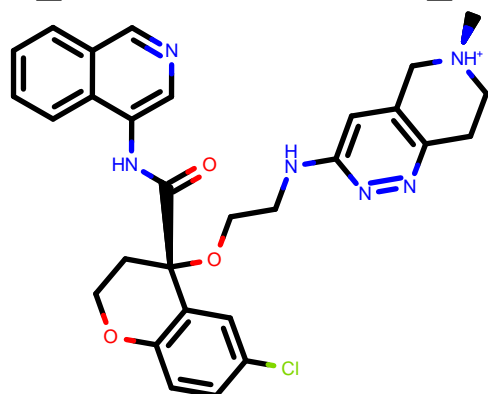
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)OC5cn[nH]5C@H6CC[C@H]6[NH3+]

RUN: RUN1470

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.34

ED_-GRI-5b13fbe2-67_2



CID: ED_-GRI-5b13fbe2-67_2

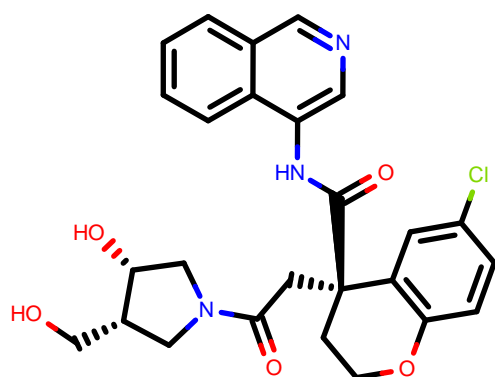
SMILES: C[N@H+]1CCc2c(cc[nH2])NCCO[C@@3](CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6)C1

RUN: RUN1480

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.34

EN300-248521_1_1_1



CID: EN300-248521_1_1_1

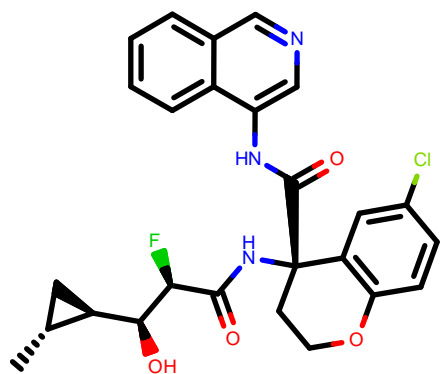
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H](C5)O[C@@H]6

RUN: RUN5927

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.36

EDG-MED-90036822-94_11



CID: EDG-MED-90036822-94_11

SMILES:

C1C=CN2C=CC=C2N1C(=O)N[C@@H](C(F)C(O)C)C(=O)Nc3ccc(Cl)cc3

RUN:

RUN1685

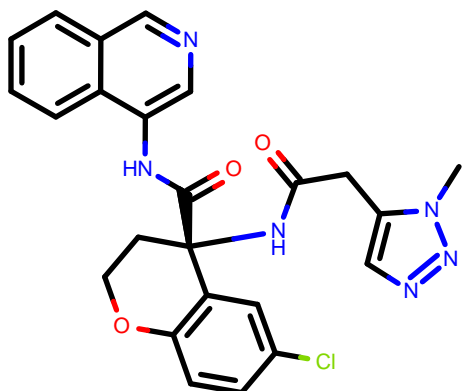
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.26

EN300-6486855_1_1_1



CID: EN300-6486855_1_1_1

SMILES:

Cn1c(cnn1)CC(=O)N[C@@H](C(=O)Nc2ccc(Cl)cc2)C(=O)Nc3ccc(Cl)cc3

RUN:

RUN4588

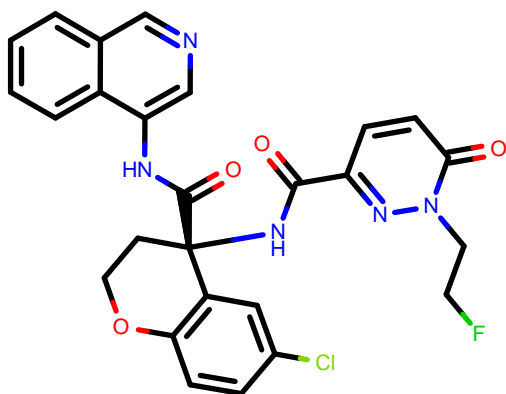
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.25

EN300-263456_1_1_1



CID: EN300-263456_1_1_1

SMILES:

C1=CC=C(C=C1)N[C@@H](C(=O)N[C@@H](C(=O)Nc2ccc(Cl)cc2)C(=O)Nc3cc(F)ccn3)C(=O)Nc4ccc(Cl)cc4

RUN:

RUN3038

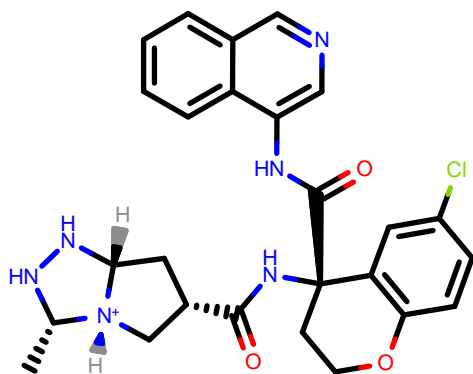
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.22

EN300-6729747_1_2_1



CID: EN300-6729747_1_2_1

SMILES:

C1C=CN2C=CC=C2N1C(=O)N[C@@H](C(=O)Nc2ccc(Cl)cc2)C(=O)Nc3ccnnc3

RUN:

RUN5123

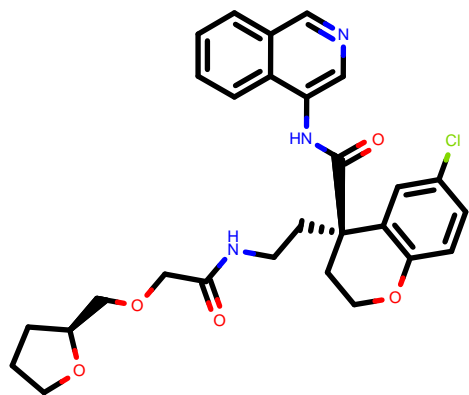
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.43

EN300-60033_3_1_1



CID: EN300-60033_3_1_1

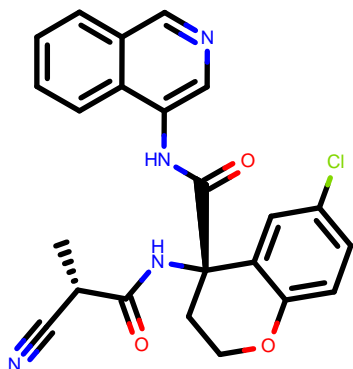
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@@H]5CCCCO5

RUN: RUN4894

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.33

EDG-MED-90036822-80_1



CID: EDG-MED-90036822-80_1

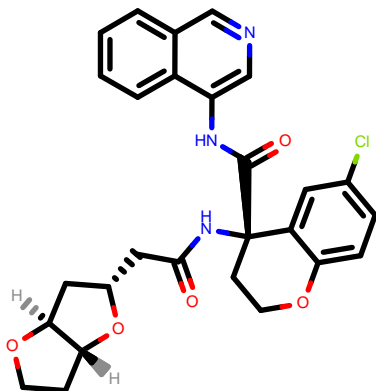
SMILES: C[C@@H](C#N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1623

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.15

EN300-735519_1_8_1



CID: EN300-735519_1_8_1

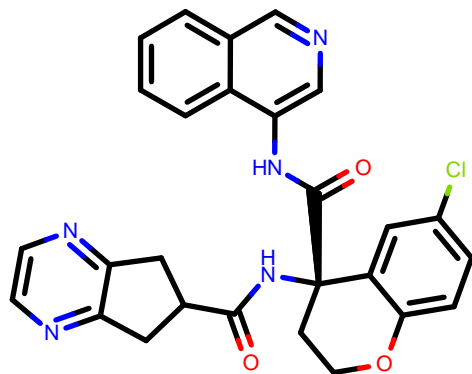
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N[C@@H]5C[C@@H]6[C@@H]7OCCCCO7

RUN: RUN4784

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.24

EN300-2011576_1_1_1



CID: EN300-2011576_1_1_1

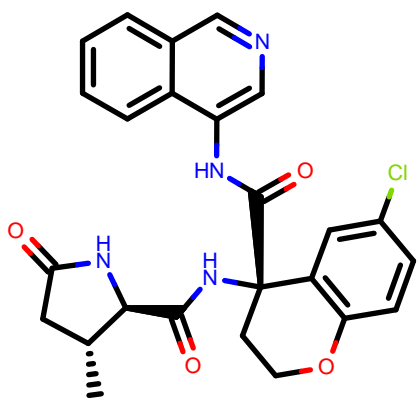
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5C6c6(nccn6)C5

RUN: RUN5956

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.24

EN300-155362_1_3_1



CID: EN300-155362_1_3_1

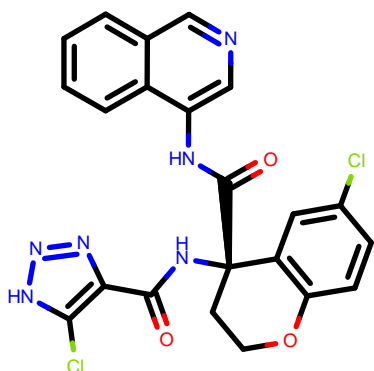
SMILES: C[C@@H]1CC(=O)N[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4620

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.23

EN300-149013_1_1_1



CID: EN300-149013_1_1_1

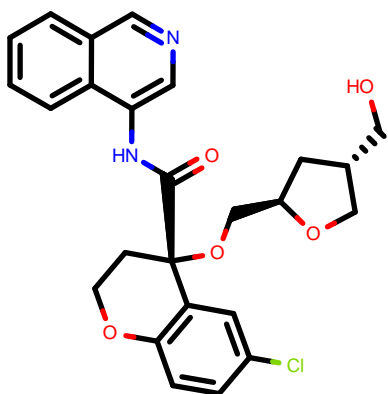
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(n[nH]n5)Cl

RUN: RUN3546

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.22

EN300-6494158_1_2_1



CID: EN300-6494158_1_2_1

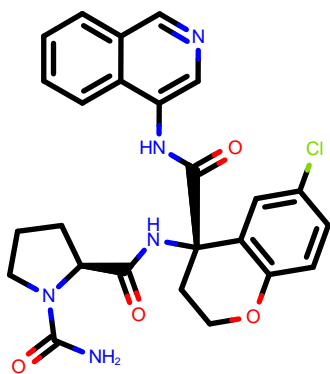
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@@H](CO)5CO

RUN: RUN3526

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.30

EN300-87536_1_1_1



CID: EN300-87536_1_1_1

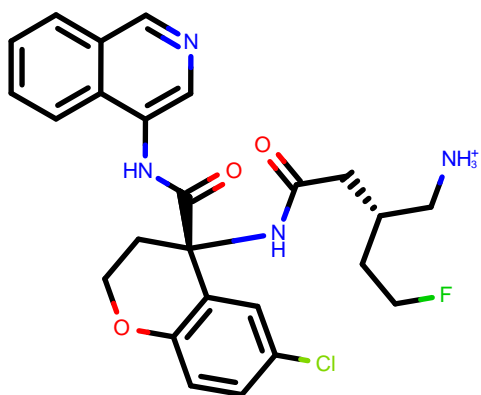
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCN5C(=O)N

RUN: RUN6864

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.27

EDG-MED-90036822-88_1



CID: EDG-MED-90036822-88_1

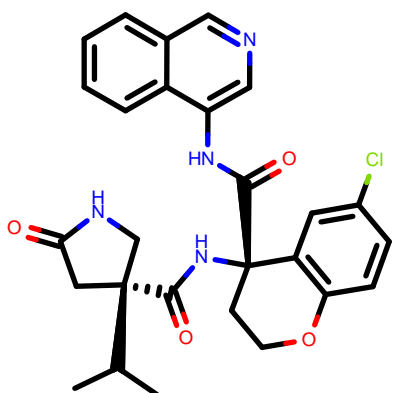
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H](CCF)C[NH3+]

RUN: RUN1681

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.30

EN300-211203_1_2_1



CID: EN300-211203_1_2_1

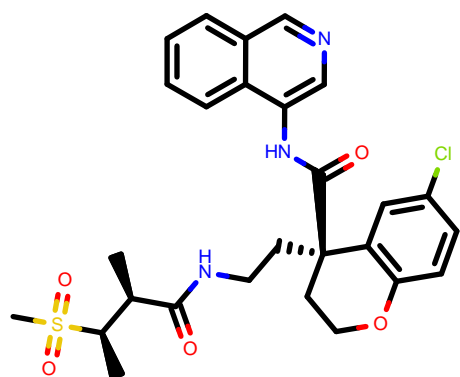
SMILES: CC(C)[C@@]1(CC(=O)NC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccc5c4cccc5

RUN: RUN5122

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-182725_3_2_1



CID: EN300-182725_3_2_1

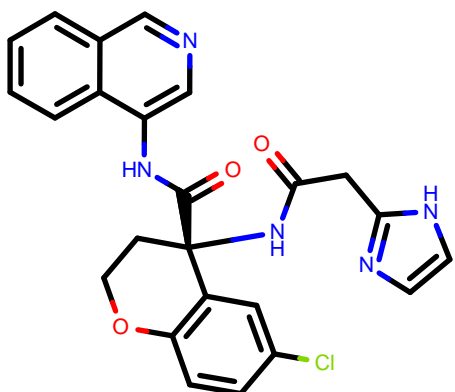
SMILES: C[C@@H](C[C@@H](C)[S](=O)(=O)C)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cccc4cccc34

RUN: RUN5618

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.43

EDG-MED-90036822-31_1



CID: EDG-MED-90036822-31_1

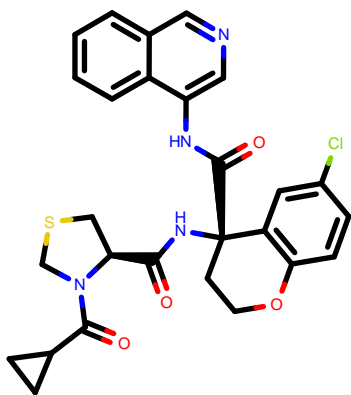
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5[nH]cn5

RUN: RUN1535

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.22

EN300-18928_1_1_1



CID: EN300-18928_1_1_1

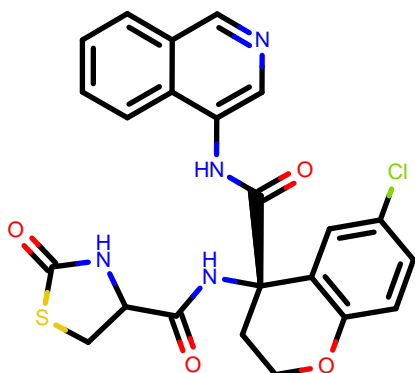
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@@@H5CSCN5C(=O)C6CC6

RUN: RUN5885

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.31

EN300-133915_1_1_1



CID: EN300-133915_1_1_1

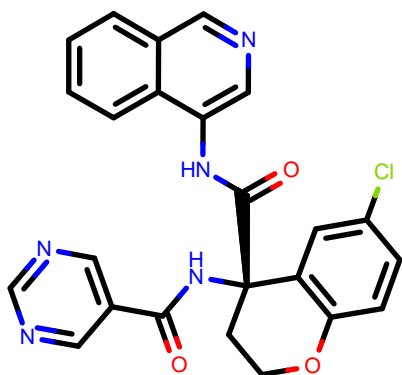
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)NC(=O)c5csc(=O)[nH]5

RUN: RUN6528

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-64297_1_1_1



CID: EN300-64297_1_1_1

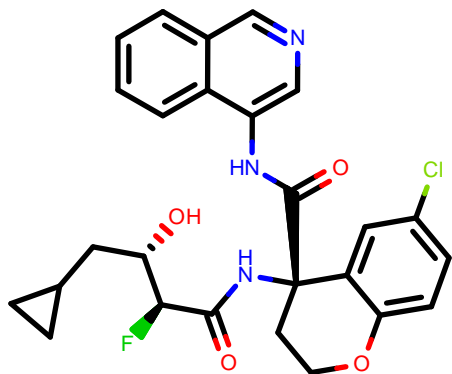
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)NC(=O)c5nncnc5

RUN: RUN4690

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.20

EDG-MED-90036822-108_4



CID: EDG-MED-90036822-108_4

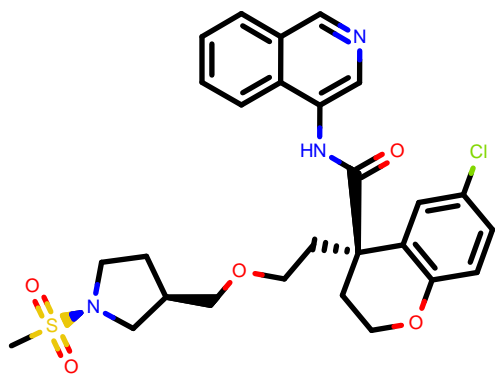
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@H(C@H)(CC5C5)O)F

RUN: RUN1754

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

KAD-UNI-8a629cb0-1_1



CID: KAD-UNI-8a629cb0-1_1

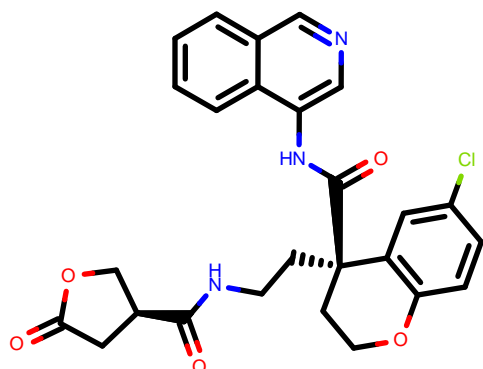
SMILES: CS(=O)(=O)N@ [1]CC[C@H](C1)COC[C@2](CCOc3c2cc(cc3)O)C(=O)Nc4cccc5c4cccc5

RUN: RUN2029

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.40

EN300-113234_3_2_1



CID: EN300-113234_3_2_1

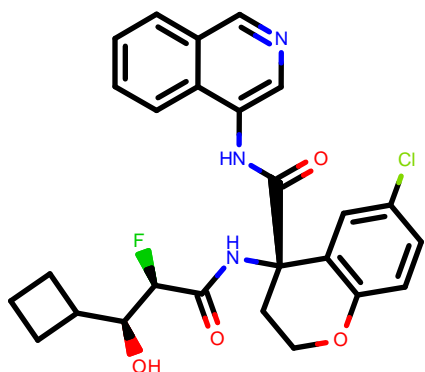
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)O)CCNC(=O)[C@H]5CC(=O)OC5

RUN: RUN4821

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

EDG-MED-90036822-99_3



CID: EDG-MED-90036822-99_3

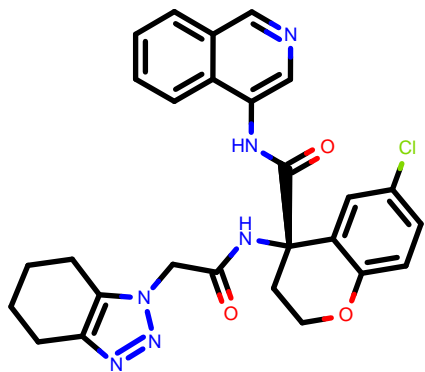
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)O)C(=O)N[C@H]5C(=O)C5)O)F

RUN: RUN1692

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.26

EN300-223187_1_1_1



CID: EN300-223187_1_1_1

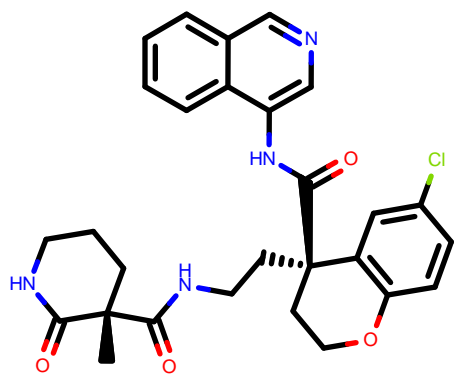
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@3](CCOc4c3cc(cc4)O)C(=O)Nc5c6c(n5)CCCC6

RUN: RUN3478

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.28

EN300-178876_3_1_1



CID: EN300-178876_3_1_1

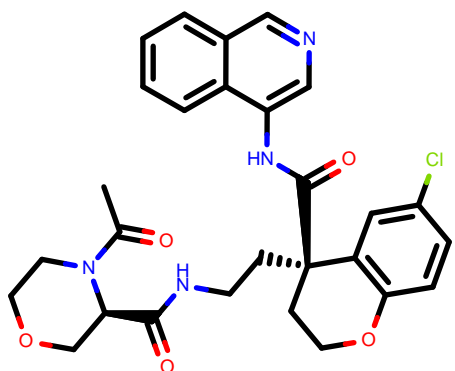
SMILES: C[C@@]1(CCCNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5109

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.40

EN300-116313_3_1_1



CID: EN300-116313_3_1_1

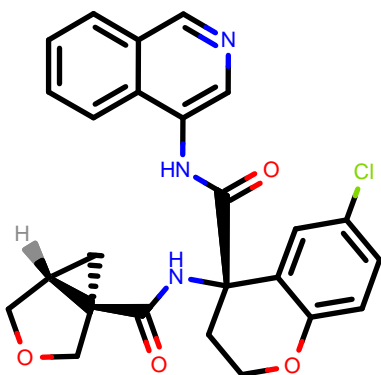
SMILES: CC(=O)N1CCOC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4487

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.31

EN300-263669_1_1_1



CID: EN300-263669_1_1_1

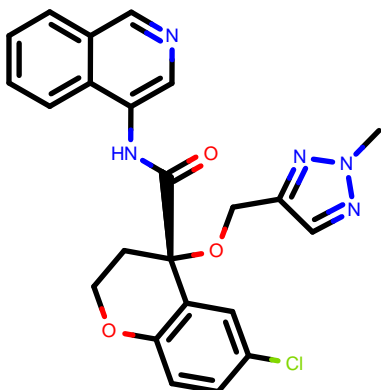
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3ccc(cc4)Cl)NC(=O)[C@]56C[C@H]5COC6

RUN: RUN4339

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.23

EN300-219020_1_1_1



CID: EN300-219020_1_1_1

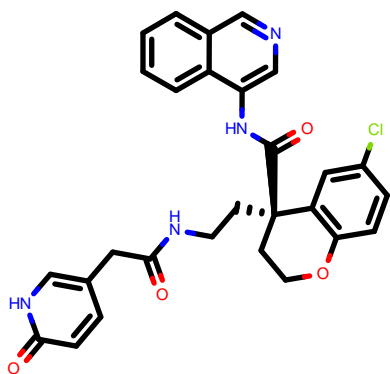
SMILES: Cn1ncc(n1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4875

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.20

EN300-189672_3_1_1



CID: EN300-189672_3_1_1

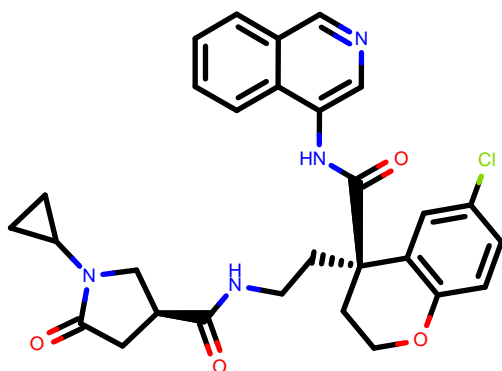
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4ccc(cc4)Cl)CCNC(=O)Cc5ccc(=O)[nH]c5

RUN: RUN4247

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.31

EN300-12440_3_2_1



CID: EN300-12440_3_2_1

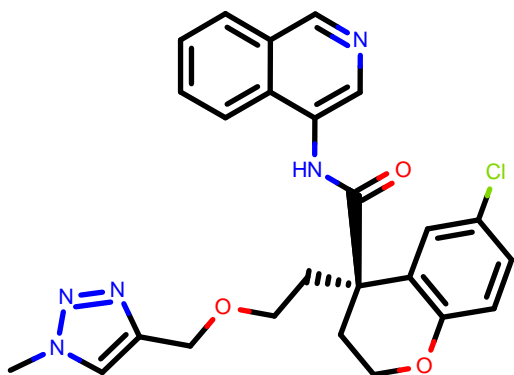
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4ccc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)N(C)CC5

RUN: RUN4451

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.43

EN300-120282_3_1_1



CID: EN300-120282_3_1_1

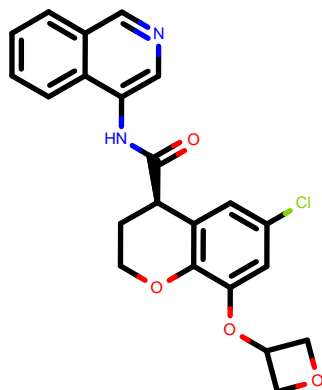
SMILES: Cn1cc(nn1)COCC[C@@H]2(COCc3ccc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3465

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.25

EDJ-MED-e4b030d8-4_1_1



CID: EDJ-MED-e4b030d8-4_1_1

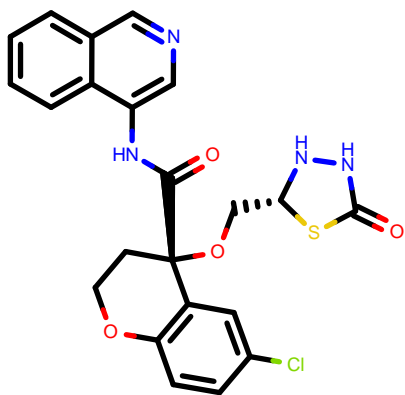
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOCc4ccc(cc4OC5COC5)Cl

RUN: RUN3965

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.19

EN300-171766_1_1_1



CID: EN300-171766_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5NNC(=O)S5

RUN:

RUN3540

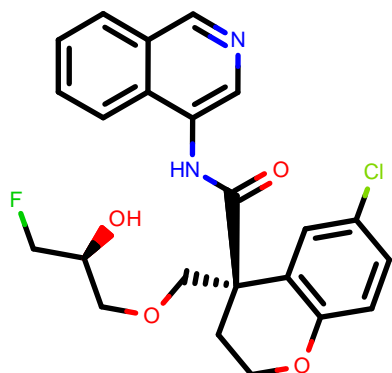
DDG (kcal/mol):

-1.62

dDDG (kcal/mol):

0.20

EN300-1968342_2_1_1



CID: EN300-1968342_2_1_1

SMILES:

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

RUN:

RUN3650

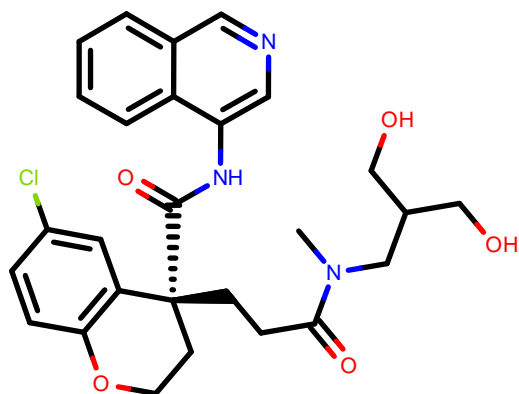
DDG (kcal/mol):

-1.61

dDDG (kcal/mol):

0.28

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)Nc3nccc4c3ccoc4

RUN:

RUN5373

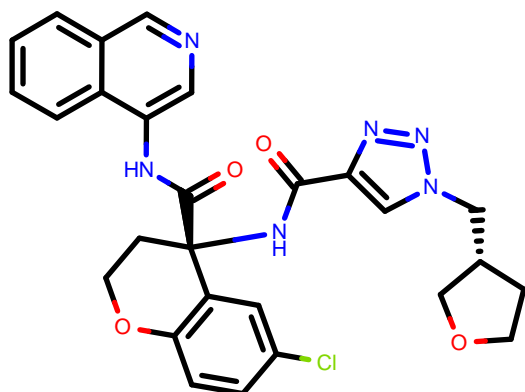
DDG (kcal/mol):

-1.61

dDDG (kcal/mol):

0.25

EN300-317272_1_1_1



CID: EN300-317272_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@H]6COC6

RUN:

RUN7490

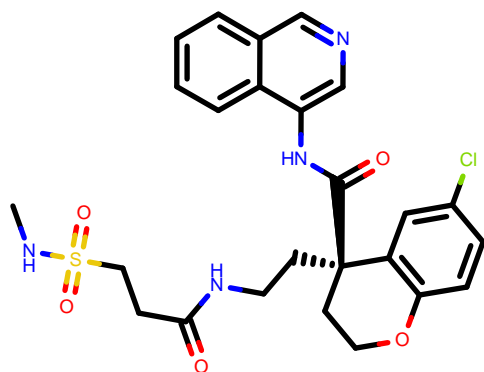
DDG (kcal/mol):

-1.61

dDDG (kcal/mol):

0.30

EN300-123205_3_1_1



CID: EN300-123205_3_1_1

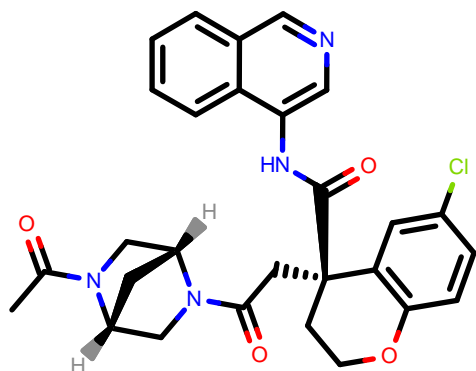
SMILES: CNS(=O)(=O)CCC(=O)NCC[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4619

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.33

KAD-UNI-80f122c8-2_2



CID: KAD-UNI-80f122c8-2_2

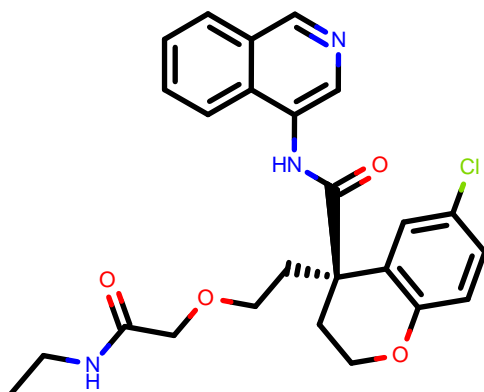
SMILES: CC(=O)N1C[C@H]2C[C@@H]1CN2C(=O)C[C@]3(C)COCc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN2201

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.32

EN300-7003350_3_1_1



CID: EN300-7003350_3_1_1

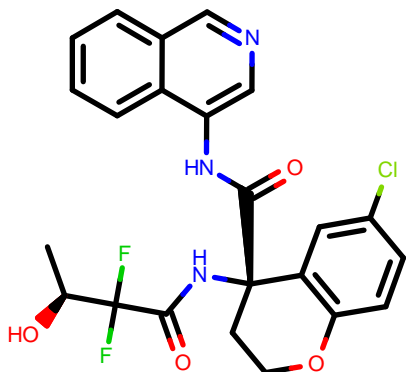
SMILES: CCNC(=O)COCC[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3833

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.25

EN300-185398_1_1_1



CID: EN300-185398_1_1_1

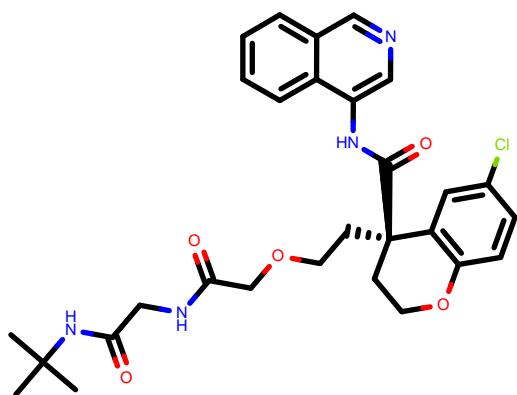
SMILES: C[C@@H](C)C(=O)N[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4(F)F)O

RUN: RUN4061

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.19

EN300-48760_3_1_1



CID: EN300-48760_3_1_1

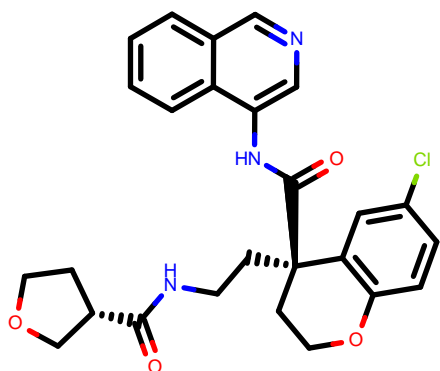
SMILES: CC(C)(C)NC(=O)CNC(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6069

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.28

EN300-170463_3_1_1



CID: EN300-170463_3_1_1

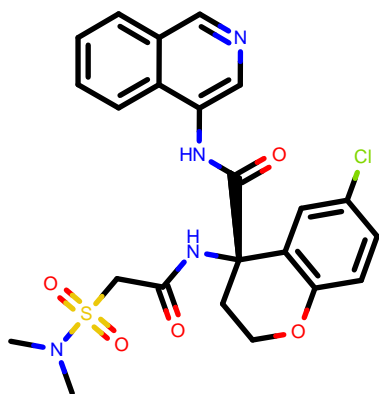
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5

RUN: RUN4696

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.27

EN300-133128_1_1_1



CID: EN300-133128_1_1_1

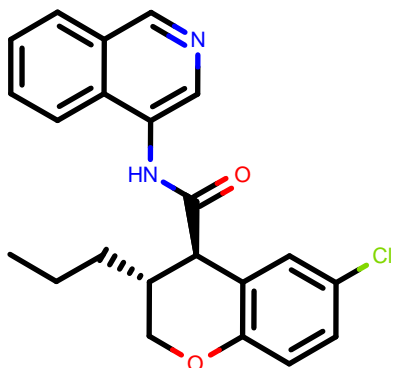
SMILES: CN(C)S(=O)(=O)CC(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3135

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.25

EDJ-MED-e4b030d8-6_1_1



CID: EDJ-MED-e4b030d8-6_1_1

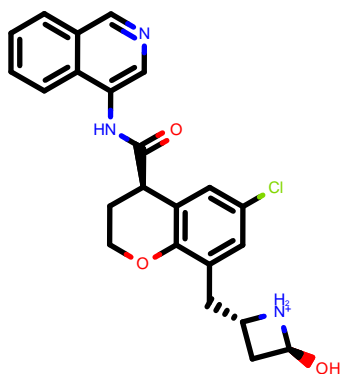
SMILES: CCC[C@H]1COc2ccc(cc2)[C@@H]1C(=O)Nc3ncc4c3cccc4)Cl

RUN: RUN3915

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.09

DAR-DIA-6a508060-5_3



CID: DAR-DIA-6a508060-5_3

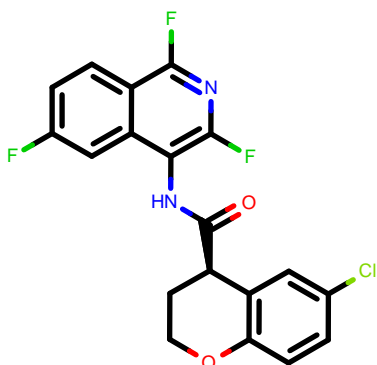
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[H]5CC(=O)N5)Cl

RUN: RUN301

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.17

JOH-SUS-a69c159d-7_1_1



CID: JOH-SUS-a69c159d-7_1_1

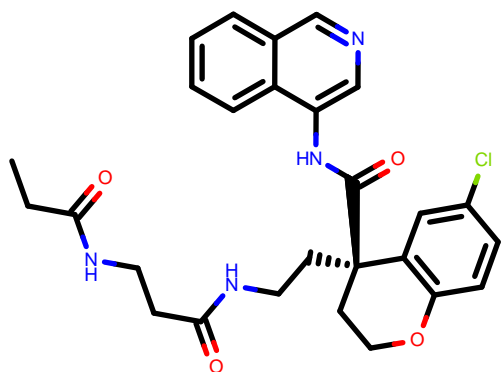
SMILES: c1cc2c(cc1F)c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN3521

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.11

EN300-31186_3_1_1



CID: EN300-31186_3_1_1

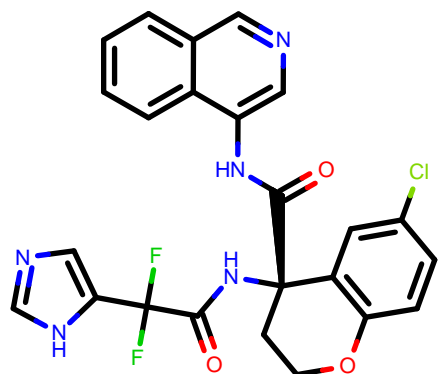
SMILES: CCC(=O)NCCC(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN7148

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.33

EDG-MED-90036822-67_1



CID: EDG-MED-90036822-67_1

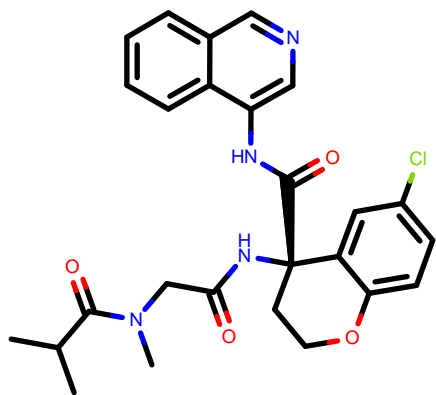
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CNc[nH]5(F)F

RUN: RUN1653

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.28

EN300-31145_1_1_1



CID: EN300-31145_1_1_1

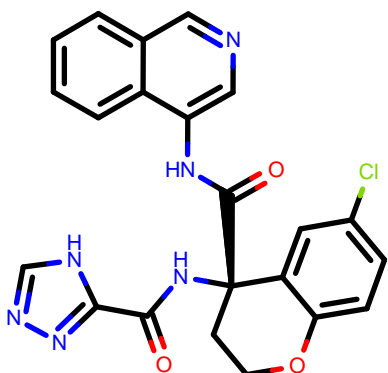
SMILES: CC(C)C(=O)N(C)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5590

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.23

EN300-100741_1_1_1



CID: EN300-100741_1_1_1

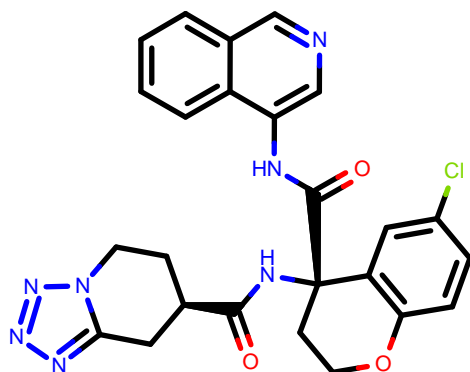
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]nnc5

RUN: RUN4163

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.19

EN300-1653482_1_1_1



CID: EN300-1653482_1_1_1

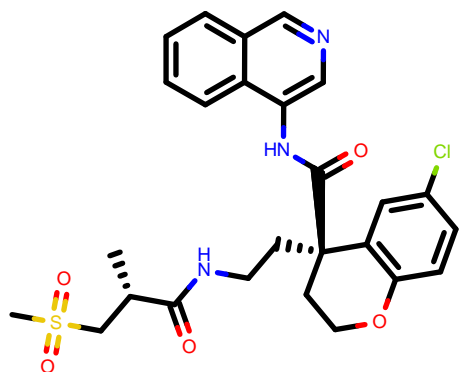
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5Cn6c[nH]n6)C5

RUN: RUN4563

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.25

EN300-97699_3_1_1



CID: EN300-97699_3_1_1

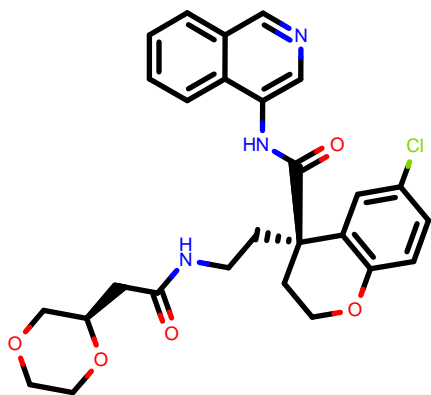
SMILES: C[C@@]H[C@@]1(CS(=O)(=O)C)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN6395

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.34

EN300-731622_3_1_1



CID: EN300-731622_3_1_1

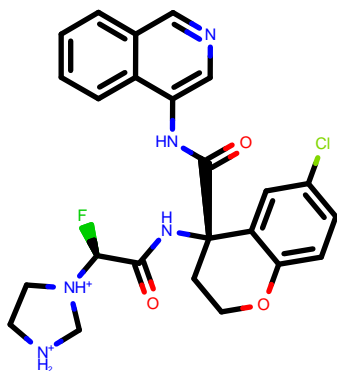
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5COCOC5

RUN: RUN6017

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.29

EDG-MED-90036822-36_1



CID: EDG-MED-90036822-36_1

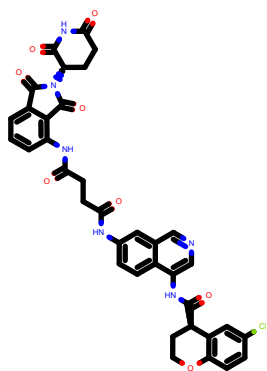
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](n5cnc5)F

RUN: RUN1575

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

DAR-DIA-9e4459de-15_7



CID: DAR-DIA-9e4459de-15_7

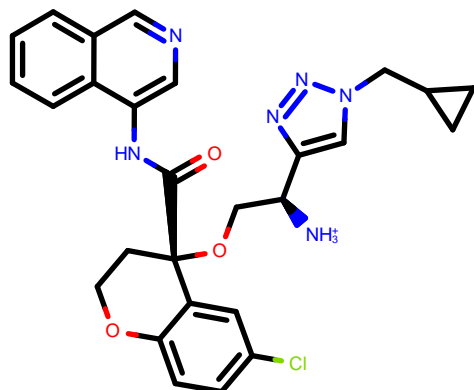
SMILES: c1cc2c(c1)NC(=O)CCCl(=O)Nc3ccc4c(c3)cnc4NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(c1c2O)[C@@H](C)C1=O)NC7=O)O

RUN: RUN1379

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-18_1



CID: ED_-GRI-5b13fbe2-18_1

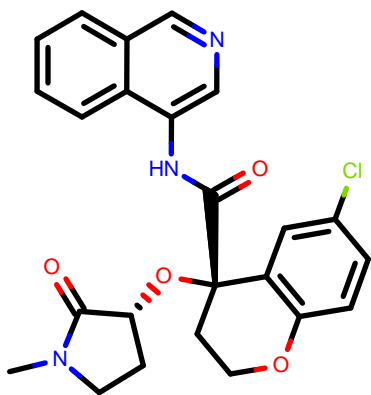
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](c5cnc6COC6C5)N3=

RUN: RUN1486

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.35

EN300-98648_1_2_1



CID: EN300-98648_1_2_1

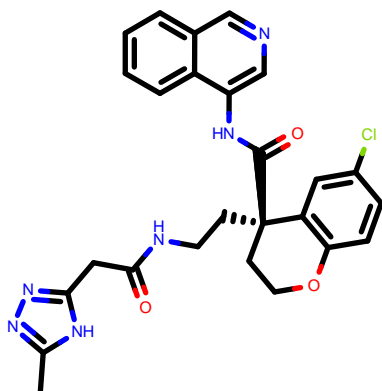
SMILES: CN1CC[C@H](C1=O)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7488

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.21

EN300-119126_3_1_1



CID: EN300-119126_3_1_1

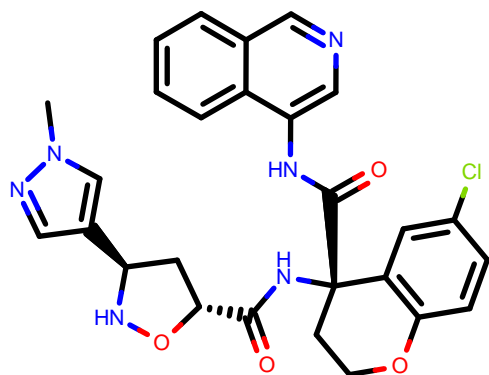
SMILES: Cc1[nH]nc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6278

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.29

EN300-92605_1_2_2



CID: EN300-92605_1_2_2

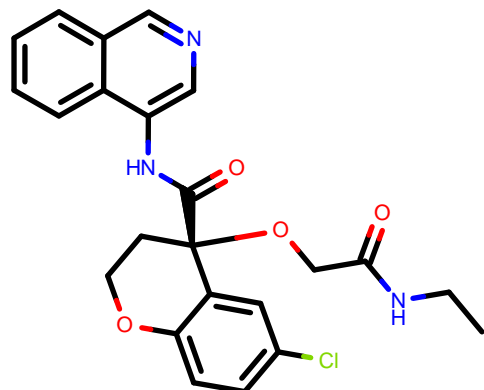
SMILES: Cn1cc[nH]1C@H2[C@@H](ON2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6

RUN: RUN4251

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.36

EN300-7003350_1_1_1



CID: EN300-7003350_1_1_1

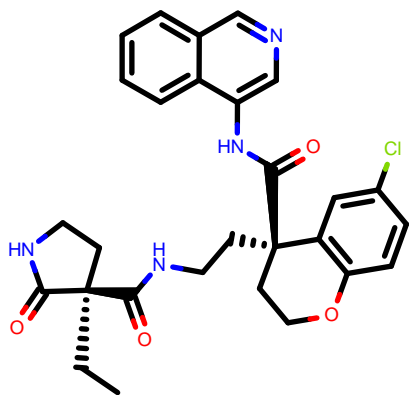
SMILES: CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3580

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.19

EN300-304135_3_2_1



CID: EN300-304135_3_2_1

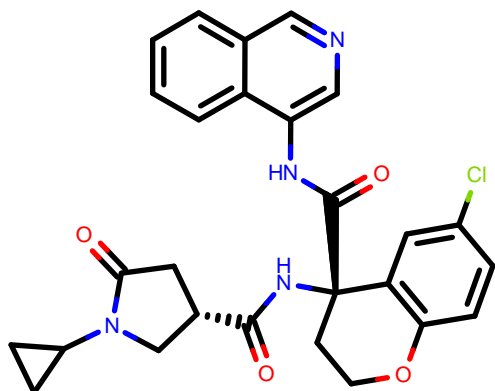
SMILES: CC[C@@]1(CNC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3663

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.34

EN300-12440_1_2_1



CID: EN300-12440_1_2_1

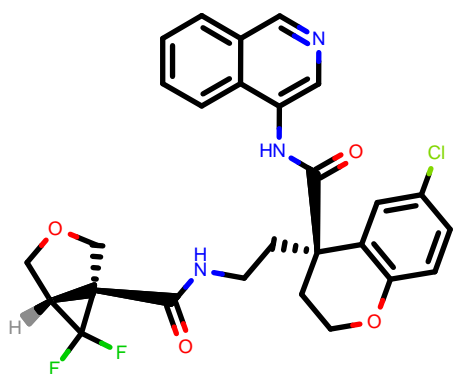
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@H]5CC(=O)N(C5)C6CC6

RUN: RUN6980

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.30

EN300-6738732_3_1_1



CID: EN300-6738732_3_1_1

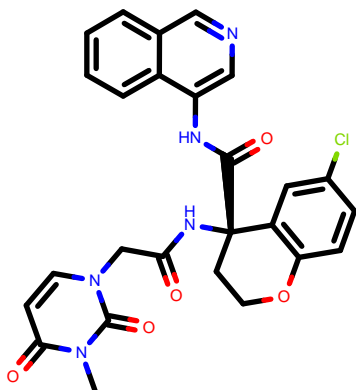
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@H]56COC[C@H]5O6(F)F

RUN: RUN4494

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.23

ALP-UNI-dbbfd3db-18_1



CID: ALP-UNI-dbbfd3db-18_1

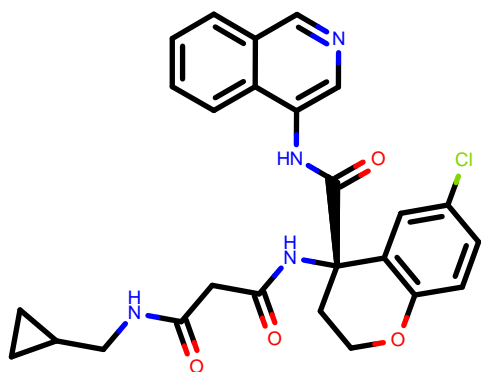
SMILES: Cn1c(=O)ccn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN2646

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.29

EN300-178829_1_1_1



CID: EN300-178829_1_1_1

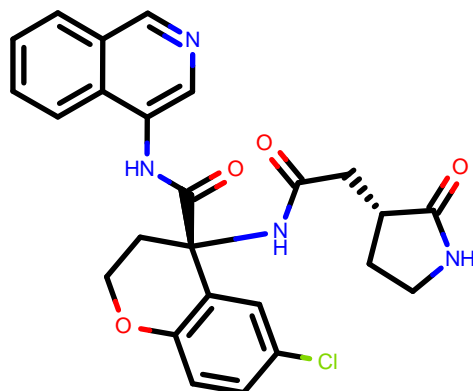
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)NCC5CC5

RUN: RUN5087

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.25

EN300-343474_1_2_1



CID: EN300-343474_1_2_1

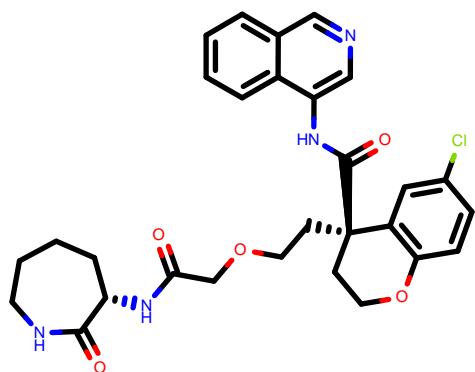
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCNC5=O

RUN: RUN5747

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.26

EN300-37195_3_2_1



CID: EN300-37195_3_2_1

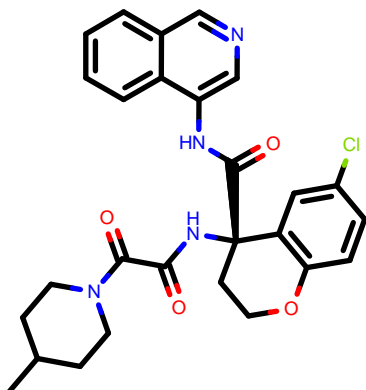
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@H]5CCCCNC5=O

RUN: RUN7401

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.32

EN300-137784_1_1_1



CID: EN300-137784_1_1_1

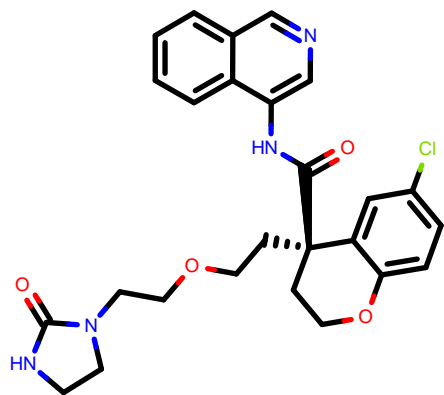
SMILES: CC1CCN(CC1)C(=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN4385

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.31

EN300-214800_3_1_1



CID: EN300-214800_3_1_1

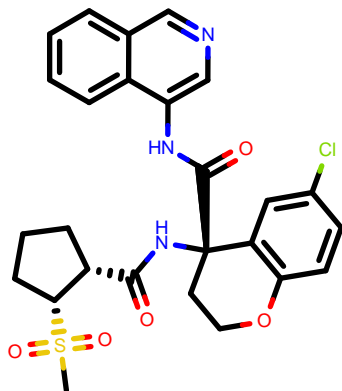
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC5N5CNC5=O

RUN: RUN3808

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-1387145_1_1_1



CID: EN300-1387145_1_1_1

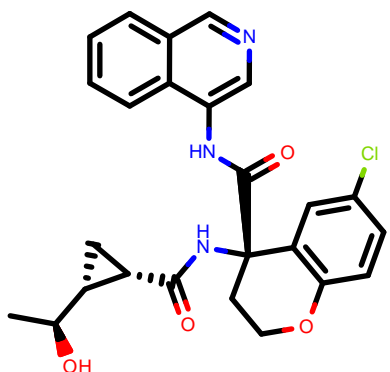
SMILES: CS(=O)(=O)[C@@]1(C)CC[C@@H]1C(=O)NC(=O)[C@@]2(CCOc3c2cc(cc3)C)C1=O)Nc4ncnc5c4ccc5=O

RUN: RUN3149

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-6729572_1_1_1



CID: EN300-6729572_1_1_1

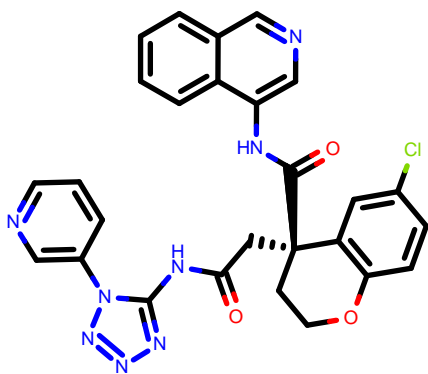
SMILES: C[C@@]1(C)CC[C@@H]1C(=O)NC(=O)[C@@]2(CCOc3c2cc(cc3)C)C1=O)Nc4ncnc5c4ccc5=O

RUN: RUN3679

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.27

EDJ-MED-d203f206-17_1



CID: EDJ-MED-d203f206-17_1

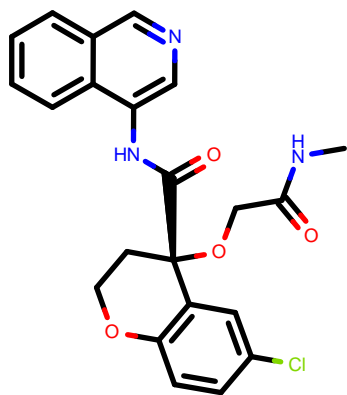
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5nnn5c6cccnc6

RUN: RUN2437

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.30

EN300-2977549_1_1_1



CID: EN300-2977549_1_1_1

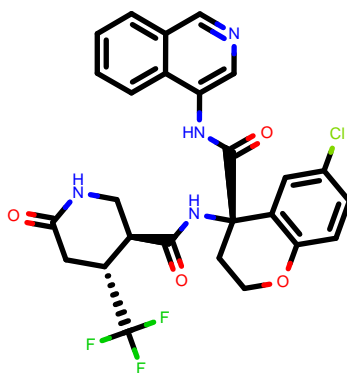
SMILES: CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5151

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.18

EN300-208959_1_3_1



CID: EN300-208959_1_3_1

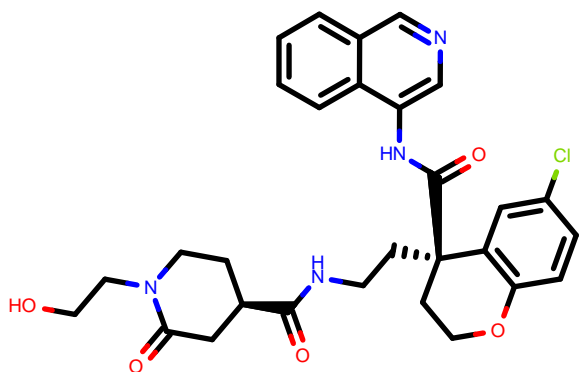
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CN(C)C(=O)C[C@H]5C(F)(F)F

RUN: RUN5084

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.27

EN300-1723663_3_1_1



CID: EN300-1723663_3_1_1

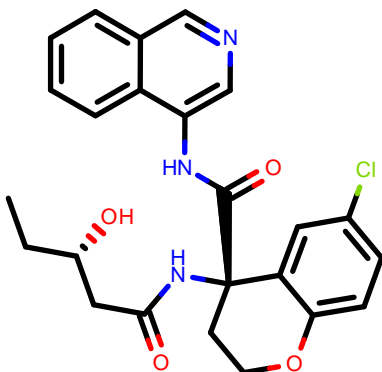
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CN(C)C(=O)C[C@@H]5CO

RUN: RUN4120

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.34

EN300-224741_1_1_1



CID: EN300-224741_1_1_1

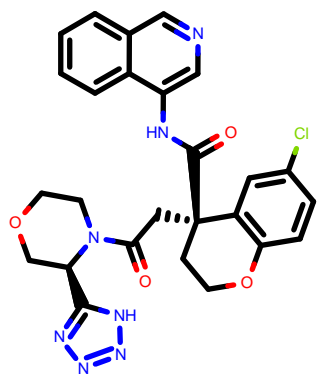
SMILES: CC[C@@H](CC(=O)N)[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4O

RUN: RUN3505

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.22

EDJ-MED-d203f206-14_1



CID: EDJ-MED-d203f206-14_1

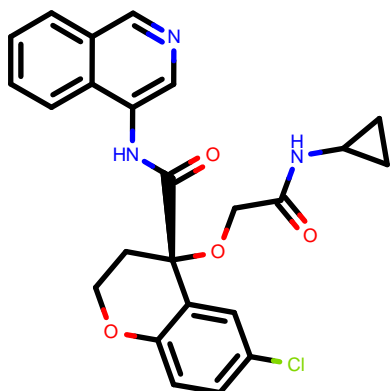
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5c6n[n-]n6

RUN: RUN2400

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.39

CHO-MSK-5891c1ff-8_1



CID: CHO-MSK-5891c1ff-8_1

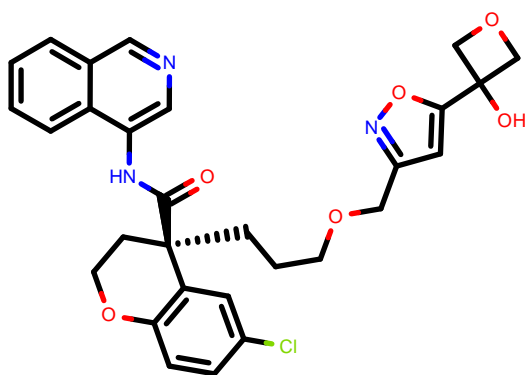
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN: RUN1718

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.19

EN300-7457159_4_1_1



CID: EN300-7457159_4_1_1

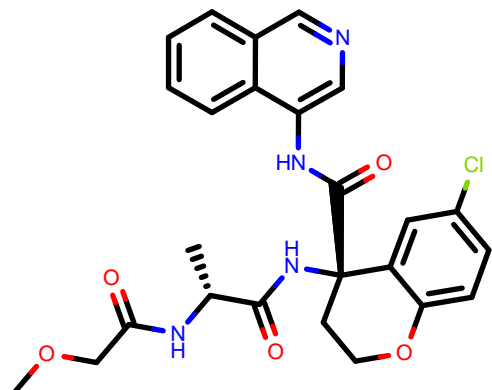
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5cc(on5)C6(COC6)O

RUN: RUN4721

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.37

EN300-31183_1_2_1



CID: EN300-31183_1_2_1

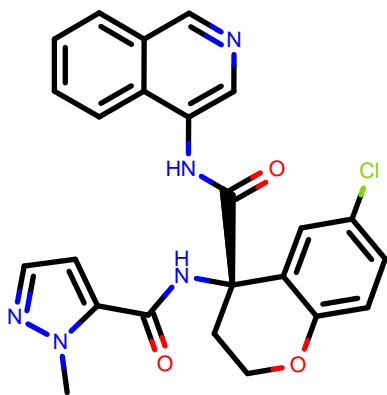
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)COC

RUN: RUN4099

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-31077_1_1_1



CID: EN300-31077_1_1_1

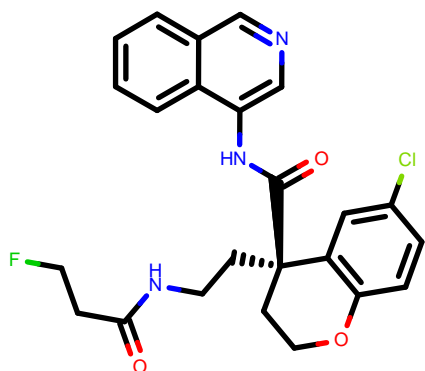
SMILES: Cn1c(ccn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4032

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.20

EN300-97758_3_1_1



CID: EN300-97758_3_1_1

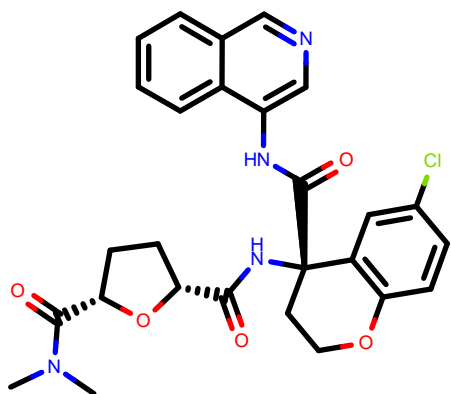
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)CCF

RUN: RUN3222

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.25

EN300-314890_1_1_1



CID: EN300-314890_1_1_1

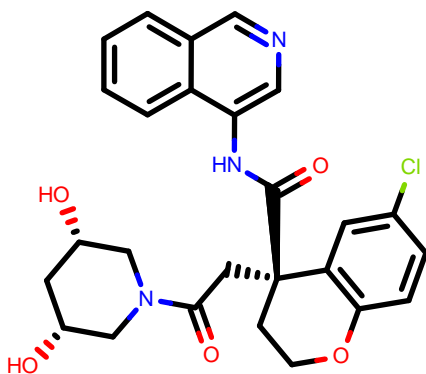
SMILES: CN(C)C(=O)N[C@@]1(C)CC[C@@H]1C[C@@H]2(C)C(=O)N[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)Nc5cnc6c4cccc65

RUN: RUN5415

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.38

EN300-96886_1_1_1



CID: EN300-96886_1_1_1

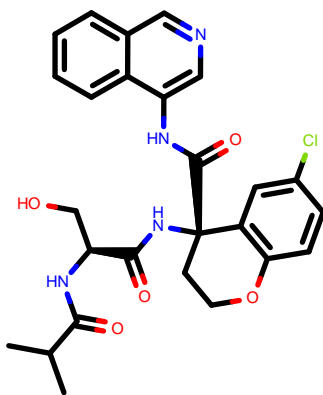
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N5C[C@@H]3[C@@H](C5)O

RUN: RUN5069

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.28

EN300-212266_1_1_1



CID: EN300-212266_1_1_1

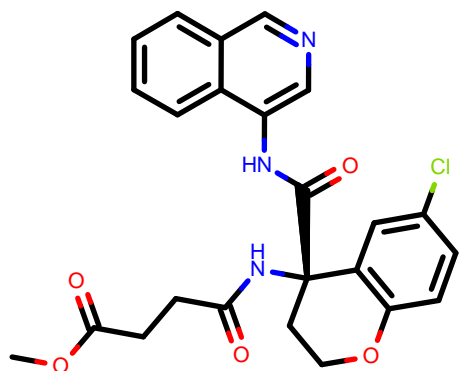
SMILES: CC(C)C(=O)N[C@@H](CO)C(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3130

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.31

EN300-24949_1_1_1



CID: EN300-24949_1_1_1

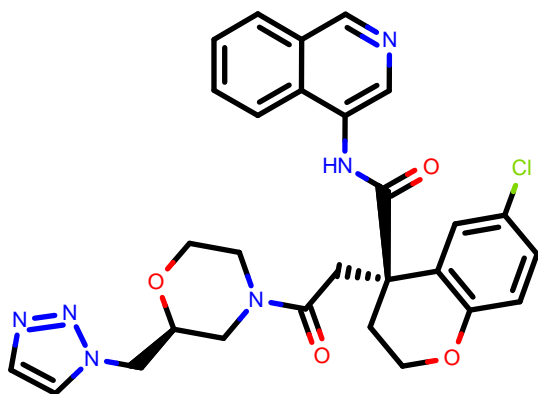
SMILES: COC(=O)CCC(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3942

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.24

EDJ-MED-d203f206-24_1



CID: EDJ-MED-d203f206-24_1

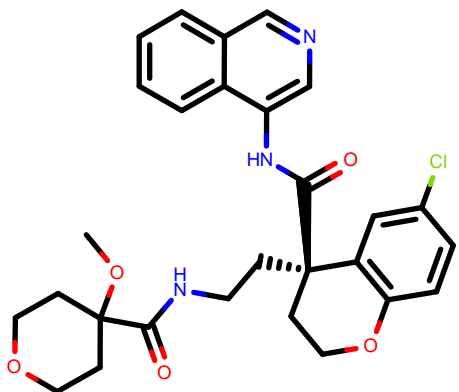
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)Cn6ccnn6

RUN: RUN2431

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.33

EN300-204133_3_1_1



CID: EN300-204133_3_1_1

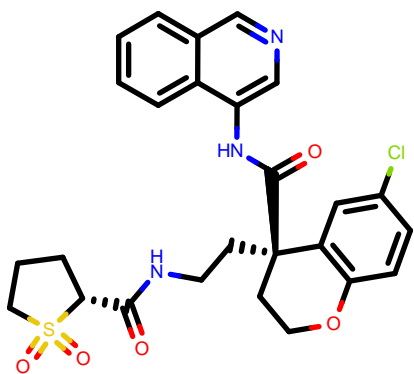
SMILES: COC1(CCOCC1)C(=O)NCC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4089

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.32

EN300-88656_3_2_1



CID: EN300-88656_3_2_1

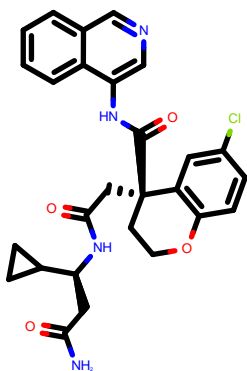
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCS5(=O)=O

RUN: RUN6033

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.28

EN300-85413_1_1_1



CID: EN300-85413_1_1_1

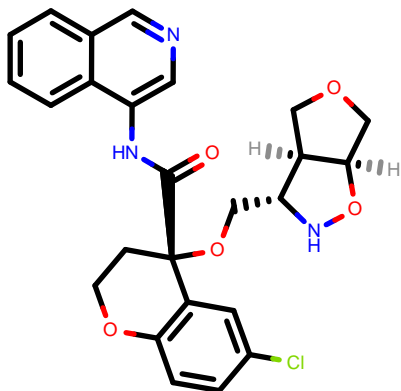
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](C(=O)N)C5CC5

RUN: RUN3467

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.32

EN300-7436306_1_1_1



CID: EN300-7436306_1_1_1

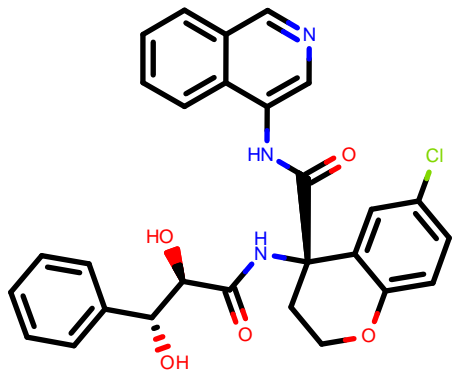
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5[C@H]6COC(C@H)6ON5

RUN: RUN5304

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.22

EN300-2923949_1_4_1



CID: EN300-2923949_1_4_1

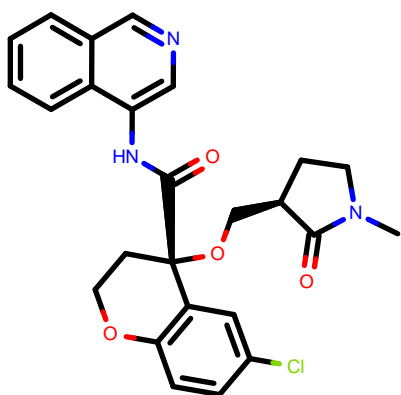
SMILES: c1ccc(cc1)C@H(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3336

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

EN300-260816_1_1_1



CID: EN300-260816_1_1_1

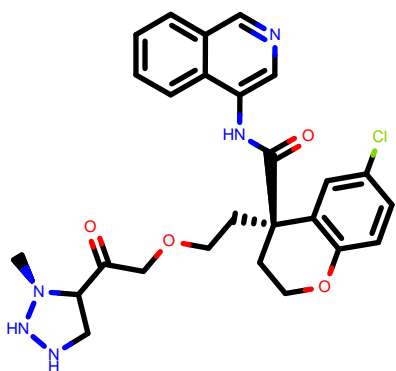
SMILES: CN1CC[C@@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3891

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.25

EN300-204936_3_1_1



CID: EN300-204936_3_1_1

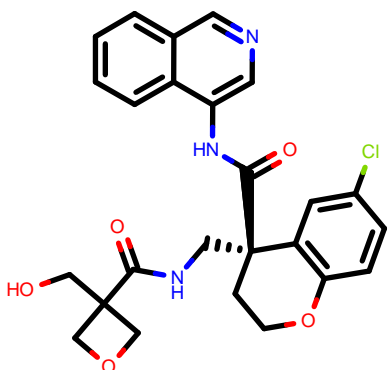
SMILES: Cn1c(cnn1)C(=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4010

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.30

EN300-105693_2_1_1



CID: EN300-105693_2_1_1

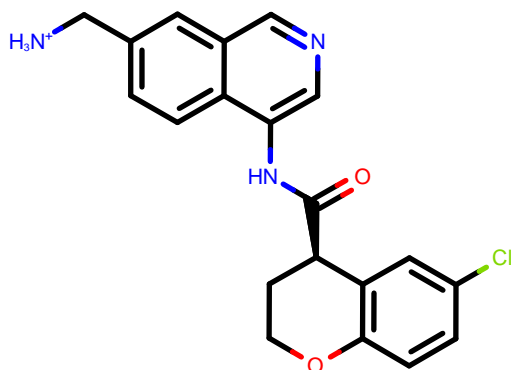
SMILES: c1cc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(COC5)CO

RUN: RUN3554

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

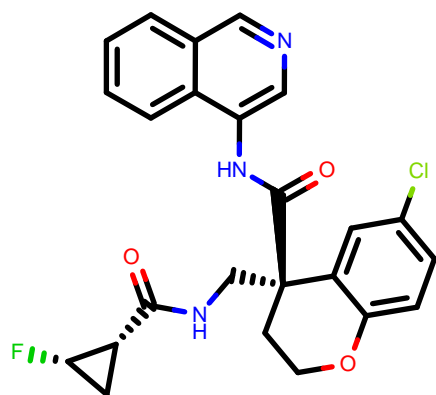
SMILES: c1cc2c(cc1C[NH3+])cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C

RUN: RUN413

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.11

EN300-97300_2_1_1



CID: EN300-97300_2_1_1

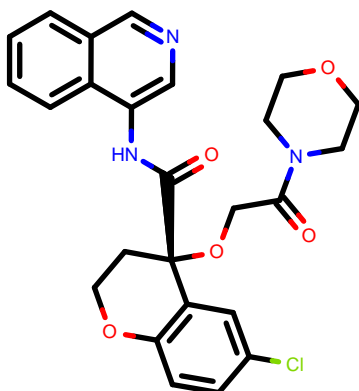
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@@H]5C[C@@H]5F

RUN: RUN6222

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-1241327_1_1_1



CID: EN300-1241327_1_1_1

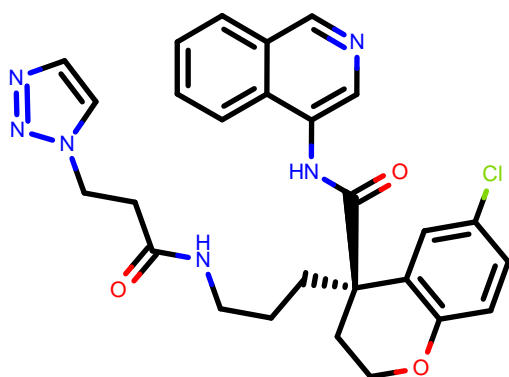
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCOCC5

RUN: RUN4943

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.26

EN300-28871_4_1_1



CID: EN300-28871_4_1_1

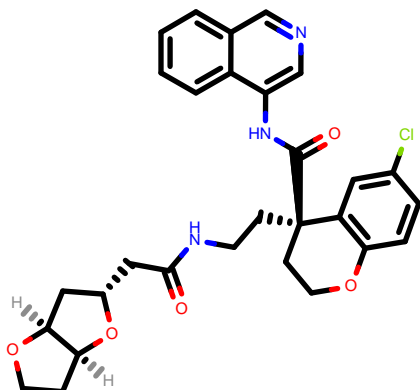
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5ccnn5

RUN: RUN5575

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.32

EN300-7355519_3_4_1



CID: EN300-7355519_3_4_1

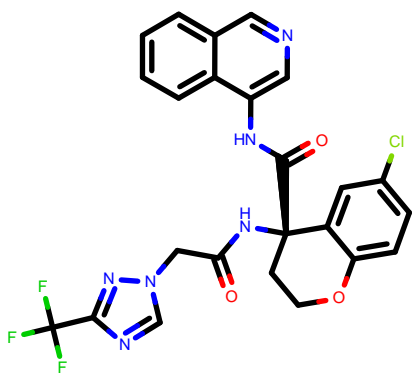
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@@H]5C[C@@H]5OC6

RUN: RUN4930

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.32

EN300-7385389_1_1_1



CID: EN300-7385389_1_1_1

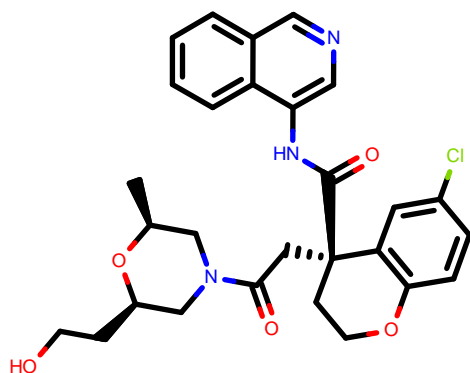
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ncnc(F)C(F)F

RUN: RUN4580

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.29

EN300-212814_1_4_1



CID: EN300-212814_1_4_1

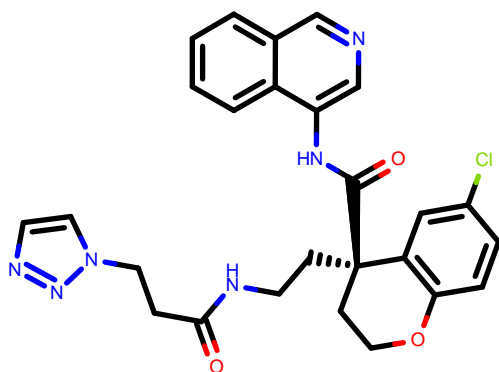
SMILES: C[C@H]1CN(C[C@H](O1)CCO)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5c4ccc5

RUN: RUN5236

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.30

EN300-28871_3_1_1



CID: EN300-28871_3_1_1

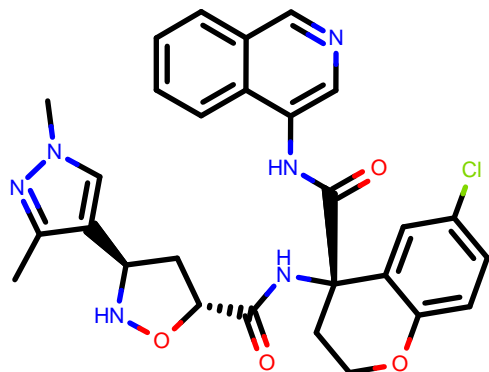
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5ncnn5

RUN: RUN3078

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.27

EN300-92684_1_2_2



CID: EN300-92684_1_2_2

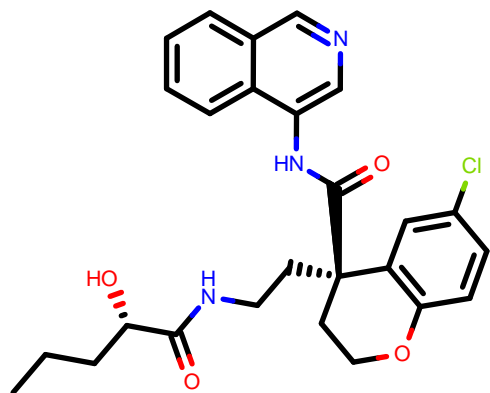
SMILES: Cc1c(c[nH]1)C(Cc2c[nH]2)C[C@@]3(CO)NC(=O)[C@@]4(CCOc5c4cc(cc5)C)C(=O)Nc6ncnc6C

RUN: RUN3026

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.40

EN300-219531_3_1_1



CID: EN300-219531_3_1_1

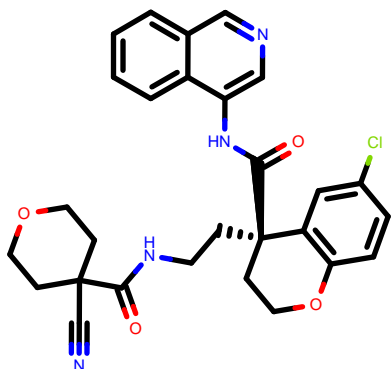
SMILES: CCC[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN3576

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.33

EN300-74089_3_1_1



CID: EN300-74089_3_1_1

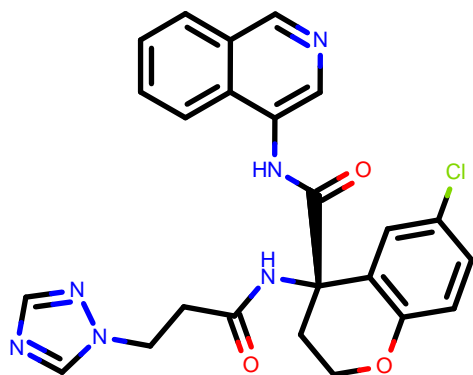
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCOCC5)C#N

RUN: RUN3769

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.38

EN300-26147_1_1_1



CID: EN300-26147_1_1_1

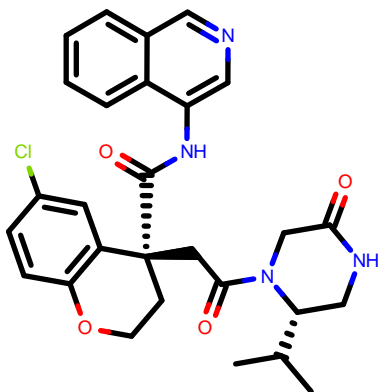
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5

RUN: RUN5308

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-2983332_1_2_1



CID: EN300-2983332_1_2_1

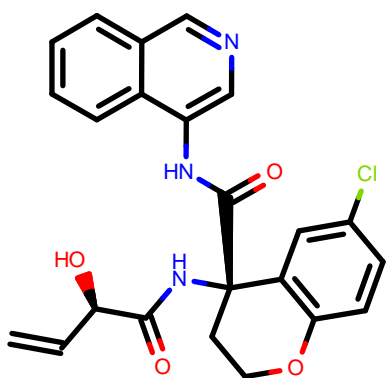
SMILES: CC(C)[C@@H]1CNC(=O)CN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN7114

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

EN300-181492_1_2_1



CID: EN300-181492_1_2_1

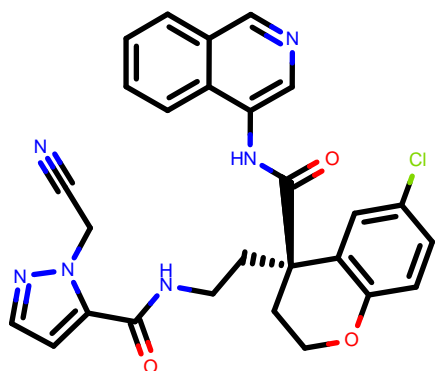
SMILES: C=C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN3167

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.23

EN300-373791_3_1_1



CID: EN300-373791_3_1_1

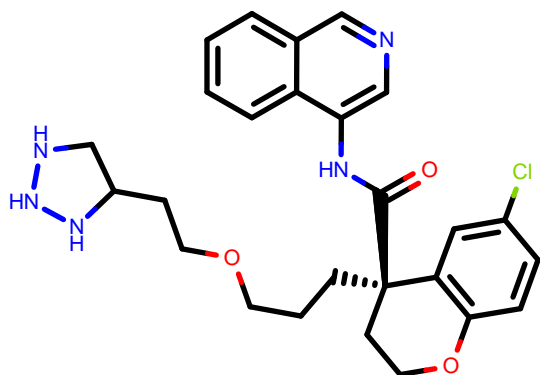
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnnc5C#N

RUN: RUN4345

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.29

EN300-222357_4_1_1



CID: EN300-222357_4_1_1

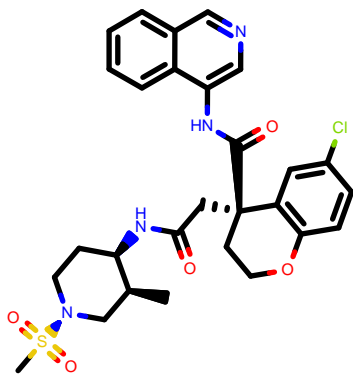
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5cn[nH]n5

RUN: RUN7368

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.35

ALP-UNI-3496895b-5_6



CID: ALP-UNI-3496895b-5_6

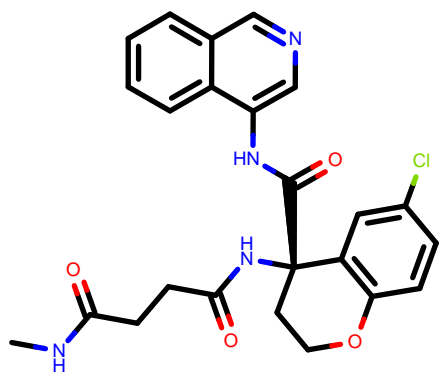
SMILES: C[C@H]1C[N@@]2CC[C@@H]1NC1=O[C@@]3(CCOc4c3cc(cc4)Cl)Nc4ncsc4C(=O)N1=O

RUN: RUN2391

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.35

EN300-1081277_1_1_1



CID: EN300-1081277_1_1_1

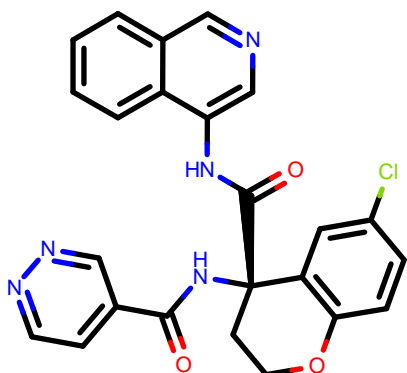
SMILES: CNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4507

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-75875_1_1_1



CID: EN300-75875_1_1_1

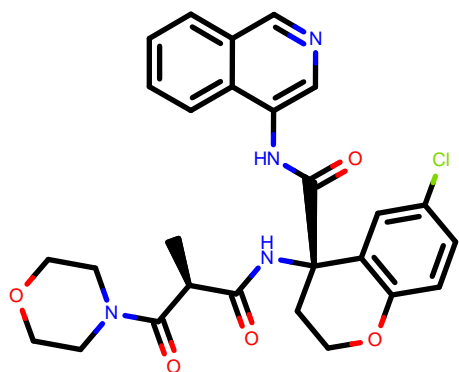
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5

RUN: RUN4346

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-2855057_1_1_1



CID: EN300-2855057_1_1_1

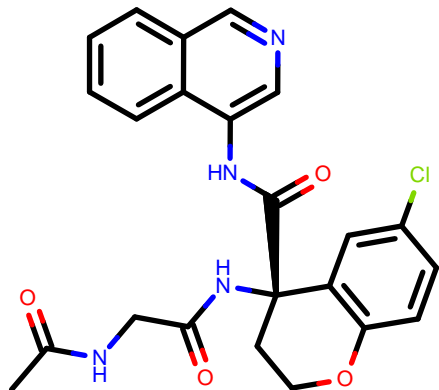
SMILES: C[C@@H](Cl)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4C(=O)N5CCOCC5

RUN: RUN6000

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.29

EN300-18561_1_1_1



CID: EN300-18561_1_1_1

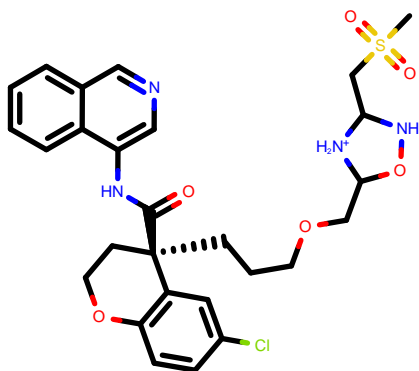
SMILES: CC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6370

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-94900_4_1_1



CID: EN300-94900_4_1_1

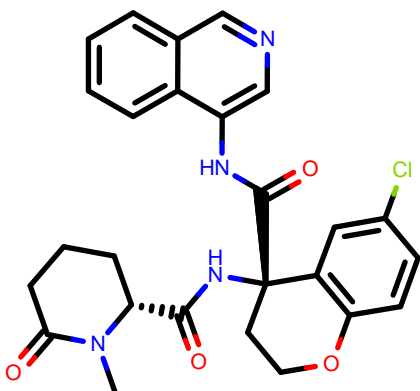
SMILES: CS(=O)(=O)Cc1nc(on1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4354

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.33

EN300-325738_1_2_1



CID: EN300-325738_1_2_1

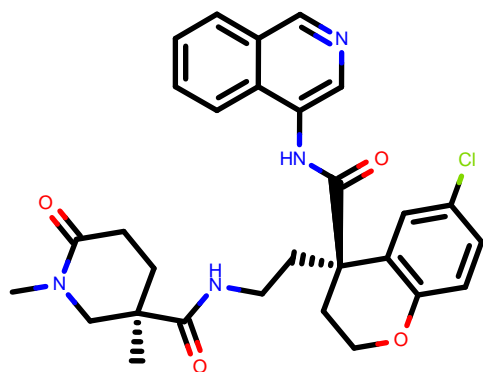
SMILES: CN1C@H](CCCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3488

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.23

EN300-6734171_3_2_1



CID: EN300-6734171_3_2_1

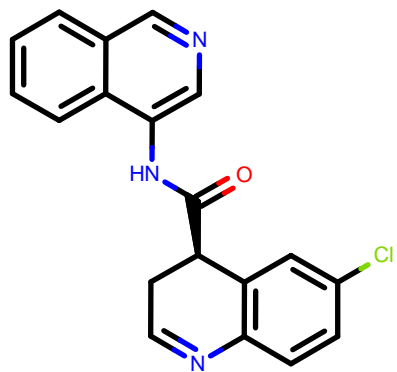
SMILES: C[C@]1(CCC(=O)N(C1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3725

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.43

BEN-BAS-c2bc0d80-1_1



CID: BEN-BAS-c2bc0d80-1_1

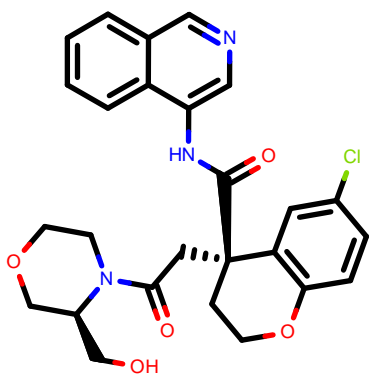
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC=Nc4c3cc(cc4)Cl

RUN: RUN997

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.28

EN300-154201_1_1_1



CID: EN300-154201_1_1_1

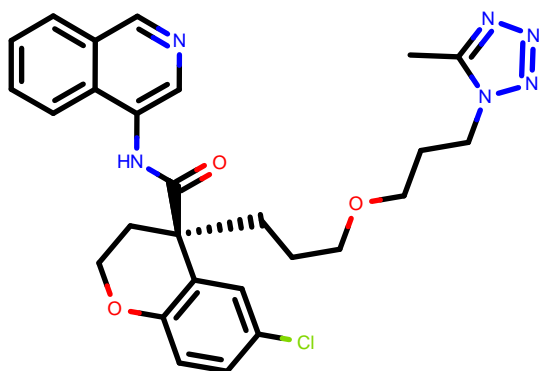
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN2999

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.31

EN300-197715_4_1_1



CID: EN300-197715_4_1_1

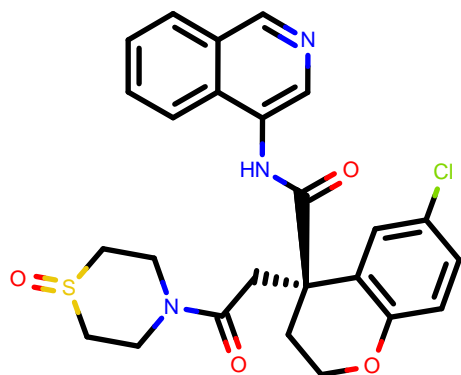
SMILES: Cc1n[nH]1CCCOCCC[C@@]2(CCOc3c2cc(cc3)Cl)CC(=O)Nc4cnc5c4cccc5

RUN: RUN5466

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.34

EDJ-MED-d203f206-37_1



CID: EDJ-MED-d203f206-37_1

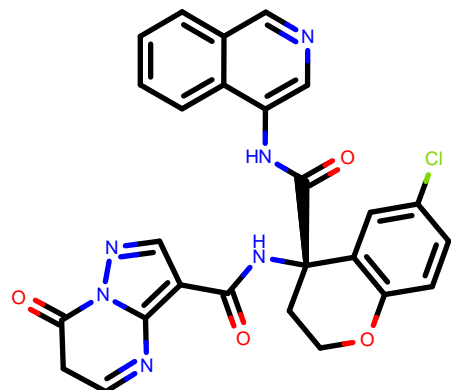
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)CC5

RUN: RUN2424

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.34

EN300-203940_1_1_1



CID: EN300-203940_1_1_1

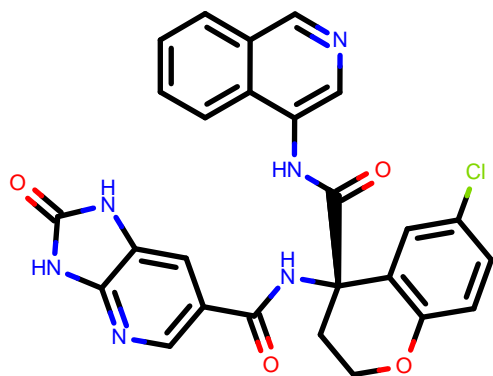
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]n6c5nnc6=O

RUN: RUN4366

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.26

EN300-214552_1_1_1



CID: EN300-214552_1_1_1

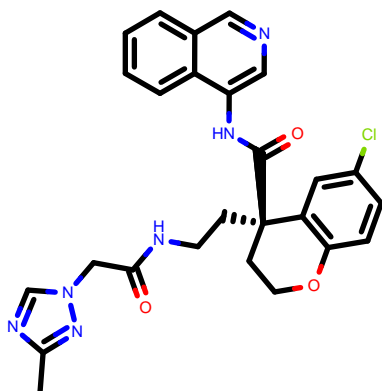
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c([nH]c(=O)[nH]6)nc5

RUN: RUN5521

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.30

EN300-7473354_3_1_1



CID: EN300-7473354_3_1_1

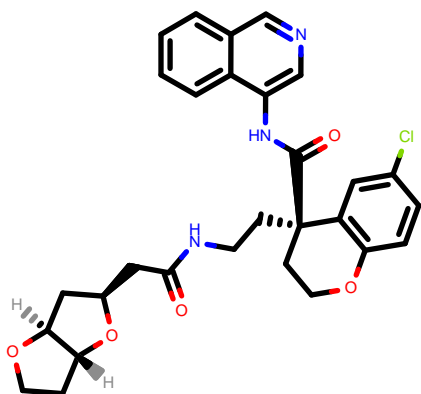
SMILES: Cc1ncn(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN3611

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.38

EN300-7355519_3_7_1



CID: EN300-7355519_3_7_1

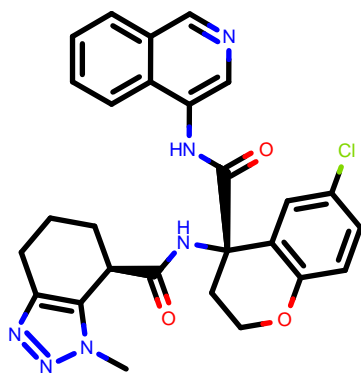
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@@]4(H)C[C@@H]5C[C@H]4O5COC6

RUN: RUN5469

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.36

EN300-1664865_1_2_1



CID: EN300-1664865_1_2_1

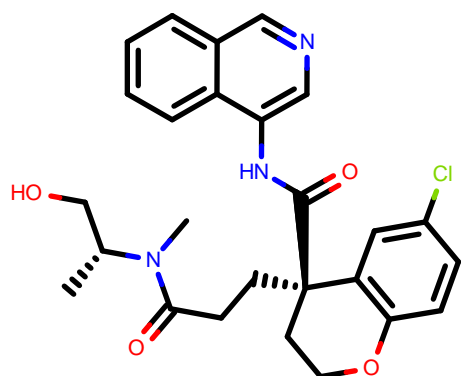
SMILES: Cn1c2c(nn1)CCC[C@@H]2C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5cnc6c5cccc6

RUN: RUN5438

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.25

EN300-205110_2_1_1



CID: EN300-205110_2_1_1

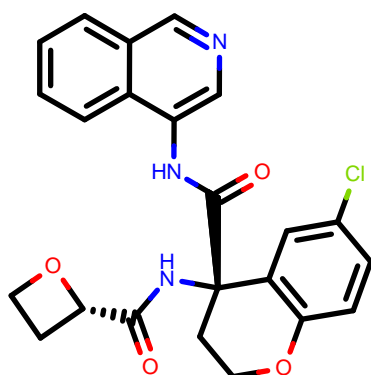
SMILES: C[C@H](CO)N(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN2742

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.24

EN300-85760_1_1_1



CID: EN300-85760_1_1_1

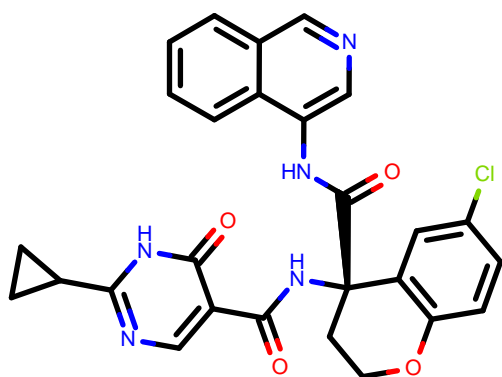
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5OC5

RUN: RUN4745

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.24

EN300-118045_1_1_1



CID: EN300-118045_1_1_1

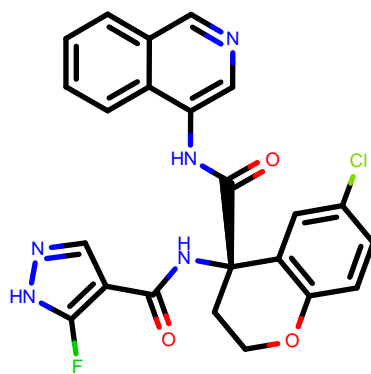
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc[nH]c5=O)C6CC6

RUN: RUN7705

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.36

EN300-7121836_1_1_1



CID: EN300-7121836_1_1_1

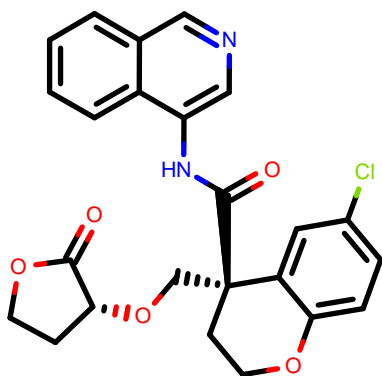
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c5F

RUN: RUN4213

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.17

EN300-20496_2_1_1



CID: EN300-20496_2_1_1

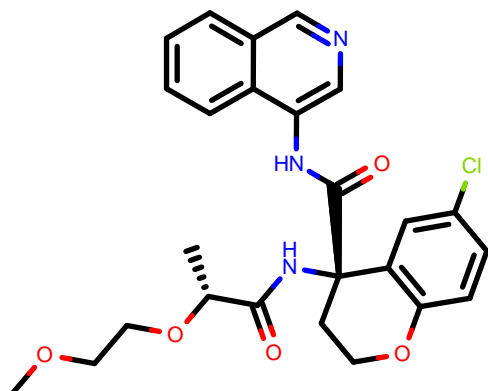
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[C@@H]5CCOC5=O

RUN: RUN4446

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.21

EN300-77359_1_2_1



CID: EN300-77359_1_2_1

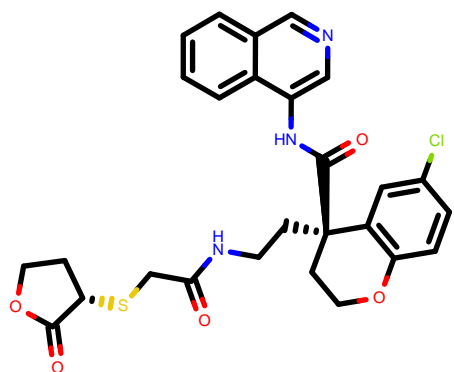
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4)OCOC

RUN: RUN4374

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.22

EN300-113218_3_2_1



CID: EN300-113218_3_2_1

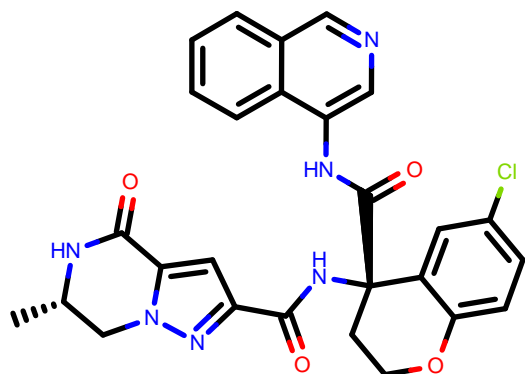
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5CCOC5=O

RUN: RUN5375

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.37

EN300-265285_1_2_1



CID: EN300-265285_1_2_1

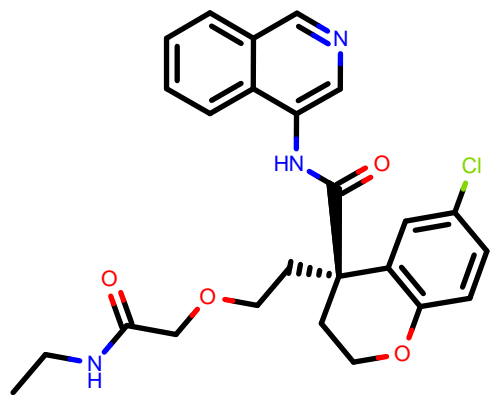
SMILES: C[C@@H]1Cn2c(cc(n2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncnc6c5ccccc6)C(=O)N1

RUN: RUN4185

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.29

EN300-7003350_3_1_1



CID: EN300-7003350_3_1_1

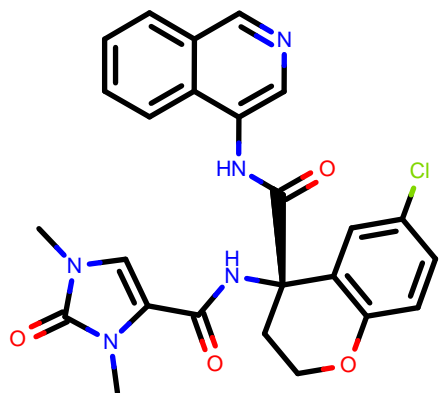
SMILES: CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN4026

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.23

EN300-312618_1_1_1



CID: EN300-312618_1_1_1

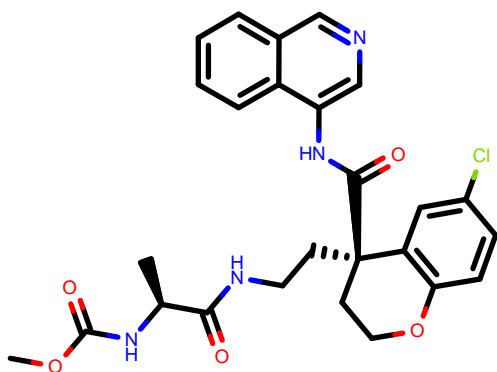
SMILES: Cn1cc(n(c1=O)C)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccc5

RUN: RUN6566

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.22

EN300-120068_3_1_1



CID: EN300-120068_3_1_1

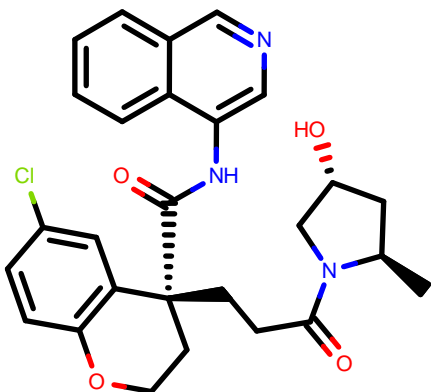
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)NC(=O)OC

RUN: RUN6181

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.28

EN300-173562_2_3_1



CID: EN300-173562_2_3_1

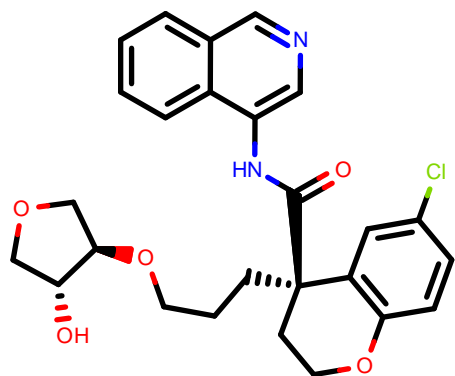
SMILES: C[C@@H]1[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN6794

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.28

EN300-331828_4_1_1



CID: EN300-331828_4_1_1

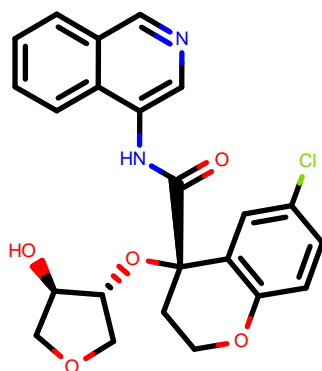
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CCCO[C@@H]5COC[C@H]5O

RUN: RUN3722

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.32

EN300-331828_1_1_1



CID: EN300-331828_1_1_1

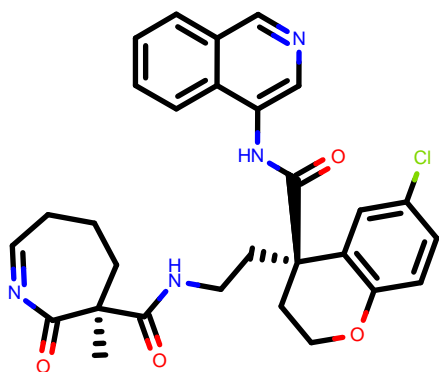
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)O[C@@H]5COC[C@H]5O

RUN: RUN7657

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.20

EN300-6745081_3_2_1



CID: EN300-6745081_3_2_1

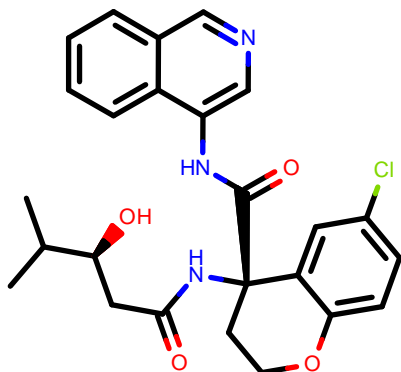
SMILES: C[C@]1(C)CCCN1=O)(C(=O)NCC[C@@]2(C)CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3241

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.45

EN300-155498_1_1_1



CID: EN300-155498_1_1_1

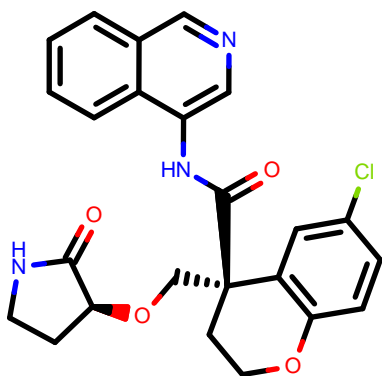
SMILES: CC(C)[C@H](CC(=O)N[C@@]1(C)CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6570

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.25

EN300-6736413_2_2_1



CID: EN300-6736413_2_2_1

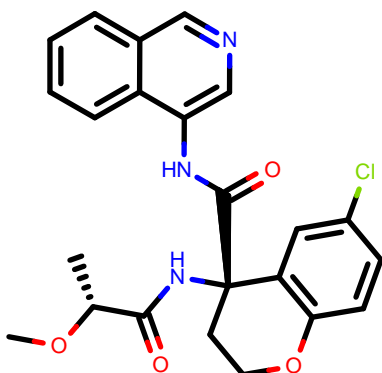
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(Cc4cc(Cl)cc4)C[C@@H]5CCNC5=O

RUN: RUN4117

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.19

EN300-247951_1_1_1



CID: EN300-247951_1_1_1

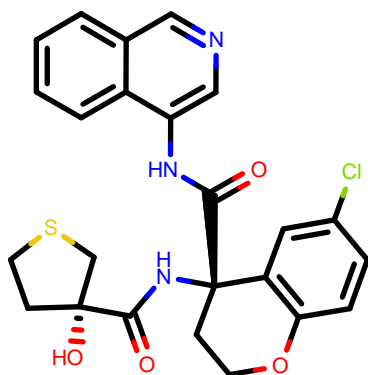
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)OC

RUN: RUN3719

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.22

EN300-122656_1_2_1



CID: EN300-122656_1_2_1

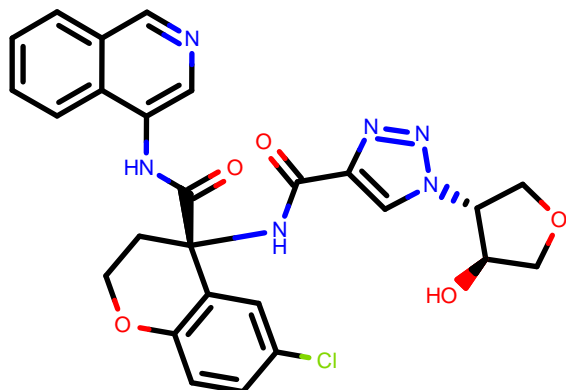
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCSC5)O

RUN: RUN2709

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.42

EN300-637424_1_1_1



CID: EN300-637424_1_1_1

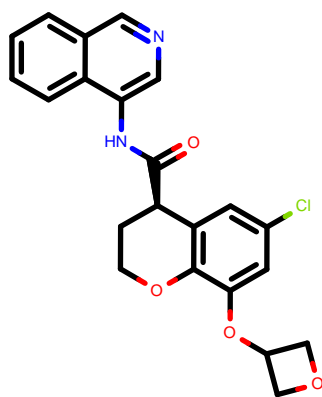
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(n5)[C@@H]6CO[C@H]6O

RUN: RUN4870

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.26

EDJ-MED-e4b030d8-4_1



CID: EDJ-MED-e4b030d8-4_1

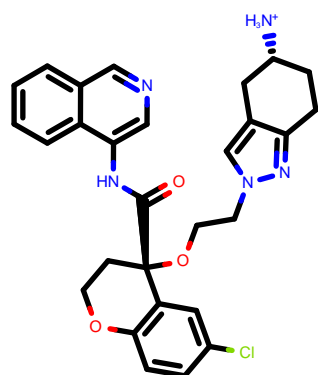
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOc4c3cc(cc4OC5COC5)Cl

RUN: RUN278

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.18

ED_-GRI-5b13fbe2-60_2



CID: ED_-GRI-5b13fbe2-60_2

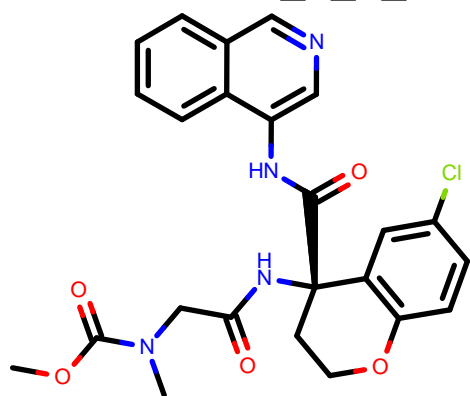
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)OCc5nc6c(n5)CC[C@H](C6)[NH3+]

RUN: RUN1450

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.35

EN300-39005_1_1_1



CID: EN300-39005_1_1_1

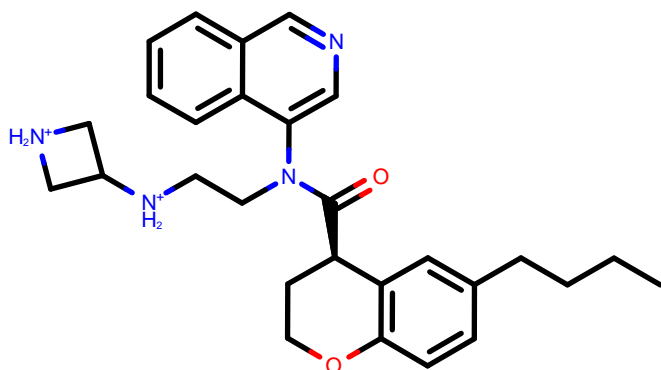
SMILES: CN(CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cc4)C(=O)OC

RUN: RUN7682

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.25

MAK-UNK-83e0a0b4-4_1_1



CID: MAK-UNK-83e0a0b4-4_1_1

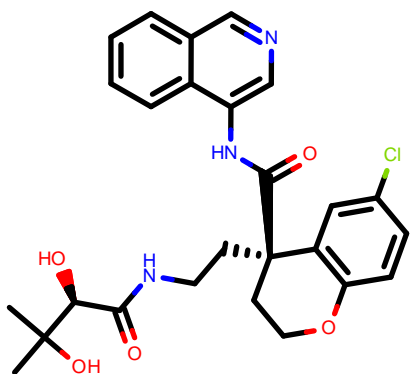
SMILES: CCCC1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCNC3C[NH2+](C3)c4nc5c4cc5)C

RUN: RUN4271

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.45

EN300-299532_3_2_1



CID: EN300-299532_3_2_1

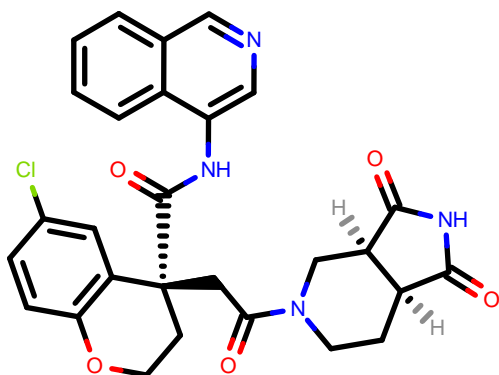
SMILES: CC(C)[C@H](C(=O)NCC[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4O)O

RUN: RUN5628

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.31

EN300-104029_1_2_1



CID: EN300-104029_1_2_1

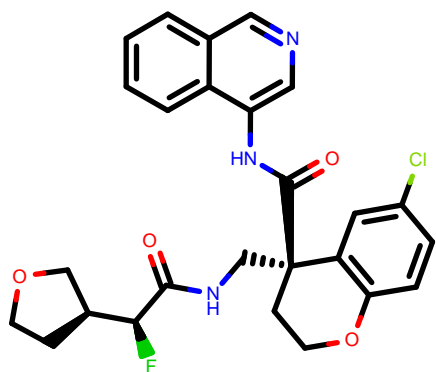
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4ccc(cc4)Cl)C(=O)N5CC[C@H]6C[C@@H](C5)C(=O)N6=O

RUN: RUN5033

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.24

EN300-783124_2_4_1



CID: EN300-783124_2_4_1

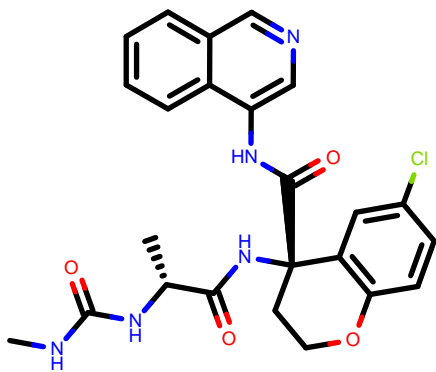
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4ccc(cc4)Cl)C(=O)N[C@@H]5COCOC5F

RUN: RUN6837

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.23

EN300-2958082_1_1_1



CID: EN300-2958082_1_1_1

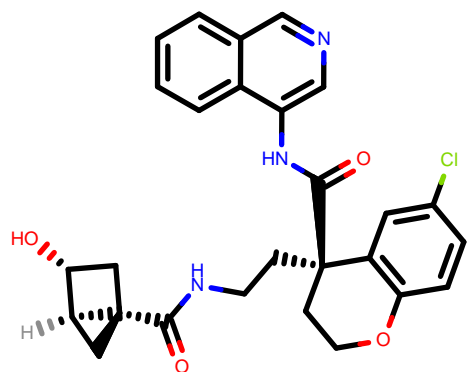
SMILES: C[C@H](C(=O)N[C@@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)NC(=O)NC

RUN: RUN4590

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-6493972_3_1_1



CID: EN300-6493972_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)O)CCNC(=O)C@]56C[C@@]5(C)O

RUN:

RUN6676

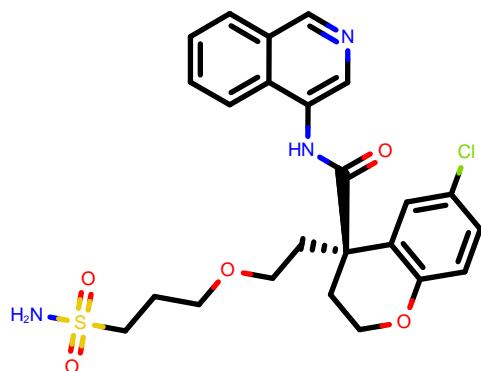
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.24

EN300-79588_3_1_1



CID: EN300-79588_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)O)CCOCCCS(=O)(=O)N

RUN:

RUN4079

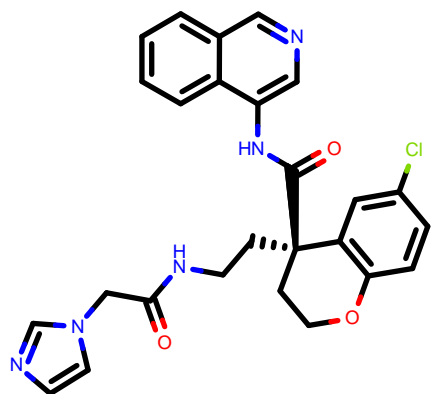
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.34

EN300-38979_3_1_1



CID: EN300-38979_3_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)O)CCNC(=O)Cn5ccnc5

RUN:

RUN5333

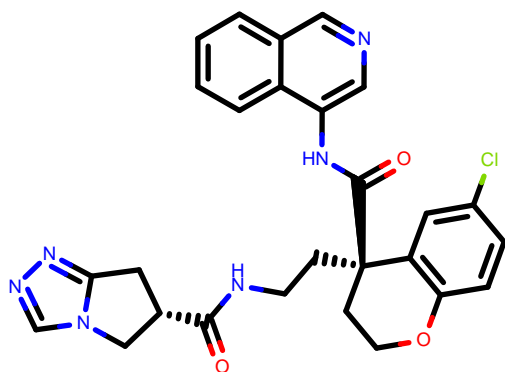
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.27

EN300-6745453_3_2_1



CID: EN300-6745453_3_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)O)CCNC(=O)[C@H]5C6nncn6C5

RUN:

RUN3047

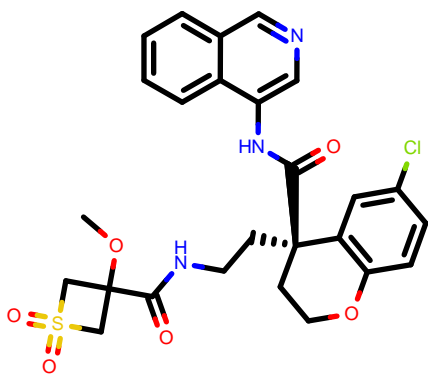
DDG (kcal/mol):

-1.46

dDDG (kcal/mol):

0.37

EN300-704025_3_1_1



CID: EN300-704025_3_1_1

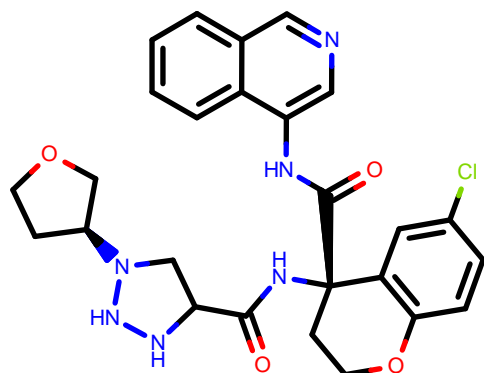
SMILES: COC1(CS(=O)(=O)C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4932

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.42

EN300-151461_1_2_1



CID: EN300-151461_1_2_1

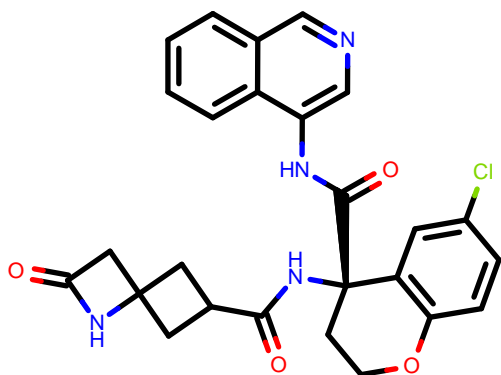
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn[nH]5[C@@H]6CCOC6

RUN: RUN5580

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EN300-1700760_1_1_1



CID: EN300-1700760_1_1_1

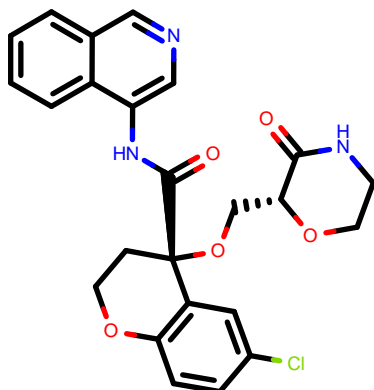
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN3176

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.22

EN300-1706036_1_1_1



CID: EN300-1706036_1_1_1

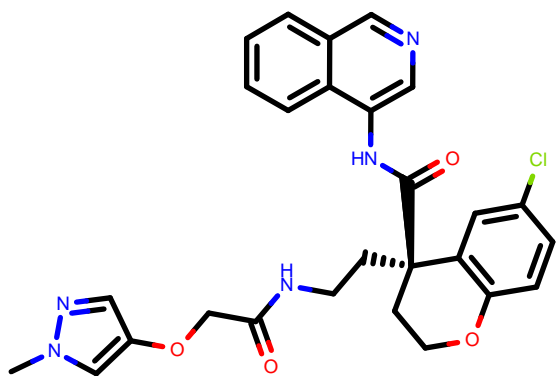
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5C(=O)NCCO5

RUN: RUN7796

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.28

EN300-201553_3_1_1



CID: EN300-201553_3_1_1

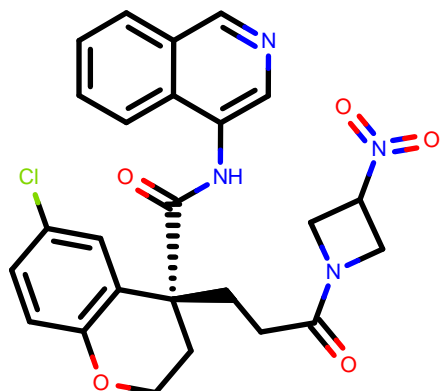
SMILES: Cn1cc(en1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4577

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.30

EN300-7461023_2_1_1



CID: EN300-7461023_2_1_1

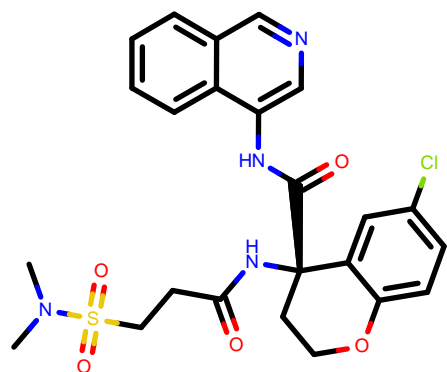
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)N(=O)=O

RUN: RUN7641

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.26

EN300-50631_1_1_1



CID: EN300-50631_1_1_1

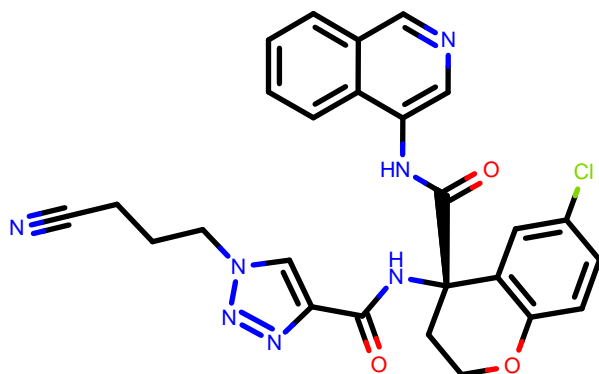
SMILES: CN(C)S(=O)(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4999

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.32

EN300-120569_1_1_1



CID: EN300-120569_1_1_1

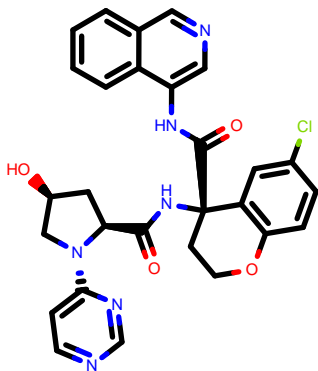
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)CCCC#N

RUN: RUN5834

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.30

EN300-310022_1_1_1



CID: EN300-310022_1_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)N1CCOC1

RUN:

RUN6196

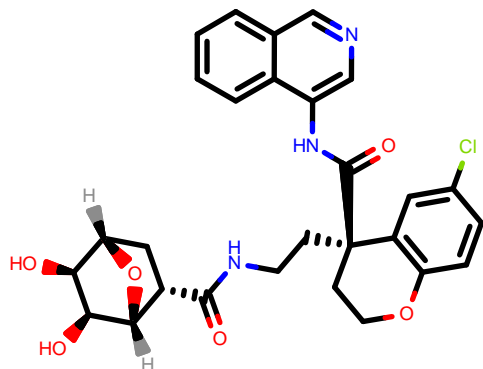
DDG (kcal/mol):

-1.45

dDDG (kcal/mol):

0.32

EN300-6764836_3_2_1



CID: EN300-6764836_3_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)N1CCOC1

RUN:

RUN5964

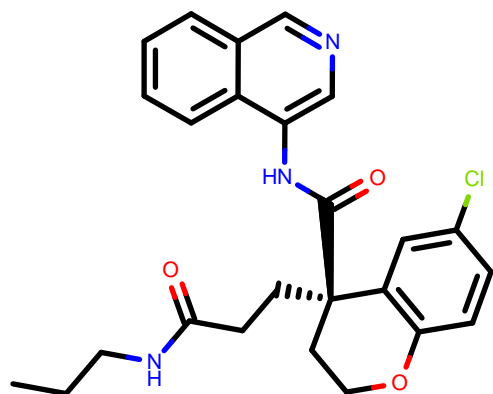
DDG (kcal/mol):

-1.45

dDDG (kcal/mol):

0.29

JAG-UCB-706446eb-2_1



CID: JAG-UCB-706446eb-2_1

SMILES:

CCCC(=O)CC[C@H]1(C)C(=O)Nc2ccc(Cl)cc21

RUN:

RUN572

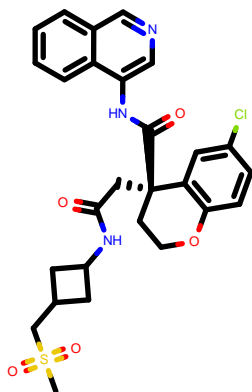
DDG (kcal/mol):

-1.44

dDDG (kcal/mol):

0.20

EN300-7430165_1_1_1



CID: EN300-7430165_1_1_1

SMILES:

CS(=O)(=O)CC1CC(C1)NC(=O)C[C@H]2(C)C(=O)Nc3ccc(Cl)cc32

RUN:

RUN7421

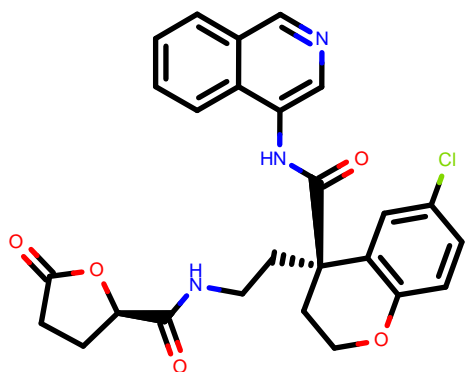
DDG (kcal/mol):

-1.44

dDDG (kcal/mol):

0.32

EN300-332606_3_1_1



CID: EN300-332606_3_1_1

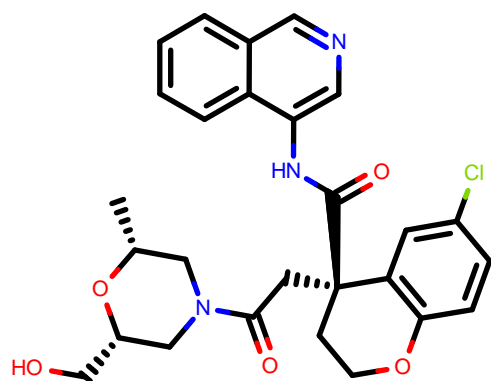
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCNC(=O)[C@@H]5CCCC(=O)O5

RUN: RUN5065

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.23

EN300-157776_1_1_1



CID: EN300-157776_1_1_1

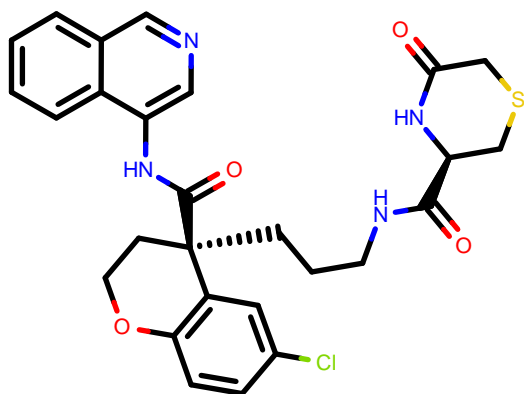
SMILES: C[C@@H]1CN[C@@H](O1)C(=O)C[C@@]2(CCOc3c2cc(cc3O)C(=O)Nc4ncc5c4ccoc5

RUN: RUN4101

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.33

EN300-657320_4_1_1



CID: EN300-657320_4_1_1

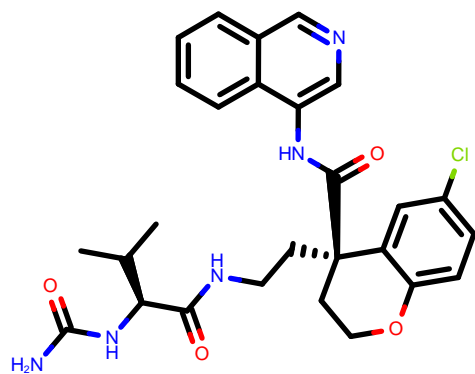
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCCCNC(=O)[C@@H]5CSCC(=O)N5

RUN: RUN6901

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.30

EN300-87528_3_1_1



CID: EN300-87528_3_1_1

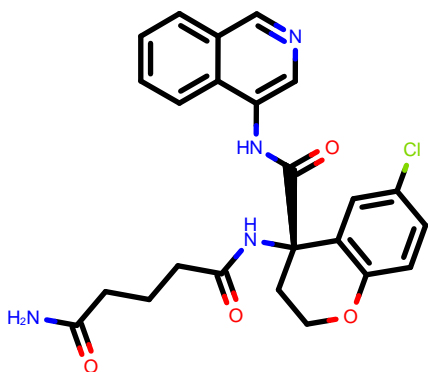
SMILES: CC(C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccoc4)NC(=O)N

RUN: RUN5401

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.34

EN300-59478_1_1_1



CID: EN300-59478_1_1_1

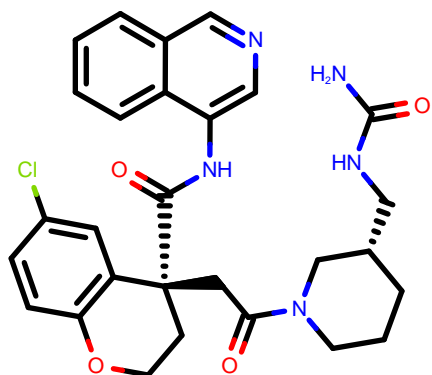
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN4330

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.29

EN300-42195_1_2_1



CID: EN300-42195_1_2_1

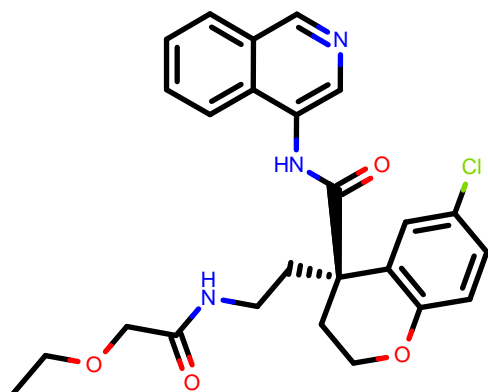
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H](C5)CNC(=O)N

RUN: RUN6277

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.32

EN300-21303_3_1_1



CID: EN300-21303_3_1_1

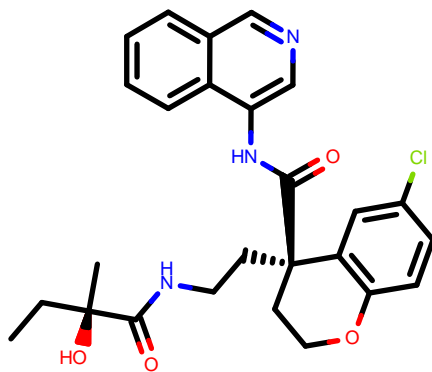
SMILES: CCOCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3691

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.25

EN300-248888_3_1_1



CID: EN300-248888_3_1_1

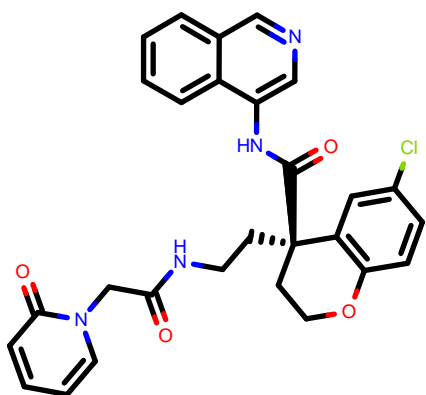
SMILES: C[C@@](C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O

RUN: RUN5887

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.31

EN300-11714_3_1_1



CID: EN300-11714_3_1_1

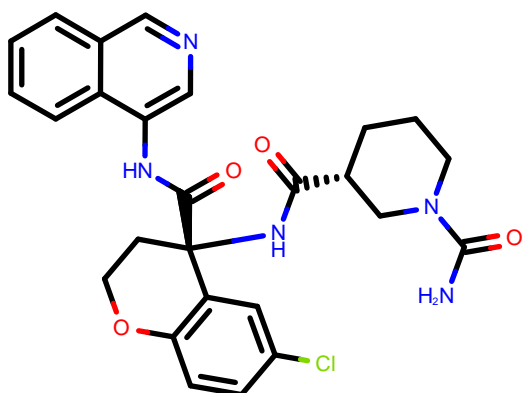
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cccc5=O

RUN: RUN5548

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.28

EN300-14767_1_1_1



CID: EN300-14767_1_1_1

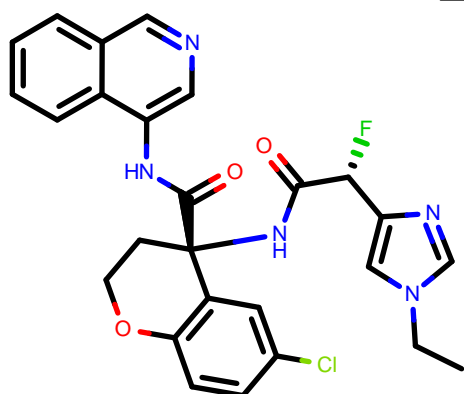
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5HJ5CCCN(C5)C(=O)N

RUN: RUN2957

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.29

EDG-MED-90036822-53_2



CID: EDG-MED-90036822-53_2

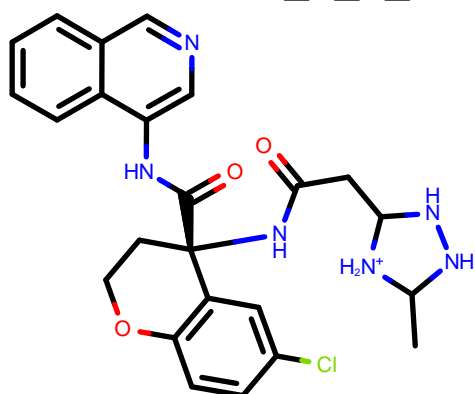
SMILES: CCn1cc(nc1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)F

RUN: RUN1643

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.24

EN300-119126_1_1_1



CID: EN300-119126_1_1_1

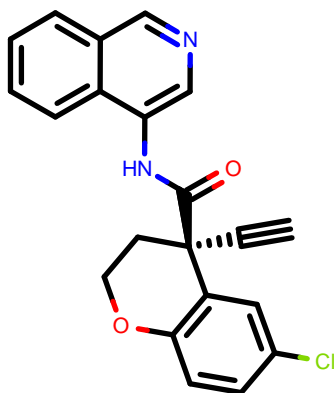
SMILES: Cc1[nH]nc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5276

DDG (kcal/mol): -1.43

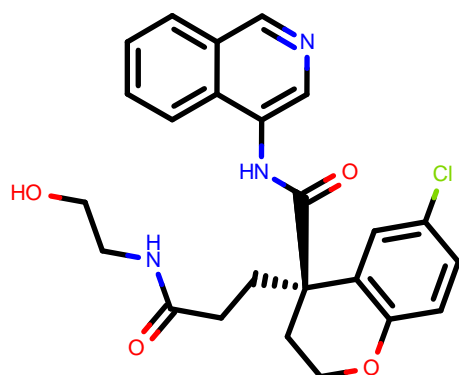
dDDG (kcal/mol): 0.21

PET-UNK-29afea89-1_1



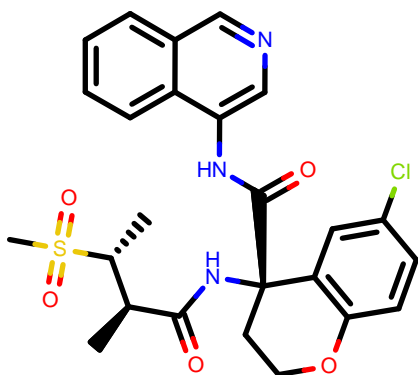
CID:	PET-UNK-29afea89-1_1
SMILES:	<chem>C#[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN583
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.11

EN300-19392_2_1_1



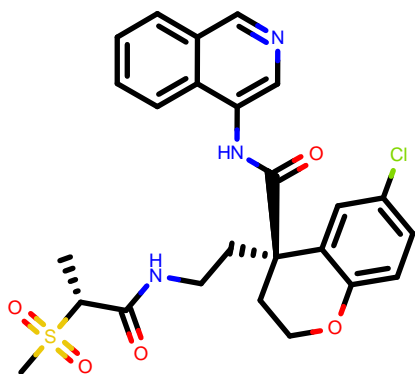
CID:	EN300-19392_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCO</chem>
RUN:	RUN6351
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.32

EN300-182725_1_1_1



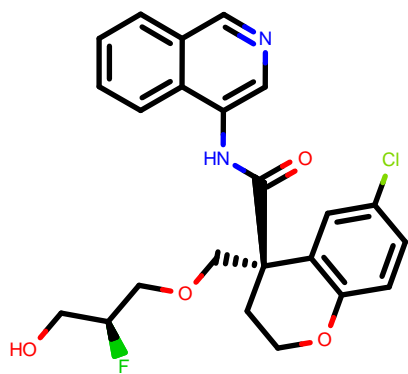
CID:	EN300-182725_1_1_1
SMILES:	<chem>CC@@H(C)S(=O)(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN6581
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.24

EN300-39405_3_2_1



CID:	EN300-39405_3_2_1
SMILES:	<chem>C[C@H](C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C</chem>
RUN:	RUN3620
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.39

EDJ-MED-fcba3f31-5_1



CID: EDJ-MED-fcba3f31-5_1

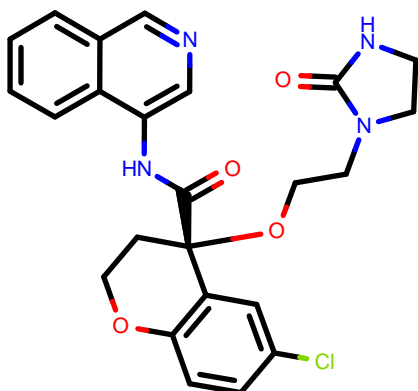
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F

RUN: RUN2402

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.25

EN300-214800_1_1_1



CID: EN300-214800_1_1_1

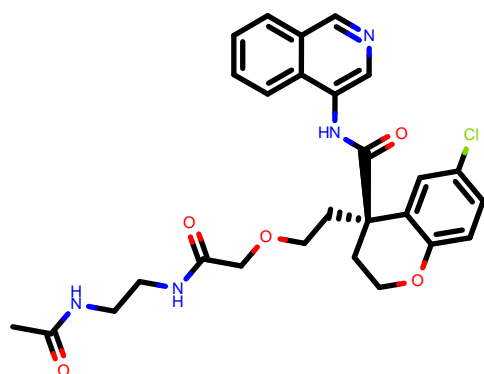
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCNC5=O

RUN: RUN3406

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.23

EN300-23129_3_1_1



CID: EN300-23129_3_1_1

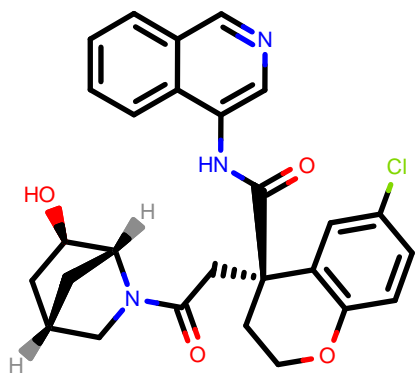
SMILES: CC(=O)NCCNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN5680

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.25

EN300-2010317_1_1_1



CID: EN300-2010317_1_1_1

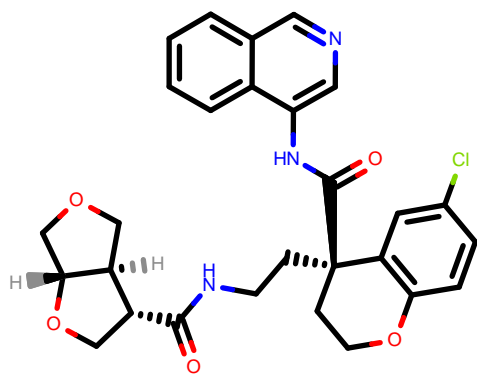
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N5C[C@H]6C[C@H]5[C@@]3(C)C6

RUN: RUN4370

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.26

EN300-6482296_3_7_1



CID: EN300-6482296_3_7_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C[C@@H]3CCOCc4ccccc4C)CCNC(=O)C[C@@H]5COC[C@@H]5COC6

RUN:

RUN5845

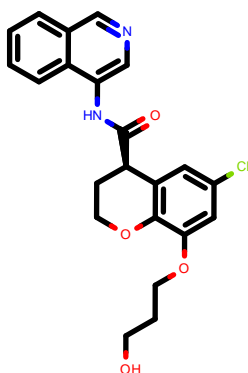
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.30

LAU-MED-88a3970a-3_1



CID: LAU-MED-88a3970a-3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C[C@@H]3CCOCc4ccccc4O)CCl

RUN:

RUN1361

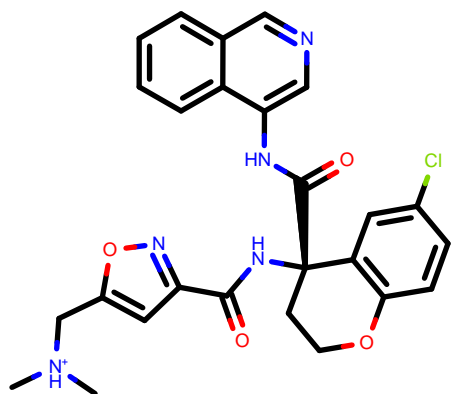
DDG (kcal/mol):

-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@@H]2(CCOc3cc2cc3)C(=O)Nc4ncnc5c4ccccc5

RUN:

RUN6607

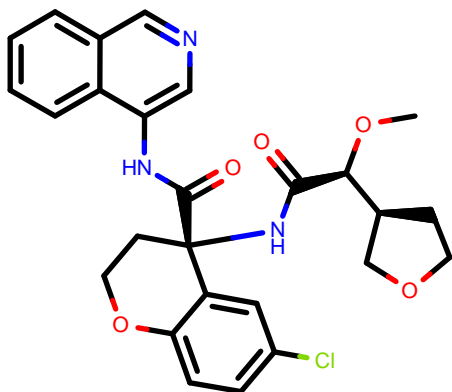
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.27

EN300-298552_1_3_1



CID: EN300-298552_1_3_1

SMILES:

CO[C@@H](C[C@@H]1CCOC1)C(=O)N[C@@H]2(CCOc3cc2cc3)C(=O)Nc4ncnc5c4ccccc5

RUN:

RUN3197

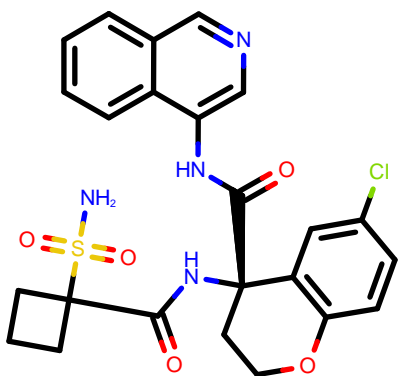
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.29

EN300-1440321_1_1_1



CID: EN300-1440321_1_1_1

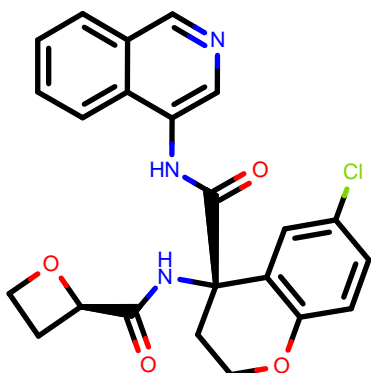
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)S(=O)(=O)N

RUN: RUN4181

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.38

EN300-85760_1_2_1



CID: EN300-85760_1_2_1

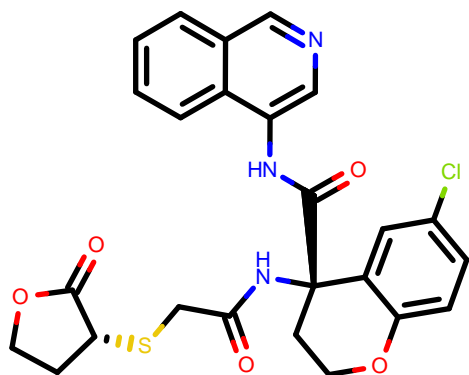
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCO5

RUN: RUN4189

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.21

EN300-113218_1_1_1



CID: EN300-113218_1_1_1

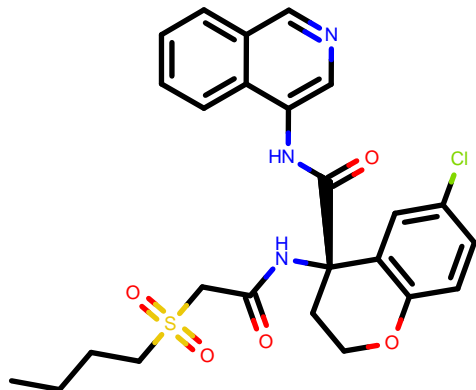
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@@]5COC5=O

RUN: RUN5023

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.28

EN300-686903_1_1_1



CID: EN300-686903_1_1_1

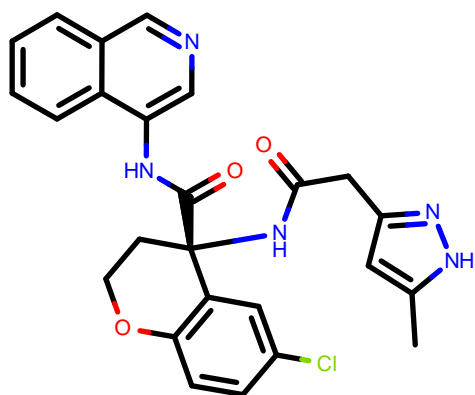
SMILES: CCCCS(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN4825

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.34

EN300-105110_1_1_1



CID: EN300-105110_1_1_1

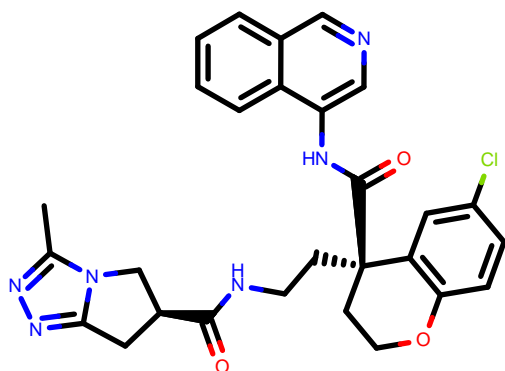
SMILES: Cc1cc(n[nH]1)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6202

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.23

EN300-6729747_3_2_1



CID: EN300-6729747_3_2_1

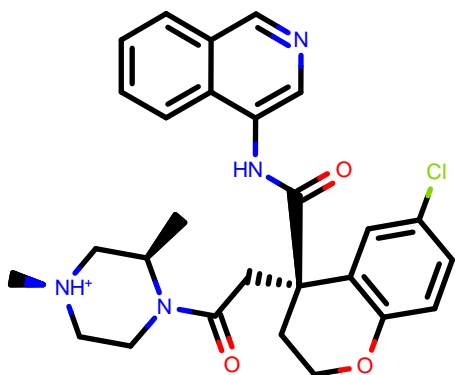
SMILES: Cc1nc2n1C[C@H](C2)C(=O)NCC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6

RUN: RUN4719

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.35

EDG-MED-ba1ac7b9-15_5



CID: EDG-MED-ba1ac7b9-15_5

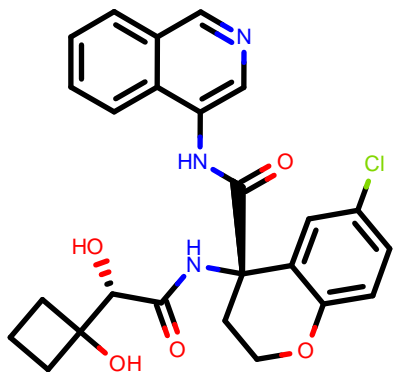
SMILES: C[C@@]1CN[C@@H]2CN1C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2520

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.36

EN300-1073320_1_2_1



CID: EN300-1073320_1_2_1

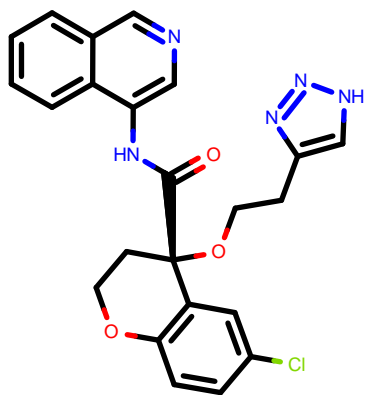
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN5890

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.30

EN300-222357_1_1_1



CID: EN300-222357_1_1_1

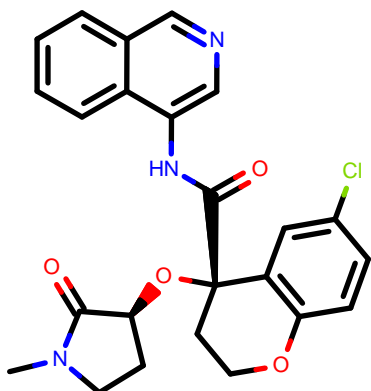
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cn[nH]n5

RUN: RUN4660

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.22

EN300-98648_1_1_1



CID: EN300-98648_1_1_1

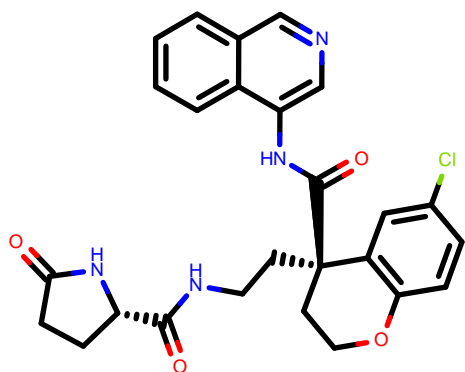
SMILES: CN1CC[C@@H](C1=O)O[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN4162

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.17

EN300-19515_3_1_1



CID: EN300-19515_3_1_1

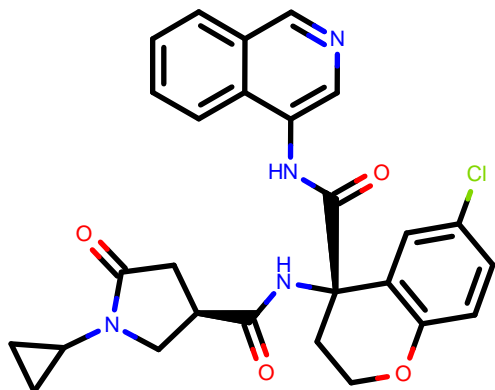
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(C)=O)N5

RUN: RUN3801

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-12440_1_1_1



CID: EN300-12440_1_1_1

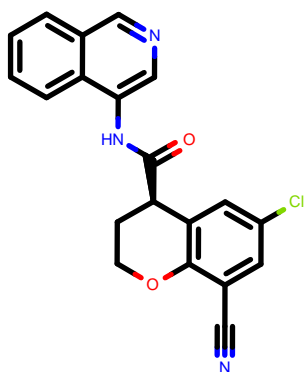
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC(=O)N(C5)C6CC6

RUN: RUN7189

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.25

RAL-THA-05e671eb-20_1



CID: RAL-THA-05e671eb-20_1

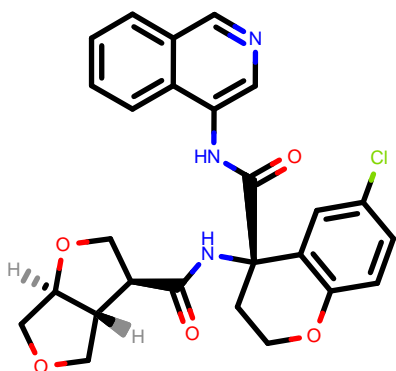
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOC4c3cc(cc4C#N)Cl

RUN: RUN1893

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.09

EN300-6482296_1_7_1



CID: EN300-6482296_1_7_1

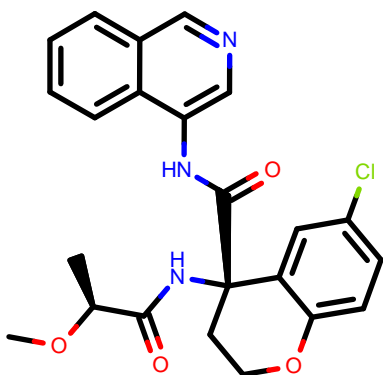
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H]4COC5C4C#N[C@@H]3C(=O)C[C@@H]5O

RUN: RUN3985

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.27

EN300-51257_1_1_1



CID: EN300-51257_1_1_1

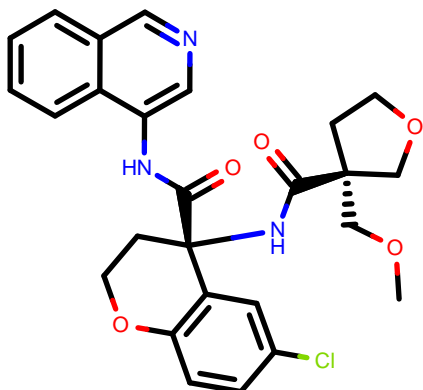
SMILES: C[C@@H](C(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)OC

RUN: RUN4525

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.23

EN300-248883_1_1_1



CID: EN300-248883_1_1_1

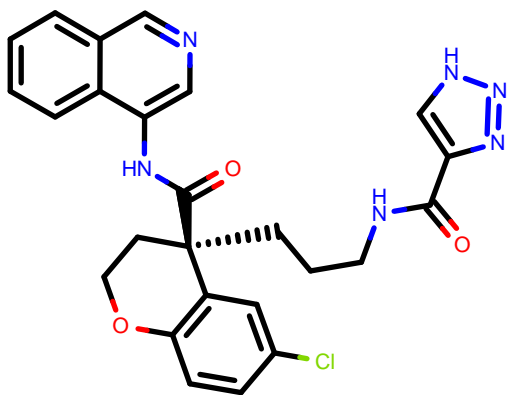
SMILES: COC[C@@H]1(CCOC1C(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3150

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.25

EN300-31998_4_1_1



CID: EN300-31998_4_1_1

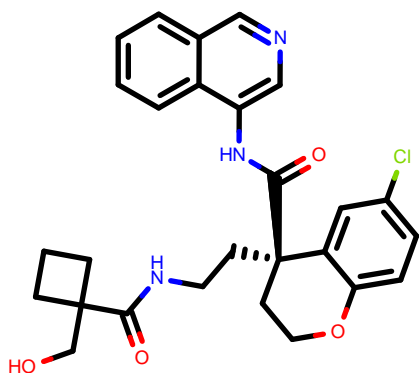
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CN([NH])N5

RUN: RUN5082

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.29

EN300-149975_3_1_1



CID: EN300-149975_3_1_1

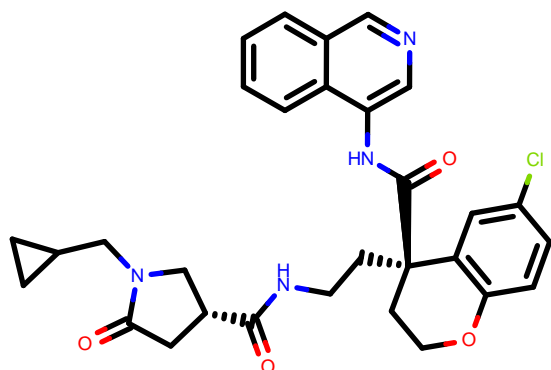
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)CO

RUN: RUN2933

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.37

EN300-31969_3_1_1



CID: EN300-31969_3_1_1

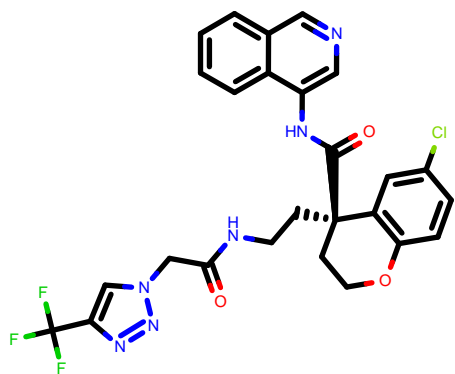
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CN(C5)C6CC6

RUN: RUN5074

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.32

EN300-2910941_3_1_1



CID: EN300-2910941_3_1_1

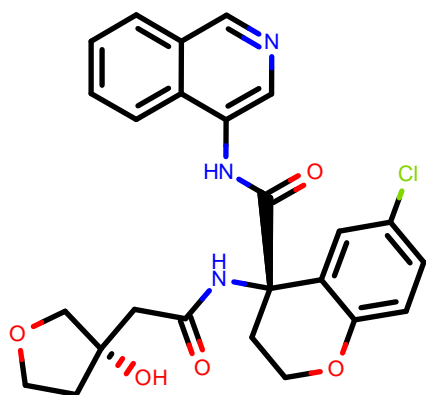
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn(n5)C(F)(F)F

RUN: RUN4544

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-360157_1_2_1



CID: EN300-360157_1_2_1

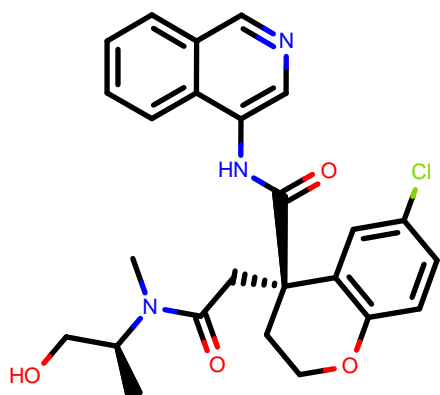
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COCc4c3cc(c4)C)NC(=O)C[C@@]5(CCOC5)O

RUN: RUN3702

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.26

EN300-204419_1_1_1



CID: EN300-204419_1_1_1

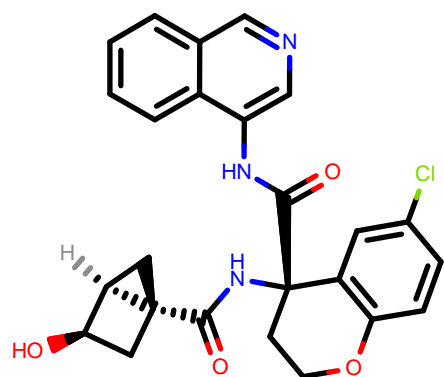
SMILES: C[C@@H](CO)N(C)C(=O)C[C@@]1(CCOCc2c1cc(c2)C)C(=O)Nc3nccc4c3cccc4

RUN: RUN4304

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.33

EN300-7433125_1_1_1



CID: EN300-7433125_1_1_1

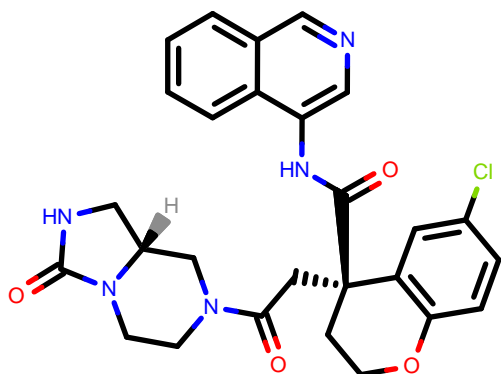
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COCc4c3cc(c4)C)NC(=O)C@@@5[C@@H](C)C@@@6[C@@H](O)C6

RUN: RUN4907

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.23

EN300-100765_1_1_1



CID: EN300-100765_1_1_1

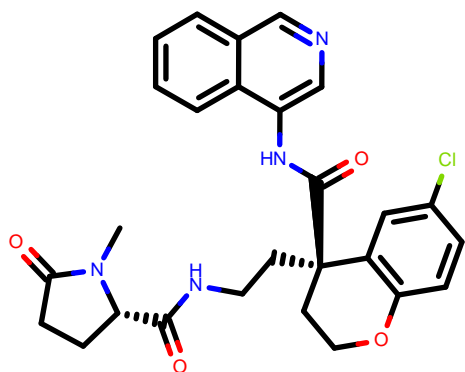
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COCc4c3cc(c4)C)CC(=O)N5CCN6[C@@H](C5)CNC6=O

RUN: RUN6057

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.28

EN300-130825_3_1_1



CID: EN300-130825_3_1_1

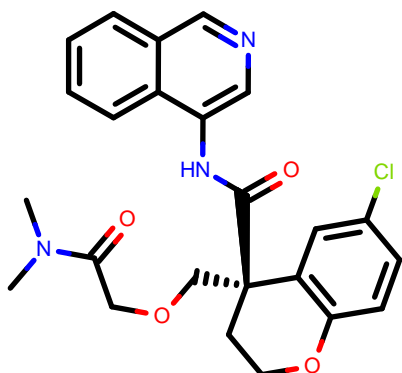
SMILES: CN1[C@@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5429

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.35

EN300-216063_2_1_1



CID: EN300-216063_2_1_1

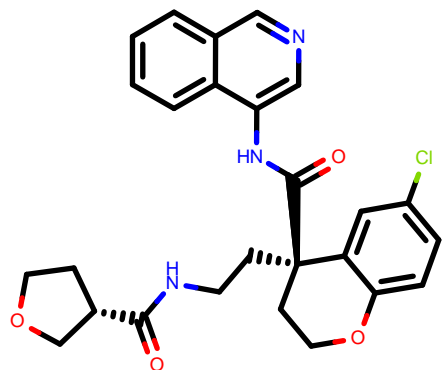
SMILES: CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4890

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.21

EN300-53423_3_2_1



CID: EN300-53423_3_2_1

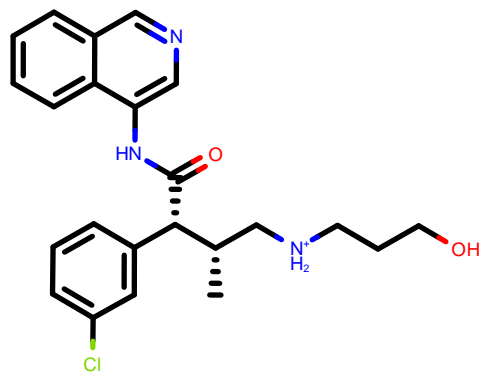
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOCC5

RUN: RUN5779

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.30

MAK-UNK-c749d764-6_3



CID: MAK-UNK-c749d764-6_3

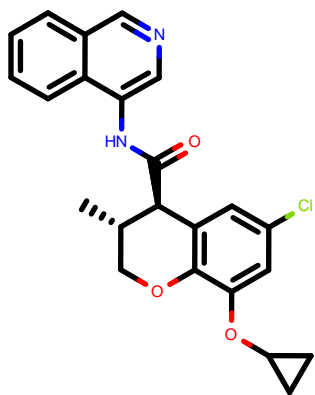
SMILES: C[C@@H](C[NH2+])CCCO[C@H](c1cccc(c1)Cl)C(=O)Nc2ccc3c2cccc3

RUN: RUN863

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.48

DAR-DIA-0d514e7d-6_1



CID: DAR-DIA-0d514e7d-6_1

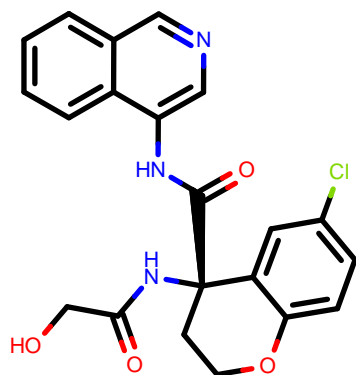
SMILES: C[C@H]1COc2c(cc2OC3CC3)Cl[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN782

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.17

EN300-19242_1_1_1



CID: EN300-19242_1_1_1

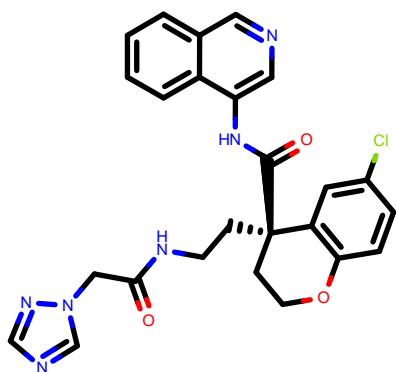
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO

RUN: RUN4963

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.17

EN300-06654_3_1_1



CID: EN300-06654_3_1_1

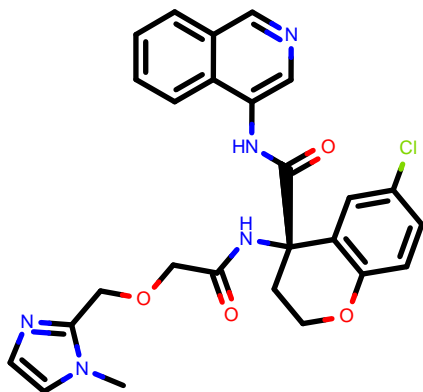
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnnc5

RUN: RUN3390

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.28

EN300-212341_1_1_1



CID: EN300-212341_1_1_1

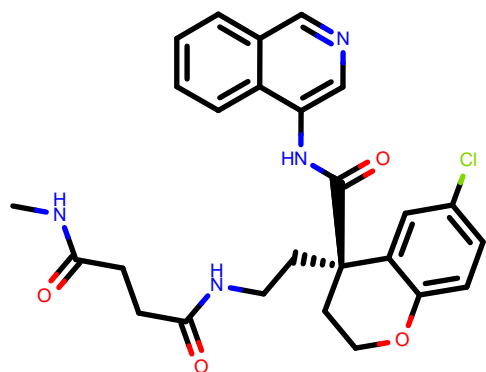
SMILES: Cn1ccnc1COCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7343

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.27

EN300-1081277_3_1_1



CID: EN300-1081277_3_1_1

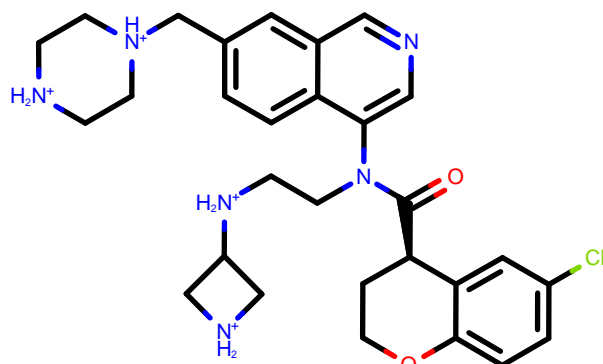
SMILES: CNC(=O)CCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN7747

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.30

MAK-UNK-83e0a0b4-2_1_1



CID: MAK-UNK-83e0a0b4-2_1_1

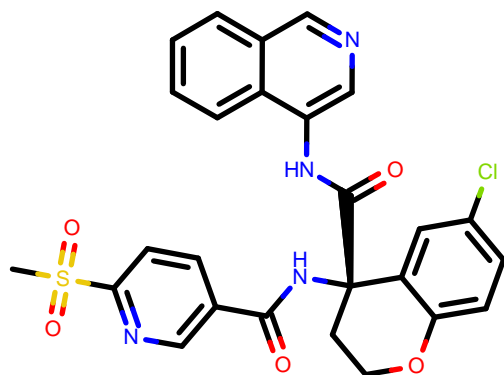
SMILES: c1cc2(ccc1CN3CC[NH2+]CC3)NCCN2C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5Cl

RUN: RUN4936

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.33

EN300-206769_1_1_1



CID: EN300-206769_1_1_1

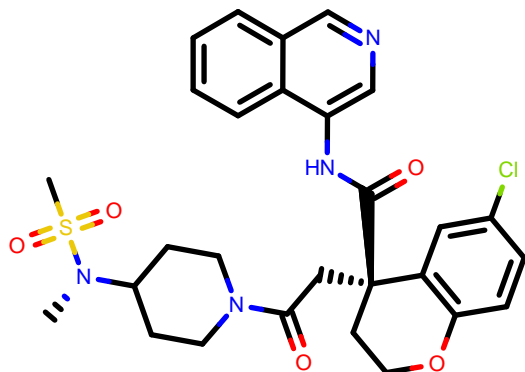
SMILES: CS(=O)(=O)c1ccc(nc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5150

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.28

ALP-UNI-3496895b-9_1



CID: ALP-UNI-3496895b-9_1

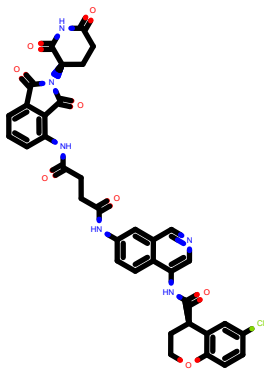
SMILES: C[N@]1(C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C

RUN: RUN2398

DDG (kcal/mol): -1.38

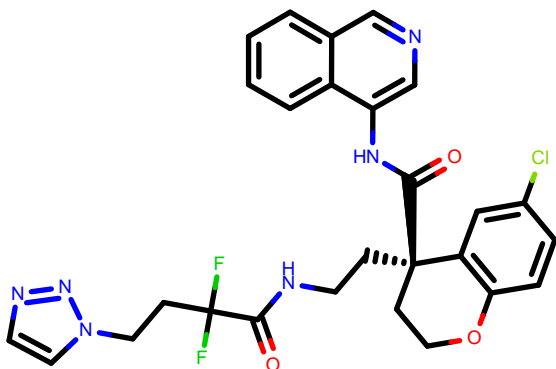
dDDG (kcal/mol): 0.30

DAR-DIA-9e4459de-15_2



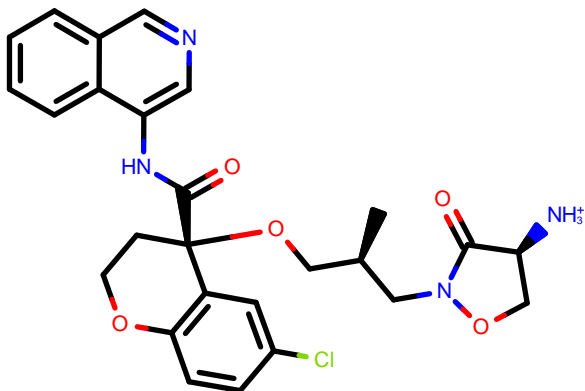
CID:	DAR-DIA-9e4459de-15_2
SMILES:	<chem>c1cc2c(c1)NC(=O)CC(=O)Nc3ccc4c(c3)nc4NC(=O)C(C@H)5CCOC6c6c(cc6)C1c1c(c2O)C(C@H)7CC(=O)NC7=O)O</chem>
RUN:	RUN1385
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.32

EN300-6474220_3_1_1



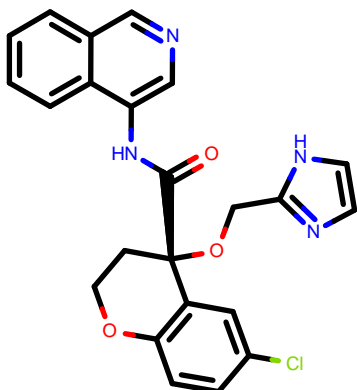
CID:	EN300-6474220_3_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)C(C@H)3(CCOc4c3cc(cc4)Cl)CNC(=O)C(Cn5ccnn5)(F)F</chem>
RUN:	RUN5385
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.47

EDG-MED-4c68219f-1_3



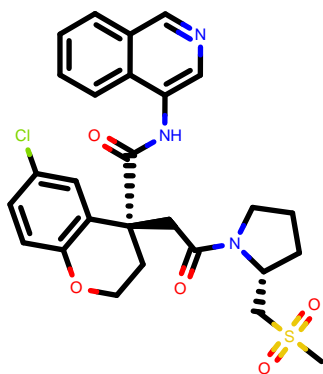
CID:	EDG-MED-4c68219f-1_3
SMILES:	<chem>C1C@H)(NC1=O)(C@H)(CO1)N#1+1)CO(C@H)2(COCc3c2cc(cc3)Cl)C1=O)N64nc5c4ccc5</chem>
RUN:	RUN1555
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.41

EDG-MED-4c68219f-17_1



CID:	EDG-MED-4c68219f-17_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)C(C@H)3(CCOc4c3cc(cc4)Cl)OCc5[nH]cnc5</chem>
RUN:	RUN1508
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.20

EN300-300294_1_1_1



CID: EN300-300294_1_1_1

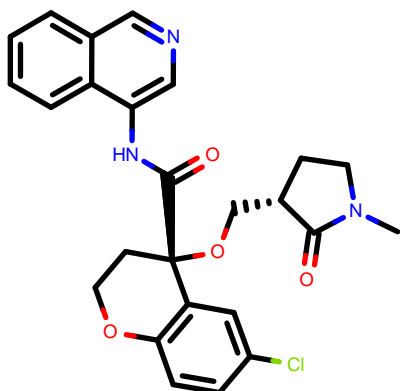
SMILES: CS(=O)(=O)C[C@H]1CCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN5060

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.30

EN300-260816_1_2_1



CID: EN300-260816_1_2_1

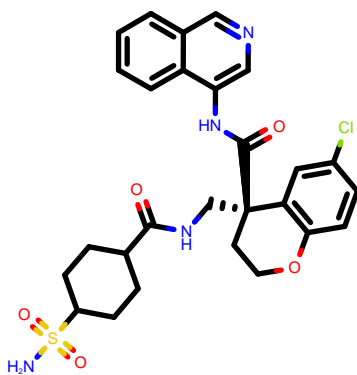
SMILES: CN1CC[C@H](C1=O)CO[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN4757

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.27

EN300-83864_2_1_1



CID: EN300-83864_2_1_1

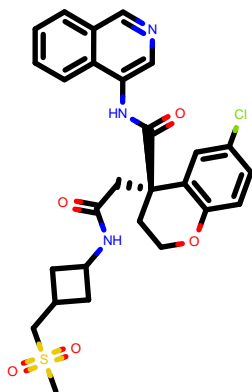
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5CCCC(C5)S(=O)(=O)N

RUN: RUN5301

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.38

EN300-7429970_1_1_1



CID: EN300-7429970_1_1_1

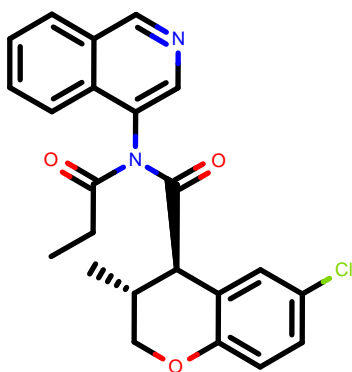
SMILES: CS(=O)(=O)CC1CC(C1)NC(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN4725

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.35

DAR-DIA-5ff57136-2_1_1



CID: DAR-DIA-5ff57136-2_1_1

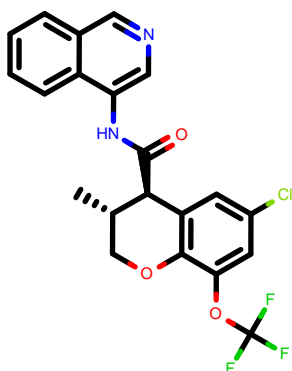
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl

RUN: RUN3807

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.19

DAR-DIA-0d514e7d-18_1



CID: DAR-DIA-0d514e7d-18_1

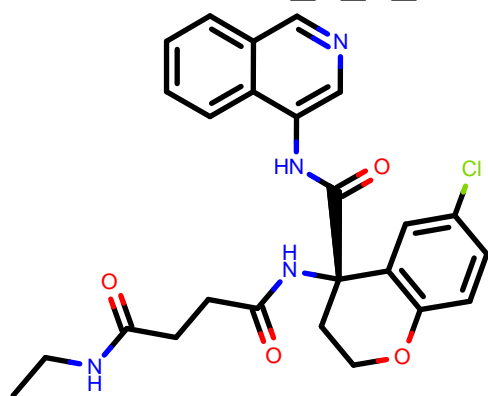
SMILES: C[C@H]1COc2c(cc(cc2OC(F)(F)F)Cl)N[C@@H]1C(=O)Nc3cncc4c3cccc4

RUN: RUN743

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.15

EN300-68889_1_1_1



CID: EN300-68889_1_1_1

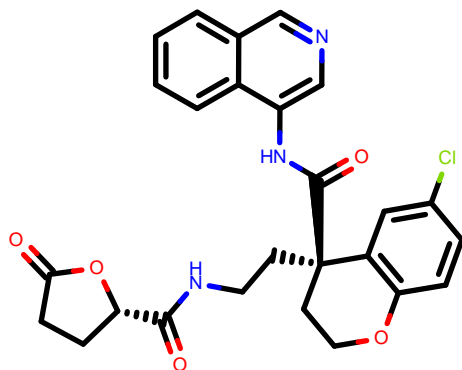
SMILES: CCNC(=O)CCC(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5073

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.27

EN300-359750_3_1_1



CID: EN300-359750_3_1_1

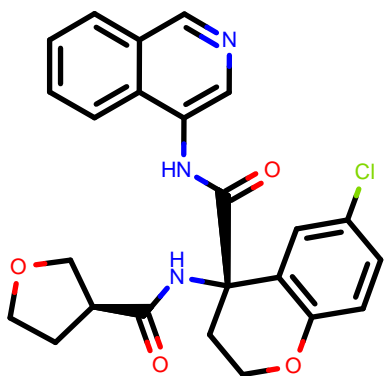
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCC(=O)O5

RUN: RUN5514

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-53423_1_2_1



CID: EN300-53423_1_2_1

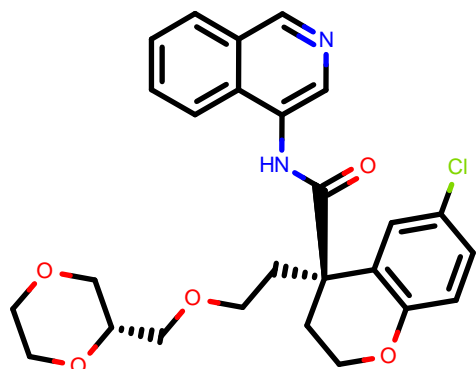
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC5

RUN: RUN3527

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.29

EN300-139167_3_2_1



CID: EN300-139167_3_2_1

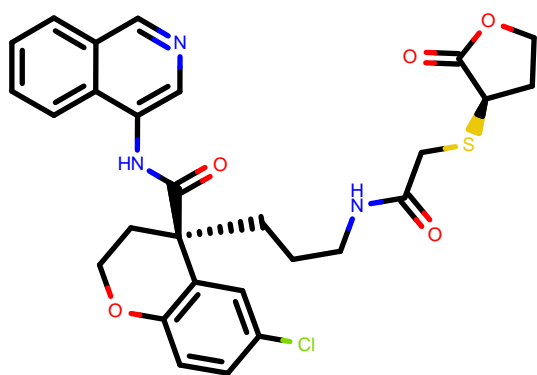
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCOC5

RUN: RUN3596

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.29

EN300-113218_4_1_1



CID: EN300-113218_4_1_1

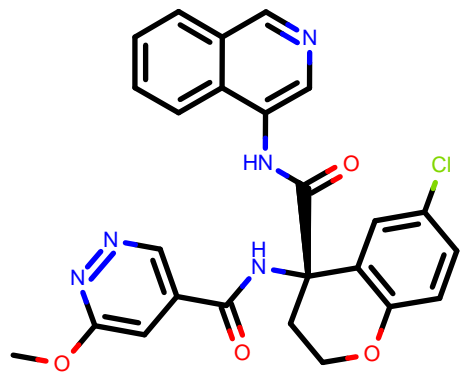
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@H]5CCOC5=O

RUN: RUN5932

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.42

EN300-252260_1_1_1



CID: EN300-252260_1_1_1

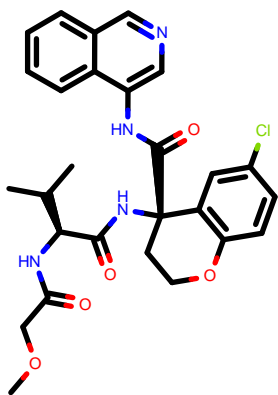
SMILES: COc1cc(cnn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5

RUN: RUN6341

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.22

EN300-83918_1_1_1



CID: EN300-83918_1_1_1

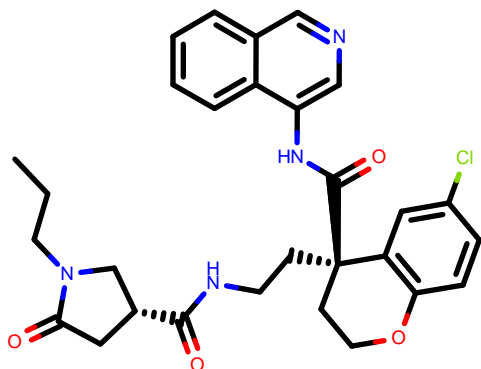
SMILES: CC(C)[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)NC(=O)COC

RUN: RUN5754

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-253443_3_1_1



CID: EN300-253443_3_1_1

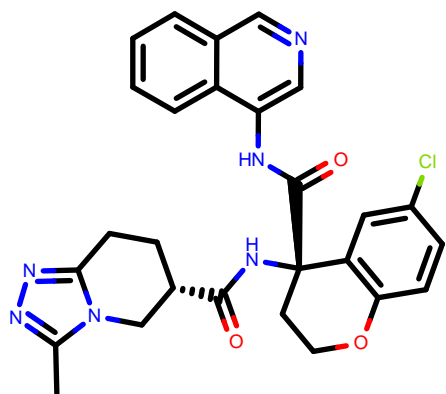
SMILES: CCCN1C[C@@H](CC1=O)C(=O)NCC[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7142

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.29

EN300-50561_1_2_1



CID: EN300-50561_1_2_1

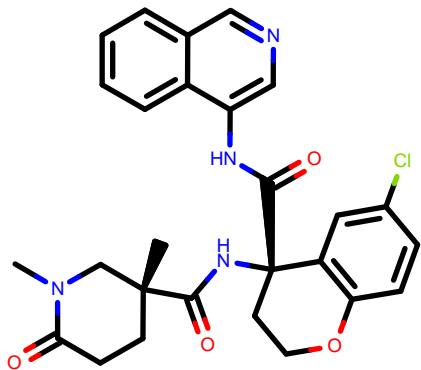
SMILES: Cc1nnc2n1C[C@@H](CC2)C(=O)N[C@@]3(CCOC4c3cc(cc4)C)C(=O)Nc5ccc6c5ccc6

RUN: RUN3542

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-6734171_1_2_1



CID: EN300-6734171_1_2_1

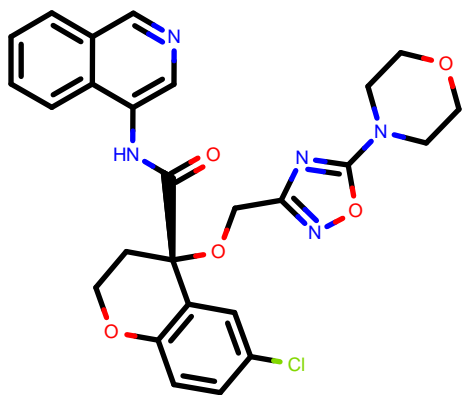
SMILES: C[C@@]1(CCC(=O)N(C1)C)C(=O)N[C@@]2(CCOC3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN6035

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.28

EN300-1608590_1_1_1



CID: EN300-1608590_1_1_1

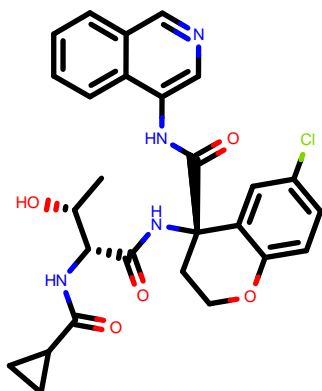
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(on5)N6CCOCC6

RUN: RUN5742

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.29

EN300-96362_1_4_1



CID: EN300-96362_1_4_1

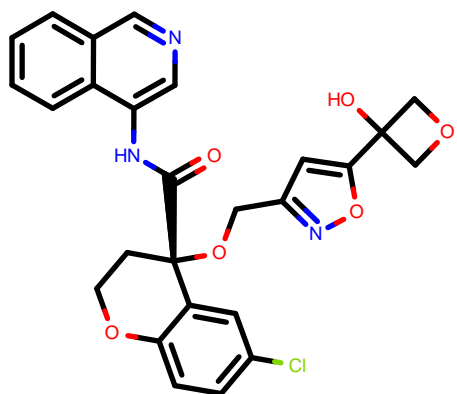
SMILES: C[C@H]([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccccc4)NC(=O)C5CC5)O

RUN: RUN4279

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.31

EN300-7457159_1_1_1



CID: EN300-7457159_1_1_1

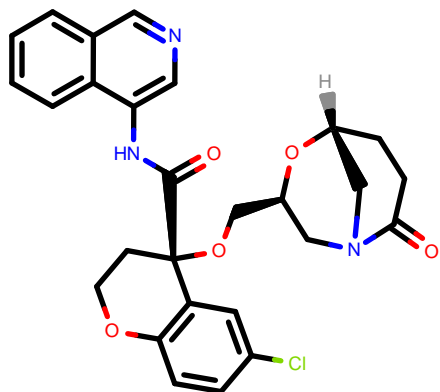
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cc(on5)C6(COC6)O

RUN: RUN3721

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.28

EN300-2008102_1_1_1



CID: EN300-2008102_1_1_1

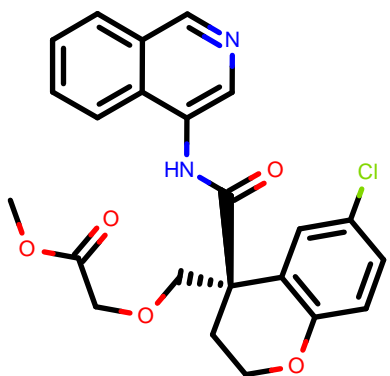
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5CN(C[C@H]5)CCC6=O

RUN: RUN4221

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.26

EN300-19700_2_1_1



CID: EN300-19700_2_1_1

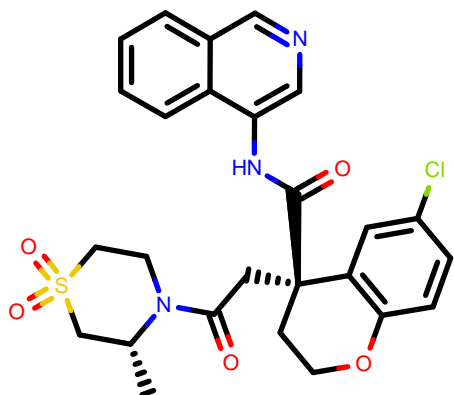
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN4743

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.19

EN300-171215_1_1_1



CID: EN300-171215_1_1_1

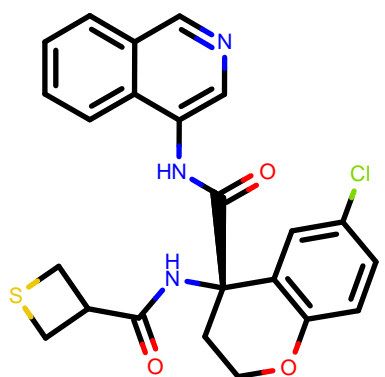
SMILES: C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN4792

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.37

EN300-95094_1_1_1



CID: EN300-95094_1_1_1

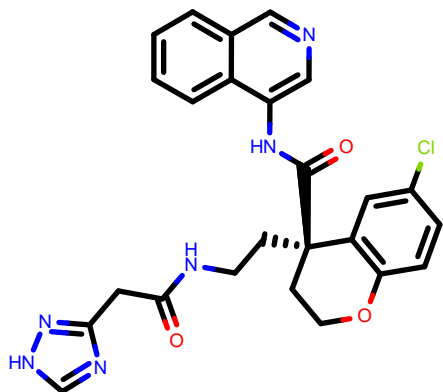
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CSC5

RUN: RUN3362

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.20

EN300-96159_3_1_1



CID: EN300-96159_3_1_1

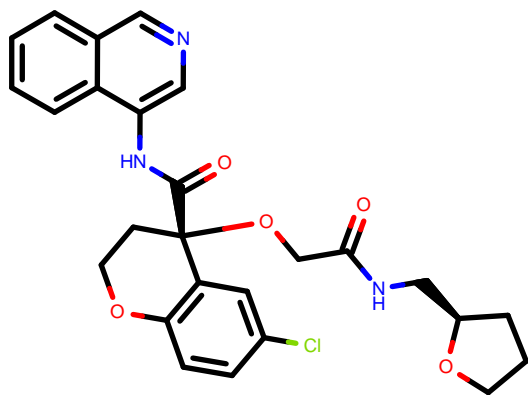
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5[nH]n5

RUN: RUN3364

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.32

EN300-01527_1_2_1



CID: EN300-01527_1_2_1

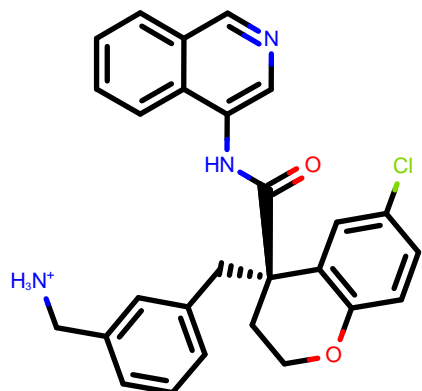
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCCCO5

RUN: RUN5606

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.30

JAG-UCB-706446eb-8_1_1



CID: JAG-UCB-706446eb-8_1_1

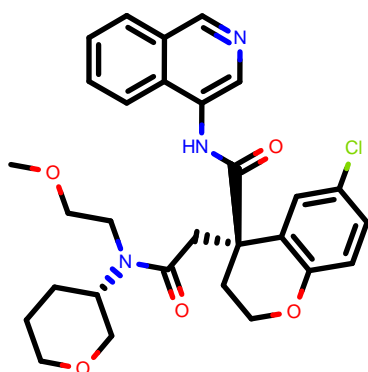
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)Cc5ccccc5[C@@H](N3+)C

RUN: RUN5393

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.25

JAG-UCB-706446eb-5_2



CID: JAG-UCB-706446eb-5_2

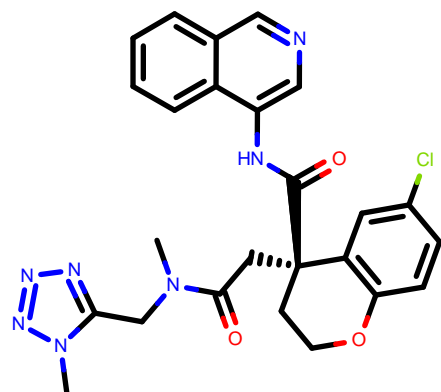
SMILES: COCCN([C@@H]1CCCCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN607

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.37

EN300-148515_1_1_1



CID: EN300-148515_1_1_1

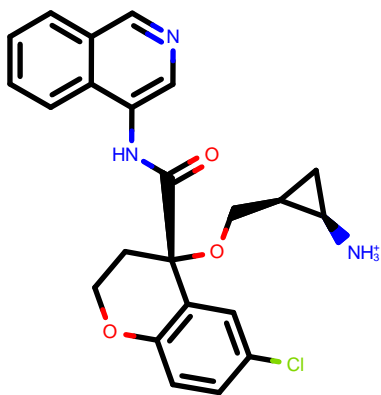
SMILES: Cn1c(nnn1)CN(C)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN5922

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-69_4



CID: ED_-GRI-5b13fbe2-69_4

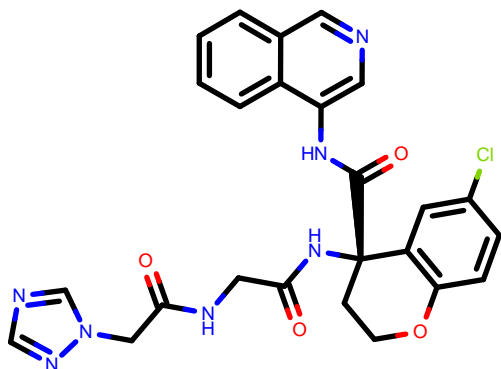
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5C[C@H]5[NH3+]

RUN: RUN1453

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

EN300-52383_1_1_1



CID: EN300-52383_1_1_1

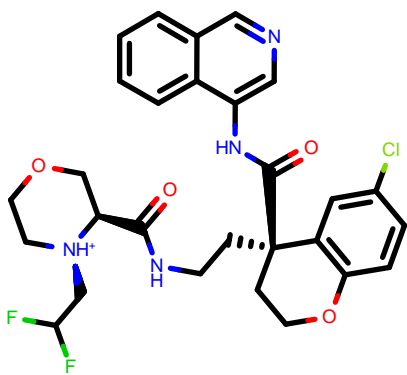
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)Cn5ncn5

RUN: RUN5321

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.30

EN300-140582_3_1_1



CID: EN300-140582_3_1_1

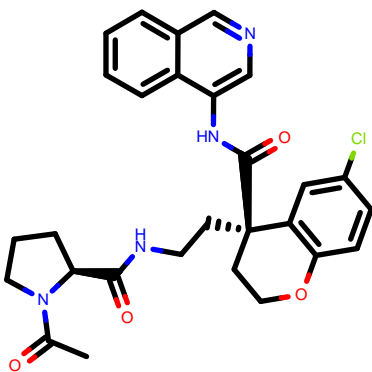
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5COC(C)N5C(F)F

RUN: RUN4029

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.30

EN300-211779_3_1_1



CID: EN300-211779_3_1_1

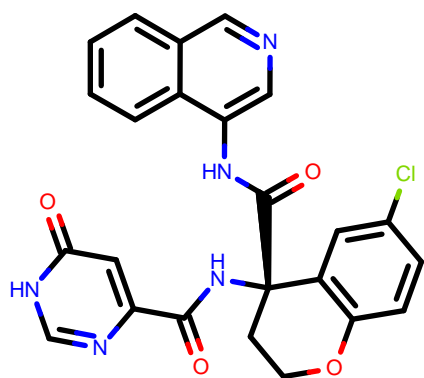
SMILES: CC(=O)N1CCC[C@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4ccc5

RUN: RUN3734

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.35

EN300-817811_1_1_1



CID: EN300-817811_1_1_1

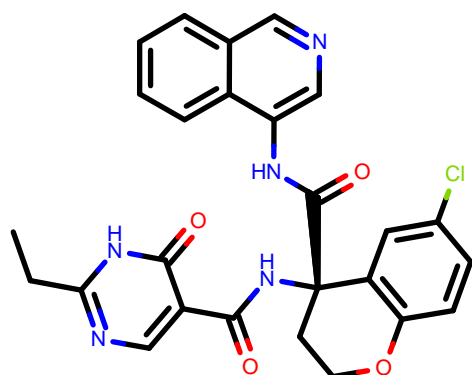
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cc(=O)[nH]jcn5

RUN: RUN3884

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

EN300-1273019_1_1_1



CID: EN300-1273019_1_1_1

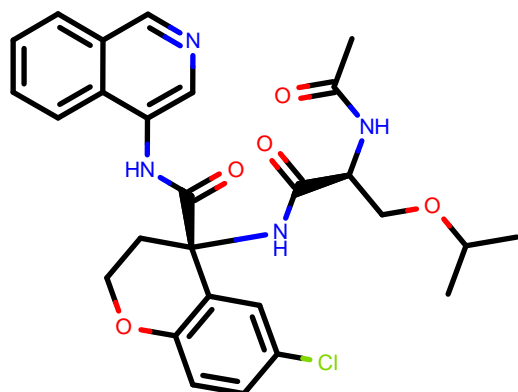
SMILES: CCc1[nH]c(=O)c(en1)C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5506

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.29

EN300-1299691_1_1_1



CID: EN300-1299691_1_1_1

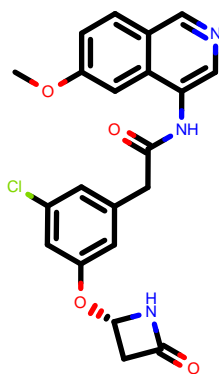
SMILES: CC(C)OC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncoc4c3ccoc4)NC(=O)C

RUN: RUN6471

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.29

ALF-EVA-0b412456-2_2



CID: ALF-EVA-0b412456-2_2

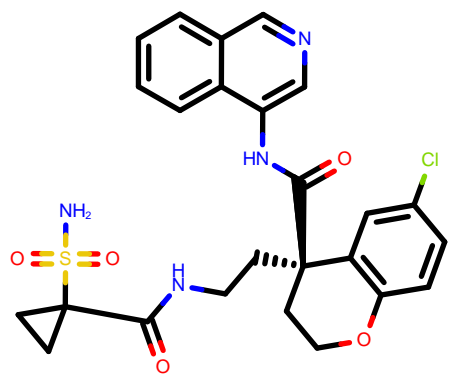
SMILES: COc1ccc2ncnc(c2c1)NC(=O)Cc3cc(cc(c3Cl)O[C@@H]4CC(=O)N4

RUN: RUN2542

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.36

EN300-223741_3_1_1



CID: EN300-223741_3_1_1

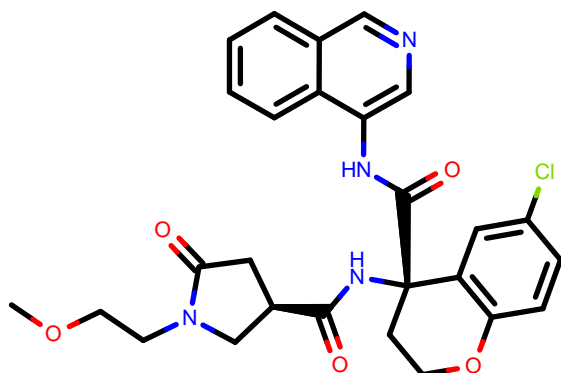
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCNC(=O)C5(C)S(=O)(=O)N

RUN: RUN5121

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.33

EN300-31845_1_1_1



CID: EN300-31845_1_1_1

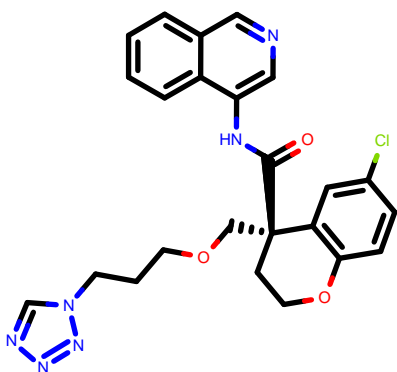
SMILES: COCCN1C[C@@H](CC1=O)C(=O)N[C@@]2(C)C(CO)C3=CC=CC=C3C1=CC=C2C(=O)N4C4=CC=CC=C4

RUN: RUN5832

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.34

EN300-1696962_2_1_1



CID: EN300-1696962_2_1_1

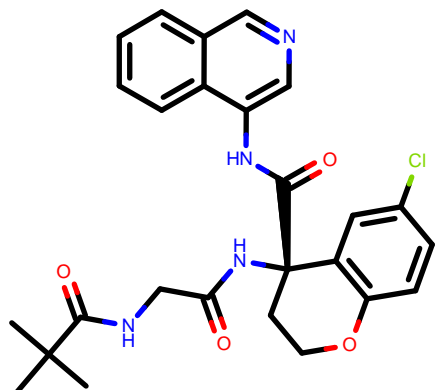
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCNC(=O)N5C5=CC=CC=C5

RUN: RUN4445

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.29

EN300-12247_1_1_1



CID: EN300-12247_1_1_1

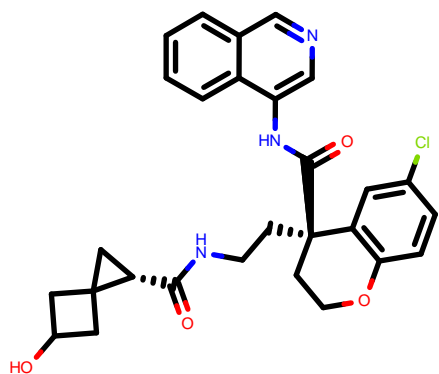
SMILES: CC(C)(C)C(=O)NCC(=O)N[C@@]1(C)C(CO)C2=CC=CC=C2C1=CC=C2C(=O)N3C3=CC=CC=C3

RUN: RUN4482

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.27

KAD-UNI-8a629cb0-35_1



CID: KAD-UNI-8a629cb0-35_1

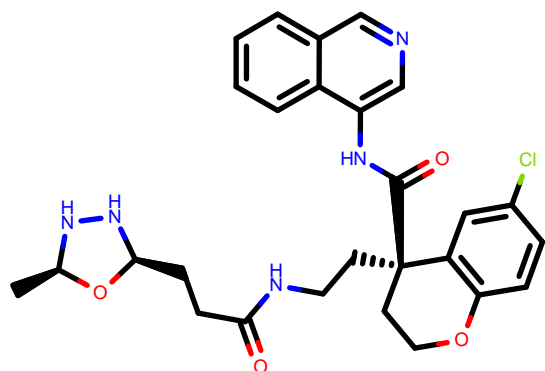
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC56C(C)C6O

RUN: RUN2018

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.33

EN300-304662_3_1_4



CID: EN300-304662_3_1_4

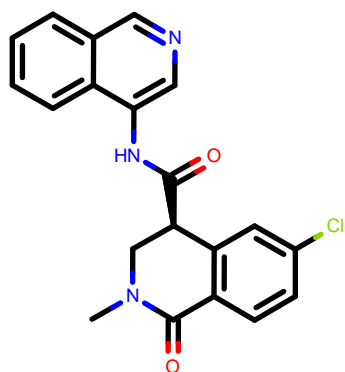
SMILES: C[C@H]1NN[C@H](O1)CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN7002

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.27

MIC-UNK-91acba05-2_2



CID: MIC-UNK-91acba05-2_2

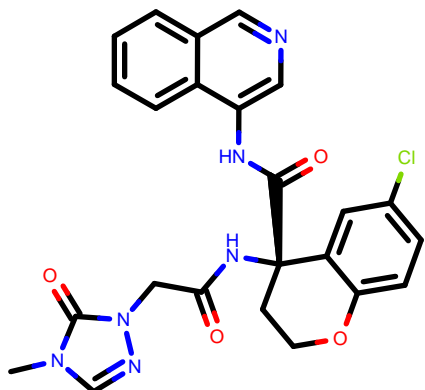
SMILES: CN1C[C@H](c2cc(ccc2C1=O)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN364

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.24

EN300-120436_1_1_1



CID: EN300-120436_1_1_1

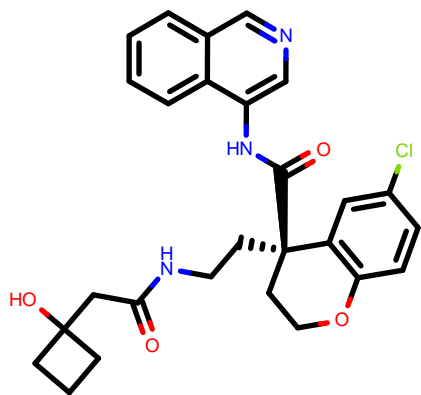
SMILES: Cn1cnn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4359

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.30

EN300-246423_3_1_1



CID: EN300-246423_3_1_1

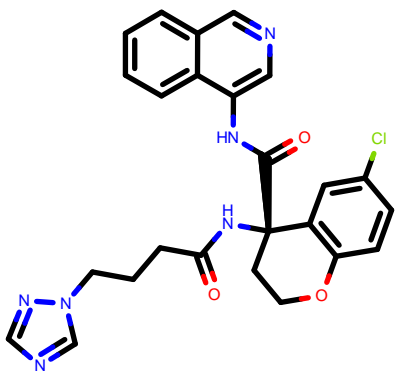
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC5(CCC5)O

RUN: RUN5773

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.25

EN300-316216_1_1_1



CID: EN300-316216_1_1_1

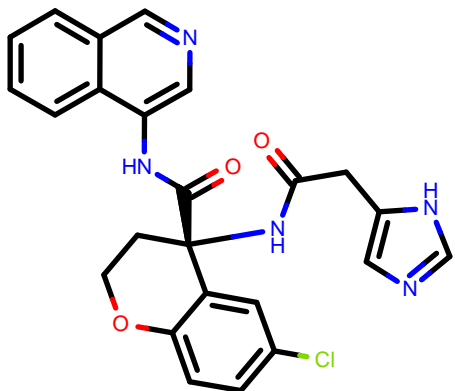
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5cnns5

RUN: RUN3507

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.23

EDG-MED-90036822-49_1



CID: EDG-MED-90036822-49_1

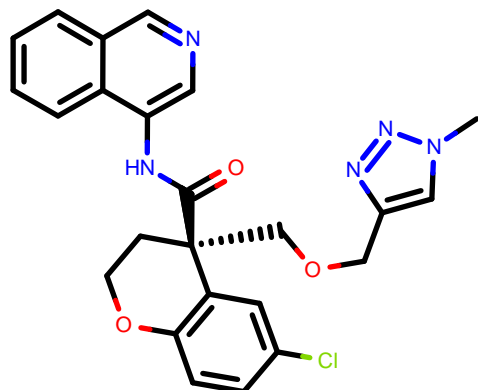
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5nc[nH]5

RUN: RUN1574

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.21

EN300-120282_2_1_1



CID: EN300-120282_2_1_1

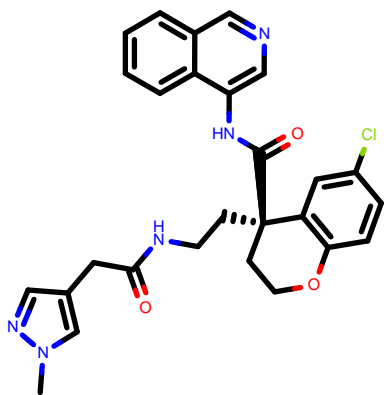
SMILES: Cn1cc(nn1)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN5593

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.23

EN300-63872_3_1_1



CID: EN300-63872_3_1_1

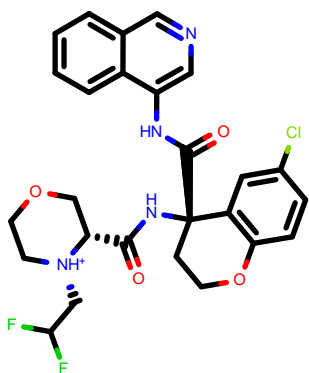
SMILES: Cn1cc(en1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4776

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.27

EN300-140582_1_2_1



CID: EN300-140582_1_2_1

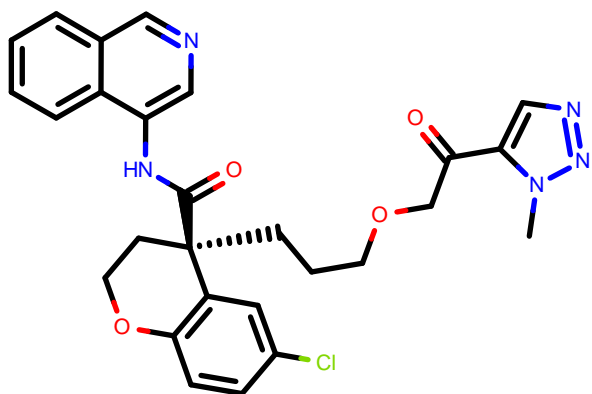
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COCC[N@]5CC(F)F

RUN: RUN3724

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.33

EN300-204936_4_1_1



CID: EN300-204936_4_1_1

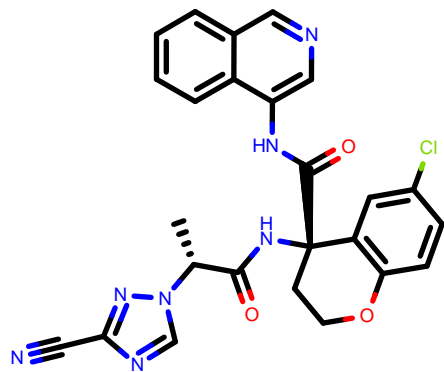
SMILES: Cn1c(cnn1)C(=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6592

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.35

EN300-198515_1_2_1



CID: EN300-198515_1_2_1

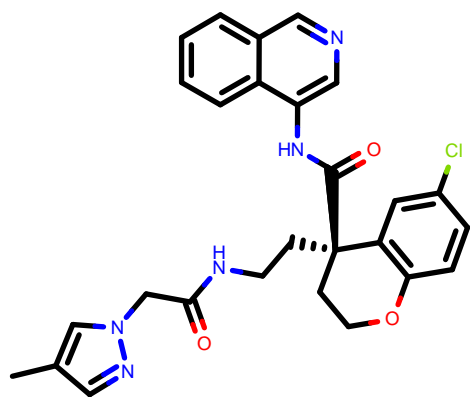
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5nc(rn5)C#N

RUN: RUN3006

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.30

EN300-51832_3_1_1



CID: EN300-51832_3_1_1

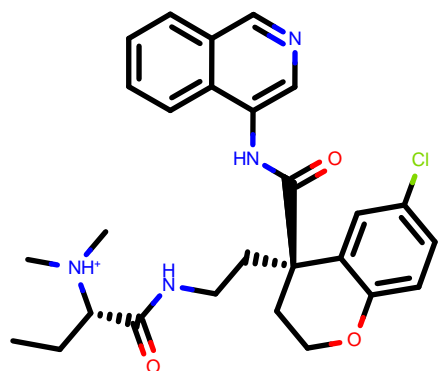
SMILES: Cc1cnn(c1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4113

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

EN300-110012_3_1_1



CID: EN300-110012_3_1_1

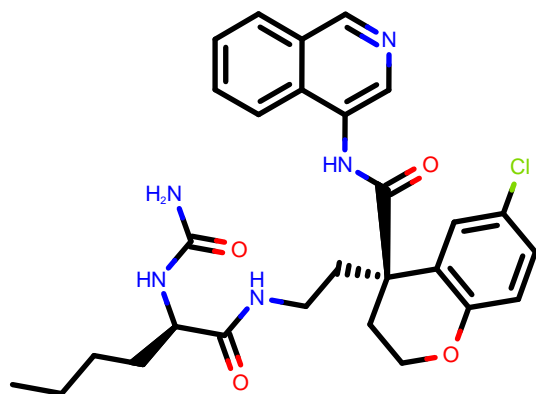
SMILES: CC[C@]([H])(C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)[NH+](C)C

RUN: RUN7124

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.40

EN300-55744_3_2_1



CID: EN300-55744_3_2_1

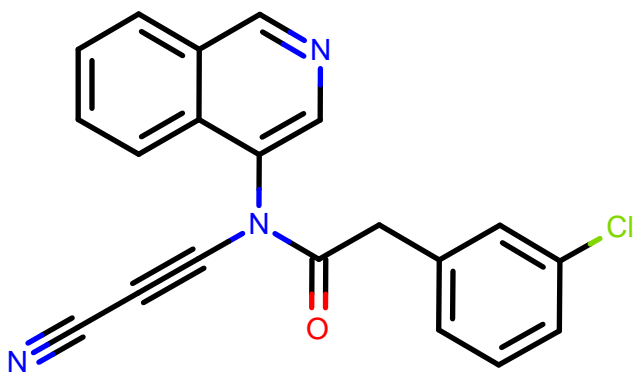
SMILES: CCCC[C@]([H])(C(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N

RUN: RUN6503

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.51

DAR-DIA-076fb6ea-5_1



CID: DAR-DIA-076fb6ea-5_1

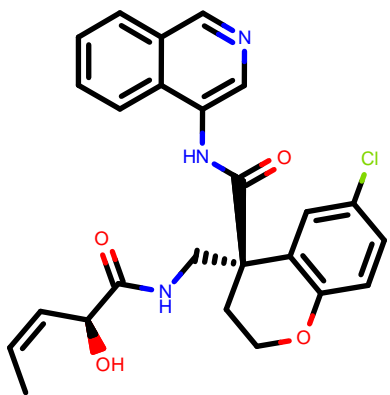
SMILES: c1ccc2c(c1)cncc2N(C#CC#N)C(=O)Cc3cccc(c3)Cl

RUN: RUN1238

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.35

EN300-300217_2_1_1



CID: EN300-300217_2_1_1

SMILES:

C=C[C@@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)O

RUN:

RUN4245

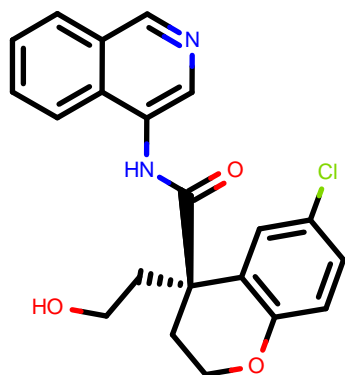
DDG (kcal/mol):

-1.31

dDDG (kcal/mol):

0.37

EDG-MED-971238d3-3_1



CID: EDG-MED-971238d3-3_1

SMILES:

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

RUN:

RUN1302

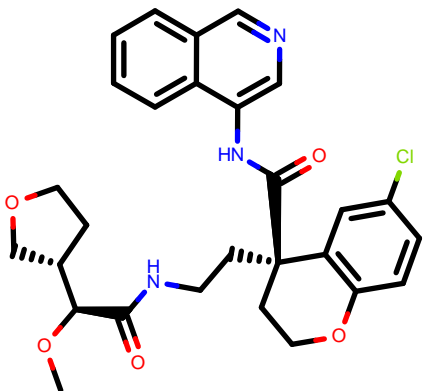
DDG (kcal/mol):

-1.31

dDDG (kcal/mol):

0.13

EN300-298552_3_3_1



CID: EN300-298552_3_3_1

SMILES:

CO[C@@H](C@H)[C@@]1(COC(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN:

RUN5291

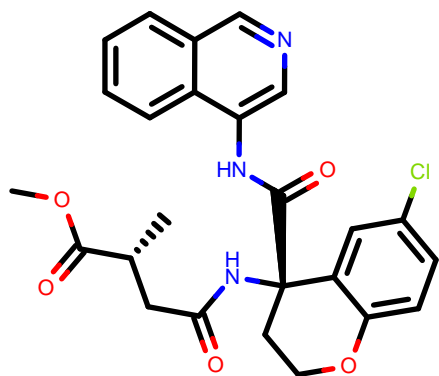
DDG (kcal/mol):

-1.31

dDDG (kcal/mol):

0.30

EN300-108413_1_2_1



CID: EN300-108413_1_2_1

SMILES:

C[C@@H](CC(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)C(=O)OC

RUN:

RUN3140

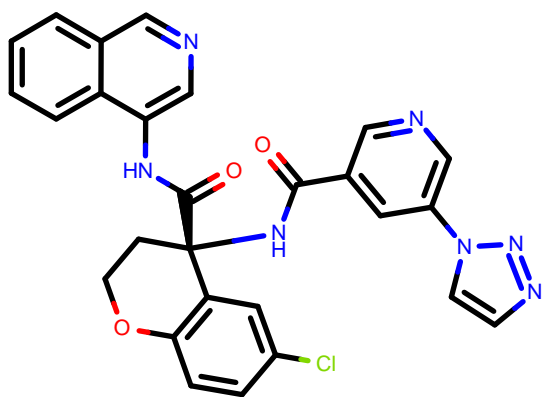
DDG (kcal/mol):

-1.31

dDDG (kcal/mol):

0.24

EN300-151298_1_1_1



CID: EN300-151298_1_1_1

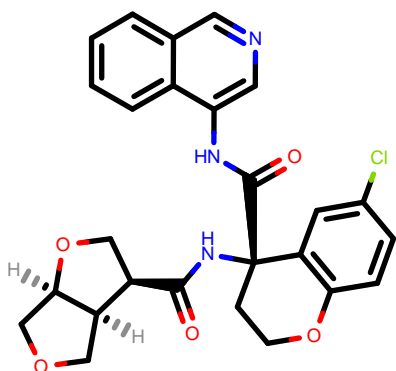
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn(cnc5)n6ccnn6

RUN: RUN3373

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-6482296_1_3_1



CID: EN300-6482296_1_3_1

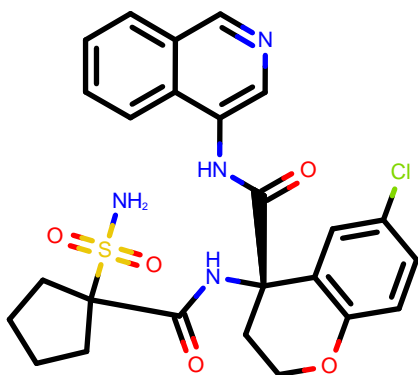
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn(cnc5)n6ccnn6

RUN: RUN4219

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.33

EN300-6486793_1_1_1



CID: EN300-6486793_1_1_1

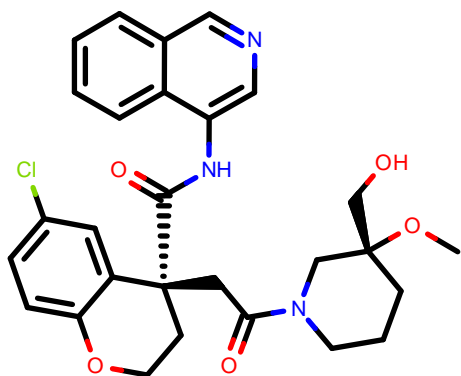
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCCC5)S(=O)(=O)N

RUN: RUN4095

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.40

EN300-299806_1_1_1



CID: EN300-299806_1_1_1

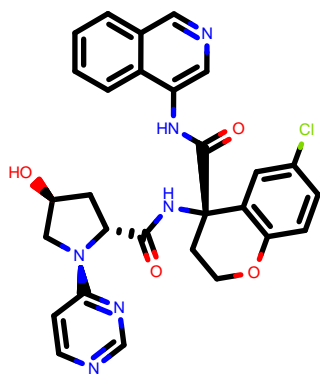
SMILES: CO[C@@]1(CCCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5)CO

RUN: RUN4441

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.37

EN300-310022_1_2_1



CID: EN300-310022_1_2_1

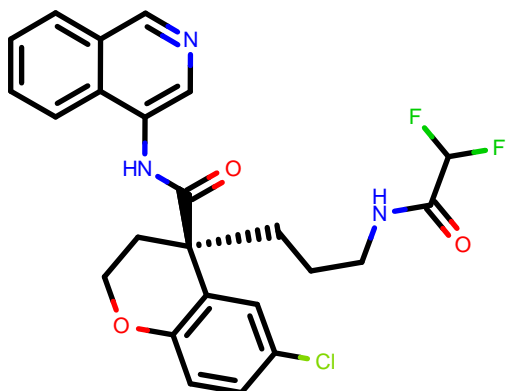
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3(C)CCOc4c3ccc4C(NC(=O)C@H5C[C@@H]CN5c6ccccc6)O

RUN: RUN3355

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.37

EN300-19507_4_1_1



CID: EN300-19507_4_1_1

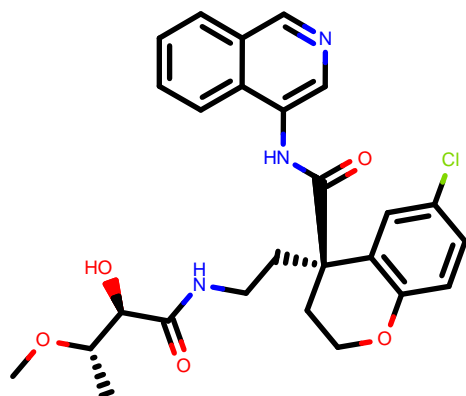
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3ccc(cc4)C)CCCN(C(=O)C(F)F)

RUN: RUN3855

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.25

EN300-220194_3_3_1



CID: EN300-220194_3_3_1

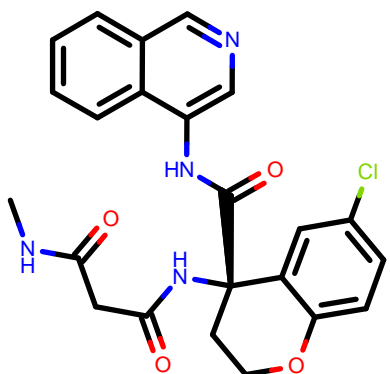
SMILES: C[C@@H]([C@@H](C(=O)NCC[C@]1(C)CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)O)O

RUN: RUN4521

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.30

EN300-128463_1_1_1



CID: EN300-128463_1_1_1

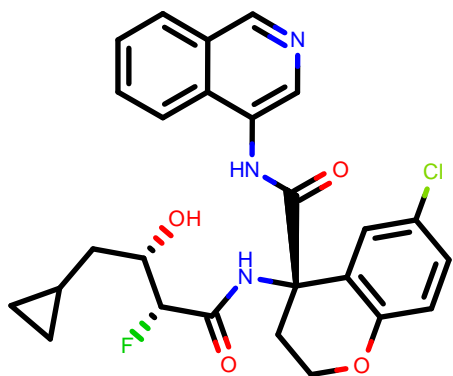
SMILES: CNC(=O)CC(=O)N[C@]1(C)CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN3735

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.21

EDG-MED-90036822-108_3



CID: EDG-MED-90036822-108_3

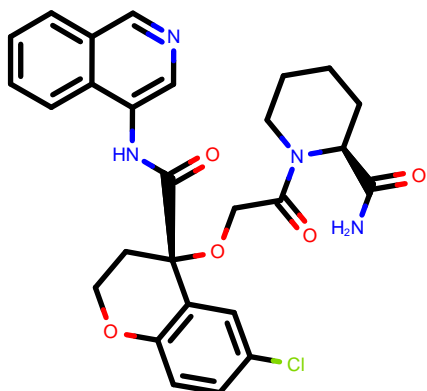
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@@H](CC5CC5)O)F

RUN: RUN1752

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.23

EN300-22879_1_2_1



CID: EN300-22879_1_2_1

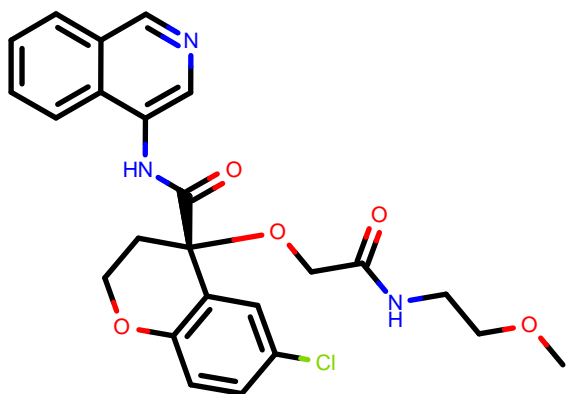
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NCC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN5967

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.28

EN300-02015_1_1_1



CID: EN300-02015_1_1_1

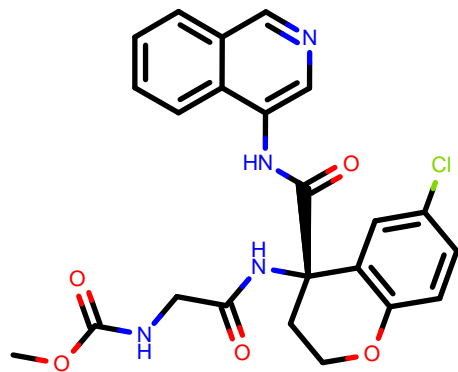
SMILES: COCCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN7334

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.26

EN300-50009_1_1_1



CID: EN300-50009_1_1_1

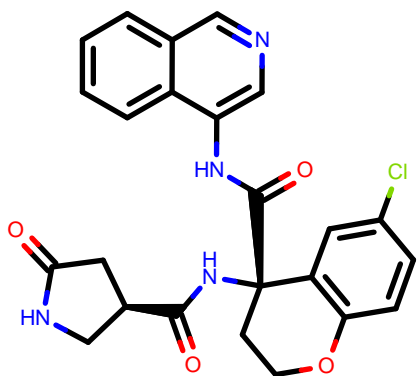
SMILES: COC(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN4406

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EN300-59487_1_1_1



CID: EN300-59487_1_1_1

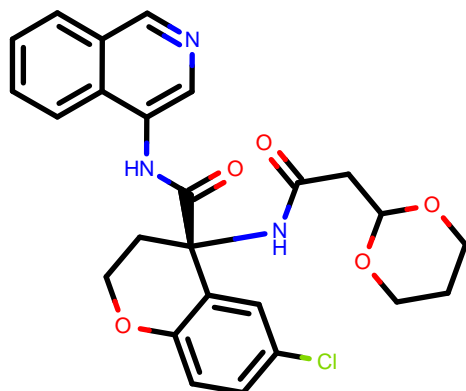
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC(=O)NCS

RUN: RUN3271

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EN300-157502_1_1_1



CID: EN300-157502_1_1_1

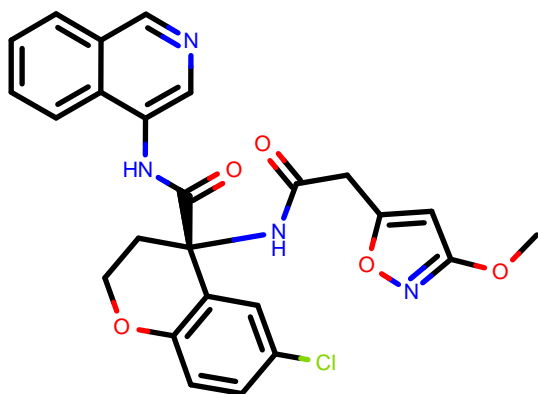
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5OCCO5

RUN: RUN4431

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.26

EN300-127197_1_1_1



CID: EN300-127197_1_1_1

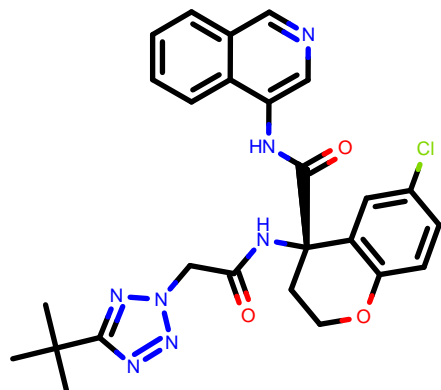
SMILES: COc1cc(on1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN3342

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

EN300-1703143_1_1_1



CID: EN300-1703143_1_1_1

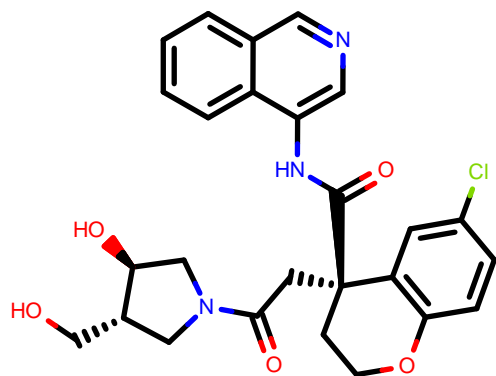
SMILES: CC(C)(C)c1nnn(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5

RUN: RUN4053

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.35

EN300-248521_1_3_1



CID: EN300-248521_1_3_1

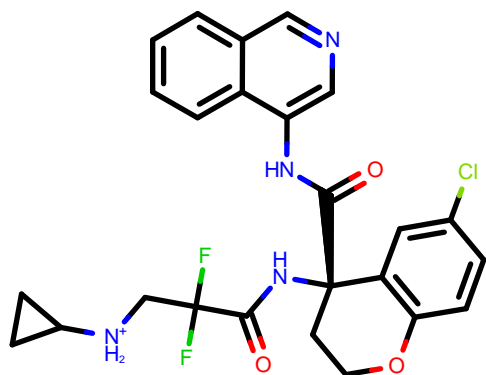
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)O)CO

RUN: RUN4655

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

EDG-MED-90036822-105_1



CID: EDG-MED-90036822-105_1

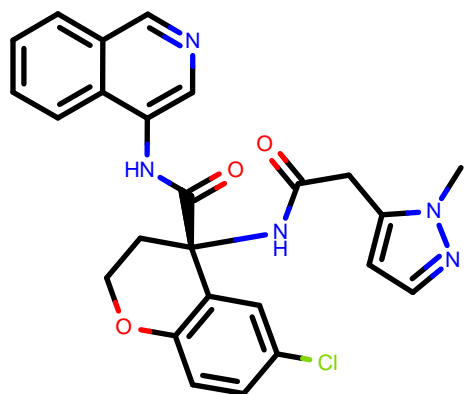
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CNC5CC5)(F)F

RUN: RUN1813

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.29

EN300-114805_1_1_1



CID: EN300-114805_1_1_1

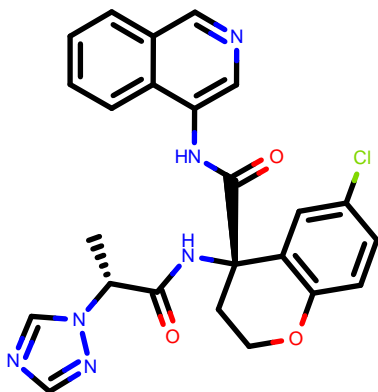
SMILES: Cn1c(ccn1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4529

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.24

EN300-30397_1_2_1



CID: EN300-30397_1_2_1

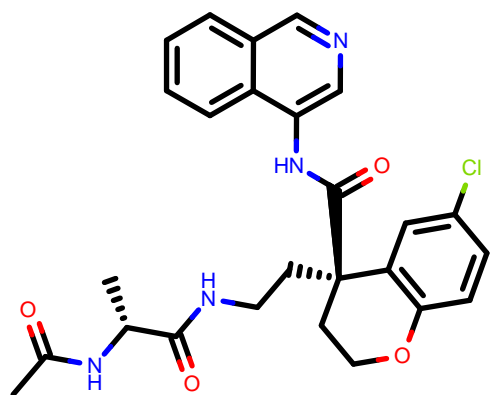
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)n5cncn5

RUN: RUN3376

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.21

EN300-18569_3_2_1



CID: EN300-18569_3_2_1

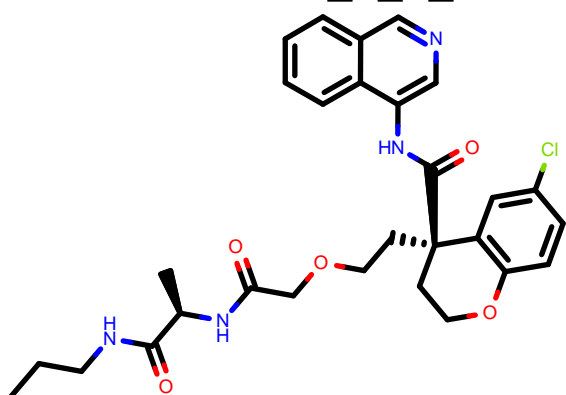
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4NC(=O)C

RUN: RUN6361

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.30

EN300-23214_3_1_1



CID: EN300-23214_3_1_1

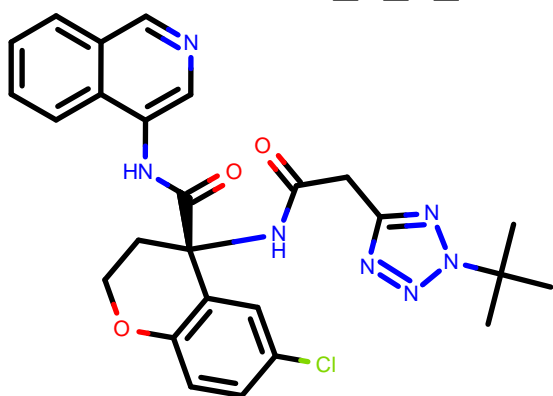
SMILES: CCCNC(=O)[C@@H](C)NC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4449

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.49

EN300-297927_1_1_1



CID: EN300-297927_1_1_1

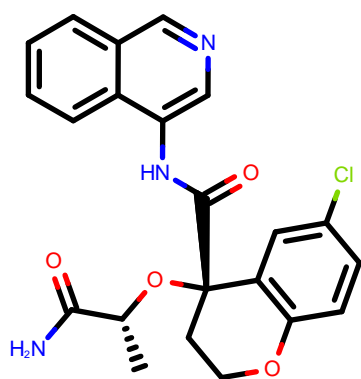
SMILES: CC(C)(C)n1nc(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4264

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.28

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

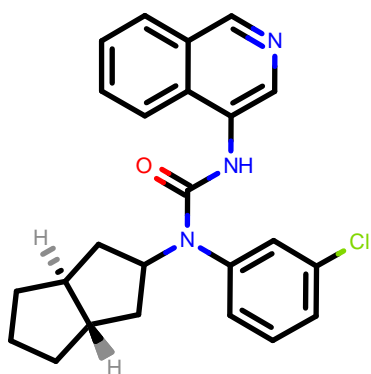
SMILES: C[C@H](C(=O)N)O[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN6234

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.19

MIC-UNK-cdc2493e-4_3



CID: MIC-UNK-cdc2493e-4_3

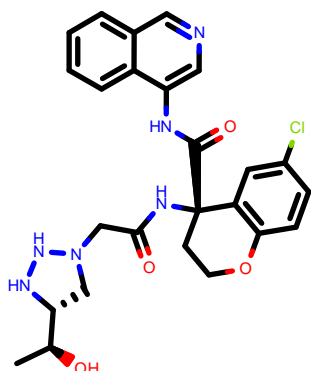
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C4C[C@@H]5CCCC[C@H]5C4

RUN: RUN448

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.29

EN300-109540_1_1_1



CID: EN300-109540_1_1_1

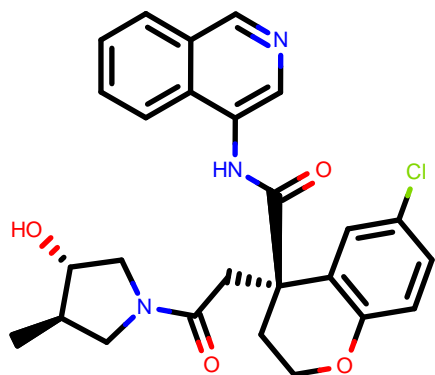
SMILES: C[C@@H](c1cn(nn1)CC(=O)N[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4cccc5c4cccc5)O

RUN: RUN4098

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.28

EN300-124052_1_3_1



CID: EN300-124052_1_3_1

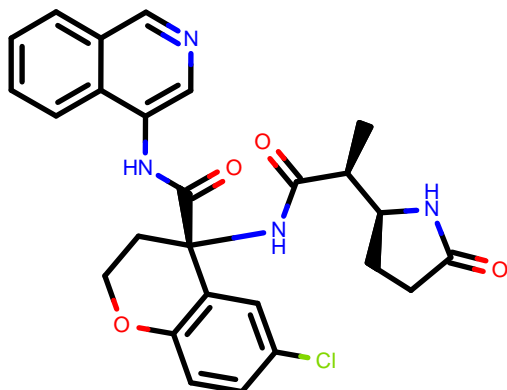
SMILES: C[C@@H]1CN(C[C@H]1O)C(=O)N[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN5608

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.26

EN300-249421_1_1_1



CID: EN300-249421_1_1_1

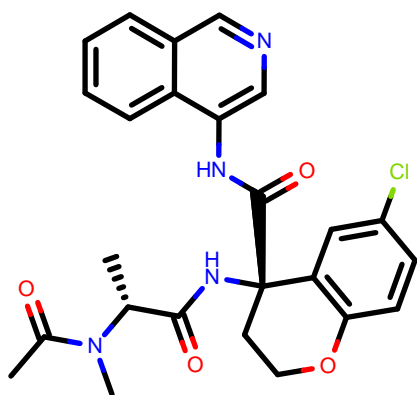
SMILES: C[C@@H]([C@@H]1CCC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(c3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN4788

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.27

EN300-863933_1_2_1



CID: EN300-863933_1_2_1

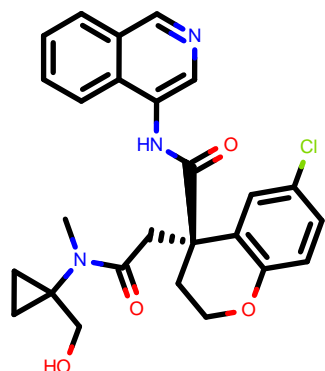
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)N(C)C(=O)C

RUN: RUN3534

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.30

EN300-211403_1_1_1



CID: EN300-211403_1_1_1

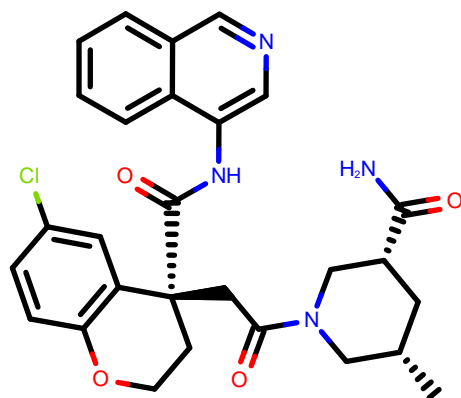
SMILES: CN(C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)C5(CC5)CO

RUN: RUN7698

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.34

EN300-1724086_1_4_1



CID: EN300-1724086_1_4_1

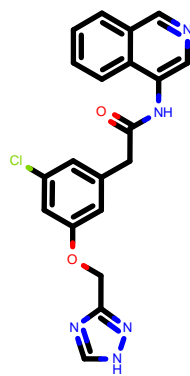
SMILES: C[C@H]1C[C@@H](CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C(=O)N

RUN: RUN3731

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.29

RAL-THA-1d44ff04-2_1



CID: RAL-THA-1d44ff04-2_1

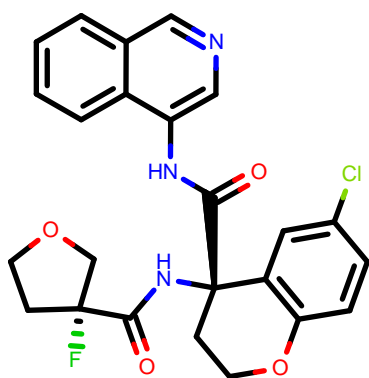
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCc4[nH]n4

RUN: RUN394

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.33

EN300-188356_1_2_1



CID: EN300-188356_1_2_1

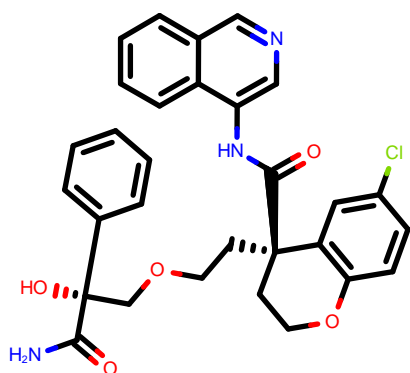
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@]5(CCOCC5)F

RUN: RUN3811

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.31

EN300-248526_3_1_1



CID: EN300-248526_3_1_1

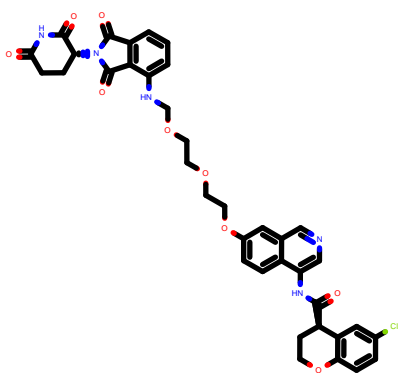
SMILES: c1ccc(cc1)[C@@]1(COCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4cccc5)C1(=O)N)O

RUN: RUN3881

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.39

DAR-DIA-9e4459de-11_3



CID: DAR-DIA-9e4459de-11_3

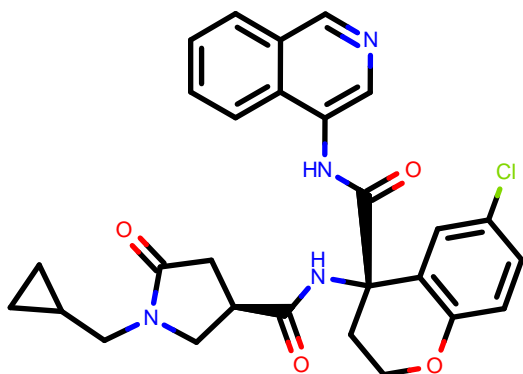
SMILES: c1ccc2c(c1)NCOCCCCOCC3CC4(C)C(=O)N(C@@)H5COOCC6CC7(C)C(=O)N(C@@)H7CC(C1=O)NC7=O)O

RUN: RUN1375

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.39

EN300-31969_1_1_1



CID: EN300-31969_1_1_1

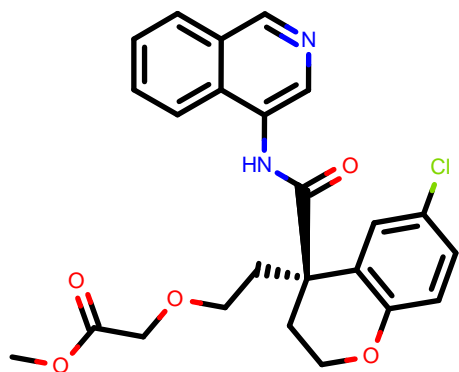
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@]5(COCC5)O)C@@H6CC(C1=O)NC7=O)O

RUN: RUN7007

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.28

EN300-19700_3_1_1



CID: EN300-19700_3_1_1

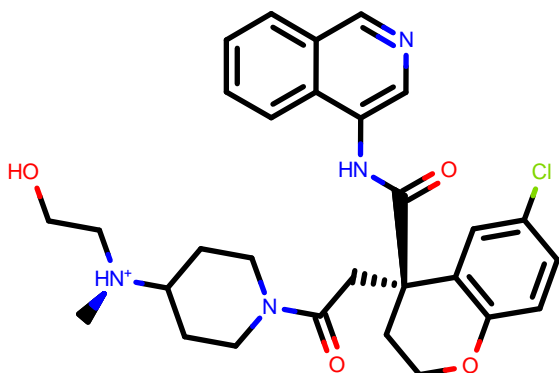
SMILES: COC(=O)COCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3957

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.21

EDG-MED-ba1ac7b9-28_3



CID: EDG-MED-ba1ac7b9-28_3

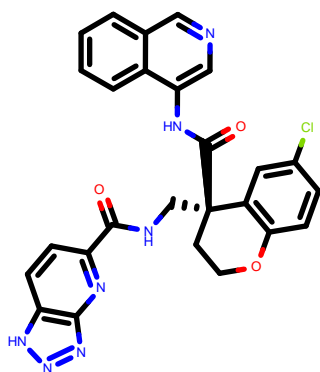
SMILES: C1N@@H+]CCO)C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2570

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.66

EN300-133058_2_1_1



CID: EN300-133058_2_1_1

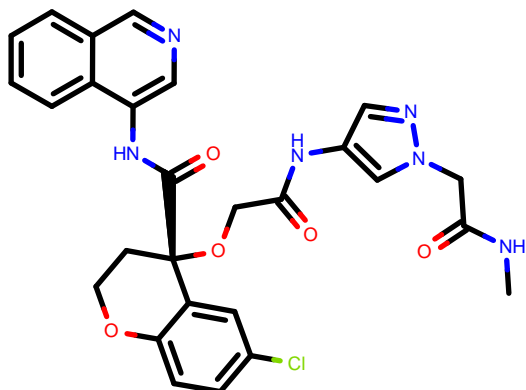
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc1cc4)Cl)CNC(=O)c5ccc6c(n5)[nH]n6

RUN: RUN4716

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-48861_1_1_1



CID: EN300-48861_1_1_1

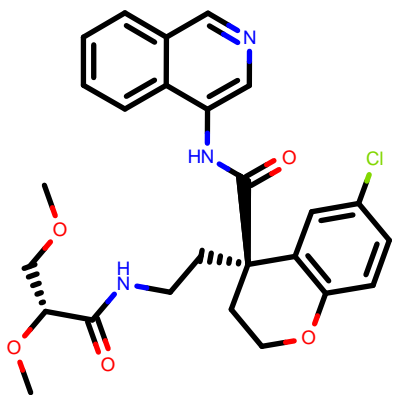
SMILES: CNC(=O)C[n+]1cc(c[nH]1)NC(=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5705

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EN300-305282_3_2_1



CID: EN300-305282_3_2_1

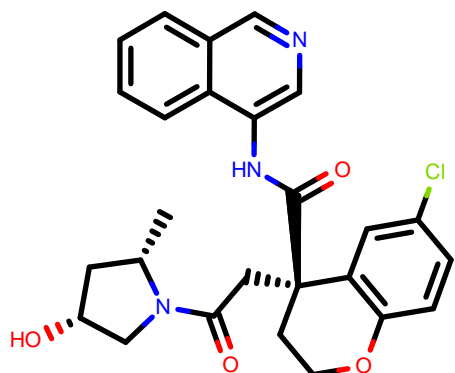
SMILES: COC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4)OC

RUN: RUN4541

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.42

EN300-173562_1_4_1



CID: EN300-173562_1_4_1

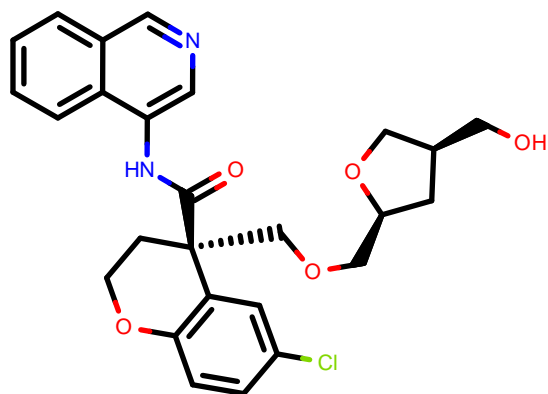
SMILES: C[C@H]1C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN5677

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.27

EDJ-MED-fcba3f31-11_1



CID: EDJ-MED-fcba3f31-11_1

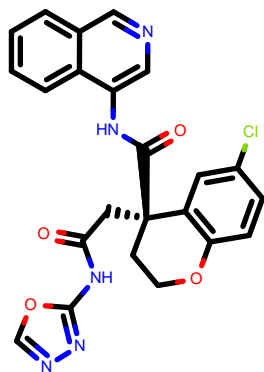
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C[C@@H](CO)C5

RUN: RUN2366

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.31

CHO-MSK-a31cca77-1_1



CID: CHO-MSK-a31cca77-1_1

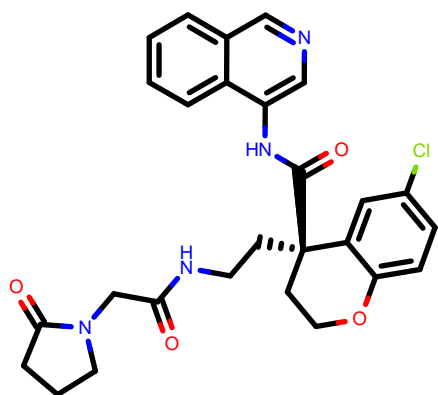
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnc5

RUN: RUN2031

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.21

EN300-11934_3_1_1



CID: EN300-11934_3_1_1

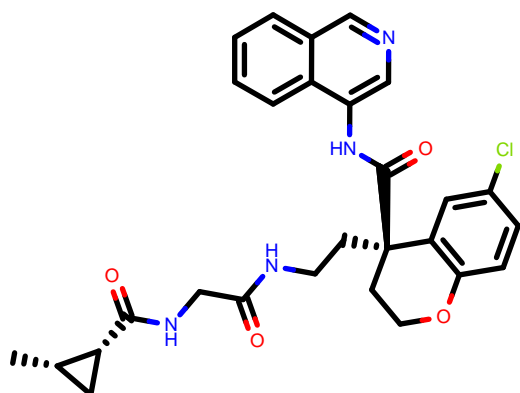
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCC5=O

RUN: RUN4770

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.28

EN300-30768_3_4_1



CID: EN300-30768_3_4_1

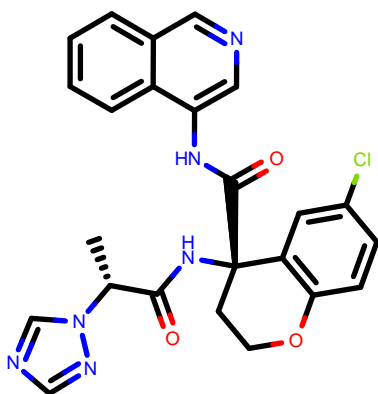
SMILES: C[C@H]1C[C@H]1C(=O)NCC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc4cccc5

RUN: RUN6496

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EN300-30397_1_2_1



CID: EN300-30397_1_2_1

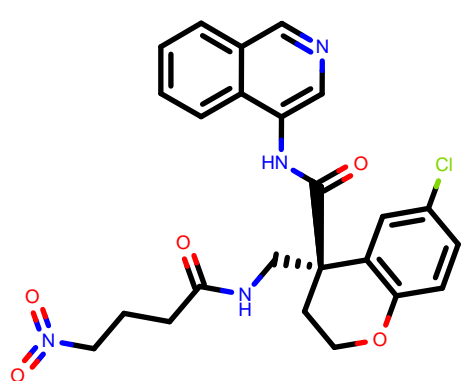
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4)n5cncn5

RUN: RUN4615

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-143449_2_1_1



CID: EN300-143449_2_1_1

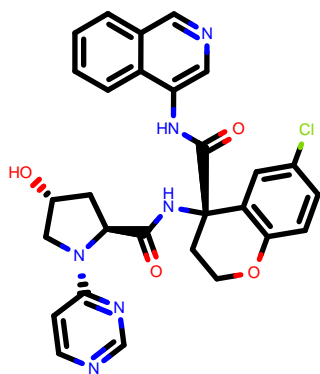
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCN(=O)=O

RUN: RUN5160

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-310022_1_3_1



CID: EN300-310022_1_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4cc3ccc4)C(NC(=O)C[C@@]5H[C@@H]CN5c6ccccc6)O

RUN:

RUN4275

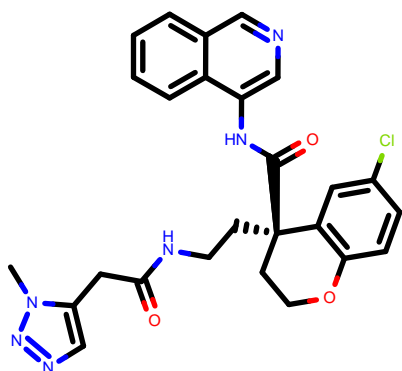
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.38

EN300-6486855_3_1_1



CID: EN300-6486855_3_1_1

SMILES:

Cn1c(cnn1)CC(=O)NCC[C@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN:

RUN5021

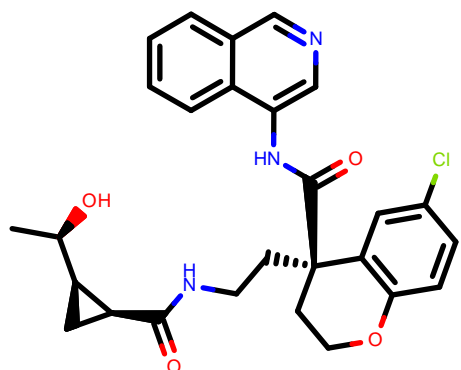
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.29

EN300-6729572_3_2_1



CID: EN300-6729572_3_2_1

SMILES:

C[C@@H]1[C@@H]2[C@@H]1[C@@H]2[C@@H]3(CO)NCC[C@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5O

RUN:

RUN5048

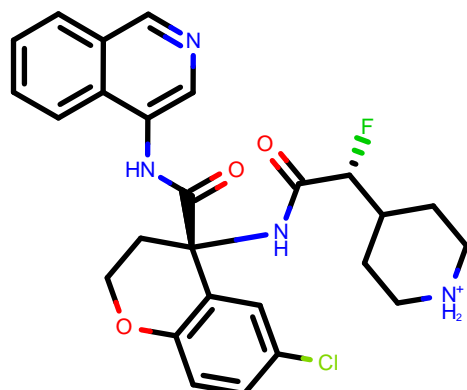
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.29

EDG-MED-90036822-95_1



CID: EDG-MED-90036822-95_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4cc3ccc4)NC(=O)C[C@@]5H[C@@H](C5CC[NH2+])CC5F

RUN:

RUN1669

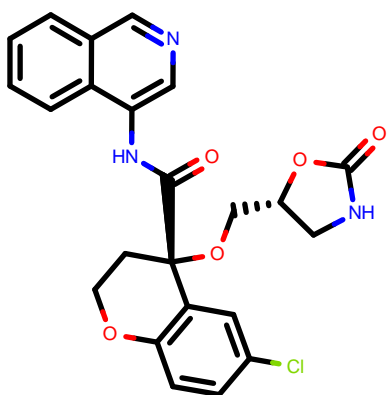
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.30

EN300-203293_1_2_1



CID: EN300-203293_1_2_1

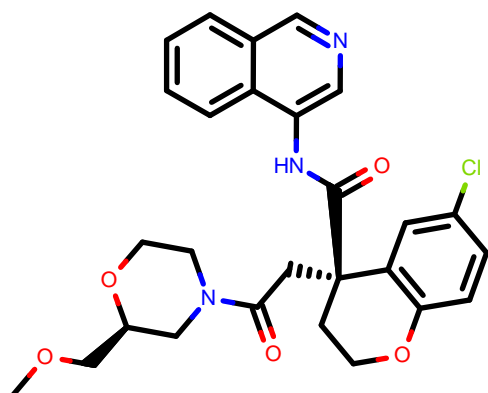
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5CNC(=O)O5

RUN: RUN6620

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EN300-6742996_1_1_1



CID: EN300-6742996_1_1_1

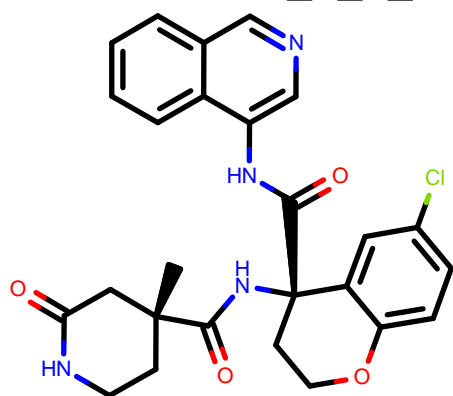
SMILES: CO[C@@H]1CN(CCO1)C(=O)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccccc5

RUN: RUN4738

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.33

EN300-315854_1_2_1



CID: EN300-315854_1_2_1

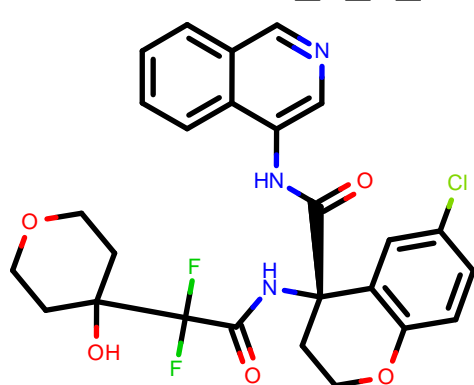
SMILES: C[C@@]1(C)CNC(=O)[C@@]2(C)C(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccccc5

RUN: RUN5066

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-706065_1_1_1



CID: EN300-706065_1_1_1

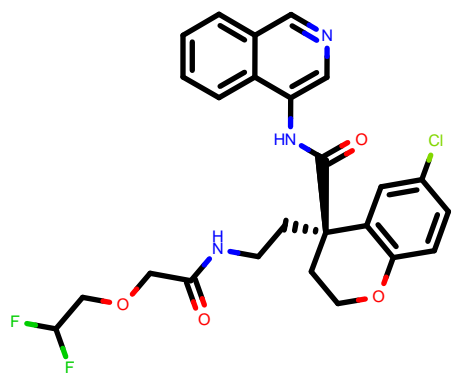
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(C5(CCOCC5)O)(F)F

RUN: RUN4503

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-315792_3_1_1



CID: EN300-315792_3_1_1

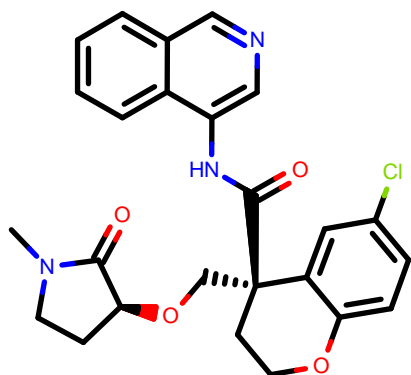
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COCC(F)F

RUN: RUN4646

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.28

EN300-98648_2_1_1



CID: EN300-98648_2_1_1

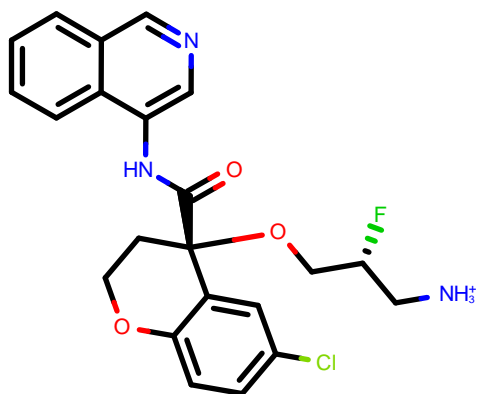
SMILES: CN1CC[C@@H](C1=O)OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3693

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.21

ED_-GRI-5b13fbe2-41_1



CID: ED_-GRI-5b13fbe2-41_1

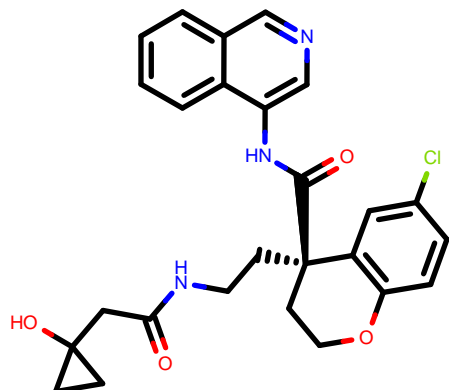
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C[NH3+])F

RUN: RUN1435

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.45

EN300-207873_3_1_1



CID: EN300-207873_3_1_1

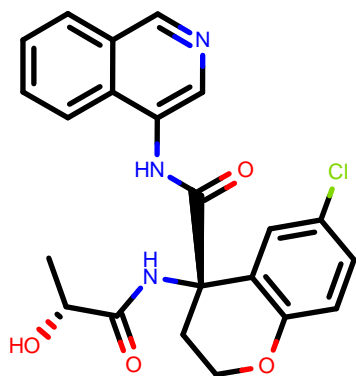
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CC5)O

RUN: RUN6695

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.26

EN300-19542_1_2_1



CID: EN300-19542_1_2_1

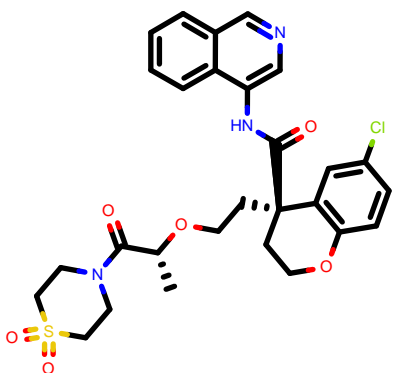
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5118

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.19

EN300-1265949_3_2_1



CID: EN300-1265949_3_2_1

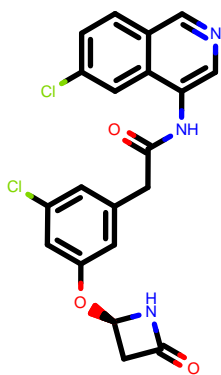
SMILES: C[C@H](C(=O)N1CCS(=O)(=O)CC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5504

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.34

ALF-EVA-0b412456-1_1



CID: ALF-EVA-0b412456-1_1

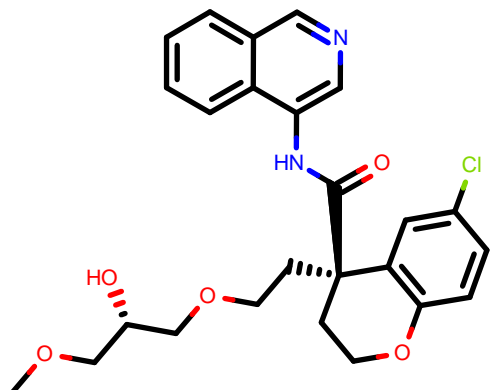
SMILES: c1cc2nccc(c2cc1Cl)NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN2535

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.34

EN300-1915260_3_1_1



CID: EN300-1915260_3_1_1

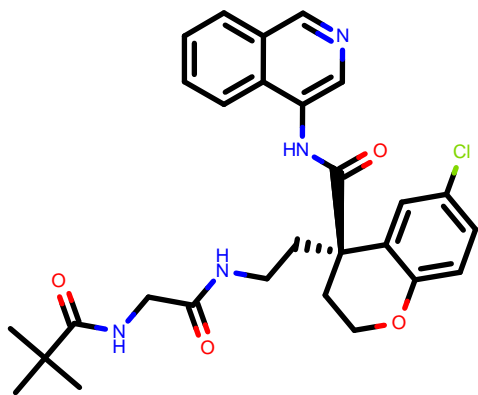
SMILES: COC[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN4908

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.43

EN300-12247_3_1_1



CID: EN300-12247_3_1_1

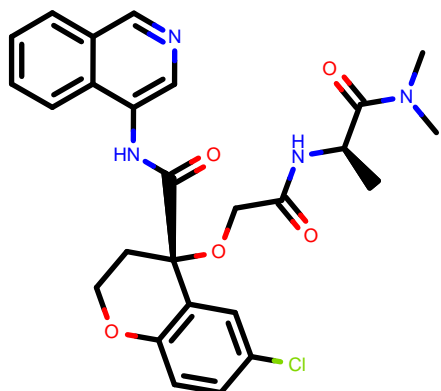
SMILES: CC(C)(C)C(=O)NCC(=O)NCC[C@]1(C)COCc2c1cc(cc2Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6994

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.27

EN300-47657_1_2_1



CID: EN300-47657_1_2_1

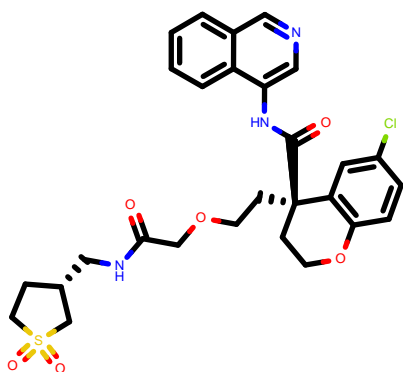
SMILES: C[C@H](C(=O)N(C)C)NC(=O)CO[C@]1(C)COCc2c1cc(cc2Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN4367

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.33

EN300-47606_3_2_1



CID: EN300-47606_3_2_1

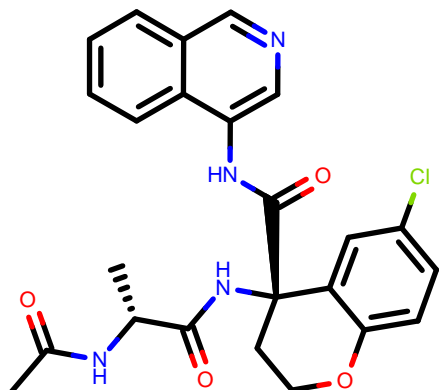
SMILES: c1ccc2c(e1)ncnc2N(C)C(=O)[C@]3(C)COCc4c3cc(cc4Cl)COC(=O)N[C@@H]5C(S(=O)(=O)C)C5

RUN: RUN5974

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.35

EN300-18569_1_2_1



CID: EN300-18569_1_2_1

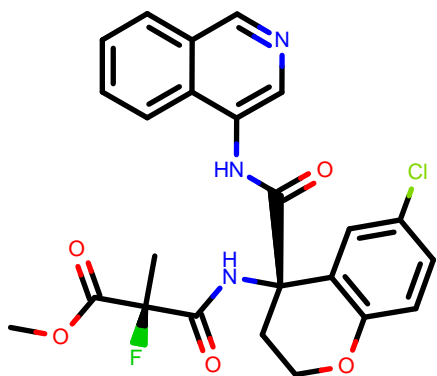
SMILES: C[C@H](C(=O)N(C)C)1(C)COCc2c1cc(cc2Cl)C(=O)Nc3nccc4c3cccc4NC(=O)C

RUN: RUN3843

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.22

EN300-7464289_1_2_1



CID: EN300-7464289_1_2_1

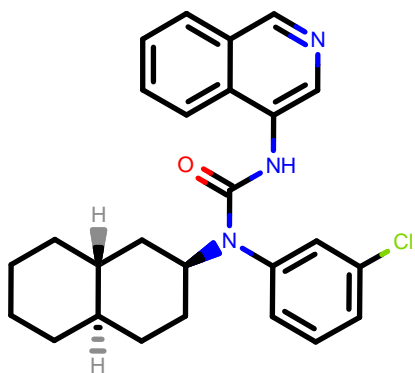
SMILES: C[C@]1C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4(C(=O)OC)F

RUN: RUN3541

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.24

MIC-UNK-cdc2493e-8_4



CID: MIC-UNK-cdc2493e-8_4

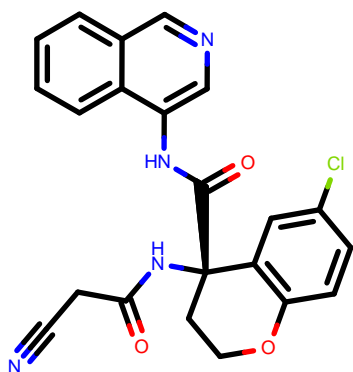
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C@H4CC[C@@H]5CCCC[C@]6[H]5C4

RUN: RUN458

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.53

EDG-MED-90036822-56_1



CID: EDG-MED-90036822-56_1

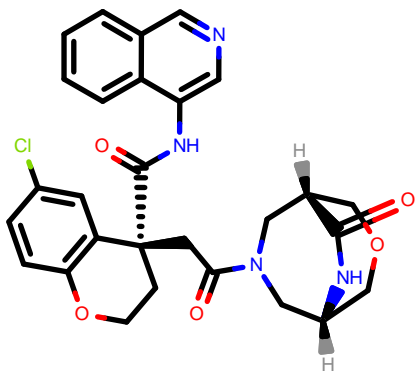
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC#N

RUN: RUN1571

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.15

EN300-6477207_1_1_1



CID: EN300-6477207_1_1_1

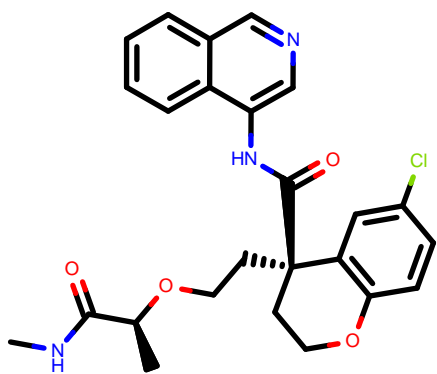
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[C@@]4(C)N[C@@]5[C@]6[H]5CO[C@]6[H]4C5N=C=O

RUN: RUN5312

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.45

EN300-211482_3_1_1



CID: EN300-211482_3_1_1

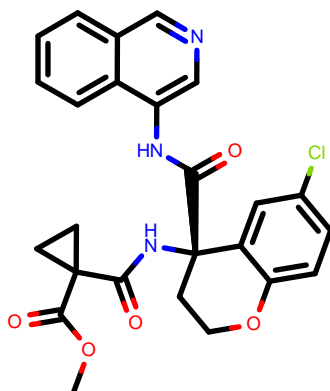
SMILES: C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN5042

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.26

EN300-138787_1_1_1



CID: EN300-138787_1_1_1

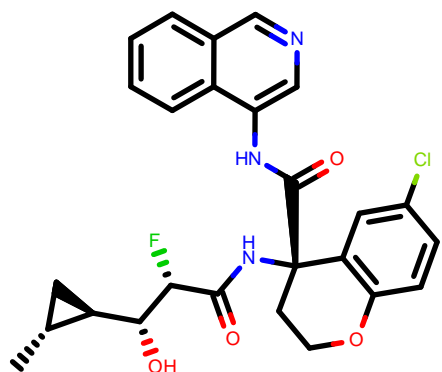
SMILES: COC(=O)C1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4165

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.21

EDG-MED-90036822-94_7



CID: EDG-MED-90036822-94_7

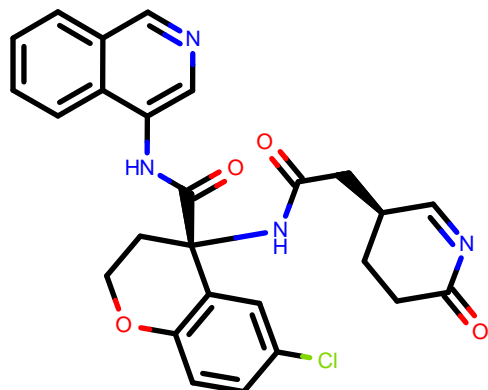
SMILES: C[C@@H]1C[C@@H]1[C@@H]2[C@@H]3[C@@H]2[C@@H]3(CCOc4c2cc(cc4)Cl)C(=O)Nc5ccc6c4cccc6F

RUN: RUN1714

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.29

EN300-246992_1_1_1



CID: EN300-246992_1_1_1

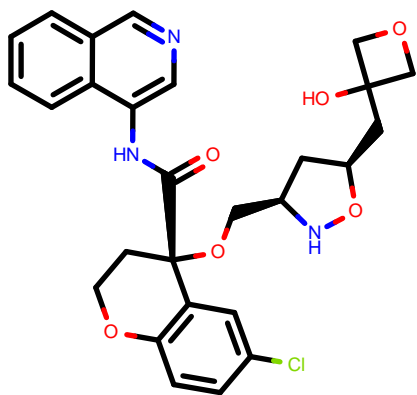
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)NCS

RUN: RUN6915

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.31

EN300-7457160_1_1_2



CID: EN300-7457160_1_1_2

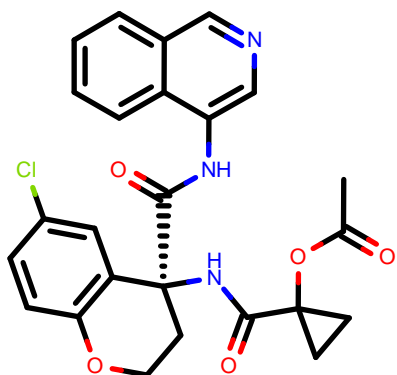
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3C(=O)C1OC[C@@H]5[C@@H]ON5COC6(COC6)O

RUN: RUN6457

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.34

EN300-173023_1_1_1



CID: EN300-173023_1_1_1

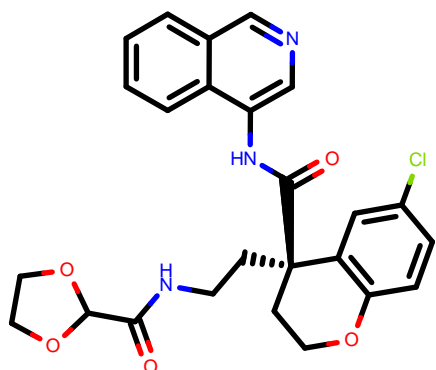
SMILES: CC(=O)OC1(CC1)C(=O)N[C@@]2(C)COC3C2C(=O)C1C(=O)N4cnc5c4ccccc5

RUN: RUN5028

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.33

EN300-154942_3_1_1



CID: EN300-154942_3_1_1

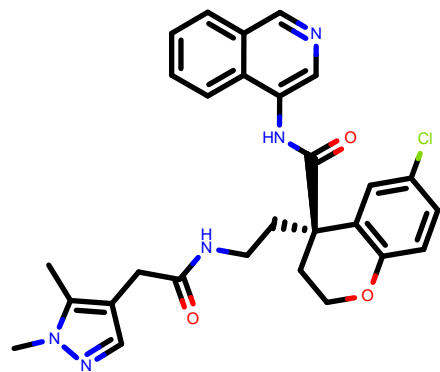
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3C(=O)C1OC[C@@H]5ON5COC6(COC6)O

RUN: RUN5124

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.28

EN300-219437_3_1_1



CID: EN300-219437_3_1_1

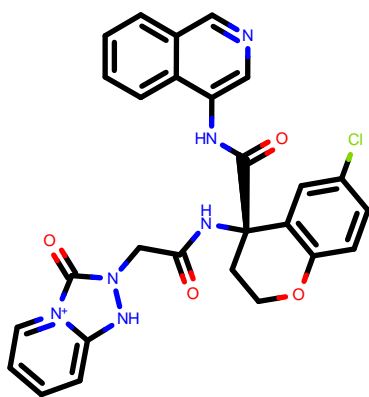
SMILES: Cc1c(cnn1C)CC(=O)NCC[C@@]2(C)COC3C2C(=O)C1C(=O)N4cnc5c4ccccc5

RUN: RUN5806

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.29

EN300-27476_1_1_1



CID: EN300-27476_1_1_1

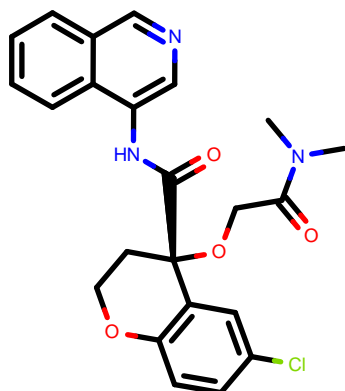
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6cccc6n5

RUN: RUN5044

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.34

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

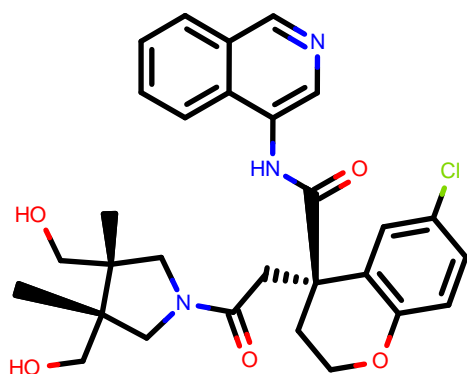
SMILES: CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4210

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.21

EN300-318058_1_1_1



CID: EN300-318058_1_1_1

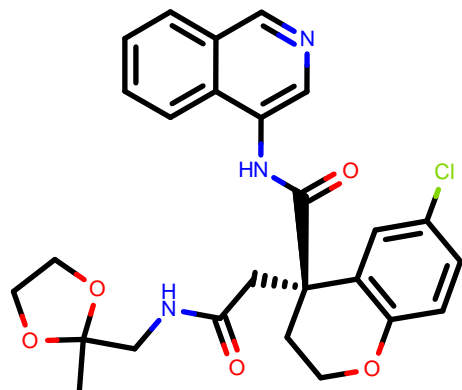
SMILES: C[C@@]1(CN(C)C[C@@]1(C)CO)C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5CO

RUN: RUN5258

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.32

EN300-114894_1_1_1



CID: EN300-114894_1_1_1

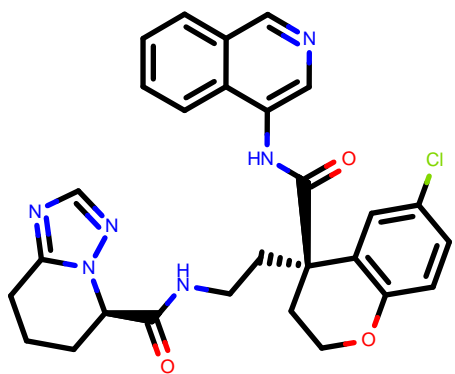
SMILES: CC1(OCCO1)CNC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN7087

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.31

EN300-1273016_3_2_1



CID: EN300-1273016_3_2_1

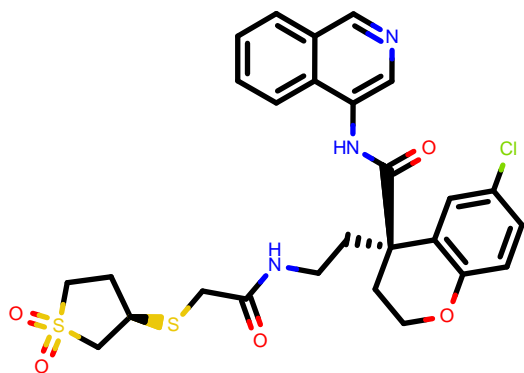
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CCc6c6n5n6

RUN: RUN4303

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.32

EN300-13890_3_1_1



CID: EN300-13890_3_1_1

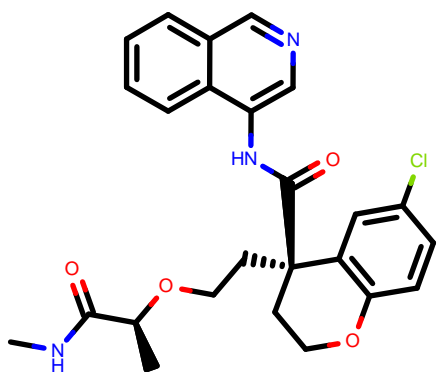
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CS(=O)S5

RUN: RUN3588

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.36

EN300-211482_3_1_1



CID: EN300-211482_3_1_1

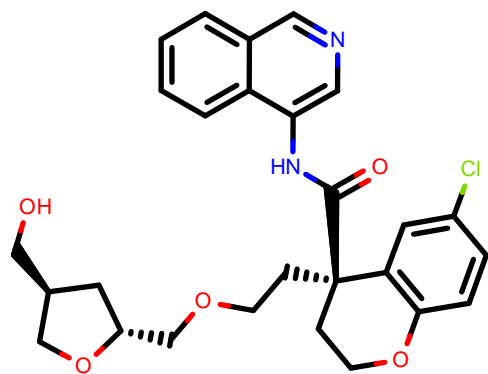
SMILES: C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nnc4c3ccoc4

RUN: RUN4447

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-6494158_3_2_1



CID: EN300-6494158_3_2_1

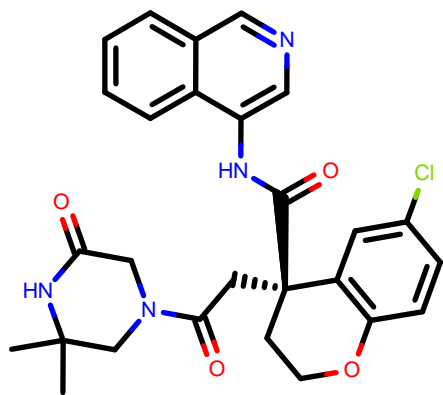
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5C[C@@H](CO)5O

RUN: RUN4290

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.31

EN300-7493939_1_1_1



CID: EN300-7493939_1_1_1

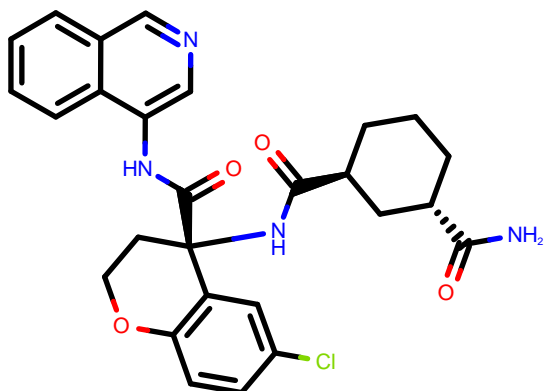
SMILES: CC1(CN(CC(=O)N1)C(=O)C)C@2(CCOc3c2cc(c3)Cl)C(=O)Nc4ncnc5c4ccc5)C

RUN: RUN4726

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.24

EN300-90142_1_2_1



CID: EN300-90142_1_2_1

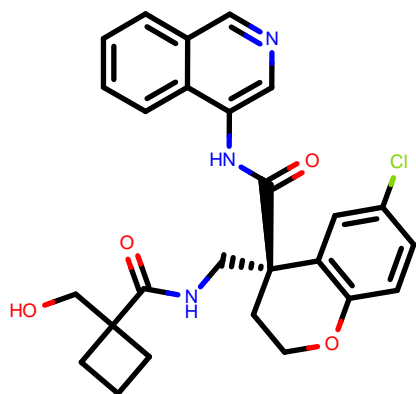
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)N)C(=O)C@H5CCC[C@@H]1C5)Cl=O

RUN: RUN3508

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.39

EDJ-MED-40433386-4_1



CID: EDJ-MED-40433386-4_1

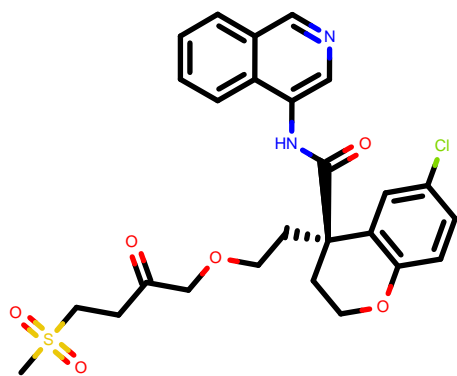
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)C(=O)CNC(=O)C5(CCC5)CO

RUN: RUN2357

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.28

EN300-1988306_3_1_1



CID: EN300-1988306_3_1_1

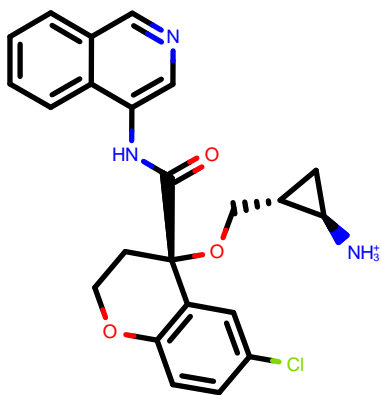
SMILES: CS(=O)(=O)CCC(=O)COCC[C@@]1(CCOc2c1cc(c2)Cl)C(=O)Nc3ncnc4c3ccc4

RUN: RUN4644

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.43

ED_-GRI-5b13fbe2-71_1



CID: ED_-GRI-5b13fbe2-71_1

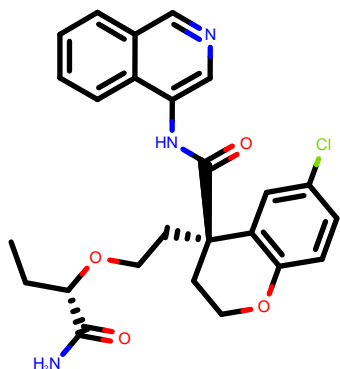
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5[C@H]5[NH3+]

RUN: RUN1485

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.27

EN300-65839_3_1_1



CID: EN300-65839_3_1_1

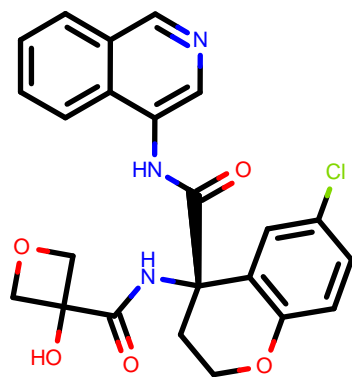
SMILES: CC[C@@H](C(=O)N)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN3007

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.31

EN300-101443_1_1_1



CID: EN300-101443_1_1_1

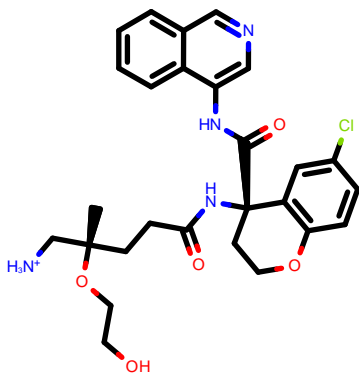
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COC5)O

RUN: RUN3823

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.21

EDG-MED-90036822-22_2



CID: EDG-MED-90036822-22_2

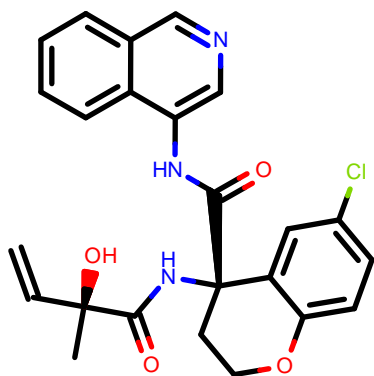
SMILES: C[C@@](CCC(=O)N)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4(C[NH3+])OCCO

RUN: RUN1625

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.50

EN300-248888_1_2_1



CID: EN300-248888_1_2_1

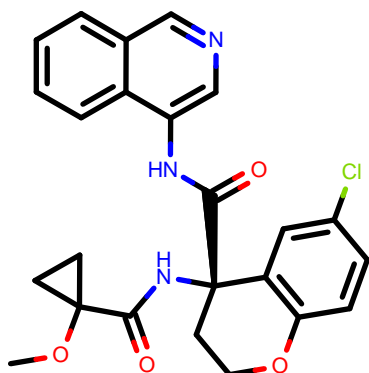
SMILES: C[C@](C=C)(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN7383

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.29

EN300-182124_1_1_1



CID: EN300-182124_1_1_1

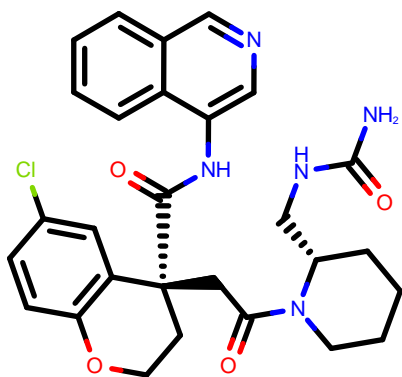
SMILES: COC1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5348

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.22

EN300-62166_1_2_1



CID: EN300-62166_1_2_1

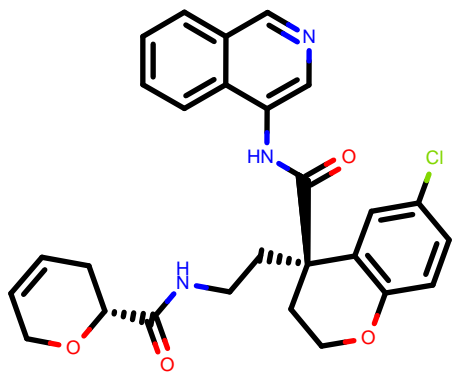
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5CNC(=O)N

RUN: RUN5981

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.28

EN300-378044_3_2_1



CID: EN300-378044_3_2_1

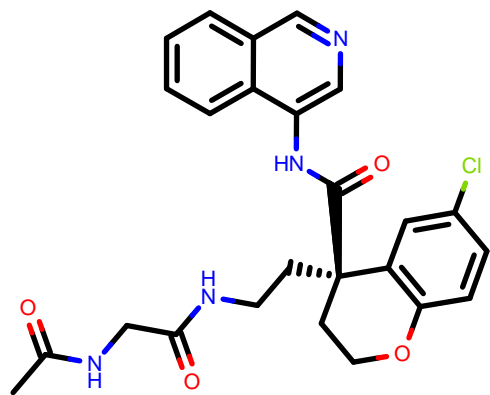
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC=CCO5

RUN: RUN4363

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.25

EN300-18561_3_1_1



CID: EN300-18561_3_1_1

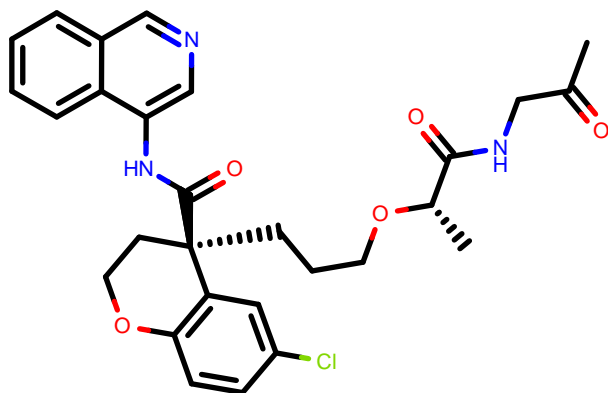
SMILES: CC(=O)NCC(=O)NCC[C@]1(C)C(CO)C2c1cc(cc2)C(=O)Nc3ccc4c3ccc4

RUN: RUN4947

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-131093_4_1_1



CID: EN300-131093_4_1_1

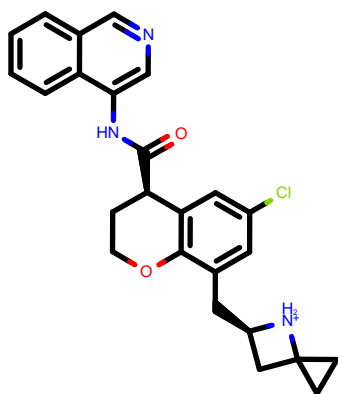
SMILES: C[C@@H](C(=O)NCC(=O)C)OCC[C@]1(C)C(CO)C2c1cc(cc2)C(=O)Nc3ccc4c3ccc4

RUN: RUN5281

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.42

DAR-DIA-23e5a6a0-10_1



CID: DAR-DIA-23e5a6a0-10_1

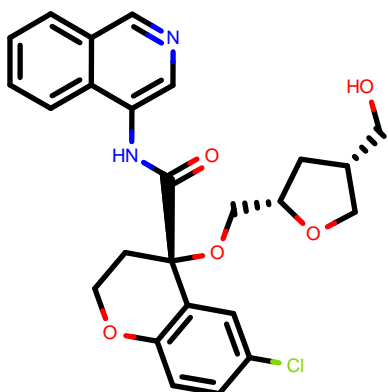
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C(=O)Nc5ccc6([NH2+][5])CC6Cl

RUN: RUN346

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.25

EN300-6494158_1_1_1



CID: EN300-6494158_1_1_1

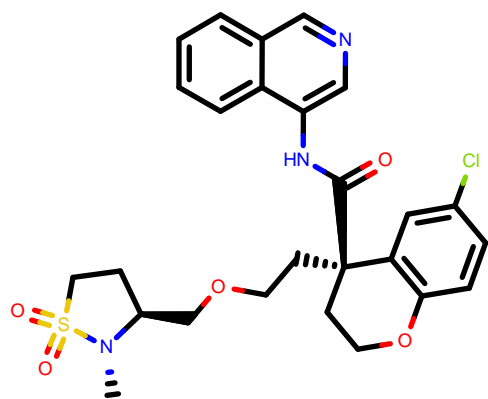
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(C)C(CO)C2c1cc(cc4)C(=O)Nc5ccc6([NH2+][5])CC6CO

RUN: RUN4621

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.33

KAD-UNI-8a629cb0-38_2



CID: KAD-UNI-8a629cb0-38_2

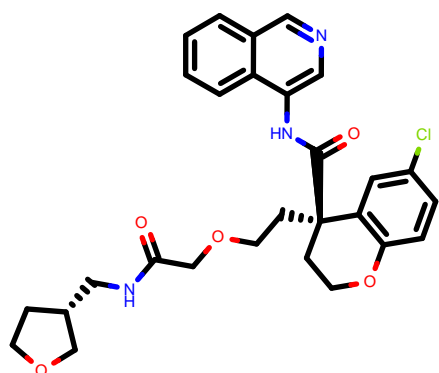
SMILES: C[N@]1[C@@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5

RUN: RUN2048

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-46832_3_2_1



CID: EN300-46832_3_2_1

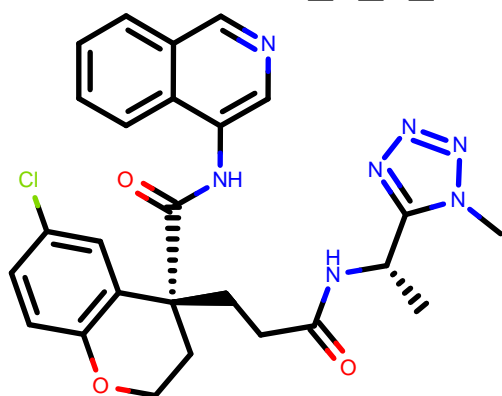
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)NC[C@H]5CCOC5

RUN: RUN5398

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.35

EN300-173020_2_1_1



CID: EN300-173020_2_1_1

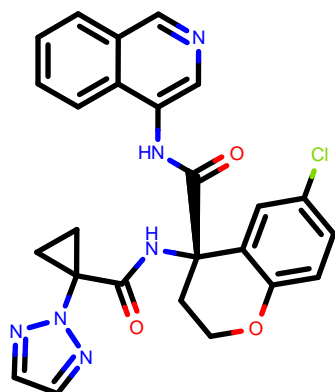
SMILES: C[C@@H](c1nmmn1C)NC(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5

RUN: RUN6168

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.32

EN300-1722017_1_1_1



CID: EN300-1722017_1_1_1

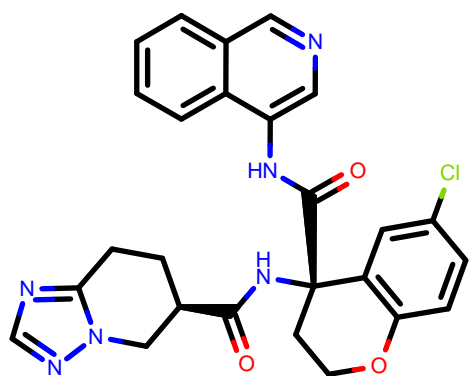
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5n6ncn6

RUN: RUN4087

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.28

EN300-1662365_1_1_1



CID: EN300-1662365_1_1_1

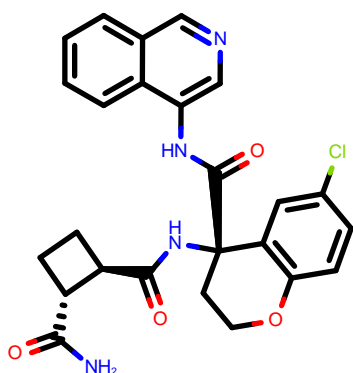
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H5CCc6nncn6C5

RUN: RUN4854

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.27

EN300-217107_1_3_1



CID: EN300-217107_1_3_1

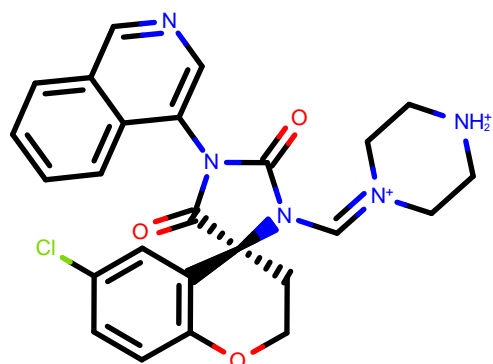
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H5CC[C@H]5C(=O)N

RUN: RUN3206

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-15_1



CID: VLA-UCB-34f3ed0c-15_1

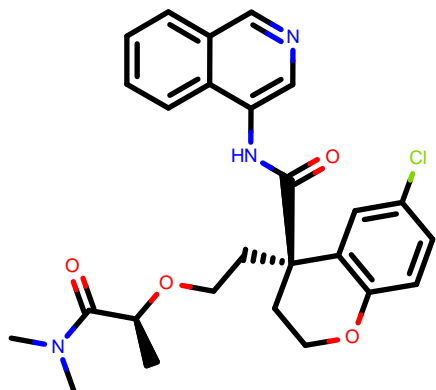
SMILES: c1ccc2c(c1)ncnc2N3C(=O)C@@4(CCOc5c4cc(cc5)Cl)N(C3=O)C6CC[NH2+][C]6

RUN: RUN543

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.46

EN300-14458_3_1_1



CID: EN300-14458_3_1_1

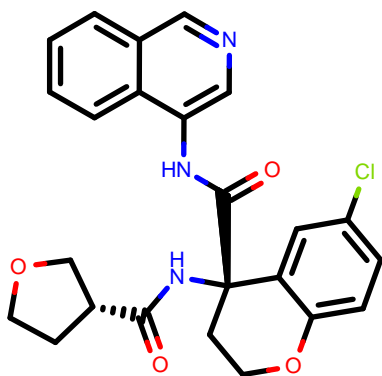
SMILES: C[C@@H](C(=O)N(C)C)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN5565

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.25

EN300-53423_1_1_1



CID: EN300-53423_1_1_1

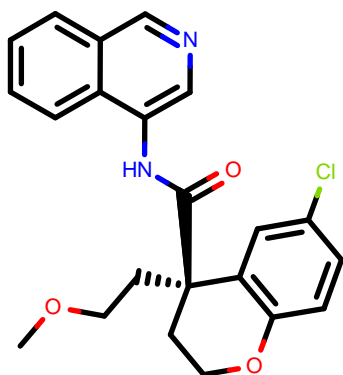
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC5

RUN: RUN4933

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.31

EDJ-MED-28ec730d-2_1



CID: EDJ-MED-28ec730d-2_1

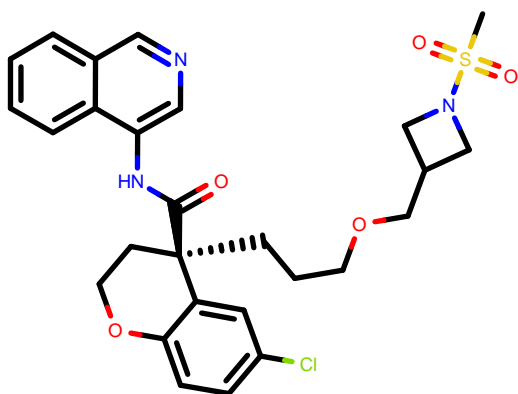
SMILES: COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN587

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.14

EN300-302290_4_1_1



CID: EN300-302290_4_1_1

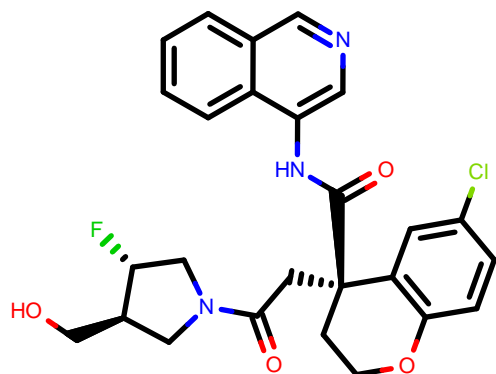
SMILES: CS(=O)(=O)N1CC(C1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN5672

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.36

EN300-1693852_1_1_1



CID: EN300-1693852_1_1_1

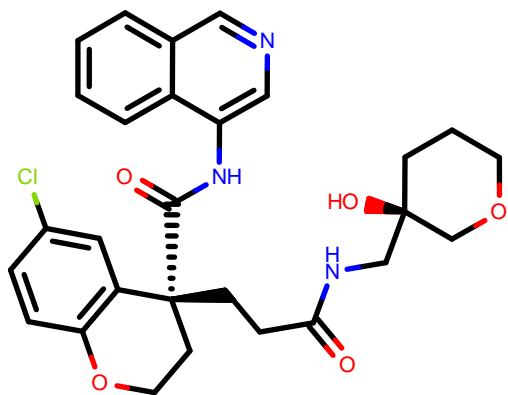
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)F)CO

RUN: RUN4741

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.25

EN300-193679_2_1_1



CID: EN300-193679_2_1_1

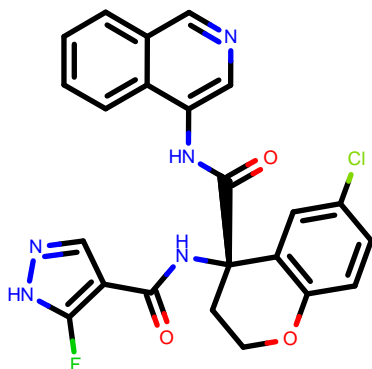
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@]5(CCCOC5)O

RUN: RUN5218

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.31

EDG-MED-90036822-66_1



CID: EDG-MED-90036822-66_1

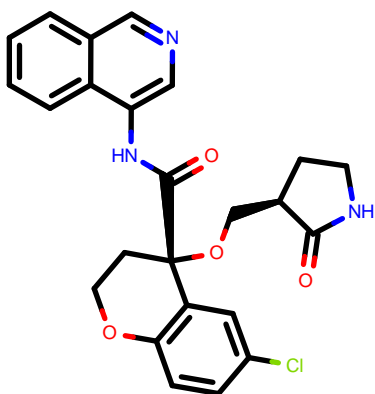
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]c5F

RUN: RUN1605

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.16

EN300-246248_1_2_1



CID: EN300-246248_1_2_1

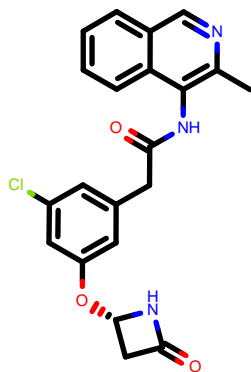
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCNC5=O

RUN: RUN3766

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.22

RAL-THA-065e0743-2_2



CID: RAL-THA-065e0743-2_2

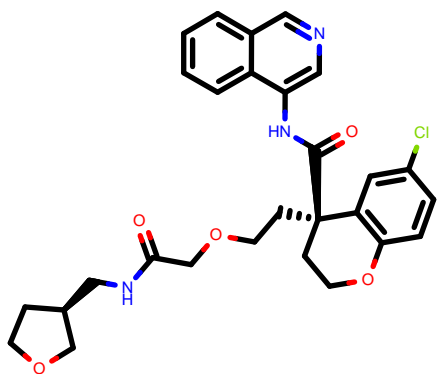
SMILES: Cc1c(c2cccc2cn1)NC(=O)Cc3ccc(cc3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN411

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.40

EN300-46832_3_1_1



CID: EN300-46832_3_1_1

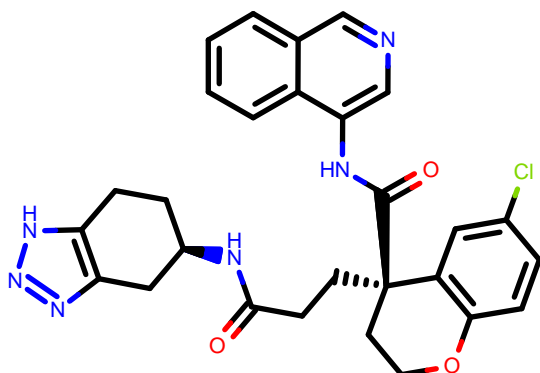
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NC[C@@H]5CCOC5

RUN: RUN3925

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.29

EN300-6491682_2_1_1



CID: EN300-6491682_2_1_1

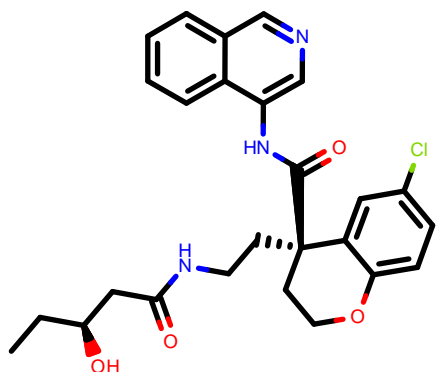
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NC[C@@H]5CCc6c[nH]5n6)C5

RUN: RUN7620

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.28

EN300-224741_3_1_1



CID: EN300-224741_3_1_1

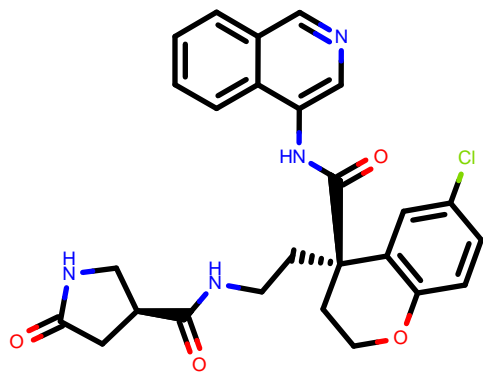
SMILES: CC[C@@H](CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3occc4)O

RUN: RUN5384

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.30

EN300-59487_3_2_1



CID: EN300-59487_3_2_1

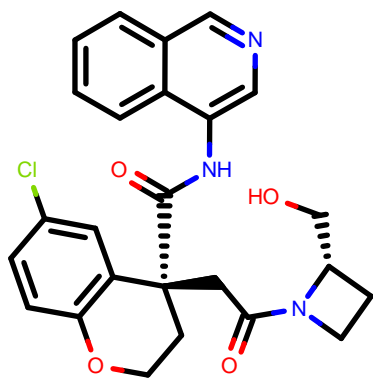
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)NCS

RUN: RUN4116

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.25

EN300-154332_1_2_1



CID: EN300-154332_1_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO

RUN:

RUN6552

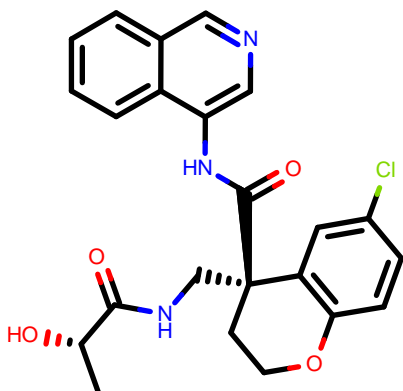
DDG (kcal/mol):

-1.18

dDDG (kcal/mol):

0.29

EN300-19542_2_1_1



CID: EN300-19542_2_1_1

SMILES:

C[C@@H](C(=O)NC[C@]1(CCCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN:

RUN5551

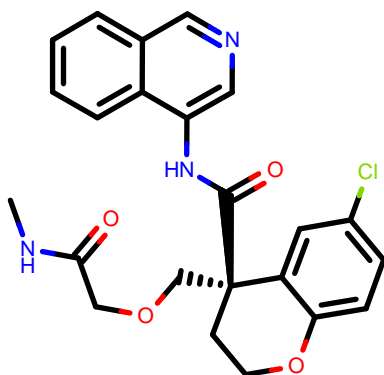
DDG (kcal/mol):

-1.18

dDDG (kcal/mol):

0.26

EN300-2977549_2_1_1



CID: EN300-2977549_2_1_1

SMILES:

CNC(=O)COC[C@]1(CCCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN:

RUN4591

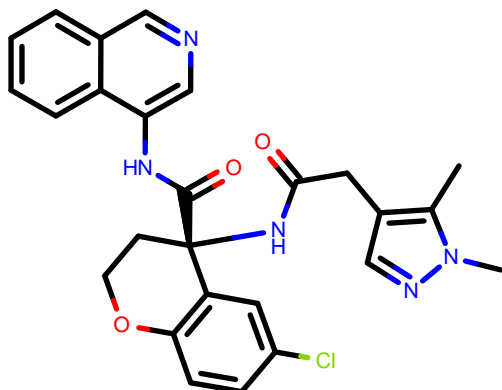
DDG (kcal/mol):

-1.18

dDDG (kcal/mol):

0.20

EN300-219437_1_1_1



CID: EN300-219437_1_1_1

SMILES:

Cc1c(cnn1C)CC(=O)N[C@@]2(CCCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN6867

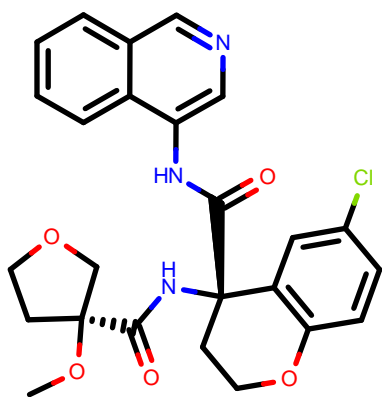
DDG (kcal/mol):

-1.18

dDDG (kcal/mol):

0.31

EN300-174668_1_2_1



CID: EN300-174668_1_2_1

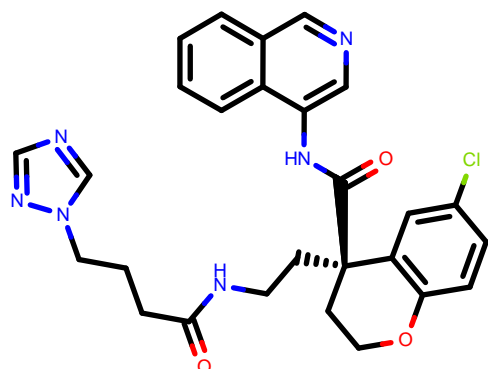
SMILES: CO[C@]1(CCOC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccoc5

RUN: RUN3002

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.38

EN300-316216_3_1_1



CID: EN300-316216_3_1_1

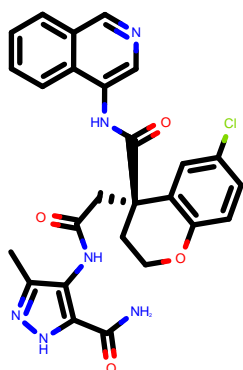
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCC5N5nn5

RUN: RUN5503

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.30

EN300-67302_1_1_1



CID: EN300-67302_1_1_1

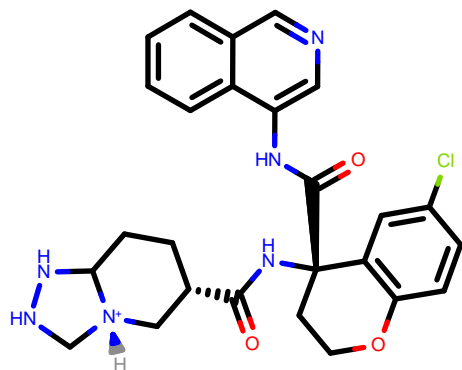
SMILES: Cc1c(c(n[nH]1)C(=O)N)NC(=O)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccoc5

RUN: RUN6532

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.30

EN300-51350_1_2_1



CID: EN300-51350_1_2_1

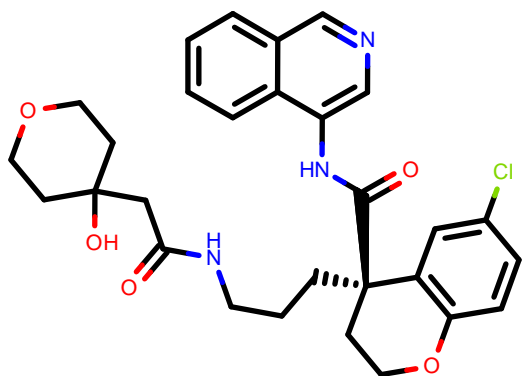
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N[C@@]C@H]5CCc6nncn6C5

RUN: RUN3451

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.23

EN300-151423_4_1_1



CID: EN300-151423_4_1_1

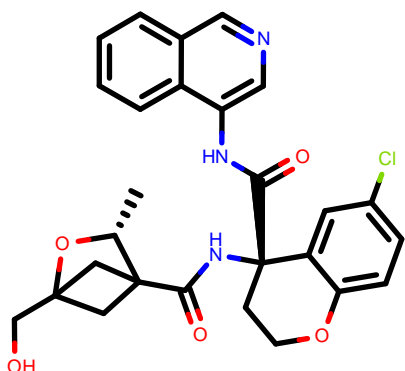
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CCOCC5)O

RUN: RUN7766

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.27

EN300-6491795_1_1_1



CID: EN300-6491795_1_1_1

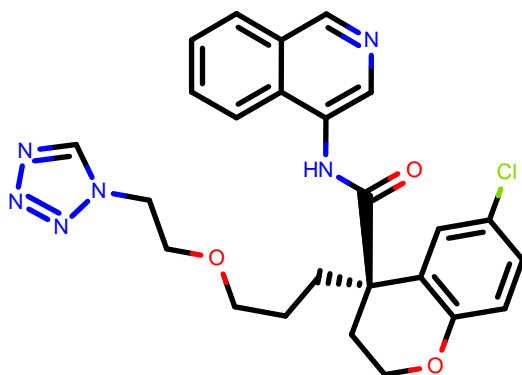
SMILES: C[C@@H]1C2(CC(C2)O1)CO)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN5043

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-364679_4_1_1



CID: EN300-364679_4_1_1

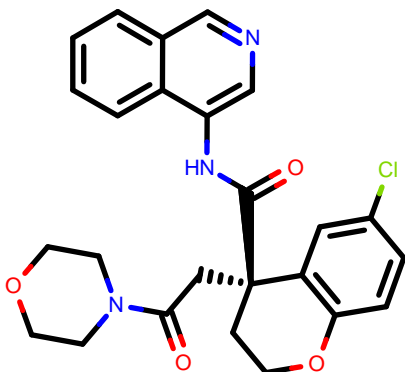
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCn5cnn5

RUN: RUN4246

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-18064_1_1_1



CID: EN300-18064_1_1_1

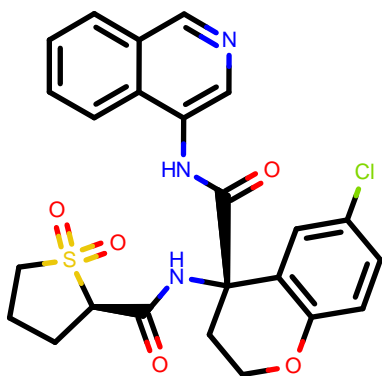
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOCC5

RUN: RUN6971

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.22

EN300-88656_1_2_1



CID: EN300-88656_1_2_1

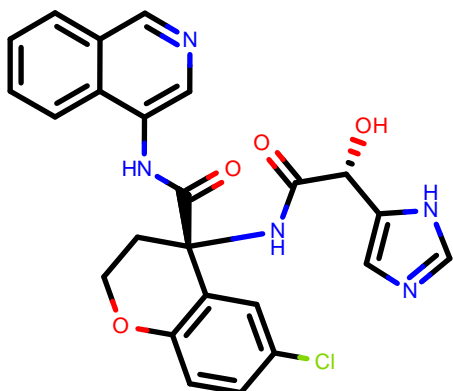
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCCS(=O)=O

RUN: RUN3357

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.32

EN300-254121_1_1_1



CID: EN300-254121_1_1_1

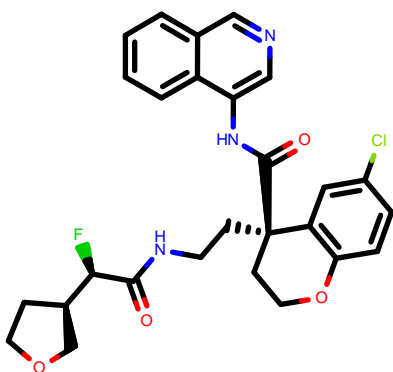
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5cnc[nH]5)O

RUN: RUN3781

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.31

EN300-783124_3_1_1



CID: EN300-783124_3_1_1

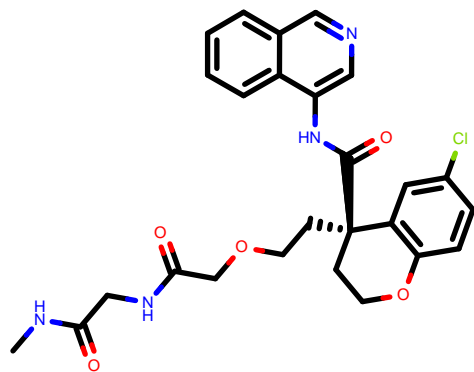
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C)F

RUN: RUN3615

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.23

EN300-23223_3_1_1



CID: EN300-23223_3_1_1

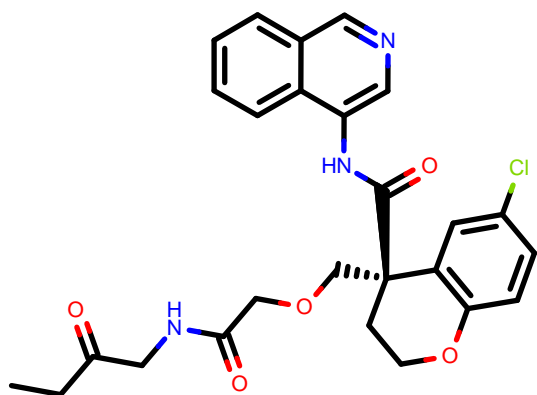
SMILES: CNC(=O)CNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4819

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.27

EN300-132624_2_1_1



CID: EN300-132624_2_1_1

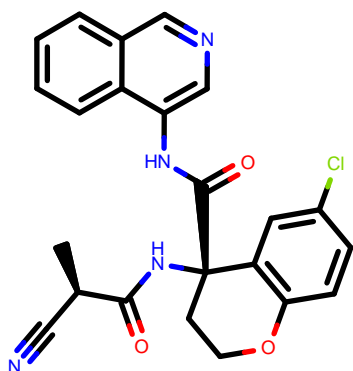
SMILES: CCC(=O)CNC(=O)COC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6301

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.35

EN300-72730_1_2_1



CID: EN300-72730_1_2_1

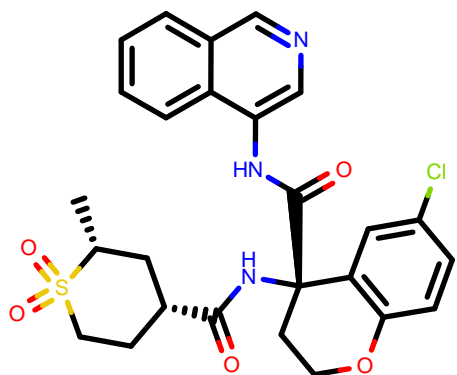
SMILES: C[C@H](C#N)C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5481

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.17

EN300-6082676_1_1_1



CID: EN300-6082676_1_1_1

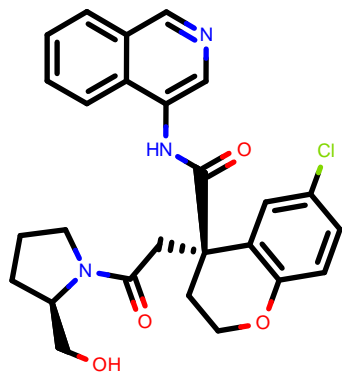
SMILES: C[C@@H]1[C@@H](C(S(=O)(=O)N1)C(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN4465

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.28

EN300-55109_1_1_1



CID: EN300-55109_1_1_1

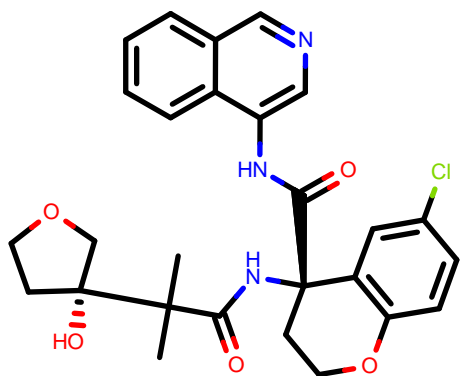
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5CO

RUN: RUN5293

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.24

EN300-1630093_1_2_1



CID: EN300-1630093_1_2_1

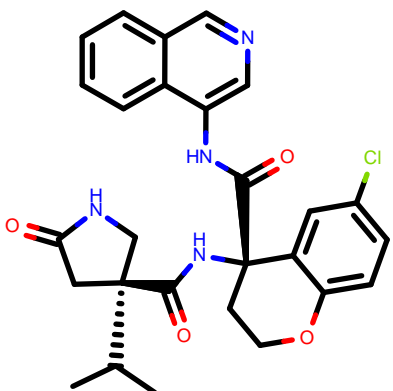
SMILES: CC(C)(C(=O)N[C@@]1(CCOC2C1CC(=O)C)C(=O)Nc3ccc4c3ccc4)[C@@]5(CCOC5)O

RUN: RUN6613

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.26

EN300-211203_1_1_1



CID: EN300-211203_1_1_1

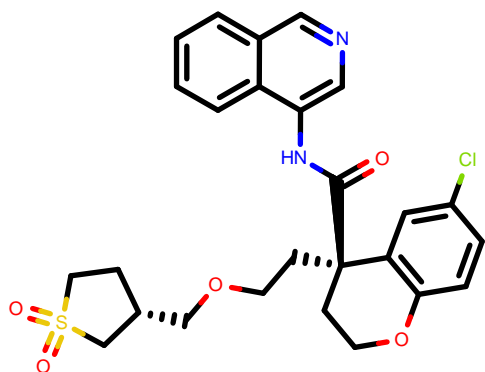
SMILES: CC(C)[C@@]1(CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN3018

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.25

EN300-1448603_3_2_1



CID: EN300-1448603_3_2_1

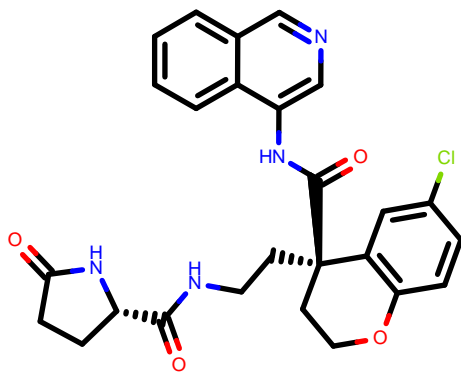
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CCOC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN4926

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.30

EN300-72896_3_1_1



CID: EN300-72896_3_1_1

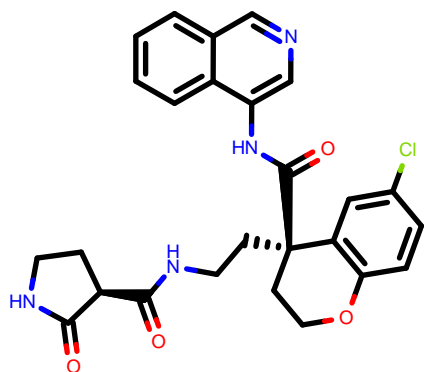
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CCNC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN5904

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-94945_3_1_1



CID: EN300-94945_3_1_1

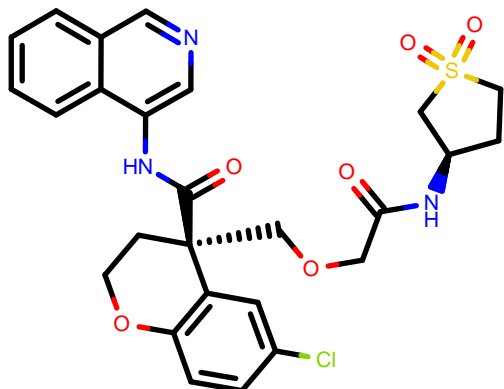
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCNC5=O

RUN: RUN6884

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.30

EN300-05512_2_1_1



CID: EN300-05512_2_1_1

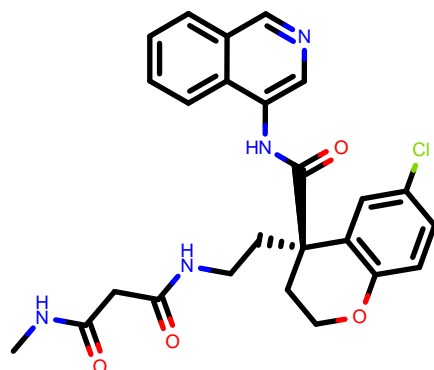
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@@H]5CCS(=O)(=O)C5

RUN: RUN5201

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.33

EN300-128463_3_1_1



CID: EN300-128463_3_1_1

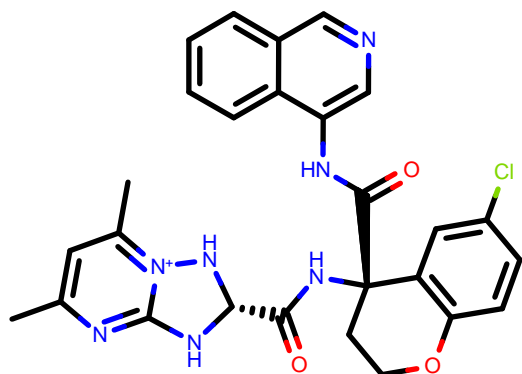
SMILES: CNC(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN3858

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.31

EN300-00904_1_1_2



CID: EN300-00904_1_1_2

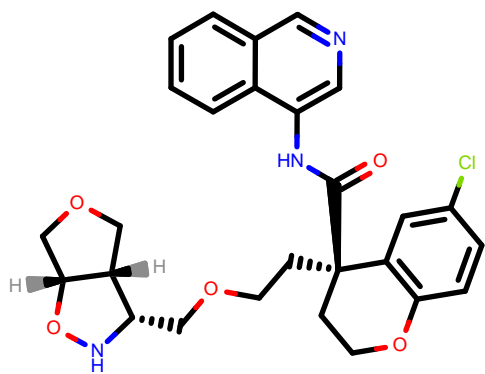
SMILES: Cc1cc([n+]2c(n1)N[C@@H](N2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6)C

RUN: RUN3381

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.35

EN300-7436306_3_1_2



CID: EN300-7436306_3_1_2

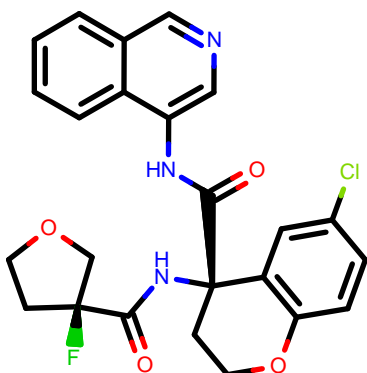
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4C)COC[C@@H]5[C@@H]6COC[C@@H]6O5

RUN: RUN3069

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.34

EN300-188356_1_1_1



CID: EN300-188356_1_1_1

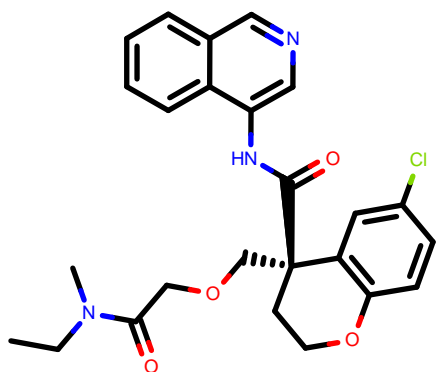
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4C)NC(=O)[C@@]5(C)C(COC)F

RUN: RUN5942

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.30

EN300-1253122_2_1_1



CID: EN300-1253122_2_1_1

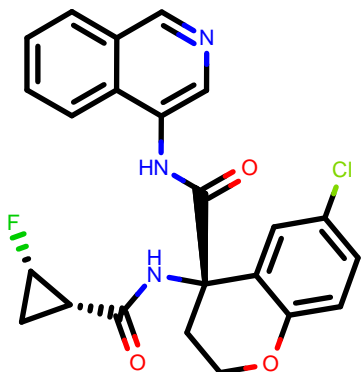
SMILES: CCN(C)C(=O)COC[C@@]1(C)CCOC2c1cc(cc2C)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3607

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-1654606_1_1_1



CID: EN300-1654606_1_1_1

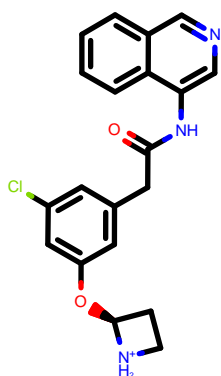
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4C)NC(=O)[C@@]5(C)C(C)F

RUN: RUN5095

DDG (kcal/mol): -1.13

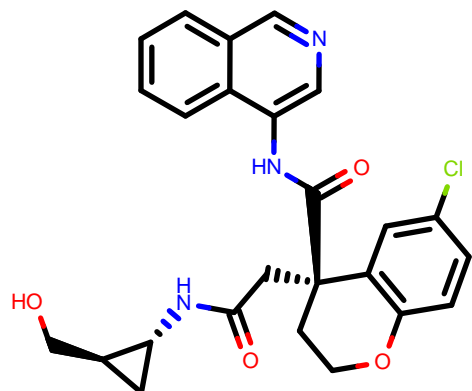
dDDG (kcal/mol): 0.17

PET-UNK-cf04cb02-1_2



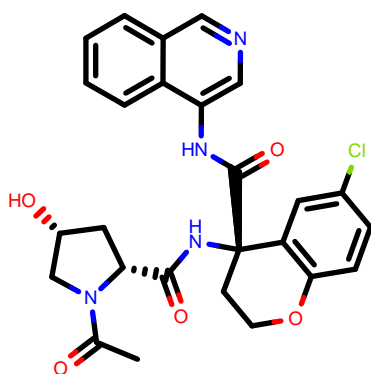
CID:	PET-UNK-cf04cb02-1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC[NH2+]4</chem>
RUN:	RUN299
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.36

EDJ-MED-d203f206-34_1



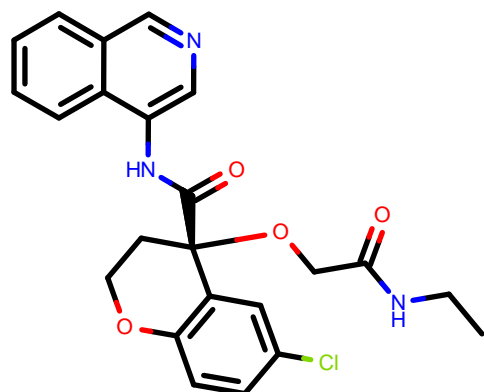
CID:	EDJ-MED-d203f206-34_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4cc3cc(c4)Cl)CC(=O)N[C@@H]5C[C@H]5CO</chem>
RUN:	RUN2458
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.29

EN300-158260_1_1_1



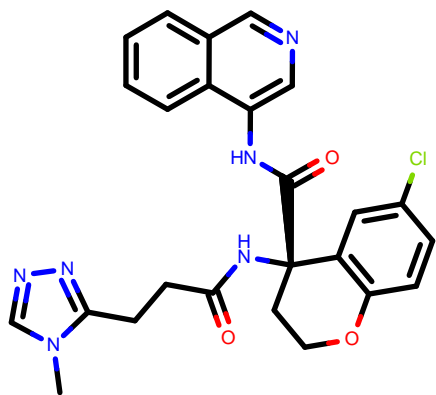
CID:	EN300-158260_1_1_1
SMILES:	<chem>CC(=O)N1C[C@@H]1[C@@H]2[C@@]3(CO)N[C@@]2(CCOc3cc2cc(c3)Cl)C1=O)Nc4ccc5c4ccc5O</chem>
RUN:	RUN4850
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.25

EN300-7003350_1_1_1



CID:	EN300-7003350_1_1_1
SMILES:	<chem>CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4</chem>
RUN:	RUN4718
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.20

EN300-1138792_1_1_1



CID: EN300-1138792_1_1_1

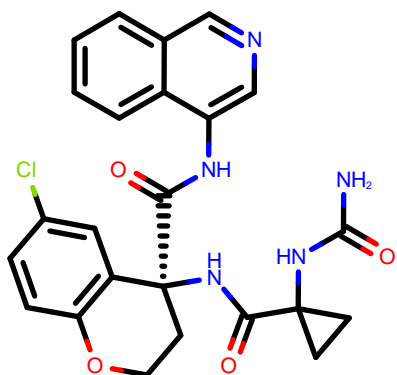
SMILES: Cn1cnc1CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3216

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.23

EN300-123614_1_1_1



CID: EN300-123614_1_1_1

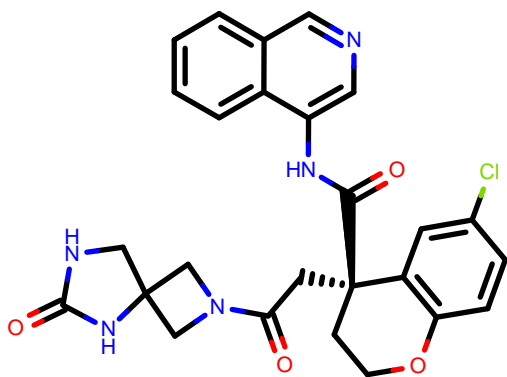
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(C)C5NC(=O)N

RUN: RUN3594

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.32

EN300-1605226_1_1_1



CID: EN300-1605226_1_1_1

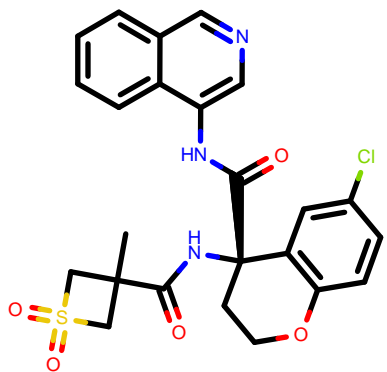
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CNC(=O)N6

RUN: RUN7140

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.30

EN300-1718364_1_1_1



CID: EN300-1718364_1_1_1

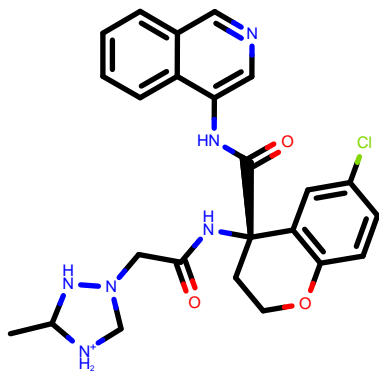
SMILES: CC1(CS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3982

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-7473354_1_1_1



CID: EN300-7473354_1_1_1

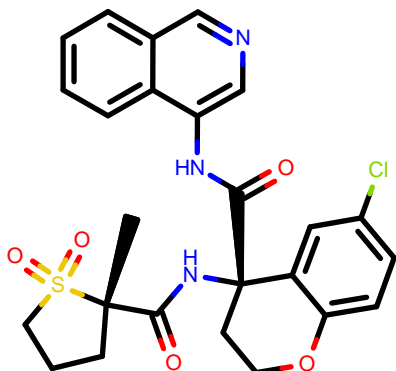
SMILES: Cc1ncn(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5780

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.25

EN300-373476_1_2_1



CID: EN300-373476_1_2_1

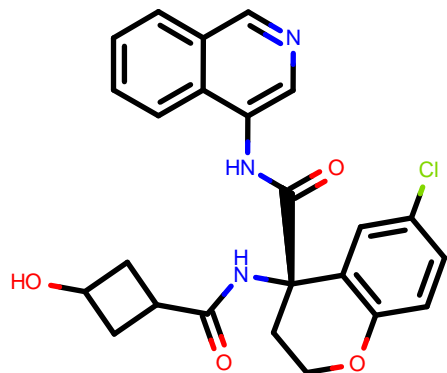
SMILES: C[C@@]1(CCCS1(=O)=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7520

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.34

EN300-306026_1_1_1



CID: EN300-306026_1_1_1

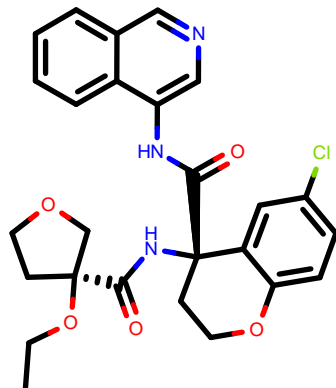
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(C5)O

RUN: RUN4203

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.22

EN300-259694_1_2_1



CID: EN300-259694_1_2_1

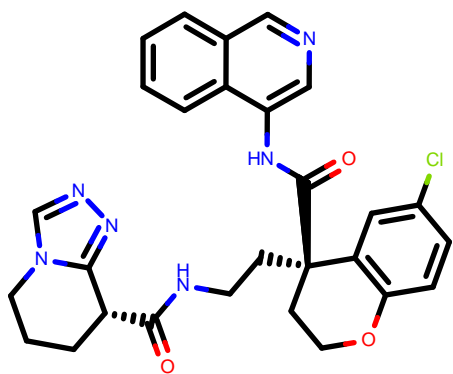
SMILES: CCOC[C@@]1(CCOc1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5248

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.35

EN300-748981_3_1_1



CID: EN300-748981_3_1_1

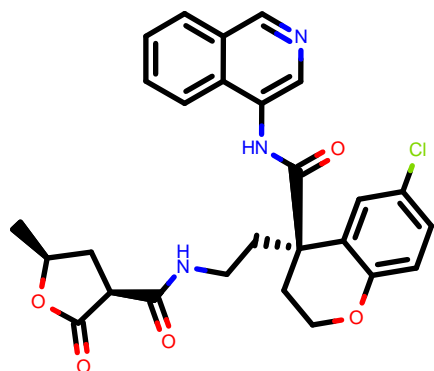
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCNC(=O)[C@@H]5CCCN6c5nc6

RUN: RUN3859

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.31

EN300-7444533_3_4_1



CID: EN300-7444533_3_4_1

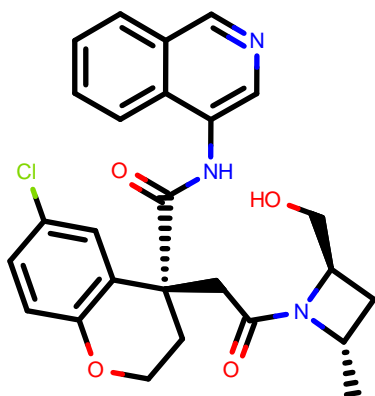
SMILES: C[C@@H]1C[C@@H](C(=O)O1)C(=O)NCC[C@@]2(CCOc3ccc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5650

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.36

EN300-1709410_1_2_1



CID: EN300-1709410_1_2_1

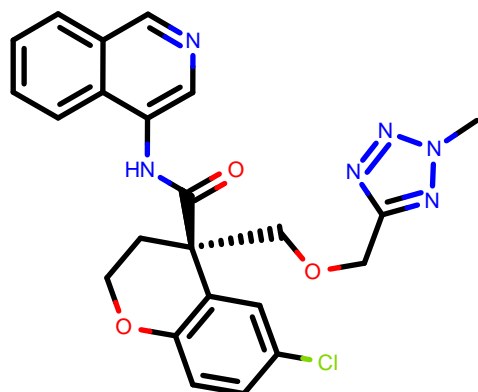
SMILES: C[C@@H]1C[C@@H](N1C(=O)C[C@@]2(CCOc3ccc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)CO

RUN: RUN4612

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.26

EN300-90225_2_1_1



CID: EN300-90225_2_1_1

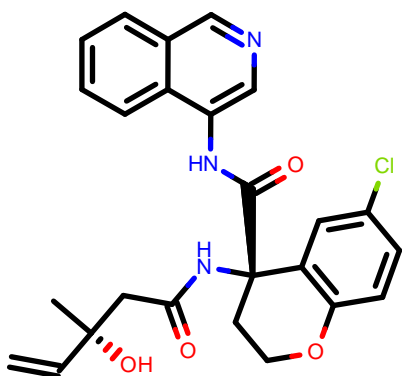
SMILES: Cn1nc(nn1)COC[C@@]2(CCOc3ccc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3327

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.24

EN300-181938_1_1_1



CID: EN300-181938_1_1_1

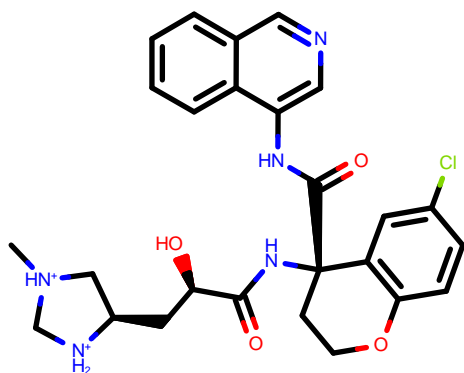
SMILES: C[C@@](C)(C(=O)N[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)(C=C)O

RUN: RUN3699

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

EN300-1725538_1_2_1



CID: EN300-1725538_1_2_1

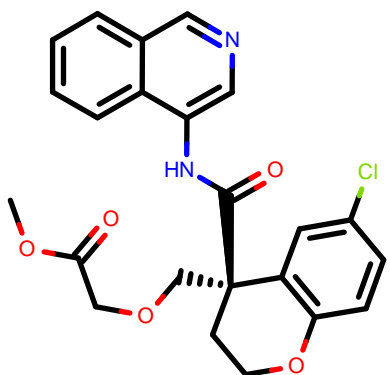
SMILES: Cn1cc(nc1)C[C@@H](C(=O)N[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccc5)O

RUN: RUN7008

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.31

EN300-19700_2_1_1



CID: EN300-19700_2_1_1

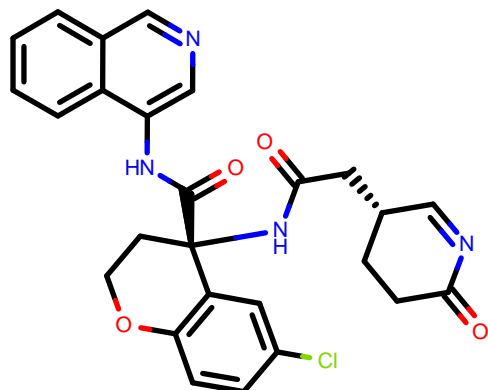
SMILES: COC(=O)COC[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN: RUN5245

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.20

EN300-246992_1_2_1



CID: EN300-246992_1_2_1

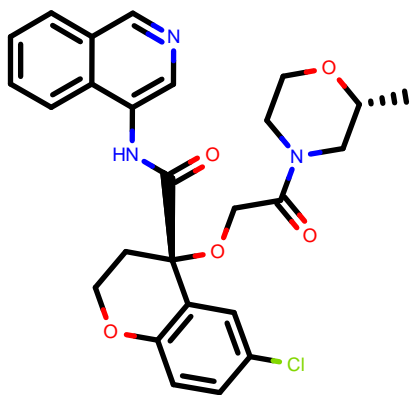
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCC(=O)NCS

RUN: RUN4329

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.22

EN300-25572_1_1_1



CID: EN300-25572_1_1_1

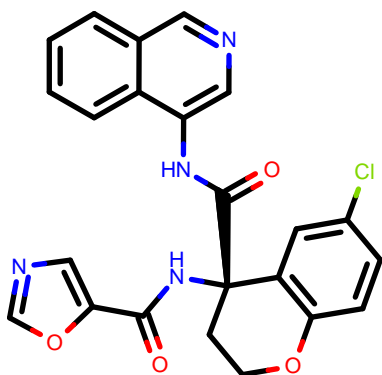
SMILES: C[C@@H]1CN(CCO1)C(=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7491

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-25446_1_1_1



CID: EN300-25446_1_1_1

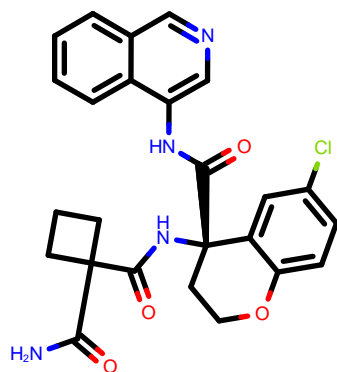
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnco5

RUN: RUN3051

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.17

EN300-68747_1_1_1



CID: EN300-68747_1_1_1

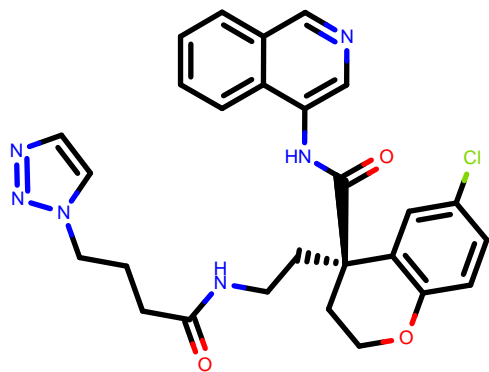
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)C(=O)N

RUN: RUN5858

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.23

EN300-124301_3_1_1



CID: EN300-124301_3_1_1

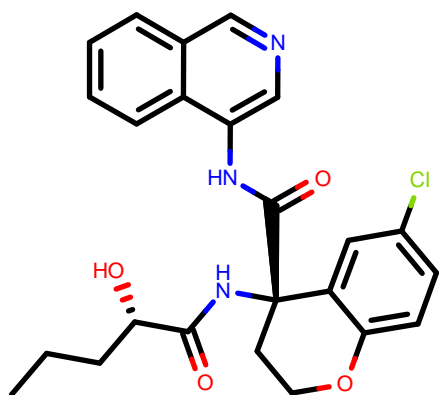
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCC5ccn5

RUN: RUN4927

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

EN300-300217_1_2_1



CID: EN300-300217_1_2_1

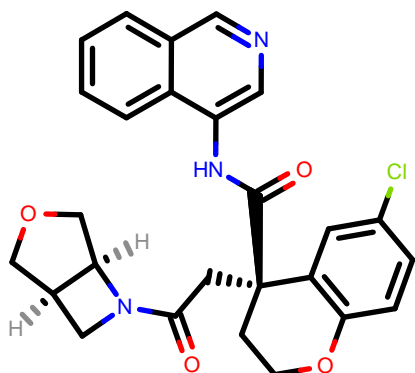
SMILES: C/C=C/[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4O

RUN: RUN4697

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.29

EN300-7493296_1_1_1



CID: EN300-7493296_1_1_1

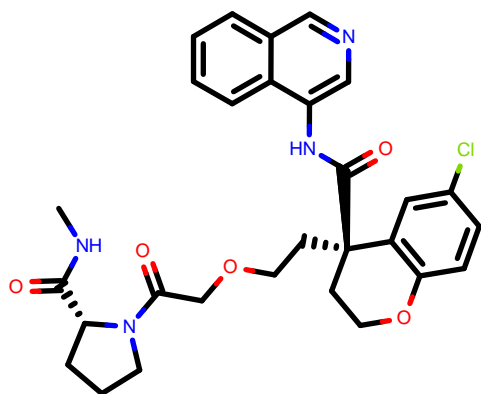
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H]5COc6

RUN: RUN6292

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.24

EN300-48902_3_2_1



CID: EN300-48902_3_2_1

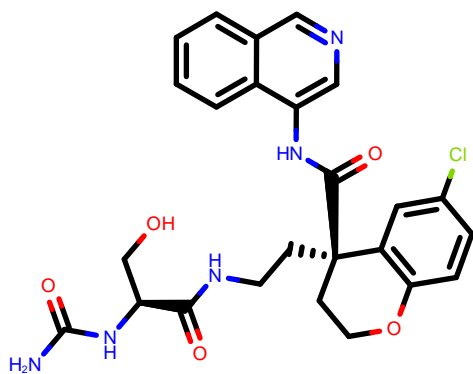
SMILES: CNC(=O)[C@@H]1CCCN1C(=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7548

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.36

EN300-10170_3_2_1



CID: EN300-10170_3_2_1

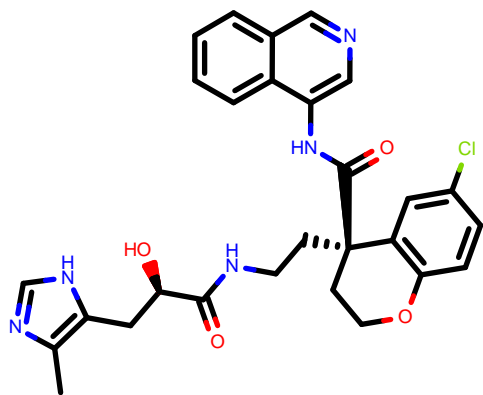
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](CO)NC(=O)N

RUN: RUN4730

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.35

EN300-7494324_3_2_1



CID: EN300-7494324_3_2_1

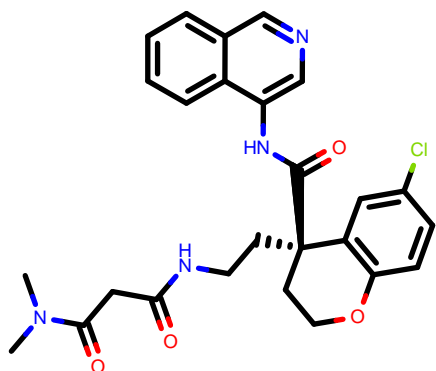
SMILES: Cc1c(nc[nH]1)C[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN6630

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.32

EN300-93573_3_1_1



CID: EN300-93573_3_1_1

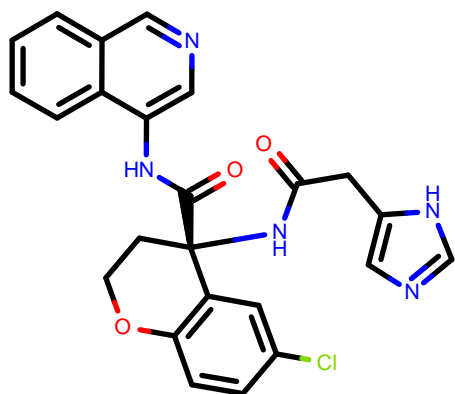
SMILES: CN(C)C(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN4238

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-342226_1_1_1



CID: EN300-342226_1_1_1

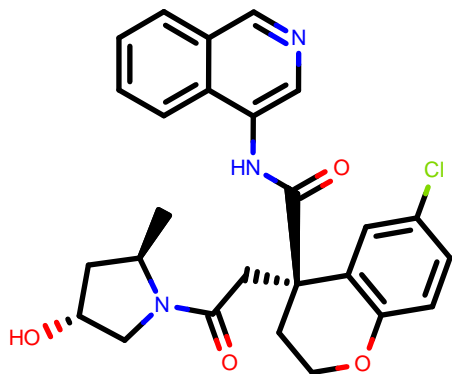
SMILES: c1ccc2c(c1)cncc2N(C(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc[nH]5)

RUN: RUN4605

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.27

EN300-173562_1_3_1



CID: EN300-173562_1_3_1

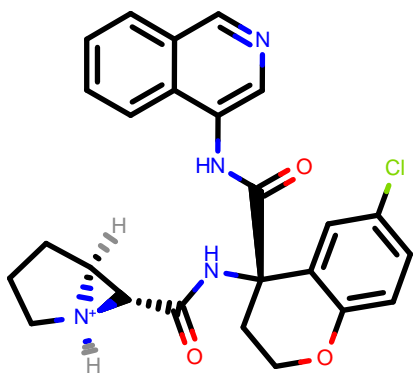
SMILES: C[C@@H]1C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3091

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.27

EDG-MED-90036822-73_2



CID: EDG-MED-90036822-73_2

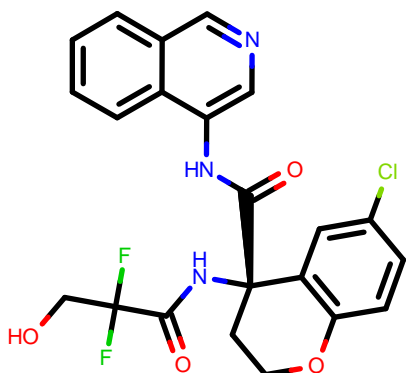
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]C@H]N@H+]5CCO5

RUN: RUN1616

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-123489_1_1_1



CID: EN300-123489_1_1_1

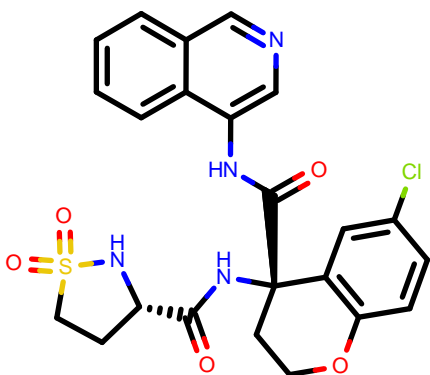
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(O)(F)F

RUN: RUN5119

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.22

EN300-45049_1_1_1



CID: EN300-45049_1_1_1

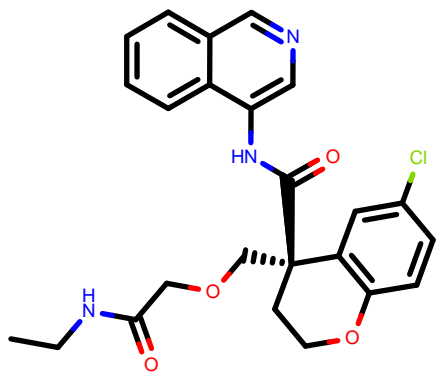
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]5CCS(=O)=O]N5

RUN: RUN4681

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.29

EN300-7003350_2_1_1



CID: EN300-7003350_2_1_1

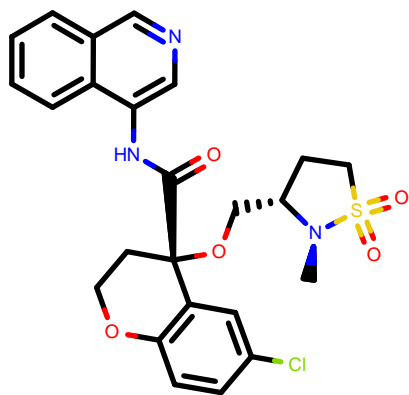
SMILES: CCNC(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6685

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.20

EN300-393148_1_1_1



CID: EN300-393148_1_1_1

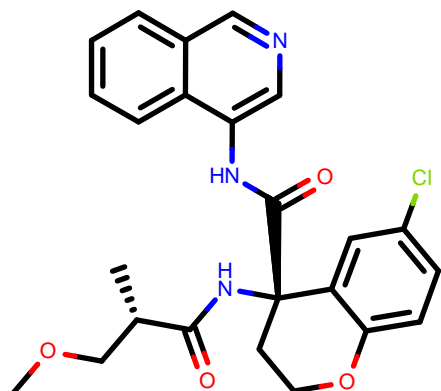
SMILES: C[N@]1[C@@H](CCS1(=O)=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6764

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-69162_1_1_1



CID: EN300-69162_1_1_1

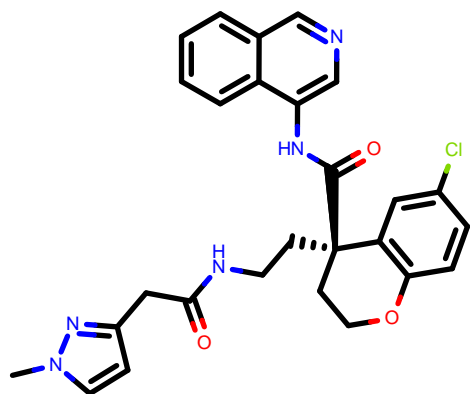
SMILES: C[C@@H](COC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN3886

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.21

EN300-258702_3_1_1



CID: EN300-258702_3_1_1

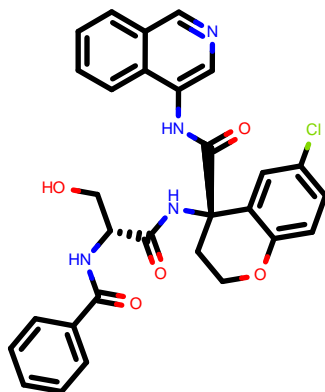
SMILES: Cn1ccc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4434

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.28

EN300-50228_1_2_1



CID: EN300-50228_1_2_1

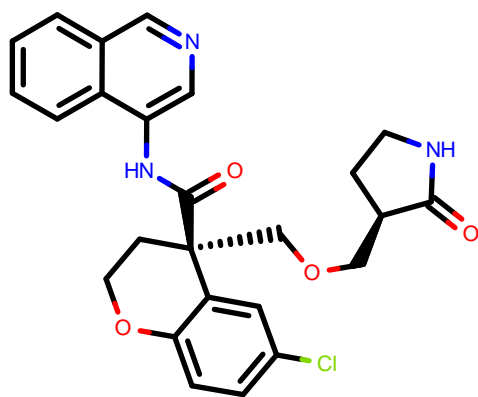
SMILES: c1ccc(cc1)C(=O)N[C@@H](CO)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5104

DDG (kcal/mol): -1.09

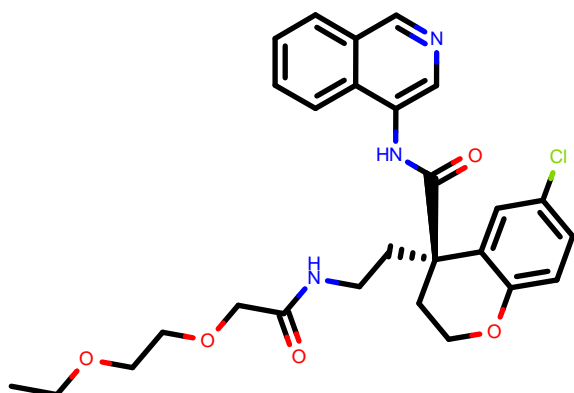
dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-6_1



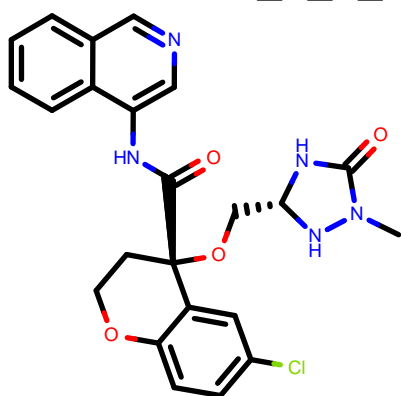
CID:	EDJ-MED-fcba3f31-6_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O</chem>
RUN:	RUN2383
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.26

EN300-54304_3_1_1



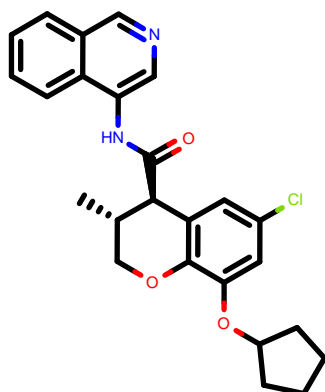
CID:	EN300-54304_3_1_1
SMILES:	<chem>CCOCCOCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN6659
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.32

EN300-124918_1_1_2



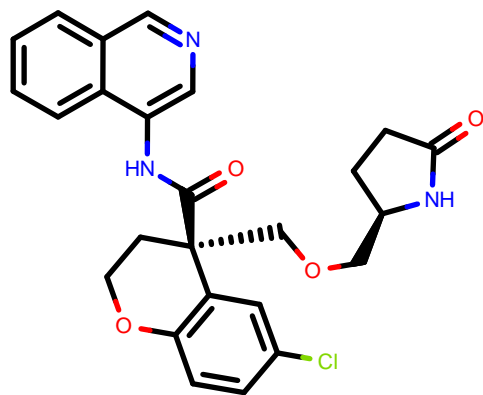
CID:	EN300-124918_1_1_2
SMILES:	<chem>CN1C(=O)N[C@@H]([NH2+][1]CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN4058
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-4_1_1



CID:	DAR-DIA-0d514e7d-4_1_1
SMILES:	<chem>C[C@@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN4177
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.24

EDJ-MED-fcba3f31-9_1



CID: EDJ-MED-fcba3f31-9_1

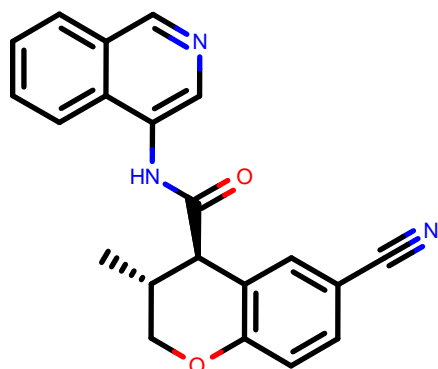
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)COC[C@H]5CCCC(=O)N5

RUN: RUN2356

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.26

DAR-DIA-0d514e7d-8_1_1



CID: DAR-DIA-0d514e7d-8_1_1

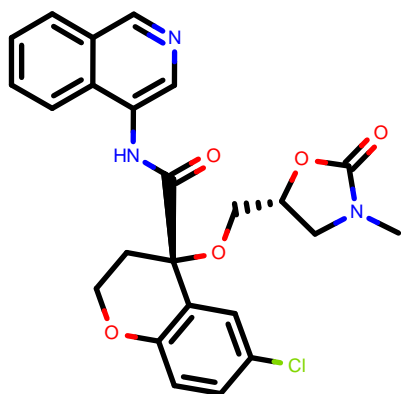
SMILES: C[C@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C#N

RUN: RUN5721

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.07

EN300-222969_1_1_1



CID: EN300-222969_1_1_1

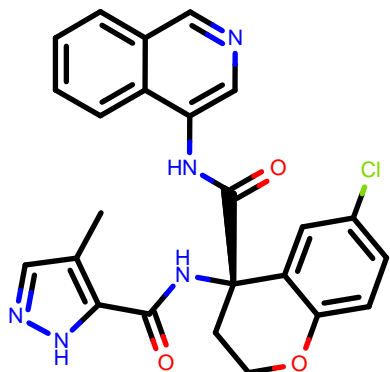
SMILES: CN1C[C@@H](OC1=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3626

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.30

EN300-248178_1_1_1



CID: EN300-248178_1_1_1

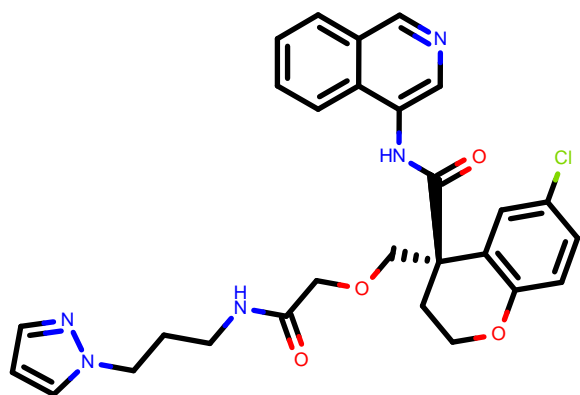
SMILES: Cc1cn[nH]c1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5045

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.21

EN300-47500_2_1_1



CID: EN300-47500_2_1_1

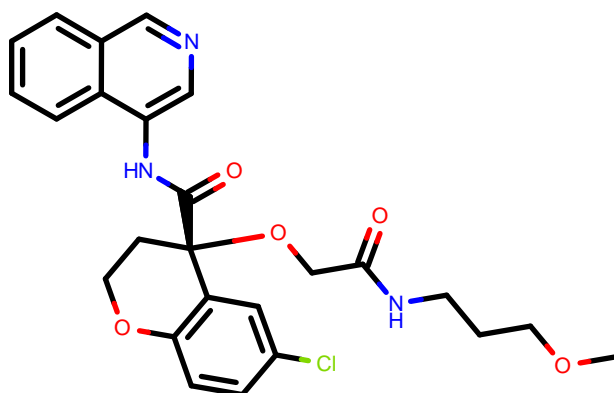
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NCCCn5cccn5

RUN: RUN5748

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.36

EN300-04492_1_1_1



CID: EN300-04492_1_1_1

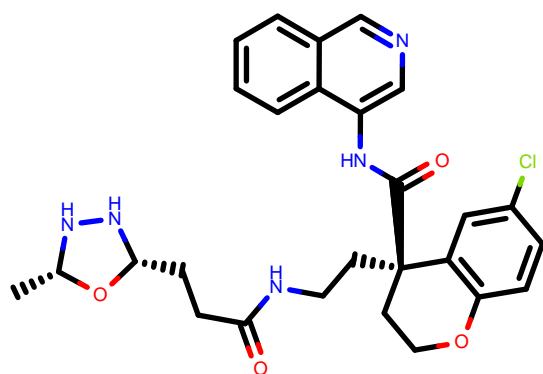
SMILES: COCCCN(C(=O)CO)[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccn4

RUN: RUN5646

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.24

EN300-304662_3_1_1



CID: EN300-304662_3_1_1

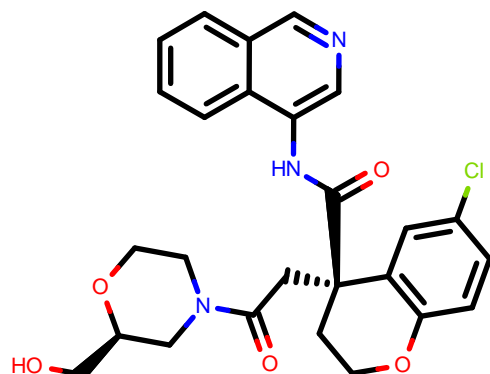
SMILES: C[C@@H]1NN[C@@H](O1)CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccn5

RUN: RUN7015

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.31

EN300-101373_1_1_1



CID: EN300-101373_1_1_1

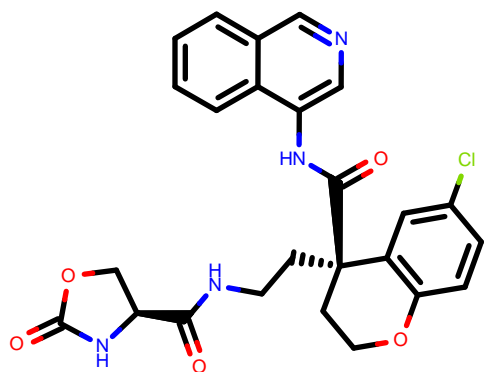
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CO

RUN: RUN4333

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.41

EN300-126389_3_1_1



CID: EN300-126389_3_1_1

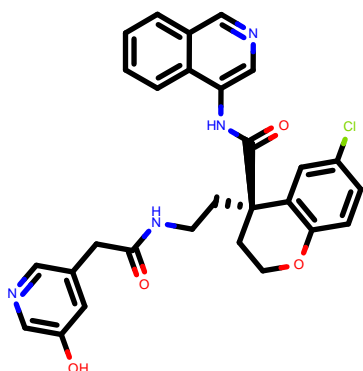
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5H5COC(=O)N5

RUN: RUN5683

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-222620_3_1_1



CID: EN300-222620_3_1_1

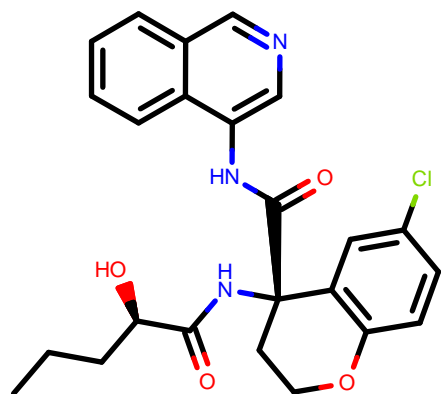
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5ccn(c5)O

RUN: RUN3428

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.43

EN300-219531_1_2_1



CID: EN300-219531_1_2_1

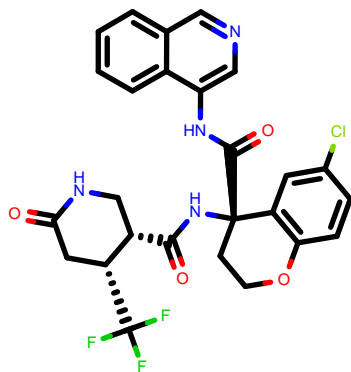
SMILES: CCC[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4)O

RUN: RUN3259

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.30

EN300-208959_1_4_1



CID: EN300-208959_1_4_1

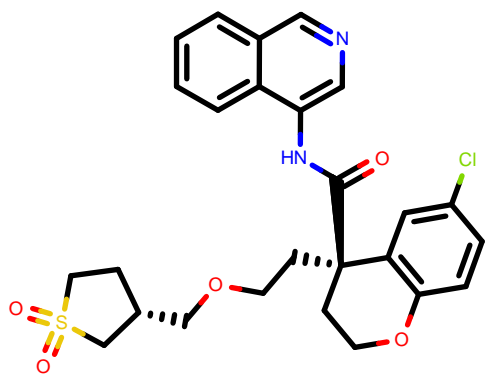
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5CNC1=O[C@H](C(F)(F)F)F5

RUN: RUN5609

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-1448603_3_2_1



CID: EN300-1448603_3_2_1

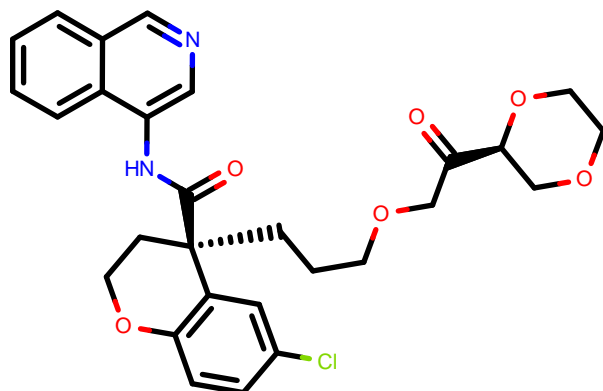
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5SCCS(=O)=O5

RUN: RUN3872

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.31

EN300-6238494_4_1_1



CID: EN300-6238494_4_1_1

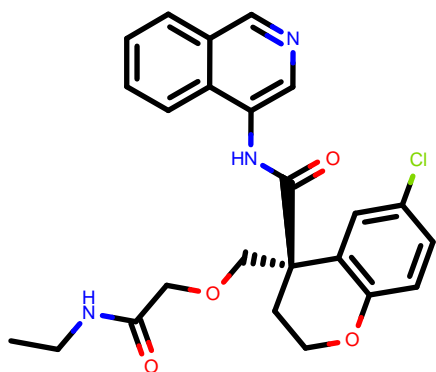
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCOCOC(=O)[C@@H]5COCOC5

RUN: RUN4485

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.33

EN300-7003350_2_1_1



CID: EN300-7003350_2_1_1

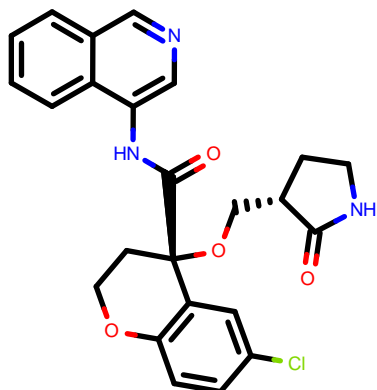
SMILES: CCNC(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6714

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-246248_1_1_1



CID: EN300-246248_1_1_1

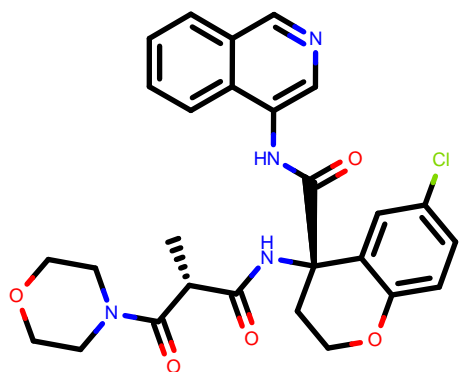
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCNC5=O

RUN: RUN5220

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-2855057_1_2_1



CID: EN300-2855057_1_2_1

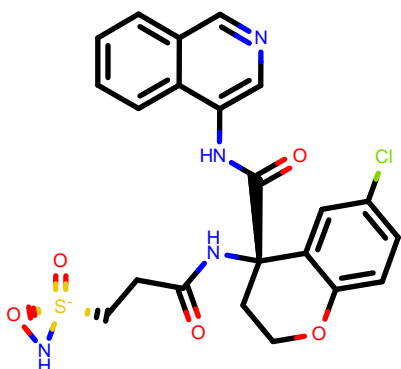
SMILES: C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)C(=O)N5CCOCC5

RUN: RUN6274

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-31553_1_1_1



CID: EN300-31553_1_1_1

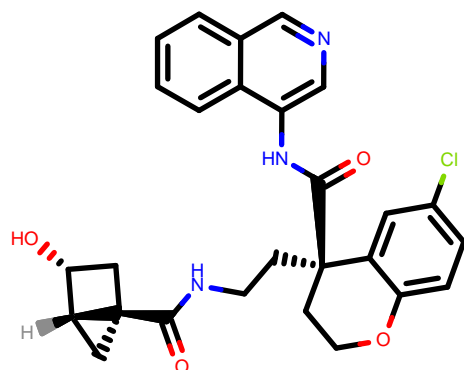
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)NC(=O)CCS(=O)(=O)N

RUN: RUN4471

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-7433125_3_1_1



CID: EN300-7433125_3_1_1

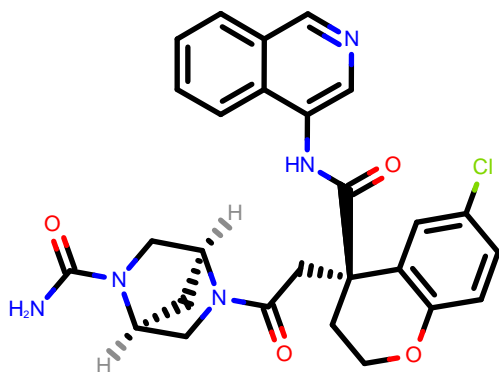
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CC(=O)C(O)C5CCN5C(=O)O

RUN: RUN6768

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.22

KAD-UNI-8a629cb0-42_1



CID: KAD-UNI-8a629cb0-42_1

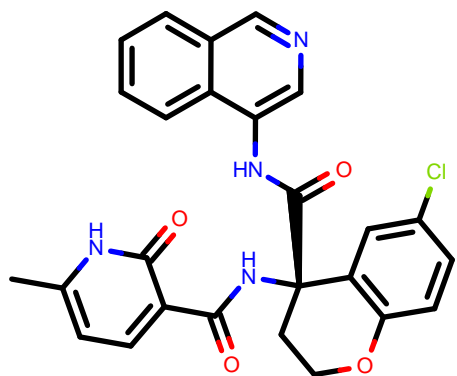
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(C)C5=O

RUN: RUN1966

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.31

EN300-39151_1_1_1



CID: EN300-39151_1_1_1

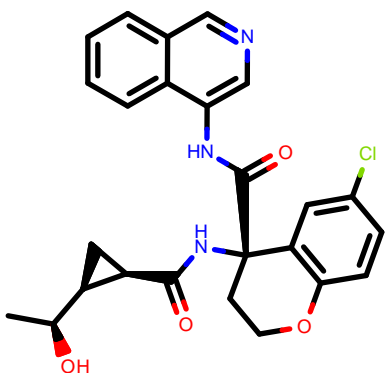
SMILES: Cc1ccc(c(O)[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN6097

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.33

EN300-6729572_1_7_1



CID: EN300-6729572_1_7_1

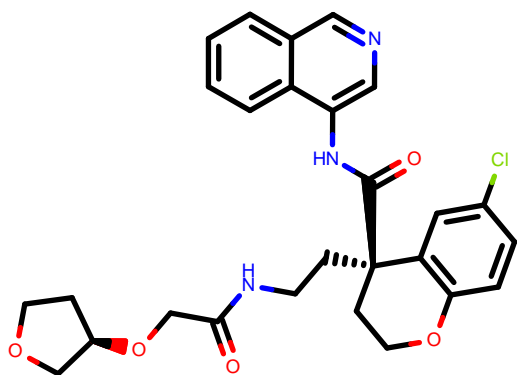
SMILES: C[C@@H]([C@H]1C[C@H]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5O

RUN: RUN5484

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.26

EN300-99391_3_1_1



CID: EN300-99391_3_1_1

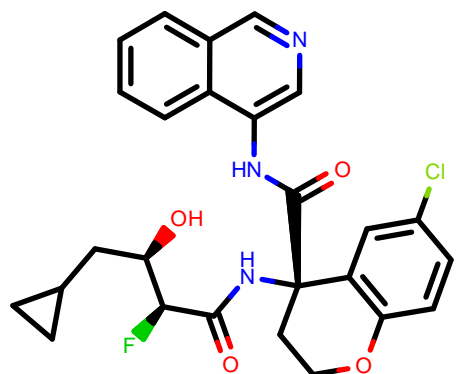
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN4035

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.34

EDG-MED-90036822-108_2



CID: EDG-MED-90036822-108_2

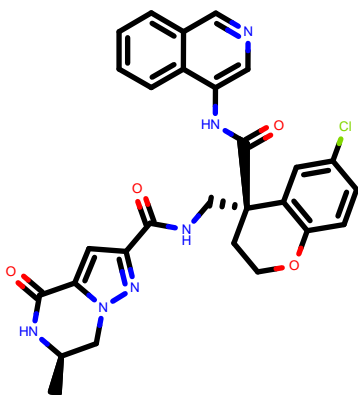
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]([C@@H](CC5CC5)O)F

RUN: RUN1715

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-265285_2_1_1



CID: EN300-265285_2_1_1

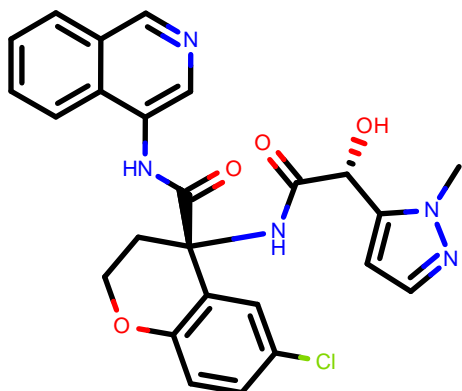
SMILES: C[C@@H]1Cn2c(cc(n2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6)C(=O)N1

RUN: RUN5147

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.36

EN300-6473273_1_2_1



CID: EN300-6473273_1_2_1

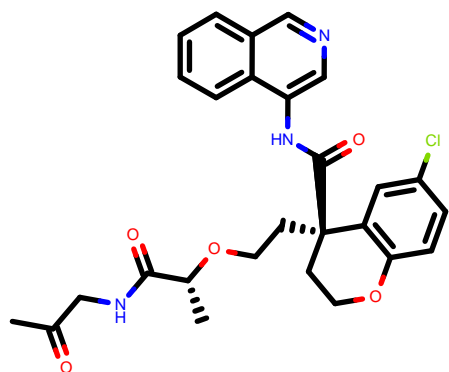
SMILES: Cn1c(ccn1)C[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN5285

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-131093_3_2_1



CID: EN300-131093_3_2_1

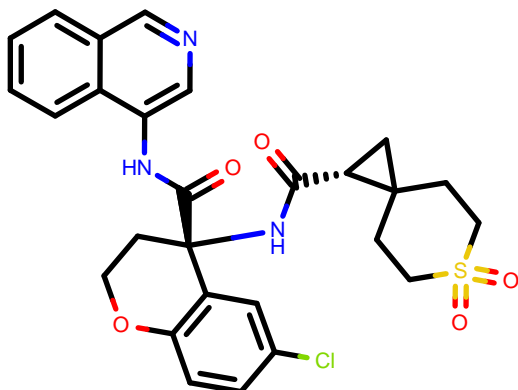
SMILES: C[C@H](C(=O)NCC(=O)C)OCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN3058

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-141809_1_1_1



CID: EN300-141809_1_1_1

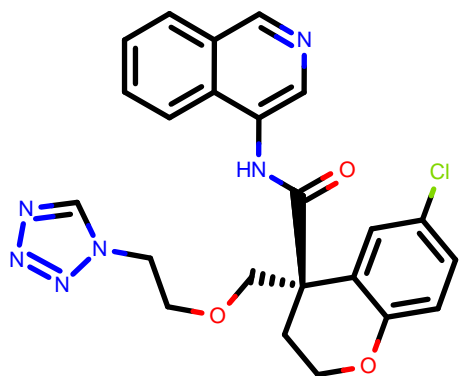
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C(=O)Nc5ccc6c5ccc6)S(=O)(=O)C6

RUN: RUN5790

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.31

EN300-364679_2_1_1



CID: EN300-364679_2_1_1

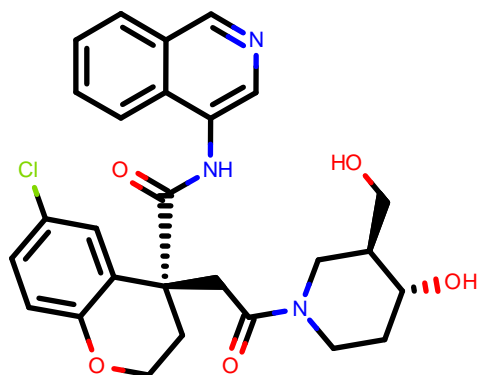
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cnnn5

RUN: RUN3246

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-233678_1_2_1



CID: EN300-233678_1_2_1

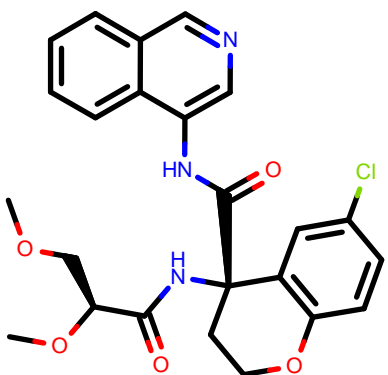
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(O)N5CC[C@H](C5)O

RUN: RUN3773

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.29

EN300-305282_1_1_1



CID: EN300-305282_1_1_1

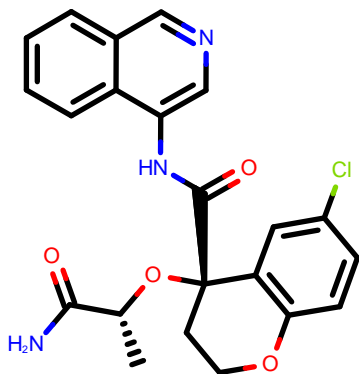
SMILES: COC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)OC

RUN: RUN5979

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.42

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

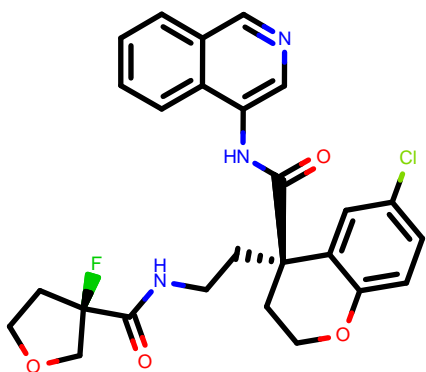
SMILES: C[C@@H](C(=O)N)O[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4

RUN: RUN5906

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.18

EN300-188356_3_2_1



CID: EN300-188356_3_2_1

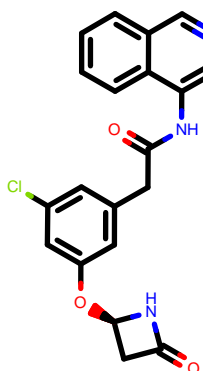
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C@5(C(COC5)F

RUN: RUN5713

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.28

EDJ-MED-7320d5d2-1_1



CID: EDJ-MED-7320d5d2-1_1

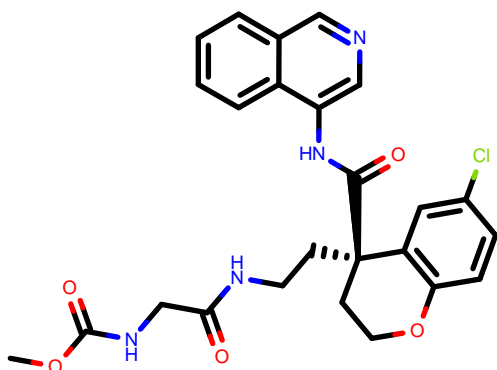
SMILES: c1ccc2c(c1)ncnc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4

RUN: RUN88

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.44

EN300-50009_3_1_1



CID: EN300-50009_3_1_1

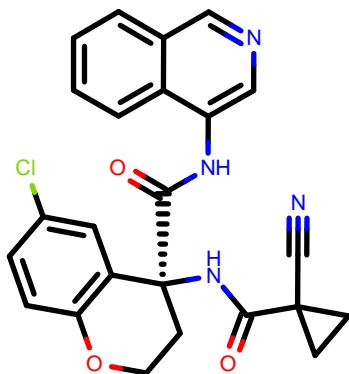
SMILES: COC(=O)NCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN3676

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.31

EN300-114082_1_1_1



CID: EN300-114082_1_1_1

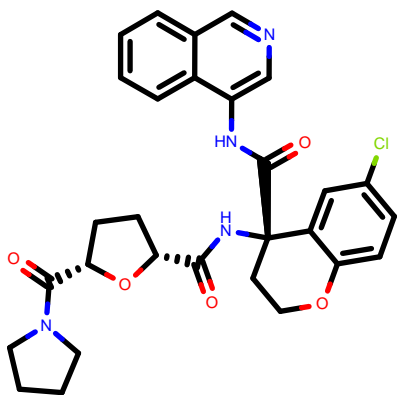
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C(C5)C#N

RUN: RUN3561

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.21

ALP-UNI-dbbfd3db-6_4



CID: ALP-UNI-dbbfd3db-6_4

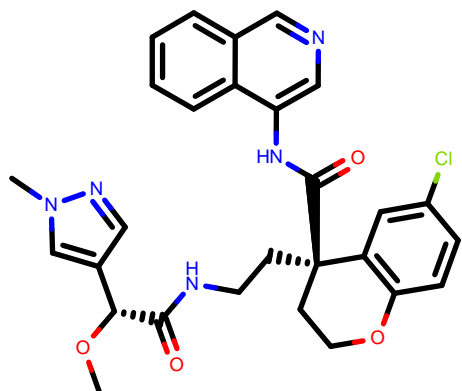
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(C)CCOc4cc3cc(c4)C)NC(=O)C@H5CC(C@H)O5(C)N6CCCC6

RUN: RUN2612

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.39

EN300-198240_3_2_1



CID: EN300-198240_3_2_1

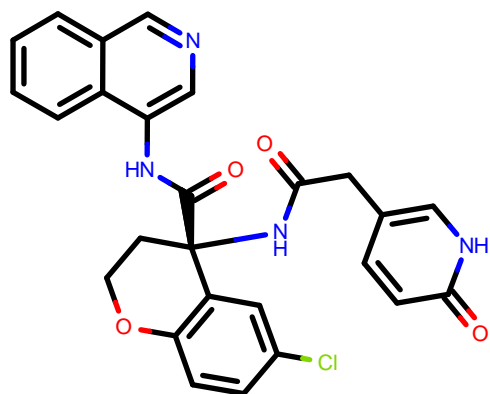
SMILES: Cn1cc(en1)[C@H](C(=O)NCC[C@@2(C)CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5)OC

RUN: RUN6390

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

EN300-189672_1_1_1



CID: EN300-189672_1_1_1

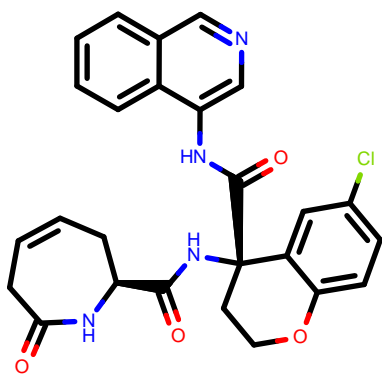
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@3(C)CCOc4c3cc(cc4)C)NC(=O)Cc5ccc(=O)[nH]5

RUN: RUN3906

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-80083_1_1_1



CID: EN300-80083_1_1_1

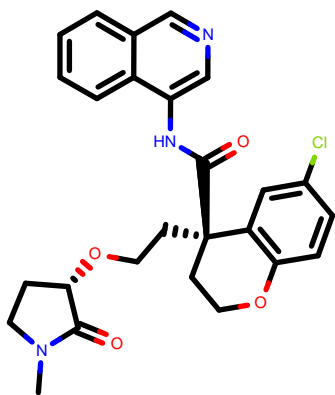
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@3(C)CCOc4c3cc(cc4)C)NC(=O)C@H5CCCCC(=O)N5

RUN: RUN4497

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.30

EN300-98648_3_1_1



CID: EN300-98648_3_1_1

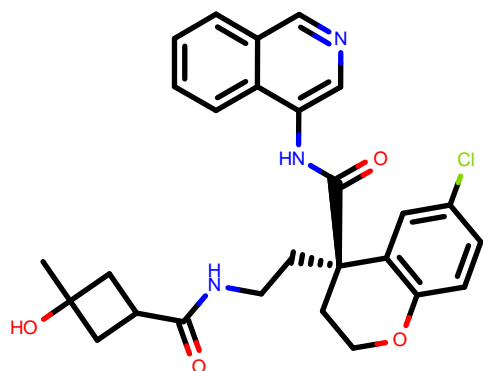
SMILES: CN1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN4013

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.24

EN300-247343_3_1_1



CID: EN300-247343_3_1_1

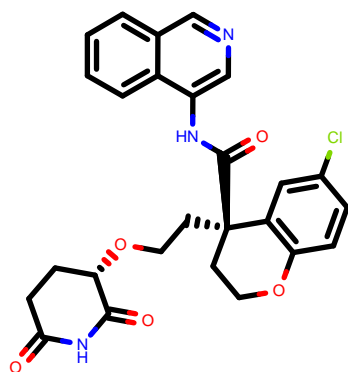
SMILES: CC1(CC(C1)C(=O)NOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5)O

RUN: RUN7043

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.29

EN300-120920_3_2_1



CID: EN300-120920_3_2_1

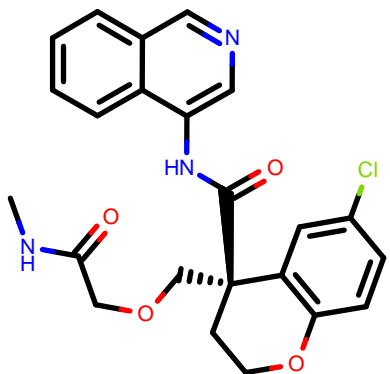
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCCC(=O)NC5=O

RUN: RUN3634

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-2977549_2_1_1



CID: EN300-2977549_2_1_1

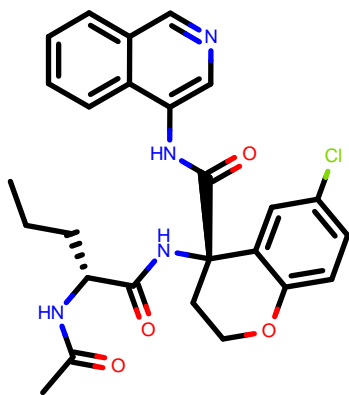
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4

RUN: RUN4642

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.20

EN300-43047_1_2_1



CID: EN300-43047_1_2_1

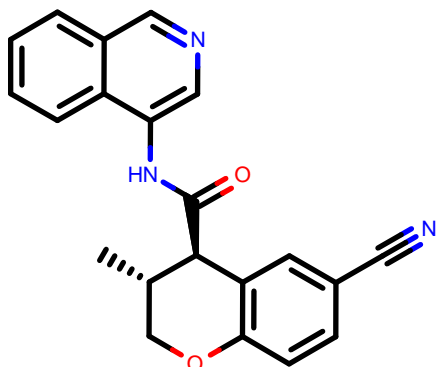
SMILES: CC(=O)N[C@@H](CC=C)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4

RUN: RUN7283

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.28

DAR-DIA-0d514e7d-8_1



CID: DAR-DIA-0d514e7d-8_1

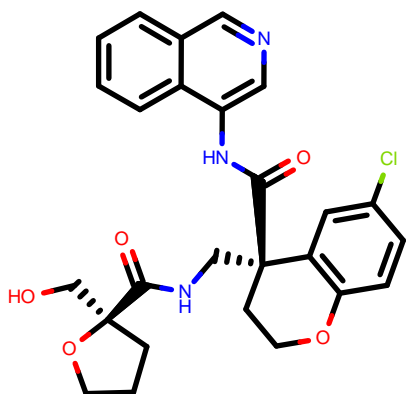
SMILES: C[C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3nccc4c3cccc4)C#N

RUN: RUN745

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.07

EN300-1425677_2_2_1



CID: EN300-1425677_2_2_1

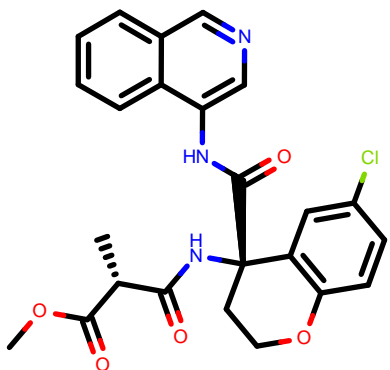
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCCO5)CO

RUN: RUN6283

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-1239522_1_2_1



CID: EN300-1239522_1_2_1

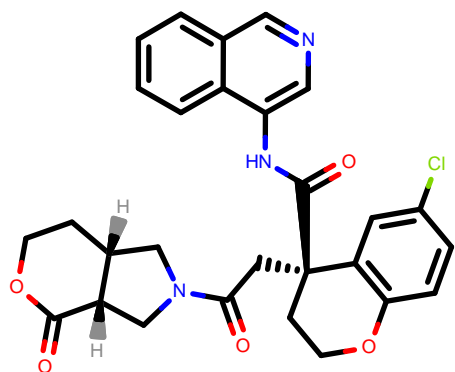
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4)C(=O)OC

RUN: RUN4023

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.25

EN300-7426520_1_1_1



CID: EN300-7426520_1_1_1

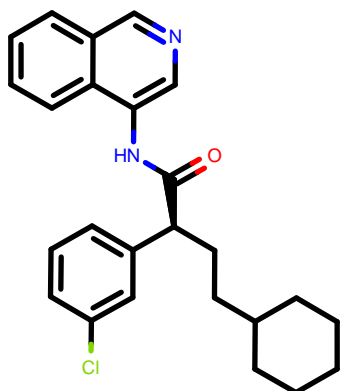
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC4=CC=C(C=C4)O)C@H3C5

RUN: RUN7240

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.25

MIC-UNK-c66144cb-3_1



CID: MIC-UNK-c66144cb-3_1

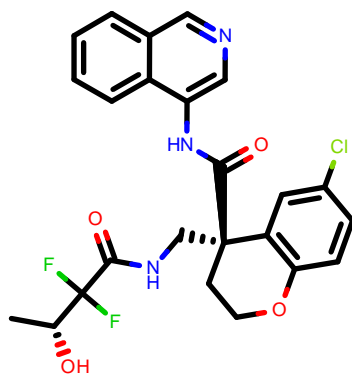
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C3CCCCC3)c4ccc(Cl)c4

RUN: RUN94

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.32

EN300-185398_2_2_1



CID: EN300-185398_2_2_1

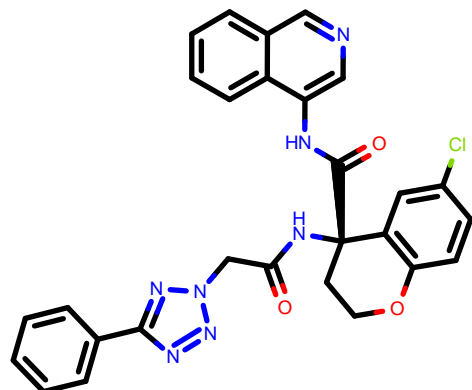
SMILES: C[C@H](C(C=O)NC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4(F)F)O

RUN: RUN5479

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.22

ALP-UNI-dbbfd3db-8_1



CID: ALP-UNI-dbbfd3db-8_1

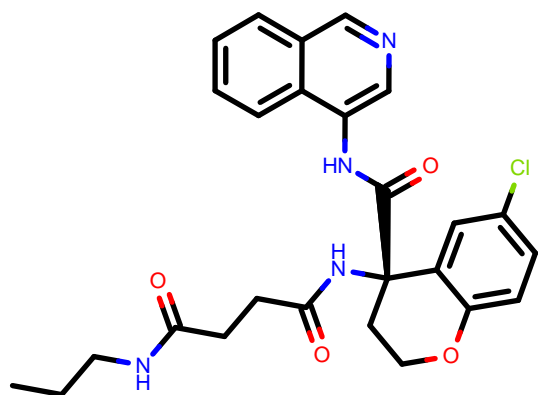
SMILES: c1ccc(cc1)c2nnn(n2)CC(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ncoc6c5ccc6

RUN: RUN2622

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.32

EN300-68740_1_1_1



CID: EN300-68740_1_1_1

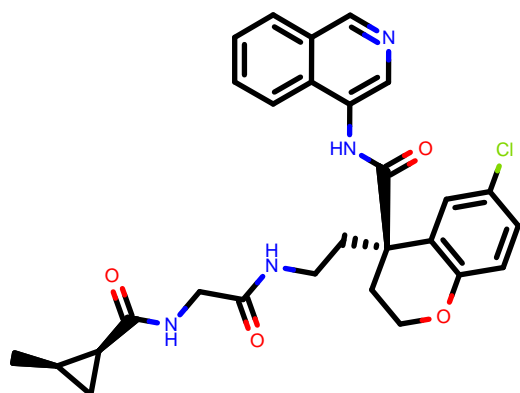
SMILES: CCCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN7659

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.30

EN300-30768_3_1_1



CID: EN300-30768_3_1_1

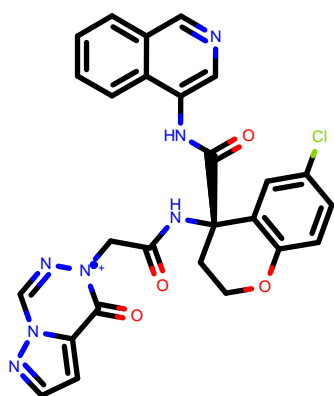
SMILES: C[C@]([H])1[C@@]([H])1C1=O)NCC1=O)NCC[C@@]2(CCOc3c2cc(c3)Cl)C1=O)Nc4ccc5c4ccc5

RUN: RUN6012

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.26

ALP-UNI-dbbfd3db-9_1



CID: ALP-UNI-dbbfd3db-9_1

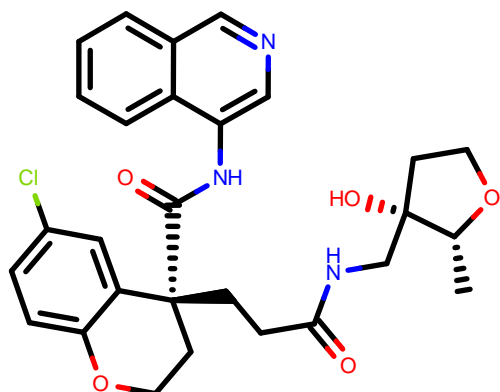
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(c=O)c6ccnn6c5

RUN: RUN2614

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.33

EN300-188324_2_3_1



CID: EN300-188324_2_3_1

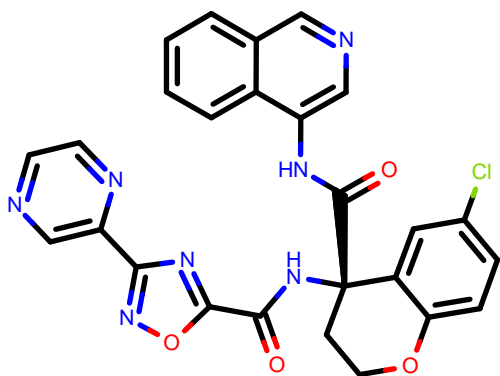
SMILES: C[C@@]([H])1[C@@]([C@@]1(CCO1)(CNC(=O)CC)C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN7431

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

EN300-239219_1_1_1



CID: EN300-239219_1_1_1

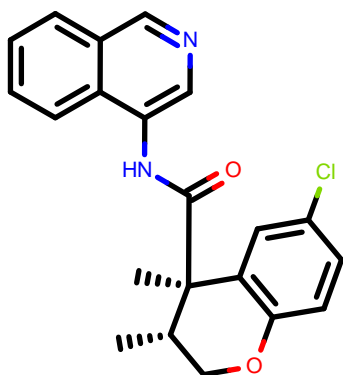
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nc(nc5)c6cncn6

RUN: RUN6300

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.20

DAR-DIA-0d514e7d-28_1_1



CID: DAR-DIA-0d514e7d-28_1_1

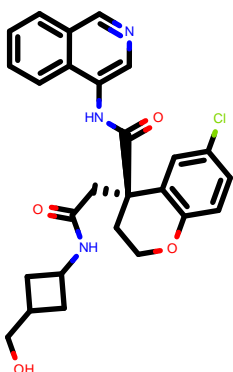
SMILES: C[C@H]1COc2ccc(cc2[C@@]1(C)C)C(=O)Nc3cnc4c3cccc4)Cl

RUN: RUN4579

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.10

EN300-331593_1_1_1



CID: EN300-331593_1_1_1

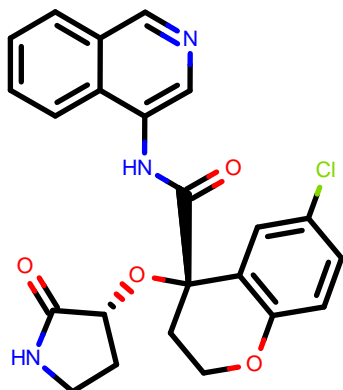
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)CO

RUN: RUN6352

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.29

EN300-6736413_1_1_1



CID: EN300-6736413_1_1_1

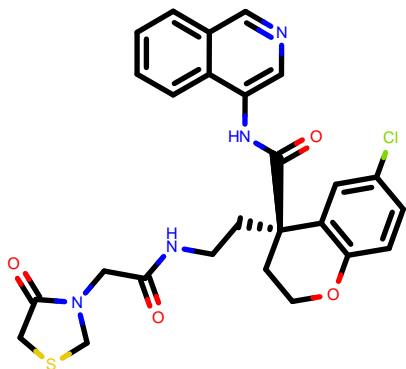
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@]5CNCNC5=O

RUN: RUN5861

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.19

EN300-10747_3_1_1



CID: EN300-10747_3_1_1

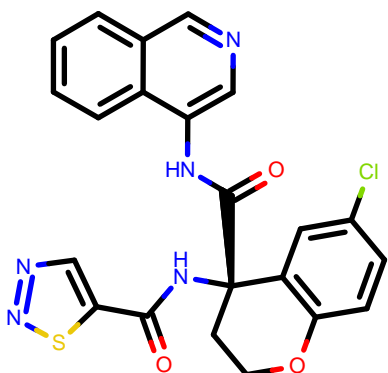
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5SCCS5=O

RUN: RUN3643

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.28

EN300-42269_1_1_1



CID: EN300-42269_1_1_1

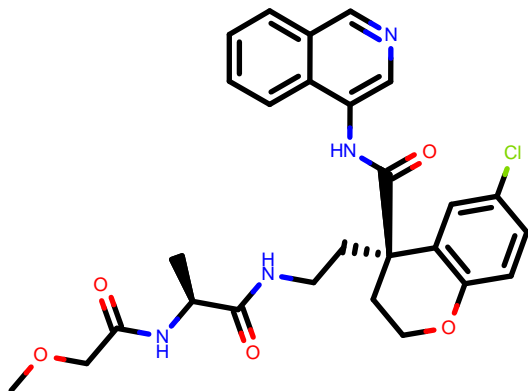
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnns5

RUN: RUN3649

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.19

EN300-31183_3_1_1



CID: EN300-31183_3_1_1

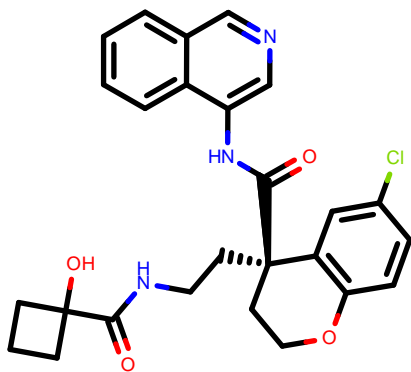
SMILES: C[C@@]H[C](=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)COCC

RUN: RUN5525

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.35

EN300-52009_3_1_1



CID: EN300-52009_3_1_1

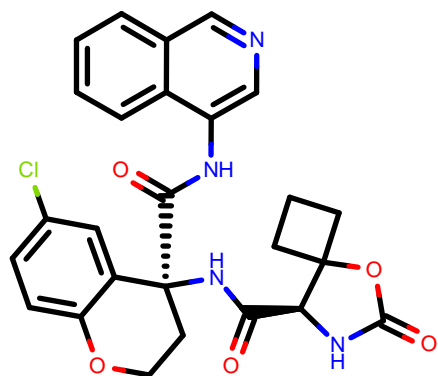
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)O

RUN: RUN4751

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-7432415_1_2_1



CID: EN300-7432415_1_2_1

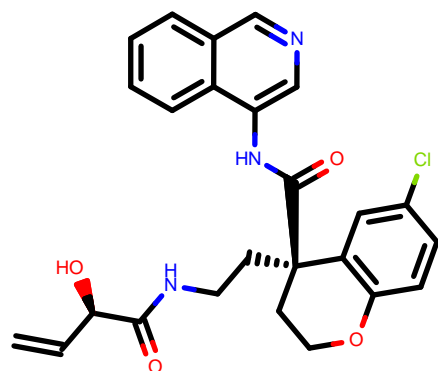
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C6(CCC6)OC(=O)N5

RUN: RUN2921

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.22

EN300-181492_3_2_1



CID: EN300-181492_3_2_1

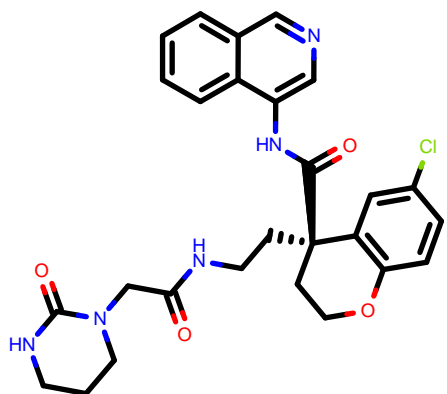
SMILES: C=C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN4439

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.30

EN300-36096_3_1_1



CID: EN300-36096_3_1_1

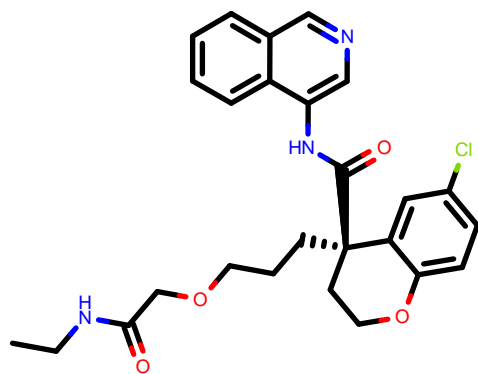
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5CCNC5=O

RUN: RUN4407

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.39

EN300-7003350_4_1_1



CID: EN300-7003350_4_1_1

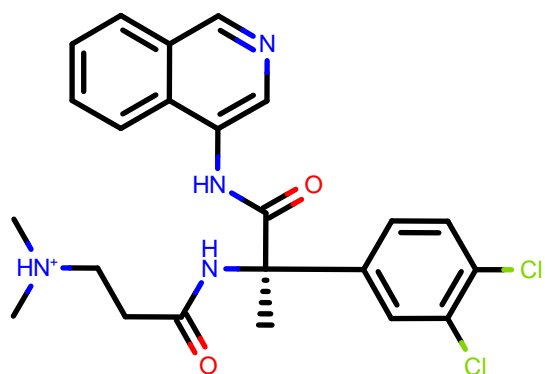
SMILES: CCNC(=O)COCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4624

DDG (kcal/mol): -1.02

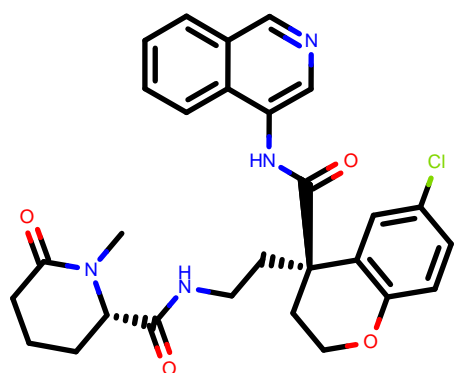
dDDG (kcal/mol): 0.28

MAT-POS-e9e99895-12_1



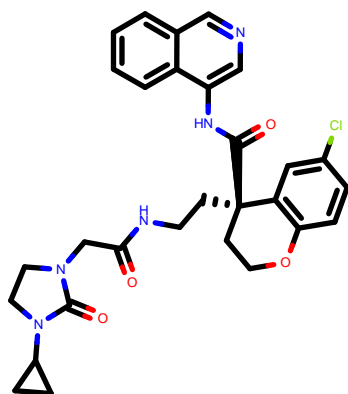
CID:	MAT-POS-e9e99895-12_1
SMILES:	<chem>C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2ccc3)NC(=O)CC[NH+](C)C</chem>
RUN:	RUN2158
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.47

EN300-325738_3_1_1



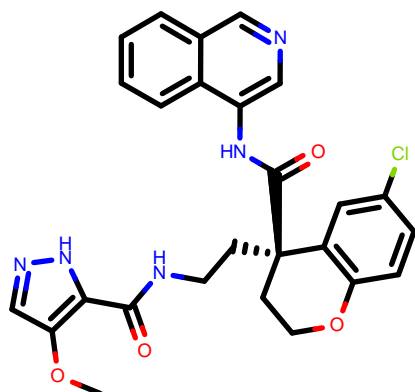
CID:	EN300-325738_3_1_1
SMILES:	<chem>CN[C@@H](CCCC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5</chem>
RUN:	RUN4626
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.27

EN300-304771_3_1_1



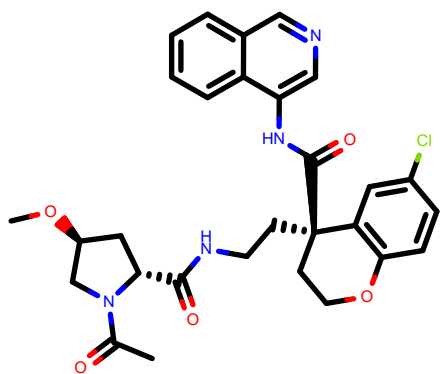
CID:	EN300-304771_3_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCN(C5=O)O6CC6</chem>
RUN:	RUN4828
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.40

EN300-7439284_3_1_1



CID:	EN300-7439284_3_1_1
SMILES:	<chem>COc1cn[nH]c1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccc5</chem>
RUN:	RUN5583
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.29

EN300-158272_3_1_1



CID: EN300-158272_3_1_1

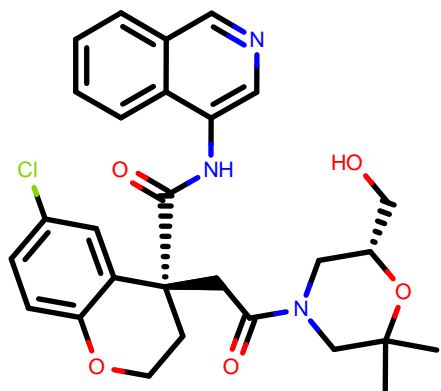
SMILES: CC(=O)N1C[C@@H](C)[C@@H](Cl)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5OC

RUN: RUN6157

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.32

EN300-158082_1_1_1



CID: EN300-158082_1_1_1

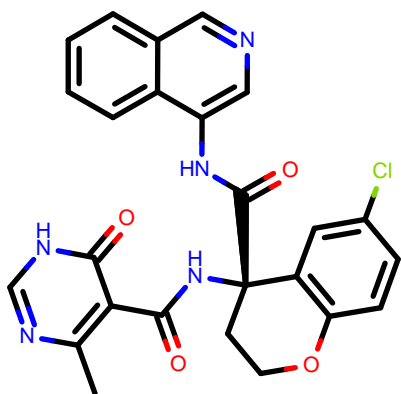
SMILES: CC1(CN(C)C[C@@H](O)CO)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5C

RUN: RUN4860

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.42

EN300-256762_1_1_1



CID: EN300-256762_1_1_1

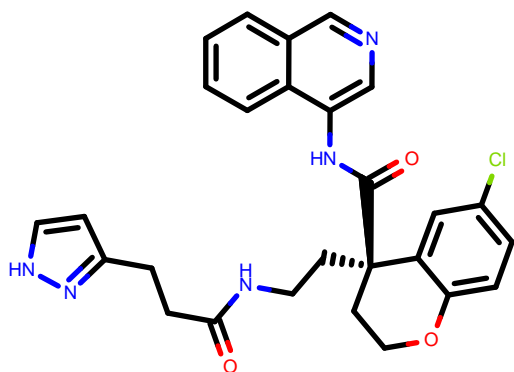
SMILES: Cc1c(c(=O)[nH]cn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5

RUN: RUN3254

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.27

EN300-1664603_3_1_1



CID: EN300-1664603_3_1_1

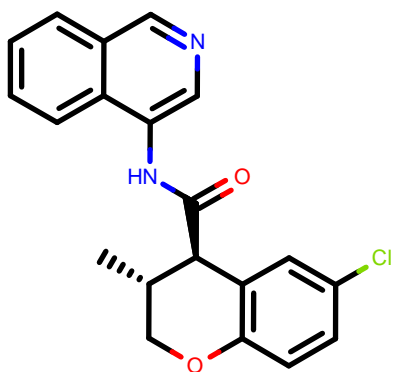
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC5cscn[nH]5

RUN: RUN4167

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.24

MAT-POS-8a69d52e-4_2



CID: MAT-POS-8a69d52e-4_2

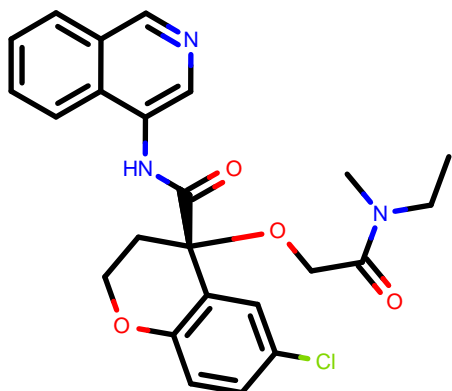
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN288

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.05

EN300-1253122_1_1_1



CID: EN300-1253122_1_1_1

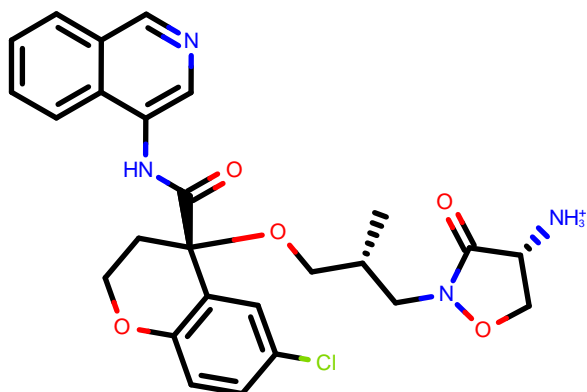
SMILES: CCN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5172

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.23

EDG-MED-4c68219f-1_2



CID: EDG-MED-4c68219f-1_2

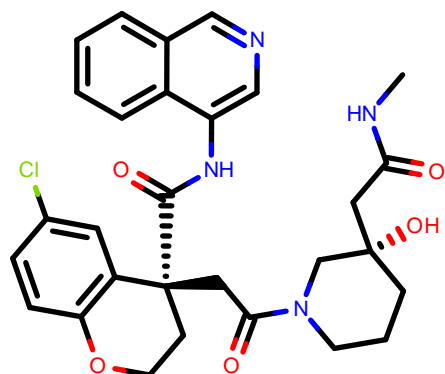
SMILES: CC(=O)N[C@@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N

RUN: RUN1513

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.40

EN300-259062_1_2_1



CID: EN300-259062_1_2_1

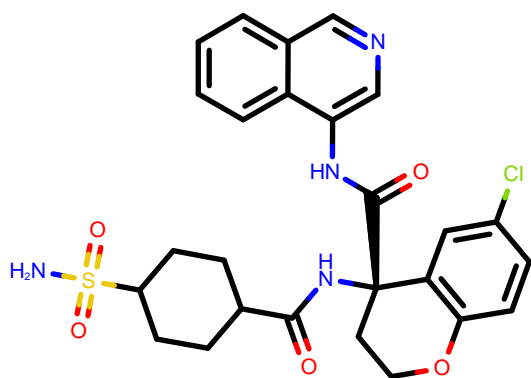
SMILES: CNC(=O)C[C@]1(CCCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN3631

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.34

EN300-83864_1_1_1



CID: EN300-83864_1_1_1

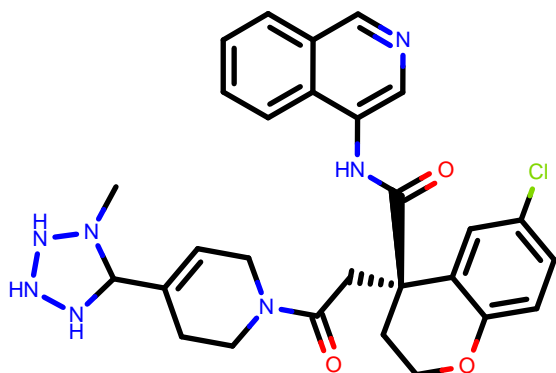
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCCC(C5)S(=O)(=O)N

RUN: RUN3212

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.38

ALP-POS-5bb456a5-3_2



CID: ALP-POS-5bb456a5-3_2

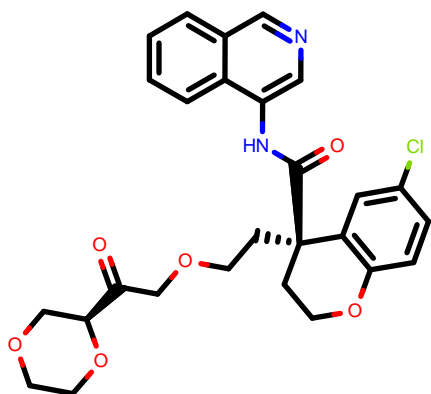
SMILES: Cn1c(nnn1)C2=CCN(CC2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccoc6

RUN: RUN2269

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.28

EN300-6238494_3_1_1



CID: EN300-6238494_3_1_1

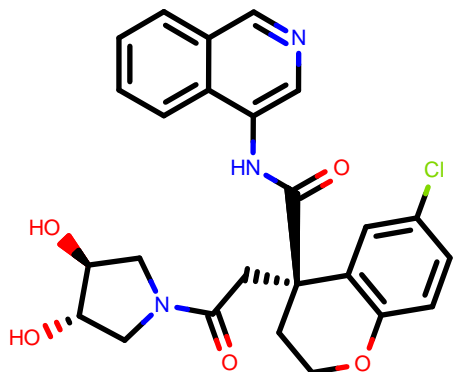
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)OC@@H]5COCOC5

RUN: RUN5381

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.25

EN300-96037_1_1_1



CID: EN300-96037_1_1_1

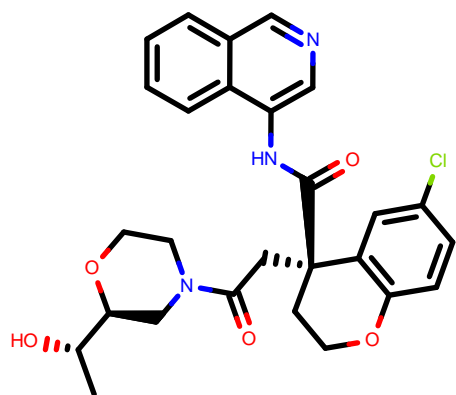
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C5)O

RUN: RUN5696

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.26

EN300-1708848_1_1_1



CID: EN300-1708848_1_1_1

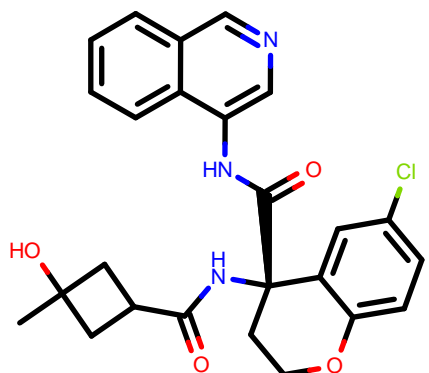
SMILES: C[C@@H]([C@@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5)O

RUN: RUN4080

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.37

EN300-7183657_1_1_1



CID: EN300-7183657_1_1_1

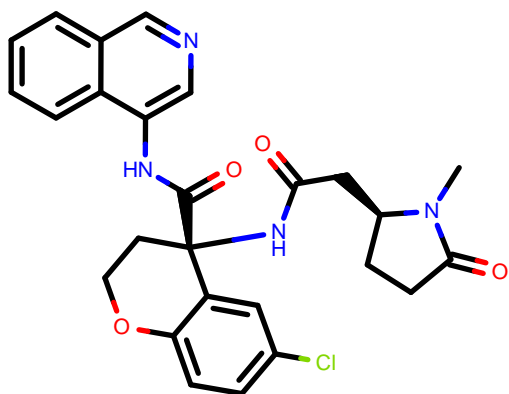
SMILES: CC1(CC(C1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C)C(=O)Nc4nc5c4cccc5)O

RUN: RUN4092

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.22

EN300-207765_1_1_1



CID: EN300-207765_1_1_1

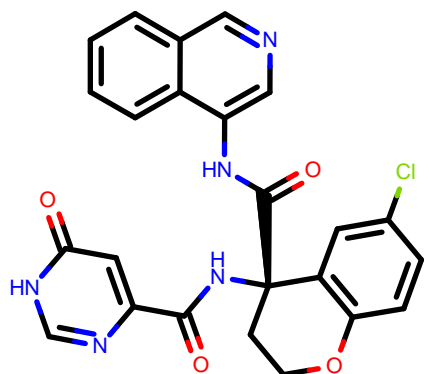
SMILES: CN1[C@@H]([C@@H]2CC1=O)CC(=O)N[C@]3(CCOc4c3c2cc(cc4)C)C)C(=O)Nc5nc6c5cccc6

RUN: RUN5439

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.27

EN300-817811_1_1_1



CID: EN300-817811_1_1_1

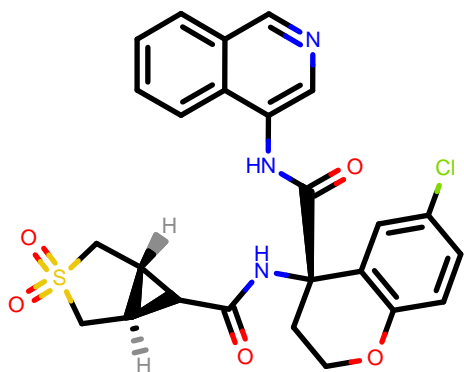
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3c2cc(cc4)C)NC(=O)c5cc(=O)[nH]jcn5

RUN: RUN5538

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.21

EN300-6779469_1_1_1



CID: EN300-6779469_1_1_1

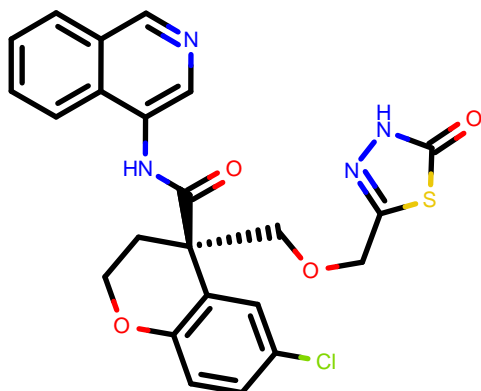
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](C(=O)Nc4ccc(Cl)cc4)C1CC(=O)Nc5cncn5

RUN: RUN5975

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.22

EDJ-MED-fcba3f31-12_1



CID: EDJ-MED-fcba3f31-12_1

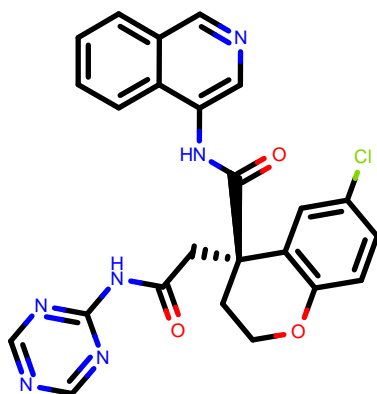
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4c[nH]s4)C1CC(=O)Nc5cncn5

RUN: RUN2387

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EDJ-MED-d203f206-20_1



CID: EDJ-MED-d203f206-20_1

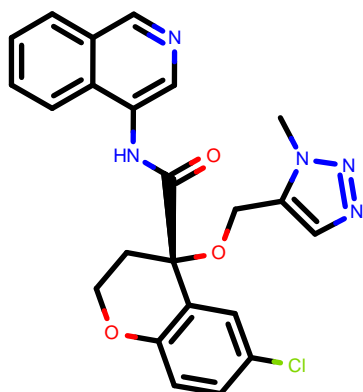
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COCc4c[nH]s4)C1CC(=O)Nc5cncn5

RUN: RUN2385

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.26

EN300-216673_1_1_1



CID: EN300-216673_1_1_1

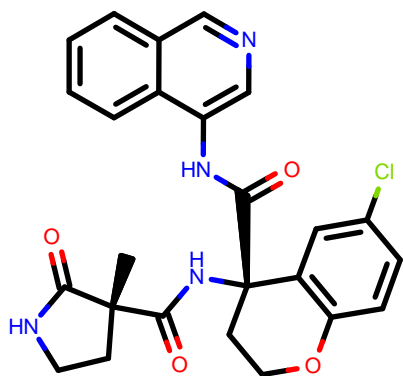
SMILES: Cn1c(cnn1)CO[C@@2](COCc3c[nH]s3)C1CC(=O)Nc4cncnc4

RUN: RUN5326

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-207959_1_2_1



CID: EN300-207959_1_2_1

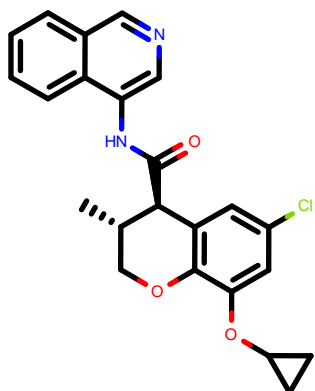
SMILES: C[C@]1(C)CNC1=O)C(=O)N[C@]2(C)COCc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3749

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.35

DAR-DIA-0d514e7d-6_1_1



CID: DAR-DIA-0d514e7d-6_1_1

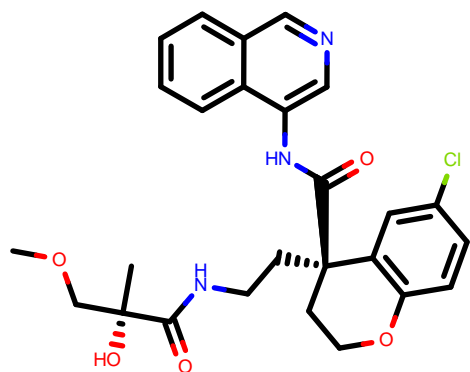
SMILES: C[C@H]1COc2c(cc2OC3CC3)C)N[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN4430

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.17

EN300-76841_3_2_1



CID: EN300-76841_3_2_1

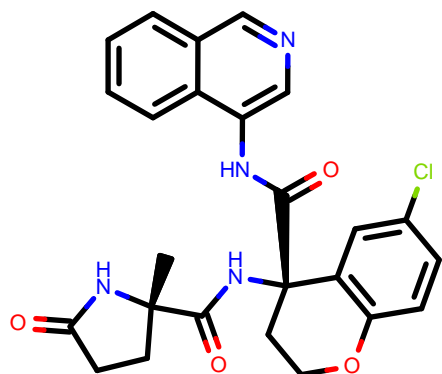
SMILES: C[C@](COC)(C(=O)N)C[C@]1(C)COCc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4O

RUN: RUN6008

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.41

EN300-177118_1_2_1



CID: EN300-177118_1_2_1

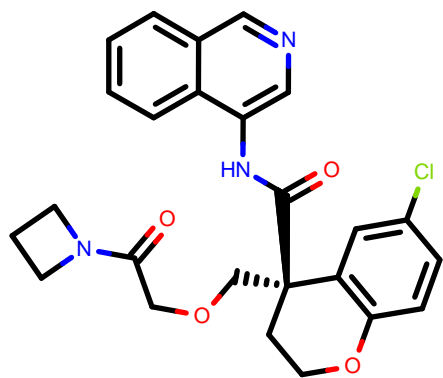
SMILES: C[C@]1(C)CNC(=O)N)C(=O)N[C@]2(C)COCc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN4899

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.23

EN300-11195_2_1_1



CID: EN300-11195_2_1_1

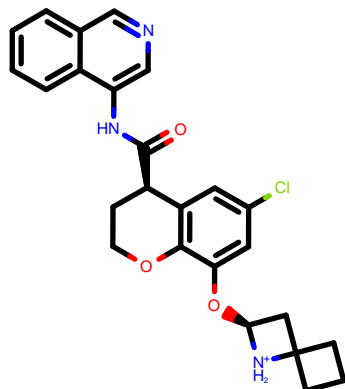
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCCC5

RUN: RUN4896

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.21

DAR-DIA-23e5a6a0-2_2



CID: DAR-DIA-23e5a6a0-2_2

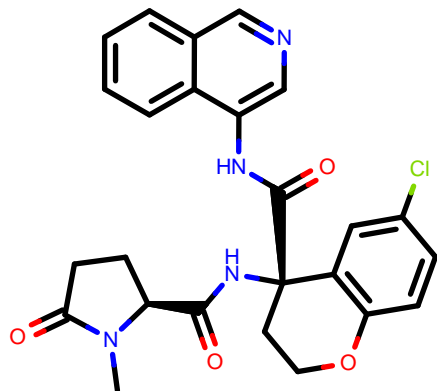
SMILES: c1ccc2c(c1)cncc2NC(=O)C@H3(CCOc4c3cc(cc4)Cl)C@H5CC6([NH2+][5])COC6Cl

RUN: RUN412

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EN300-132963_1_1_1



CID: EN300-132963_1_1_1

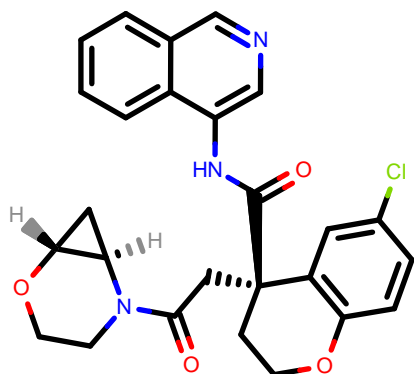
SMILES: CN1C@@H(CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccc5

RUN: RUN7580

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

EN300-91609_1_4_1



CID: EN300-91609_1_4_1

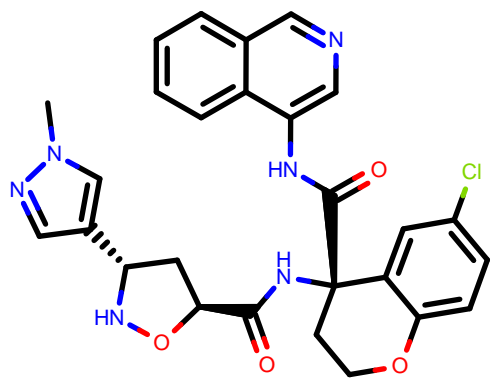
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H]6[C@@H]5C6

RUN: RUN4470

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EN300-92605_1_1_1



CID: EN300-92605_1_1_1

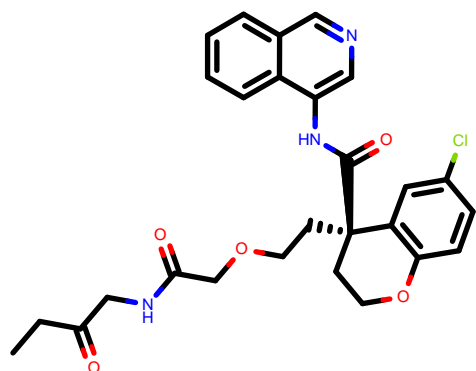
SMILES: Cn1cc(m1)[C@@H]2[C@@H](O)N2[C@@H](O)N[C@@H]3(CCOc4c3cc(c54)Cl)C1=O)Nc5nc6c5ccccc6

RUN: RUN4196

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.40

EN300-132624_3_1_1



CID: EN300-132624_3_1_1

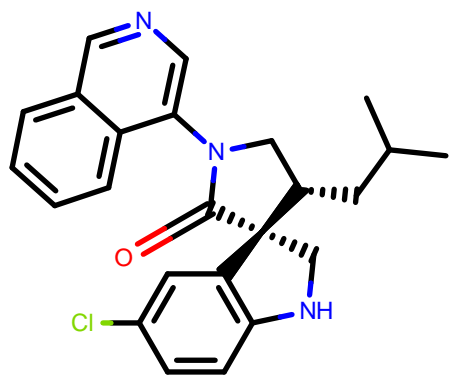
SMILES: CCC(=O)N[C@@H](O)COC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN4556

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.33

DAR-DIA-6be260fc-2_1



CID: DAR-DIA-6be260fc-2_1

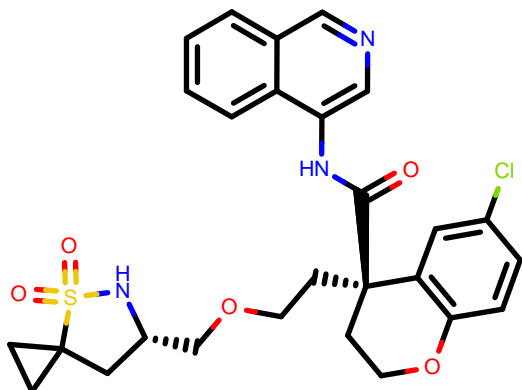
SMILES: CC(C)C[C@@H]1CN(C(=O)[C@@H]2CCNc3c2cc(cc3)Cl)c4ncc5c4ccccc5

RUN: RUN1935

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.32

KAD-UNI-8a629cb0-29_1



CID: KAD-UNI-8a629cb0-29_1

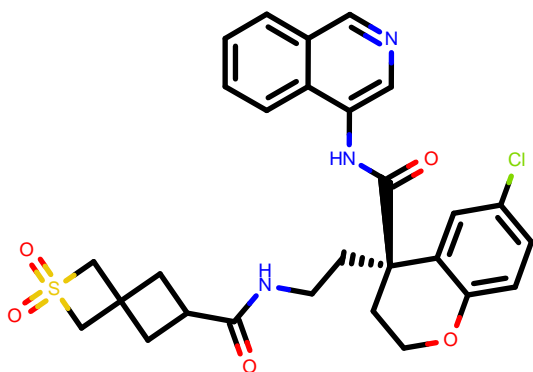
SMILES: c1ccc2c(1)ncoc2N[C@@H](O)C[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COC6(C6)S(=O)(=O)N5

RUN: RUN2030

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

KAD-UNI-8a629cb0-24_1



CID: KAD-UNI-8a629cb0-24_1

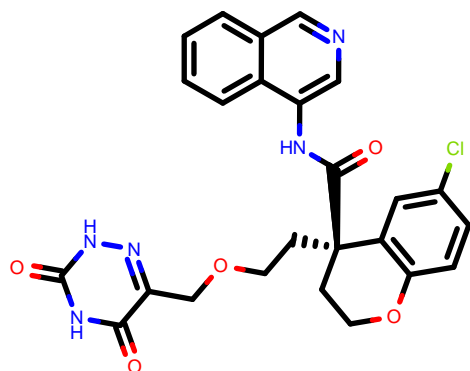
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)CCNC(=O)C5CC6(C5)CS(=O)(=O)C6

RUN: RUN1975

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-761746_3_1_1



CID: EN300-761746_3_1_1

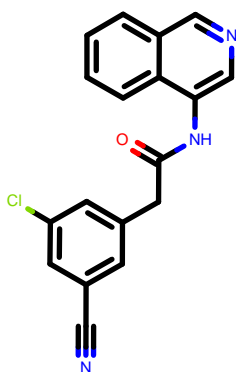
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)CCOCc5c(=O)[nH]c(=O)[nH]n5

RUN: RUN3473

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.31

RAL-THA-2d450e86-17_1



CID: RAL-THA-2d450e86-17_1

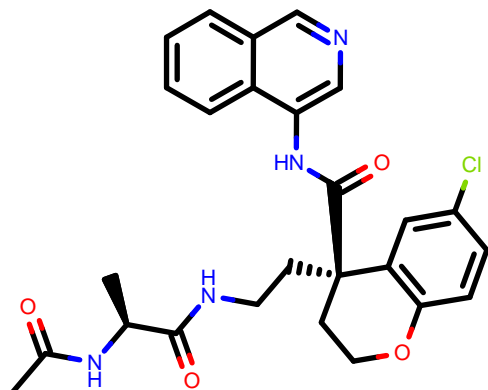
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C#N

RUN: RUN1796

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-862647_3_1_1



CID: EN300-862647_3_1_1

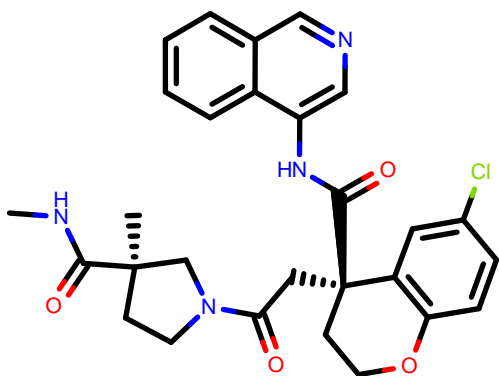
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)C

RUN: RUN4783

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

EN300-196140_1_2_1



CID: EN300-196140_1_2_1

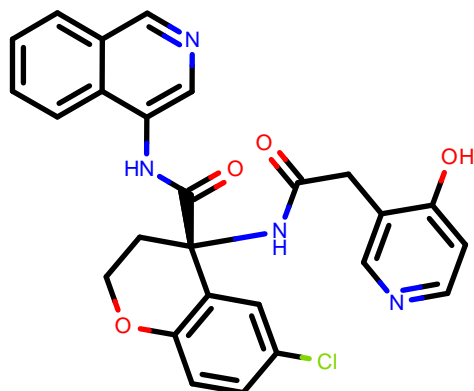
SMILES: C[C@]1(CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5)C(=O)NC

RUN: RUN4596

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.42

EN300-205486_1_1_1



CID: EN300-205486_1_1_1

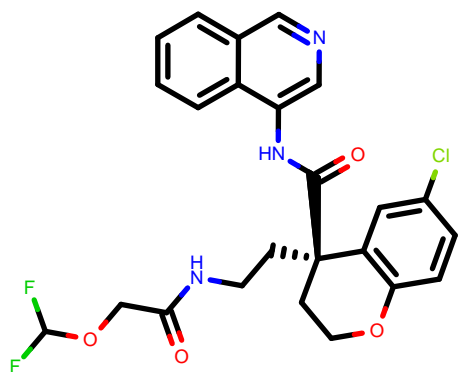
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]c5=O

RUN: RUN6855

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-179091_3_1_1



CID: EN300-179091_3_1_1

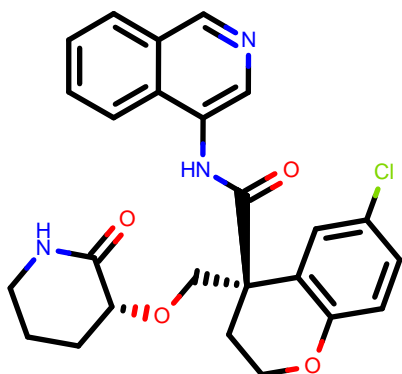
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC(F)F

RUN: RUN3933

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EDJ-MED-fcba3f31-1_1



CID: EDJ-MED-fcba3f31-1_1

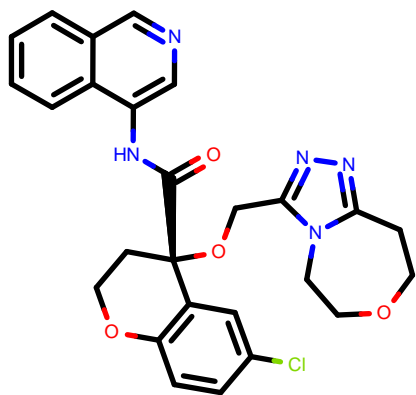
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNCC5=O

RUN: RUN2353

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-310888_1_1_1



CID: EN300-310888_1_1_1

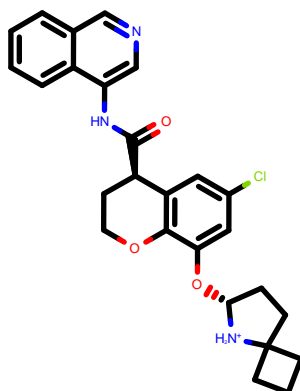
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nnc6n5CCOC6

RUN: RUN5478

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.26

DAR-DIA-23e5a6a0-1_1



CID: DAR-DIA-23e5a6a0-1_1

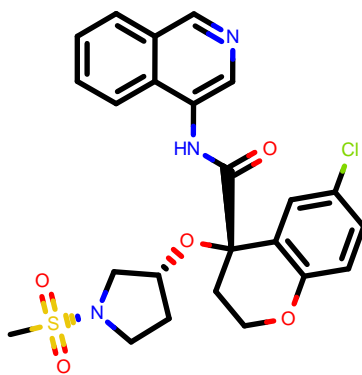
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3C[C@@]4(COCC4)C@H5CCCC6([NH2+5])COC6)Cl

RUN: RUN417

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.34

EN300-301690_1_2_1



CID: EN300-301690_1_2_1

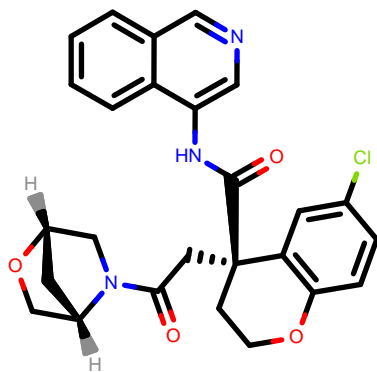
SMILES: CS(=O)(=O)[N@]1CC[C@H]1C1O[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN7564

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.31

EN300-321790_1_1_1



CID: EN300-321790_1_1_1

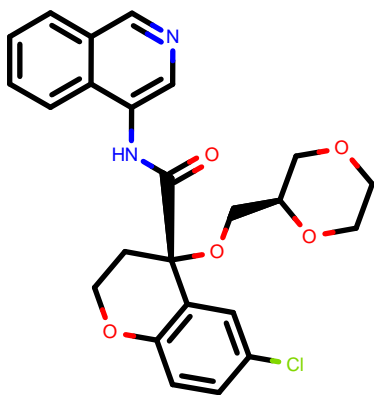
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]H6C[C@H]5CO6

RUN: RUN4861

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.25

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

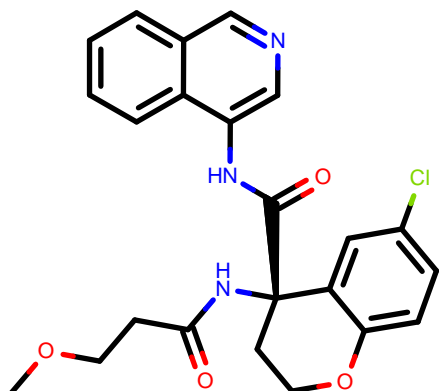
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5COCCO5

RUN: RUN3817

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-64536_1_1_1



CID: EN300-64536_1_1_1

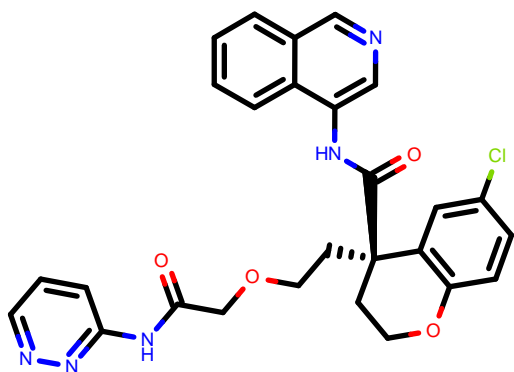
SMILES: COCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN4565

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-761618_3_1_1



CID: EN300-761618_3_1_1

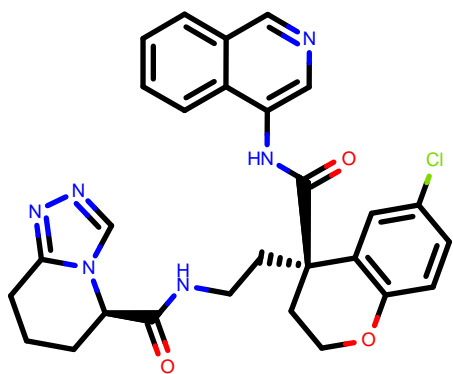
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5ccnnc5

RUN: RUN3931

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.27

EN300-6478631_3_2_1



CID: EN300-6478631_3_2_1

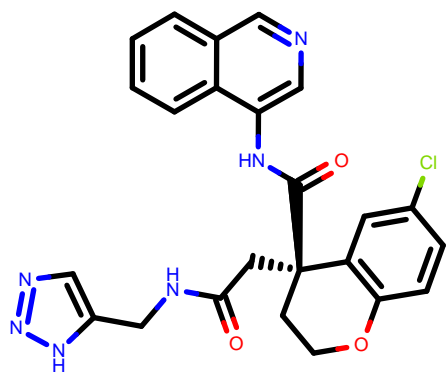
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC5Cn6nnc6

RUN: RUN6328

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.29

EN300-98429_1_1_1



CID: EN300-98429_1_1_1

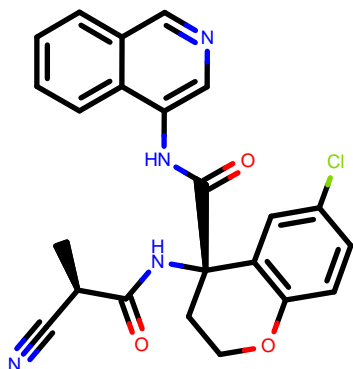
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5cn[nH]n5

RUN: RUN5190

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.29

EDG-MED-90036822-80_2



CID: EDG-MED-90036822-80_2

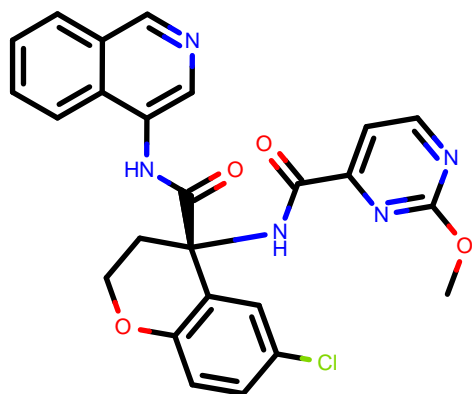
SMILES: C[C@H](C#N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1636

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.17

EN300-154912_1_1_1



CID: EN300-154912_1_1_1

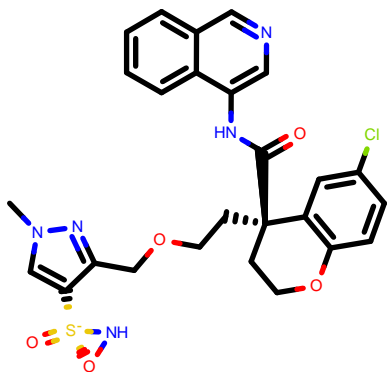
SMILES: COc1nccc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5464

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.26

EN300-7355737_3_1_1



CID: EN300-7355737_3_1_1

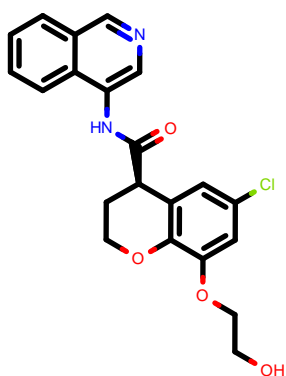
SMILES: Cn1cc(c(n1)C)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5S(=O)(=O)N

RUN: RUN6414

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.42

LAU-MED-88a3970a-1_1



CID: LAU-MED-88a3970a-1_1

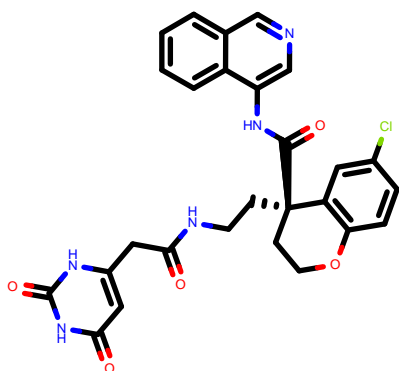
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4cc(cc4OCCO)Cl

RUN: RUN1314

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-11441_3_1_1



CID: EN300-11441_3_1_1

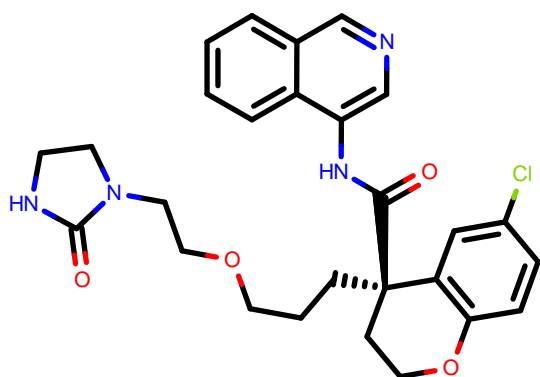
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN4538

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.31

EN300-214800_4_1_1



CID: EN300-214800_4_1_1

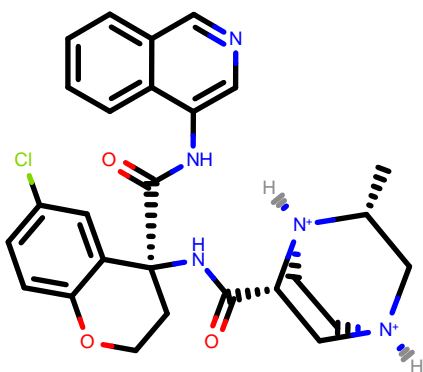
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCN5CCNC5=O

RUN: RUN4340

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.32

EN300-120562_1_3_1



CID: EN300-120562_1_3_1

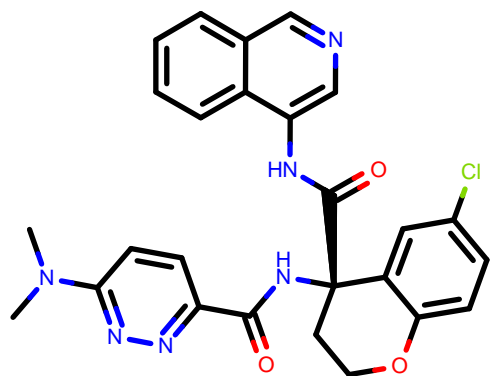
SMILES: C[C@@H]1CN[C@@]2CC[N@@H]1[C@@H](C2)C(=O)N[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5c6cc6c5cc6

RUN: RUN7494

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.34

EN300-7535922_1_1_1



CID: EN300-7535922_1_1_1

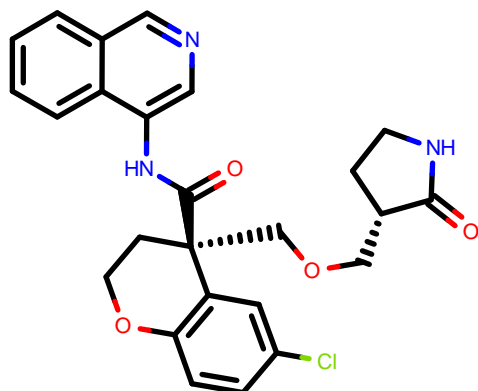
SMILES: CN(C)c1ccc(nn1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4206

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.25

EN300-246248_2_1_1



CID: EN300-246248_2_1_1

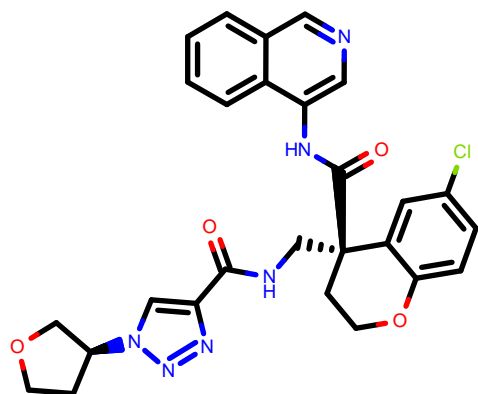
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O

RUN: RUN4589

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.24

EN300-151461_2_2_1



CID: EN300-151461_2_2_1

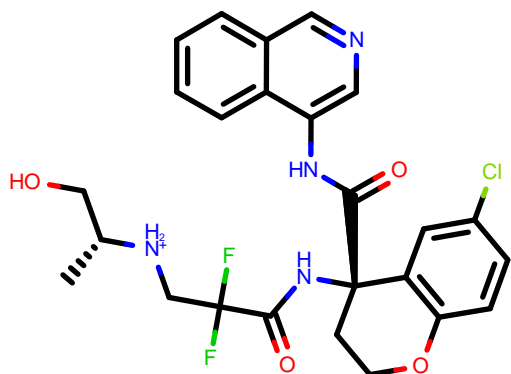
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nc5)[C@@H]6CCOC6

RUN: RUN6605

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.37

EDG-MED-90036822-39_2



CID: EDG-MED-90036822-39_2

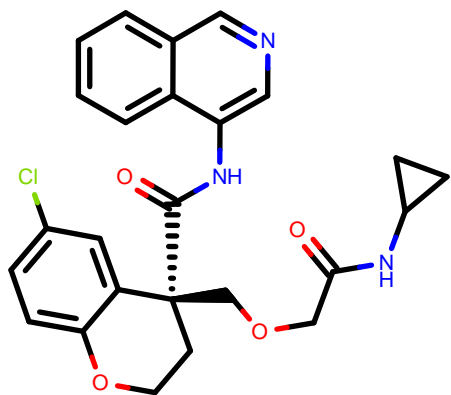
SMILES: C[C@@H](CO)NCC(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)F)F

RUN: RUN1678

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.36

EN300-1253178_2_1_1



CID: EN300-1253178_2_1_1

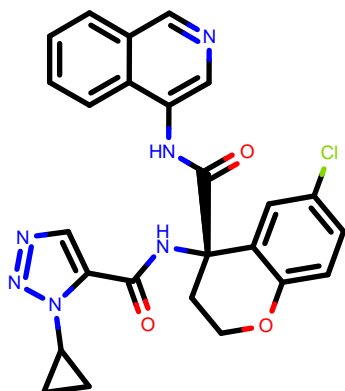
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CC5

RUN: RUN4656

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EN300-1718675_1_1_1



CID: EN300-1718675_1_1_1

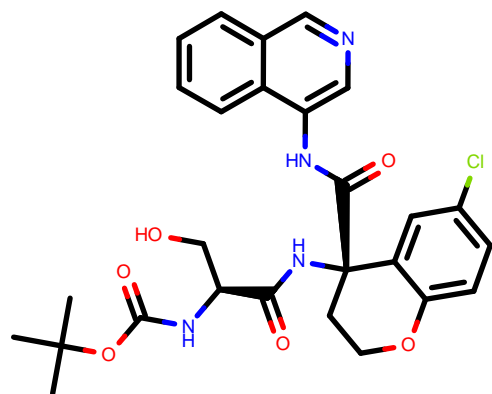
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnnn5C6CC6

RUN: RUN5686

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EN300-72109_1_1_1



CID: EN300-72109_1_1_1

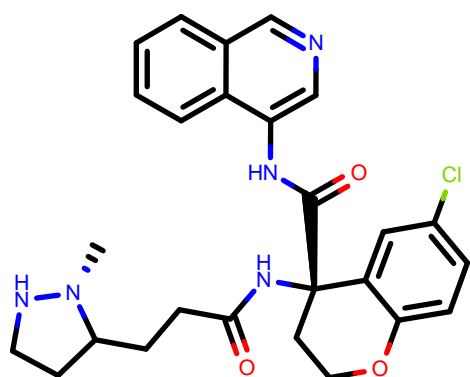
SMILES: CC(C)(C)OC(=O)N[C@@]H(CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4

RUN: RUN5228

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.29

EN300-92662_1_1_1



CID: EN300-92662_1_1_1

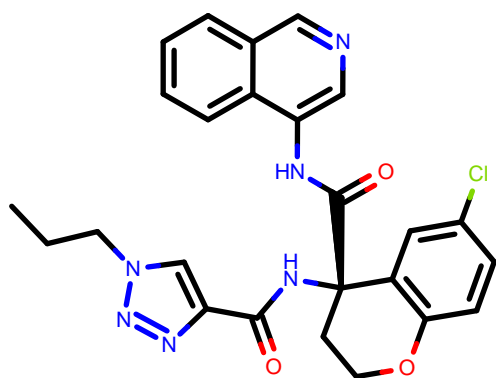
SMILES: Cn1c(ccn1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5006

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.25

EN300-261596_1_1_1



CID: EN300-261596_1_1_1

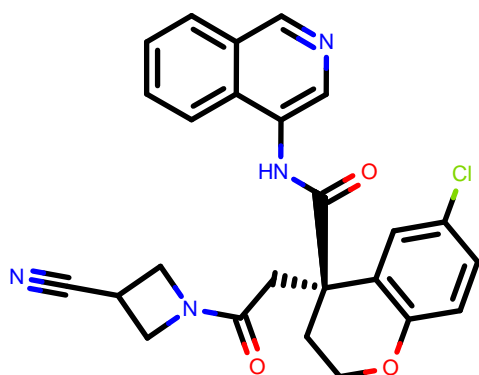
SMILES: C=CCn1cc(nn1)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN2820

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.22

EN300-206282_1_1_1



CID: EN300-206282_1_1_1

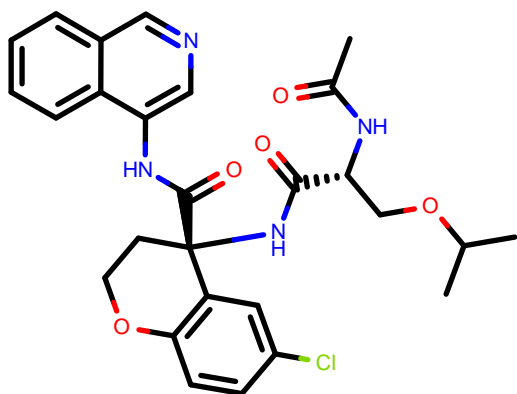
SMILES: c1ccc2c(c1)cncc2N[C@@]([C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N5CC(C5)C#N

RUN: RUN5434

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.24

EN300-1299691_1_2_1



CID: EN300-1299691_1_2_1

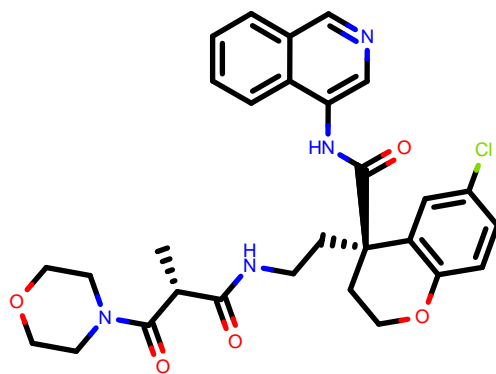
SMILES: CC(C)OC[C@@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C(=O)C

RUN: RUN6402

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-2855057_3_2_1



CID: EN300-2855057_3_2_1

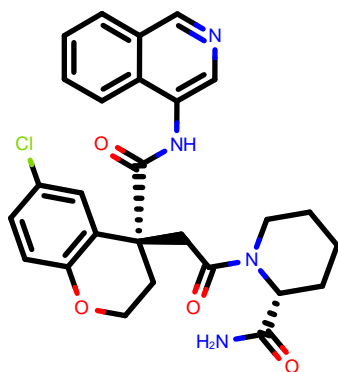
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)N5COCOC5

RUN: RUN5659

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.42

EDJ-MED-d203f206-30_1



CID: EDJ-MED-d203f206-30_1

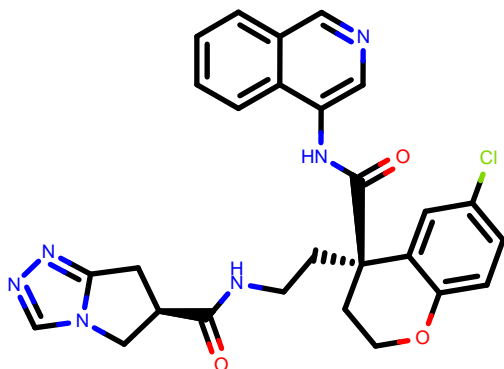
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN2428

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

EN300-6745453_3_1_1



CID: EN300-6745453_3_1_1

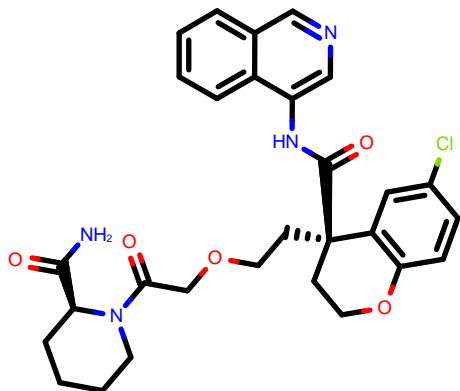
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C6Nnnc6C5

RUN: RUN5539

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.30

EN300-22879_3_2_1



CID: EN300-22879_3_2_1

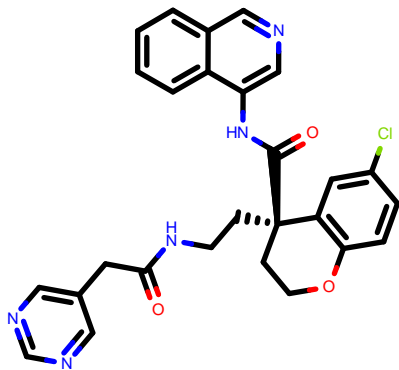
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN4025

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.37

EN300-185751_3_1_1



CID: EN300-185751_3_1_1

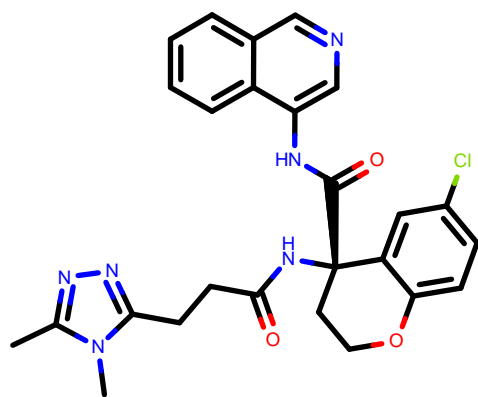
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cncnc5

RUN: RUN3969

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.27

EN300-1721328_1_1_1



CID: EN300-1721328_1_1_1

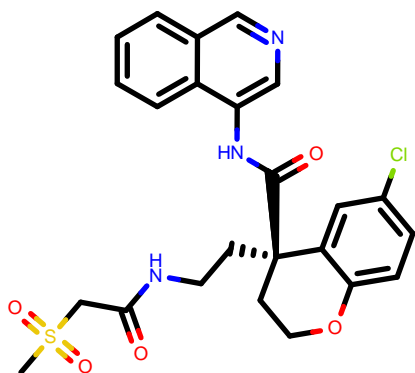
SMILES: Cc1nnc(n1C)CCC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3971

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-53677_3_1_1



CID: EN300-53677_3_1_1

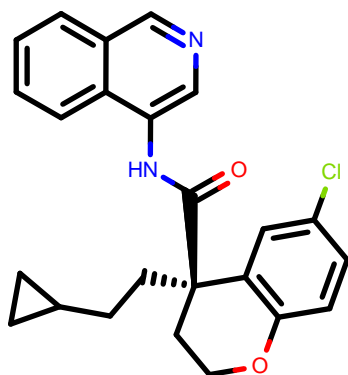
SMILES: CS(=O)(=O)CC(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6221

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

ALP-POS-477dc5b7-3_1



CID: ALP-POS-477dc5b7-3_1

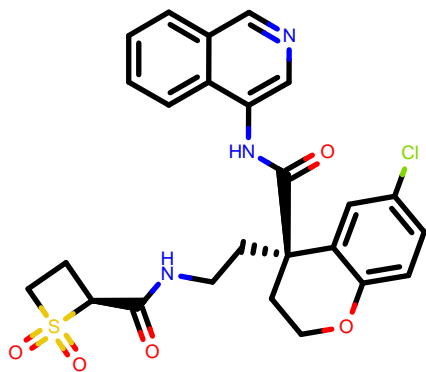
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC5CC5

RUN: RUN249

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.20

EN300-1387104_3_1_1



CID: EN300-1387104_3_1_1

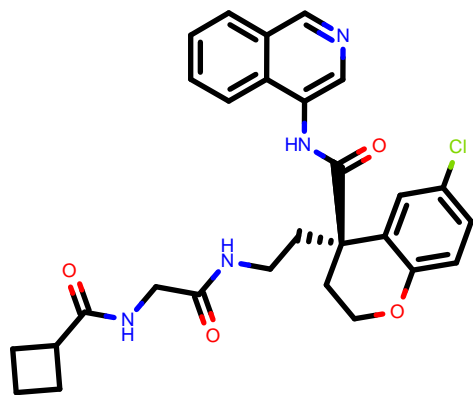
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)[C@@]5CCS5(=O)=O

RUN: RUN3786

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.24

EN300-62448_3_1_1



CID: EN300-62448_3_1_1

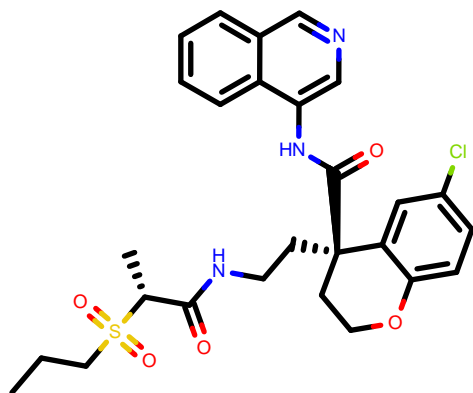
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CC5C5

RUN: RUN4652

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.34

EN300-52768_3_2_1



CID: EN300-52768_3_2_1

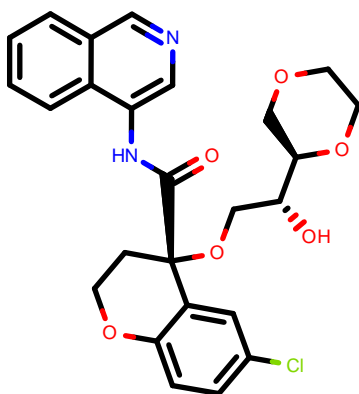
SMILES: CCCS(=O)(=O)[C@H](C)C(=O)NCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN6032

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.47

EN300-6238494_1_2_2



CID: EN300-6238494_1_2_2

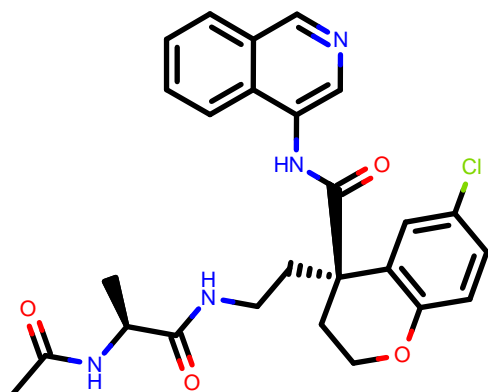
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)OC[C@H](C)O5COCCO5O

RUN: RUN5103

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.46

EN300-18569_3_1_1



CID: EN300-18569_3_1_1

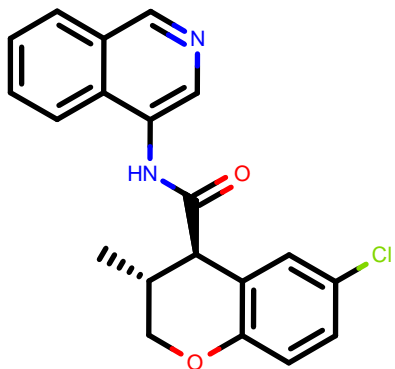
SMILES: C[C@@]H(C)C(=O)NCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)C

RUN: RUN5687

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.29

MAT-POS-8a69d52e-4_2_1



CID: MAT-POS-8a69d52e-4_2_1

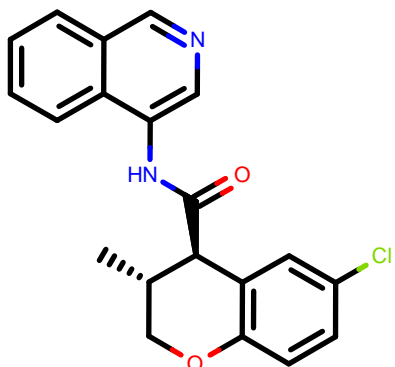
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cnccc4c3cccc4)Cl

RUN: RUN5655

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.05

EDJ-MED-e4b030d8-11_1



CID: EDJ-MED-e4b030d8-11_1

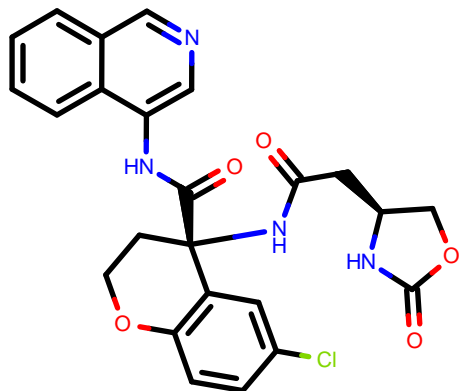
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cnccc4c3cccc4)Cl

RUN: RUN248

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.05

EN300-1703852_1_1_1



CID: EN300-1703852_1_1_1

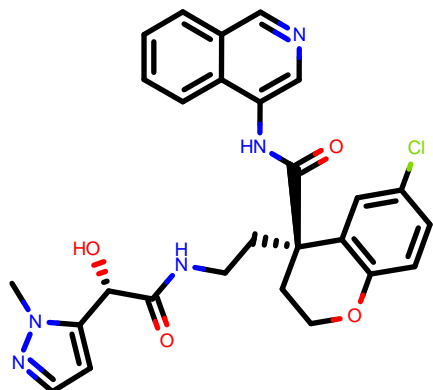
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](COC(=O)N5C(=O)C@H5)C(=O)C[C@@H]3COC(=O)N5

RUN: RUN4722

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.29

EN300-6473273_3_1_1



CID: EN300-6473273_3_1_1

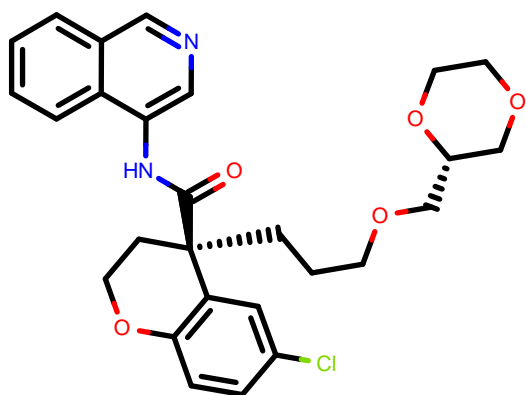
SMILES: Cn1c(cnn1)[C@@H](C(=O)NCC[C@@H]2(COC(=O)N3C(=O)C@H3)C(=O)N4cnc5c4cccc5)O

RUN: RUN4399

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.33

EN300-139167_4_2_1



CID: EN300-139167_4_2_1

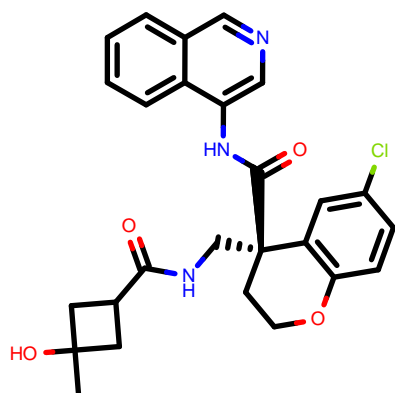
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5COCOC5

RUN: RUN7141

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.36

EN300-247343_2_1_1



CID: EN300-247343_2_1_1

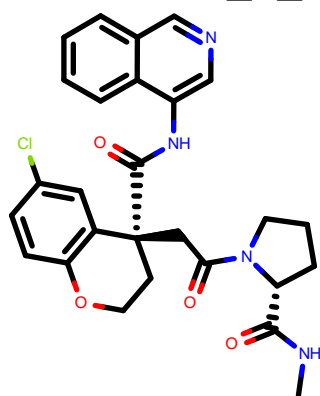
SMILES: CC1(CC(C1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)O

RUN: RUN5371

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.21

EN300-6492197_1_1_1



CID: EN300-6492197_1_1_1

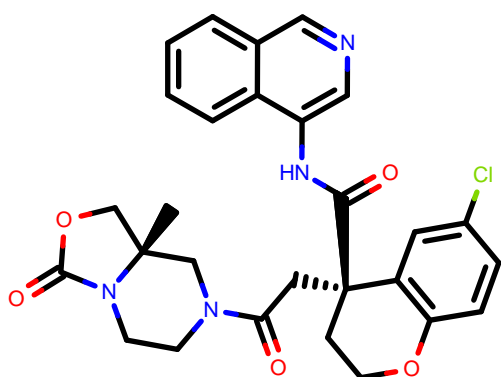
SMILES: CNC(=O)[C@H]1CCCN1C(=O)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6461

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.32

EN300-395954_1_1_1



CID: EN300-395954_1_1_1

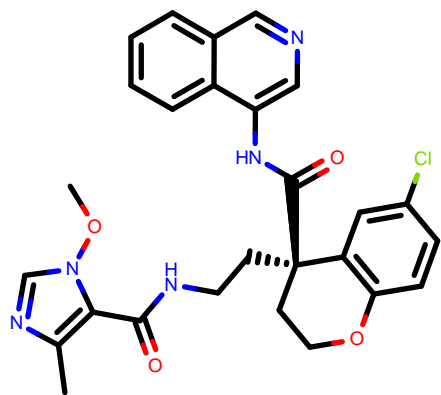
SMILES: C[C@@]12CN(CGN1C(=O)OC2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6

RUN: RUN4717

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.33

EN300-7442332_3_1_1



CID: EN300-7442332_3_1_1

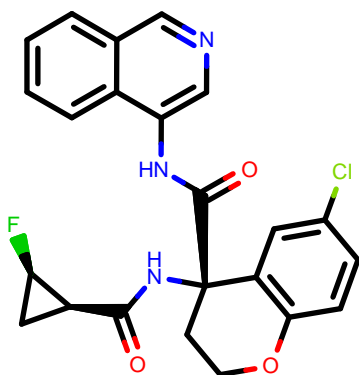
SMILES: Cc1c(n(n1)OC)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN5558

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-6953121_1_1_1



CID: EN300-6953121_1_1_1

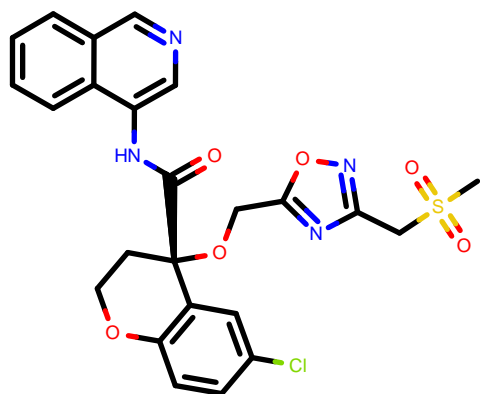
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[C@H]5F

RUN: RUN5647

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.20

EN300-94900_1_1_1



CID: EN300-94900_1_1_1

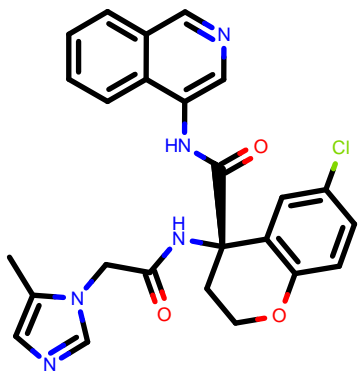
SMILES: CS(=O)(=O)Cc1nc(n1)CO[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN6464

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.35

EN300-315453_1_1_1



CID: EN300-315453_1_1_1

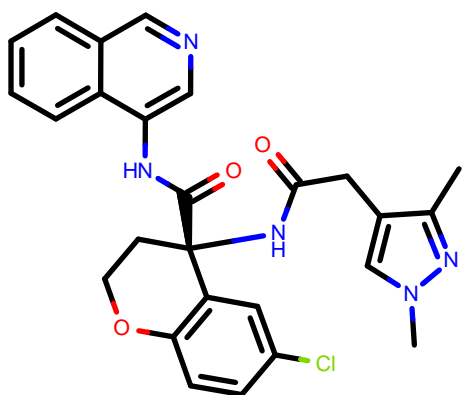
SMILES: Cc1cn(n1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncoc5c4cccc5

RUN: RUN4508

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.23

EN300-245061_1_1_1



CID: EN300-245061_1_1_1

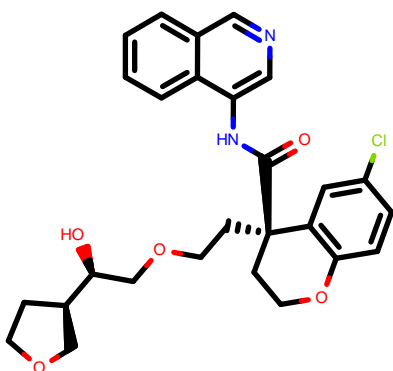
SMILES: Cc1c(cn(n1)C)CC(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6483

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.24

EN300-1911992_3_1_1



CID: EN300-1911992_3_1_1

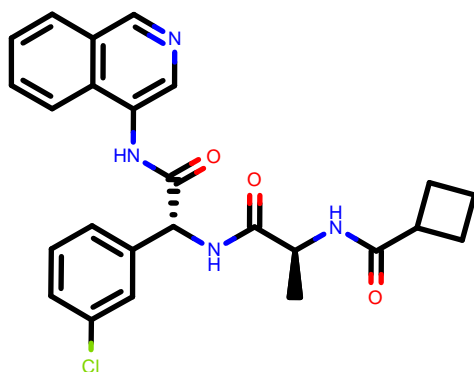
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COC[C@@H](C)[C@@H]5COCOC5O

RUN: RUN5682

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.30

EDJ-MED-ee07cf00-4_3



CID: EDJ-MED-ee07cf00-4_3

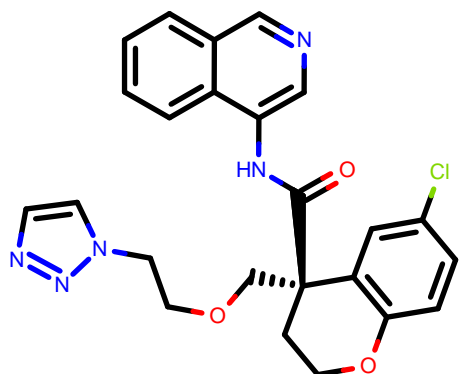
SMILES: C[C@@H](C=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)NC(=O)C4CCCC4

RUN: RUN2645

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.45

EN300-1715993_2_1_1



CID: EN300-1715993_2_1_1

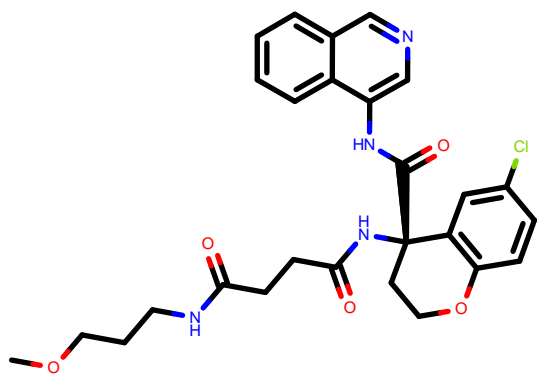
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COC[C@H]5cnn5

RUN: RUN5131

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.25

EN300-175251_1_1_1



CID: EN300-175251_1_1_1

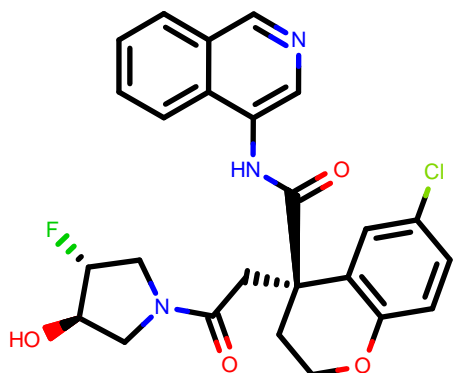
SMILES: COCCNC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN7453

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.35

EN300-317085_1_1_1



CID: EN300-317085_1_1_1

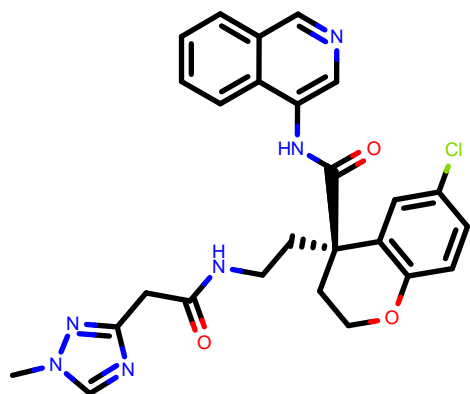
SMILES: c1ccc2c(c1)cncc2N[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)F)O

RUN: RUN6121

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-7493922_3_1_1



CID: EN300-7493922_3_1_1

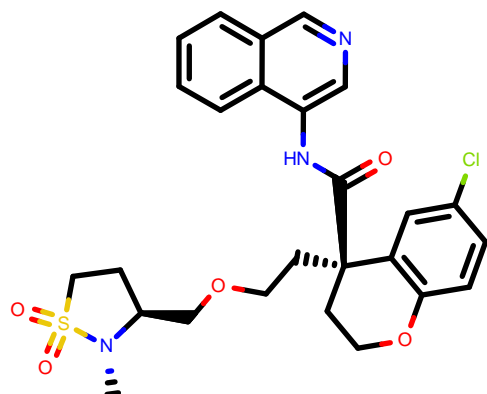
SMILES: Cn1cnc(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4341

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

EN300-393148_3_1_1



CID: EN300-393148_3_1_1

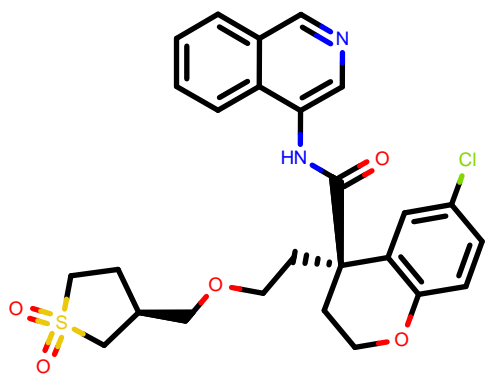
SMILES: C[N@@]1[C@@H]([C@@H](CCS1(=O)=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4517

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

EN300-1448603_3_1_1



CID: EN300-1448603_3_1_1

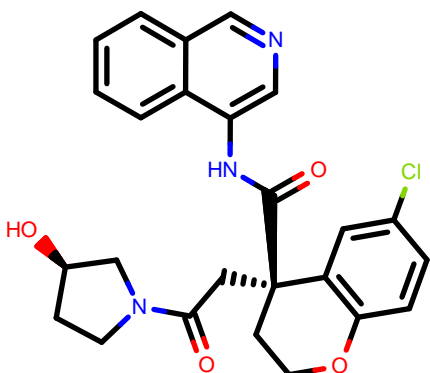
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)C5

RUN: RUN7025

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.29

EN300-69313_1_1_1



CID: EN300-69313_1_1_1

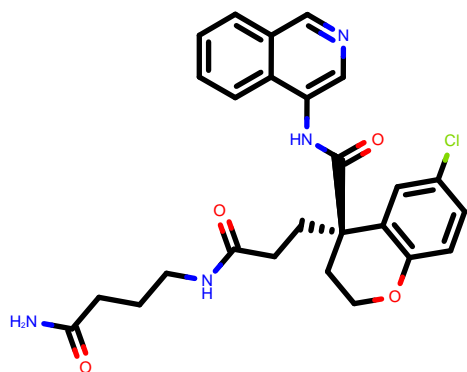
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O

RUN: RUN5547

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-39439_2_1_1



CID: EN300-39439_2_1_1

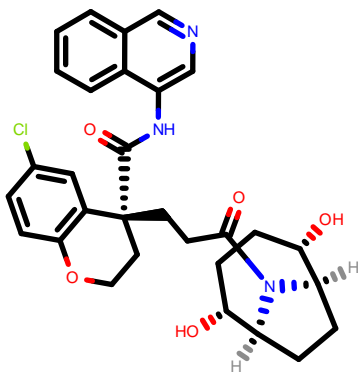
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCCC(=O)N

RUN: RUN2756

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-6738887_2_1_1



CID: EN300-6738887_2_1_1

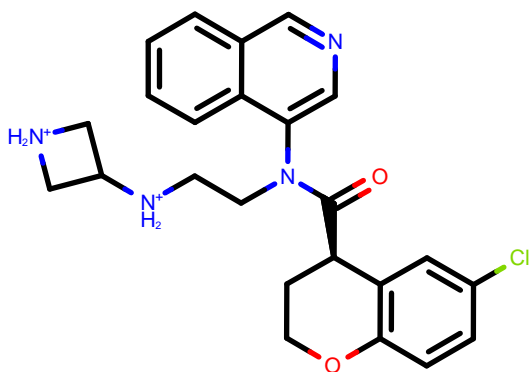
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5[C@@H](C[C@@H]5[C@@H](O)O)O

RUN: RUN7100

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

MAK-UNK-83e0a0b4-3_1



CID: MAK-UNK-83e0a0b4-3_1

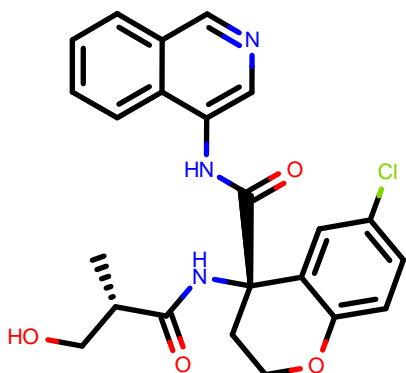
SMILES: c1ccc2c(c1)cncc2N(CCN(C)C)C(=O)N[C@@H](C)C(=O)O

RUN: RUN755

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.31

EN300-55072_1_1_1



CID: EN300-55072_1_1_1

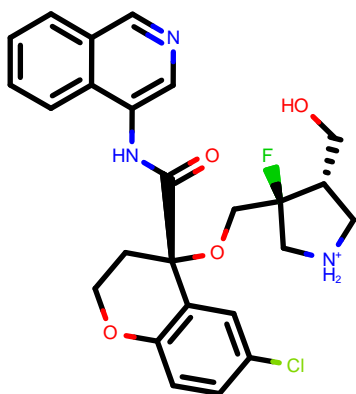
SMILES: C[C@@H](CO)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)O

RUN: RUN4343

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.27

ED_-GRI-5b13fbe2-55_4



CID: ED_-GRI-5b13fbe2-55_4

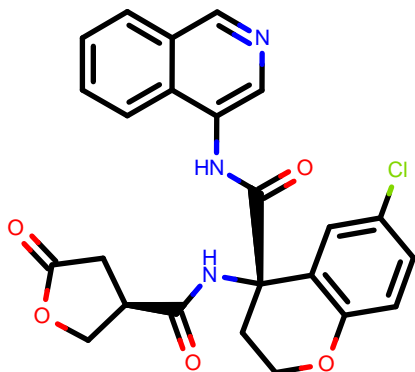
SMILES: c1ccc2c(c1)cncc2N(C)C(=O)N[C@@H](C)C(=O)O

RUN: RUN1487

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.35

EN300-113234_1_1_1



CID: EN300-113234_1_1_1

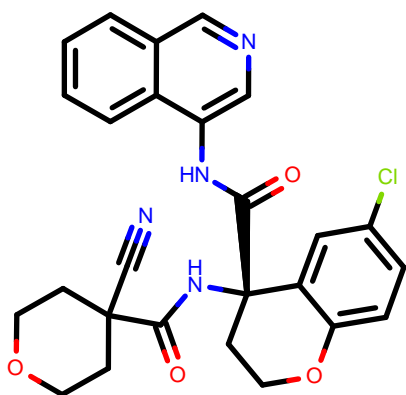
SMILES: c1ccc2c(c1)cncc2N(C)C(=O)N[C@@H](C)C(=O)O

RUN: RUN3574

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-74089_1_1_1



CID: EN300-74089_1_1_1

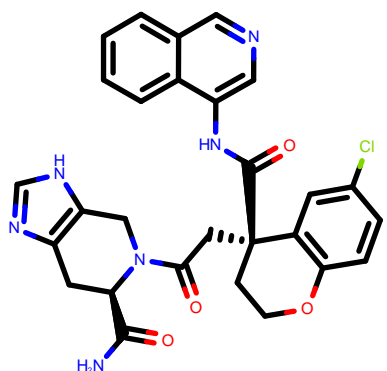
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)C#N

RUN: RUN2771

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EDG-MED-ba1ac7b9-22_1



CID: EDG-MED-ba1ac7b9-22_1

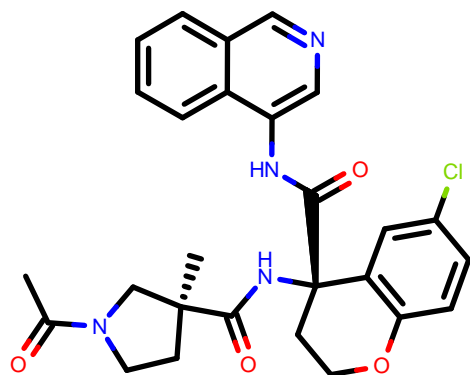
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6cnc6c1#9[C@@]#H5C(=O)N

RUN: RUN2547

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.36

EN300-98018_1_2_1



CID: EN300-98018_1_2_1

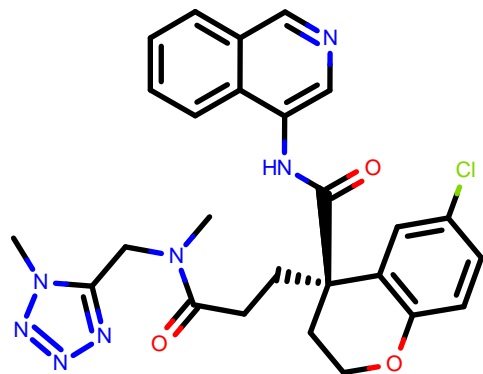
SMILES: CC(=O)N1CC[C@](C1)(C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc5

RUN: RUN4282

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.27

EN300-148515_2_1_1



CID: EN300-148515_2_1_1

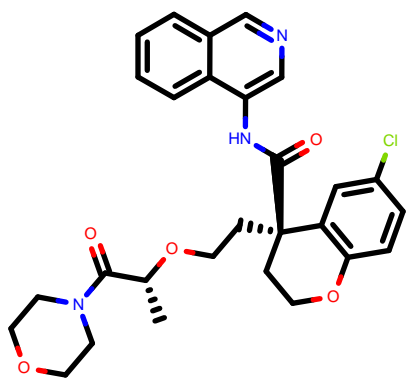
SMILES: Cn1c(nnn1)CN(C)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccoc5

RUN: RUN6900

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-05754_3_2_1



CID: EN300-05754_3_2_1

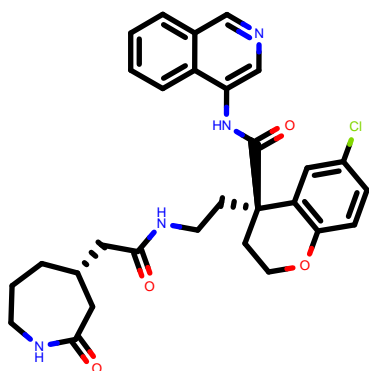
SMILES: C[C@H](C(=O)N1CCOCC1)OCC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4072

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.34

EN300-195590_3_2_1



CID: EN300-195590_3_2_1

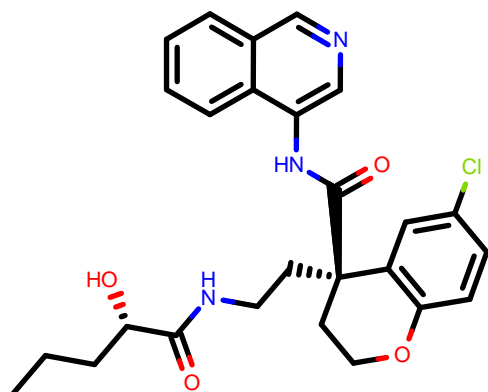
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C[C@H]5CCNC(=O)C5

RUN: RUN5735

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.32

EN300-316679_3_1_1



CID: EN300-316679_3_1_1

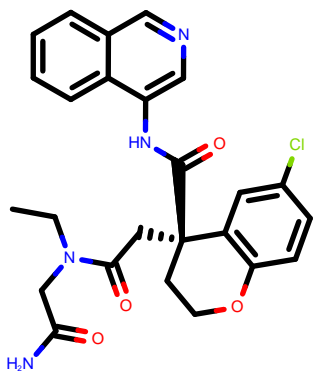
SMILES: CCC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN6961

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.37

EN300-174763_1_1_1



CID: EN300-174763_1_1_1

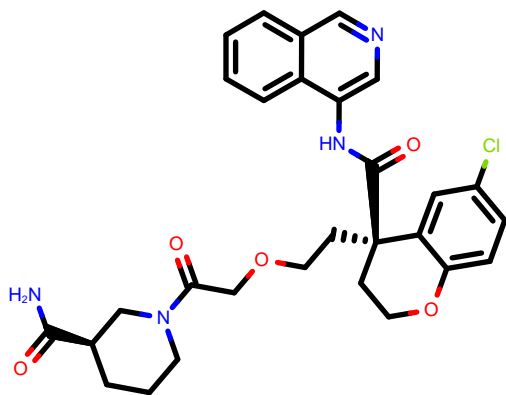
SMILES: CCN(CC(=O)N)C(=O)C[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3275

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

EN300-22880_3_2_1



CID: EN300-22880_3_2_1

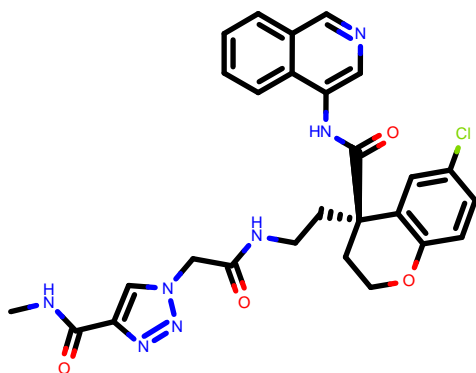
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc1cc4)Cl)COC(=O)N5CCC[C@H](C5)C(=O)N

RUN: RUN6237

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.31

EN300-2617222_3_1_1



CID: EN300-2617222_3_1_1

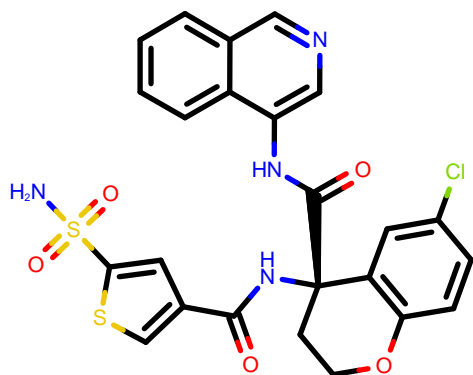
SMILES: CNC(=O)c1cn(nn1)CC(=O)NCC[C@@]2(CCOc3c2cc1cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4807

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

EN300-23792_1_1_1



CID: EN300-23792_1_1_1

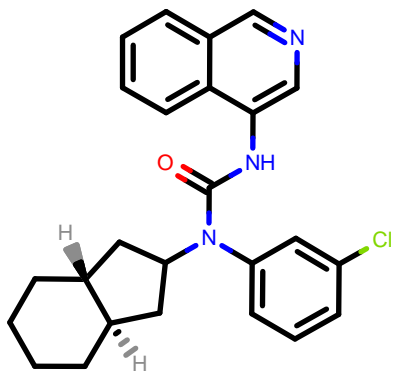
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc1cc4)Cl)NC(=O)c5cc1sc5)S(=O)(=O)N

RUN: RUN6259

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.23

MIC-UNK-cdc2493e-5_2



CID: MIC-UNK-cdc2493e-5_2

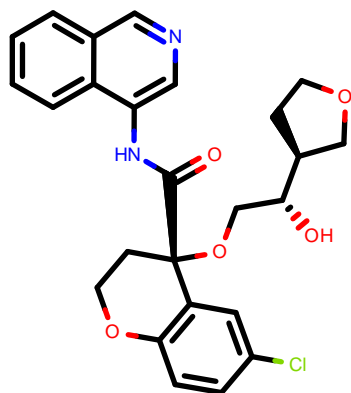
SMILES: c1ccc2c(c1)ncnc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCCC[C@H]5C4

RUN: RUN478

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.41

EN300-1911992_1_4_1



CID: EN300-1911992_1_4_1

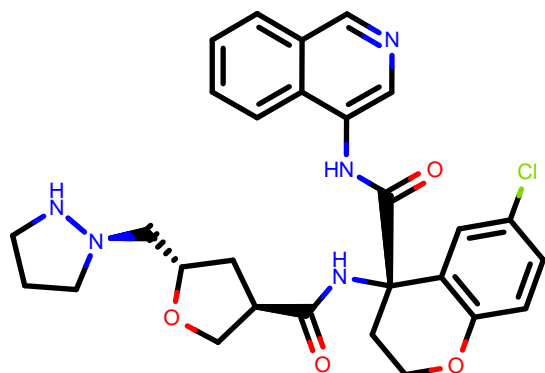
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)OC[C@@H]([C@@H]5CCOC5)O

RUN: RUN4272

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.30

EN300-6494859_1_3_1



CID: EN300-6494859_1_3_1

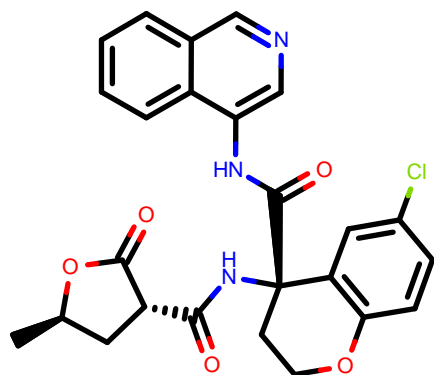
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)[C@@H]5C[C@H]OC5

RUN: RUN3850

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.31

EN300-7444533_1_3_1



CID: EN300-7444533_1_3_1

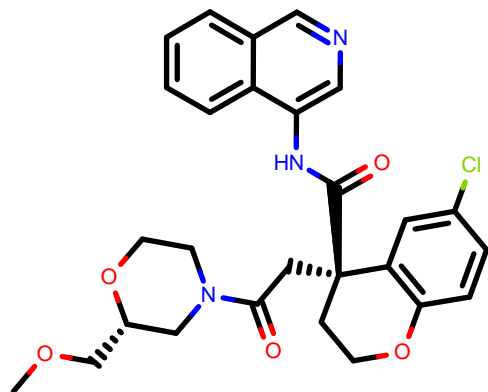
SMILES: C[C@@H]1C[C@@H](C(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN6183

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.25

EN300-85707_1_2_1



CID: EN300-85707_1_2_1

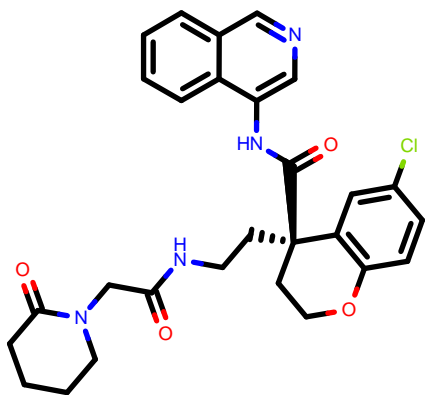
SMILES: COC[C@@H]1CN(CCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN4561

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.32

EN300-36111_3_1_1



CID: EN300-36111_3_1_1

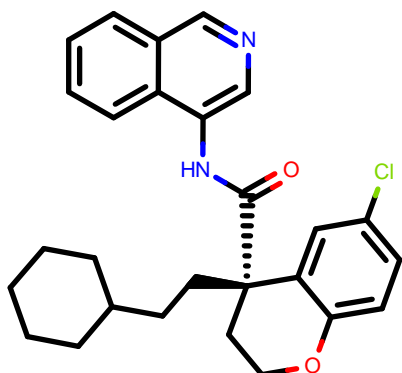
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCCC5=O

RUN: RUN5940

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

VLA-UCB-05e51b3f-13_1



CID: VLA-UCB-05e51b3f-13_1

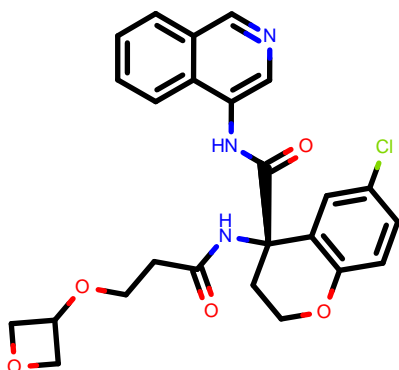
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5

RUN: RUN267

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.38

EN300-321703_1_1_1



CID: EN300-321703_1_1_1

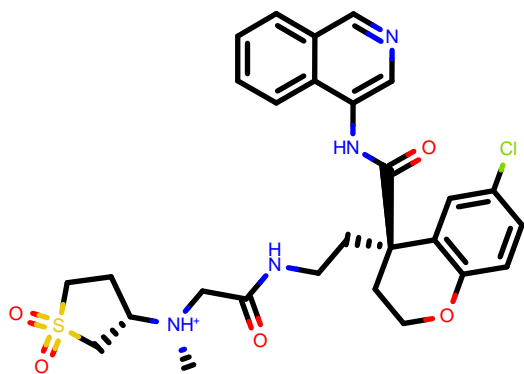
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCOC5C0C5

RUN: RUN4201

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.25

EN300-14628_3_2_1



CID: EN300-14628_3_2_1

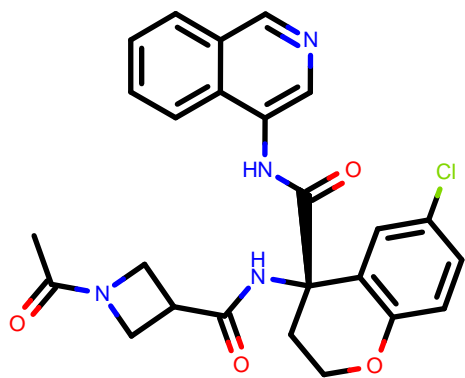
SMILES: C[N+]([O-])CC(O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4[C@@]5H5CCS1(=O)=O

RUN: RUN6896

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.46

EN300-74876_1_1_1



CID: EN300-74876_1_1_1

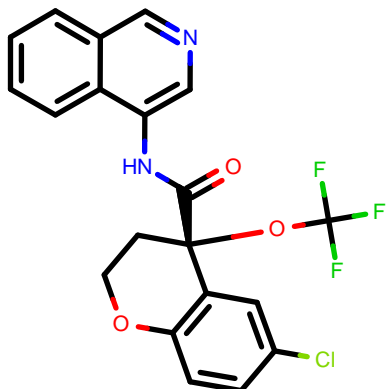
SMILES: CC(=O)N1CC(C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN5022

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

DAR-DIA-e7614d05-2_1



CID: DAR-DIA-e7614d05-2_1

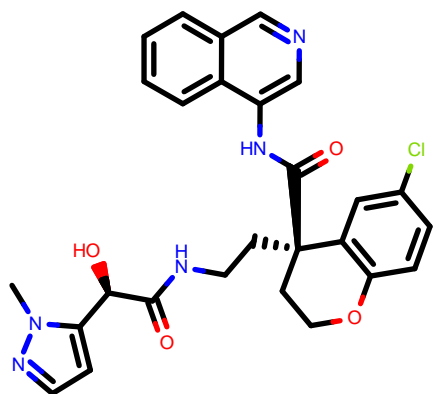
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC(F)(F)F

RUN: RUN2293

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.17

EN300-6473273_3_2_1



CID: EN300-6473273_3_2_1

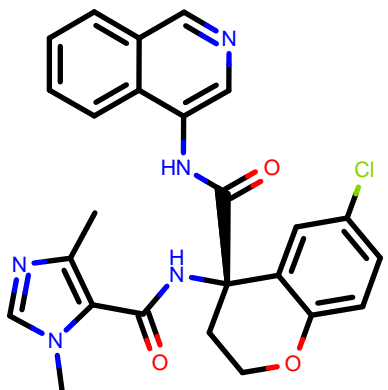
SMILES: Cn1c(cn1)[C@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5)O

RUN: RUN6591

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.33

EN300-6498351_1_1_1



CID: EN300-6498351_1_1_1

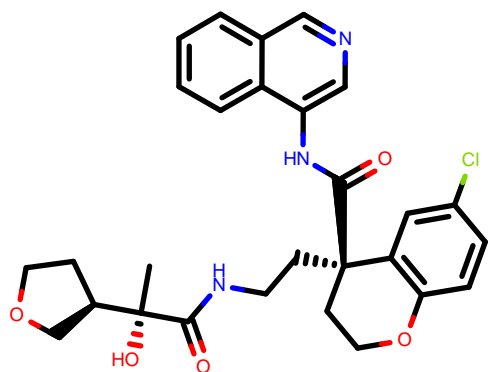
SMILES: Cc1c(n(cn1)C(=O)N)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN5572

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-217494_3_2_1



CID: EN300-217494_3_2_1

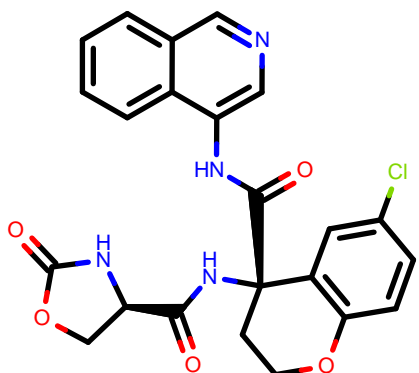
SMILES: C[C@@]([C@@H]1CCOC1)(C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN4182

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.33

EN300-201346_1_2_1



CID: EN300-201346_1_2_1

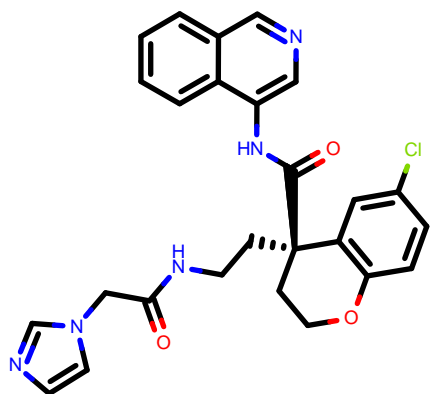
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COC(=O)N5

RUN: RUN4091

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.19

EN300-38979_3_1_1



CID: EN300-38979_3_1_1

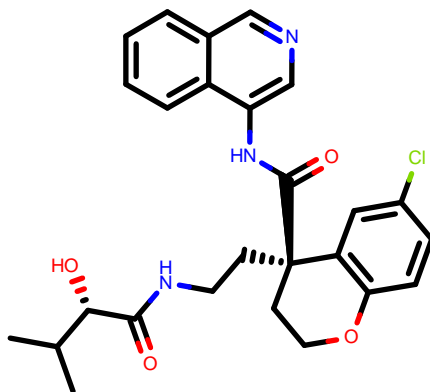
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc5

RUN: RUN3754

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.27

EN300-199359_3_1_1



CID: EN300-199359_3_1_1

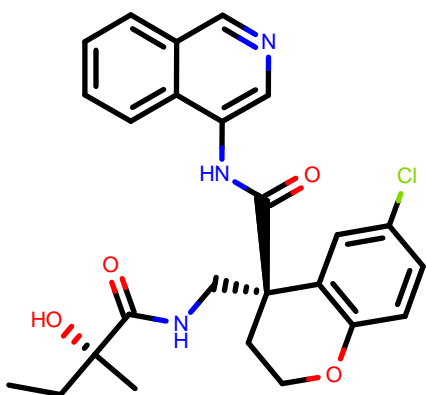
SMILES: CC(C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN7702

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.30

EN300-104746_2_2_1



CID: EN300-104746_2_2_1

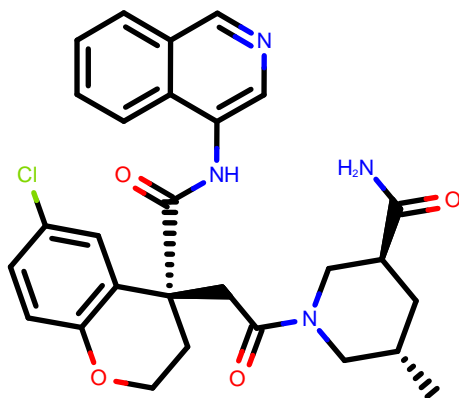
SMILES: CC[C@](C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN5893

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.28

EN300-1724086_1_2_1



CID: EN300-1724086_1_2_1

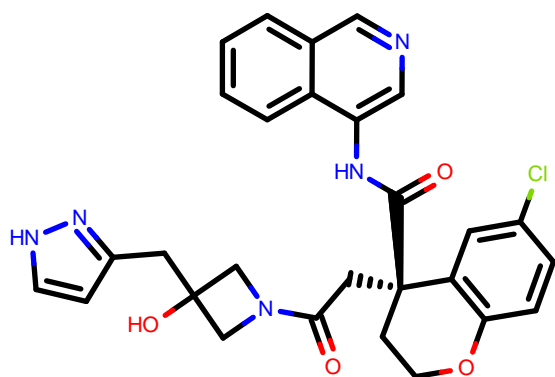
SMILES: C[C@@H]1C[C@@H]2(CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5)Cl=O

RUN: RUN5430

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-6489696_1_1_1



CID: EN300-6489696_1_1_1

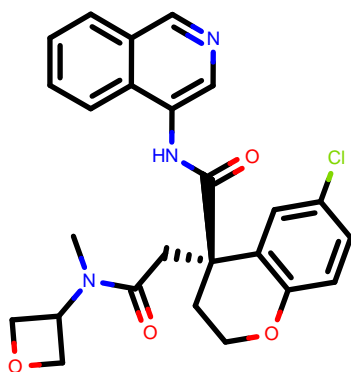
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5CC(C5)(C6c6cn[nH]6)O

RUN: RUN5284

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-1091444_1_1_1



CID: EN300-1091444_1_1_1

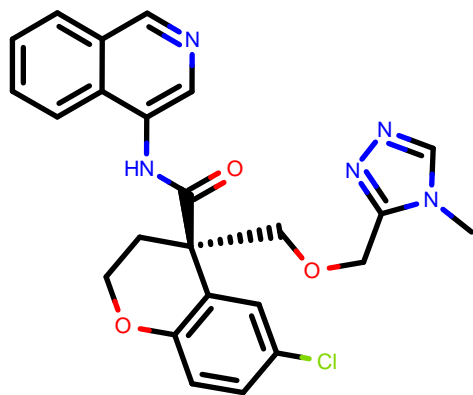
SMILES: CN(C1CO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN3832

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.28

EN300-113112_2_1_1



CID: EN300-113112_2_1_1

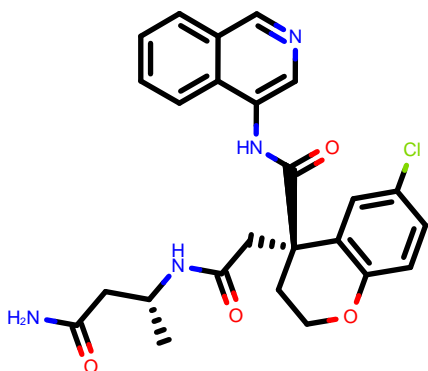
SMILES: Cn1cnnc1COC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3170

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.22

EN300-84785_1_2_1



CID: EN300-84785_1_2_1

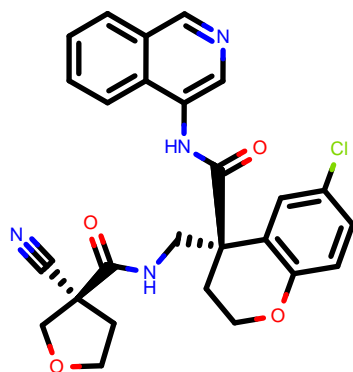
SMILES: C[C@@H](CC(=O)N)NC(=O)[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3301

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EDJ-MED-40433386-8_1



CID: EDJ-MED-40433386-8_1

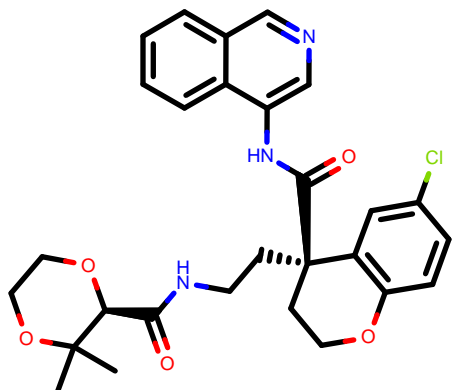
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOC5)C#N

RUN: RUN2386

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.29

EN300-1601684_3_1_1



CID: EN300-1601684_3_1_1

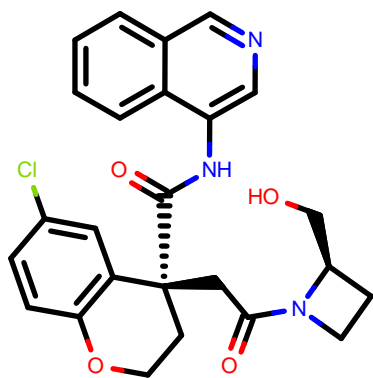
SMILES: CC1([C@@H](OCCO1)C(=O)N)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN5184

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.40

EN300-154332_1_1_1



CID: EN300-154332_1_1_1

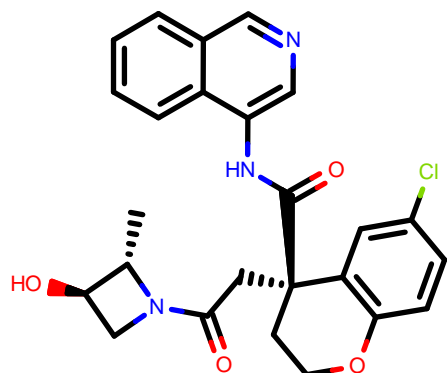
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H]5CO

RUN: RUN5797

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-7471076_1_2_1



CID: EN300-7471076_1_2_1

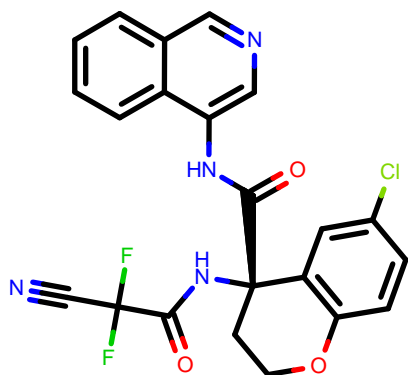
SMILES: C[C@H]1[C@@H](CN1C(=O)[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccc5)O

RUN: RUN5423

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EDG-MED-90036822-84_1



CID: EDG-MED-90036822-84_1

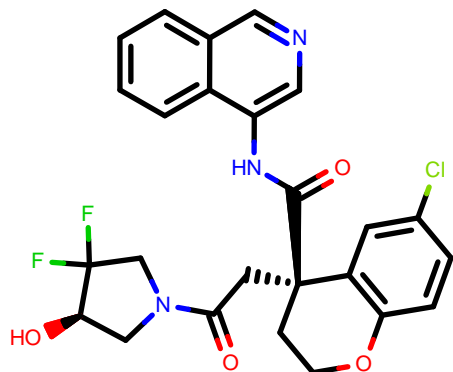
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(C#N)(F)F

RUN: RUN1622

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.22

EN300-1710153_1_2_1



CID: EN300-1710153_1_2_1

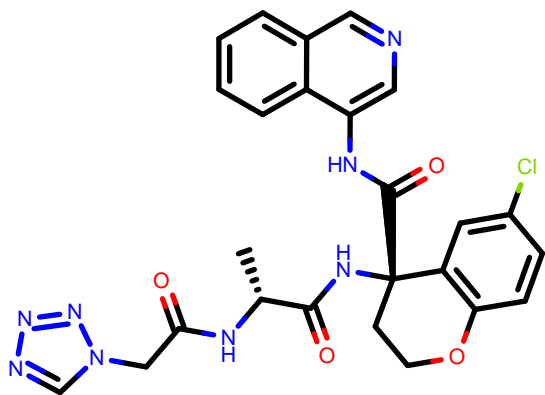
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C5)(F)F)O

RUN: RUN7384

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.23

EN300-649743_1_1_1



CID: EN300-649743_1_1_1

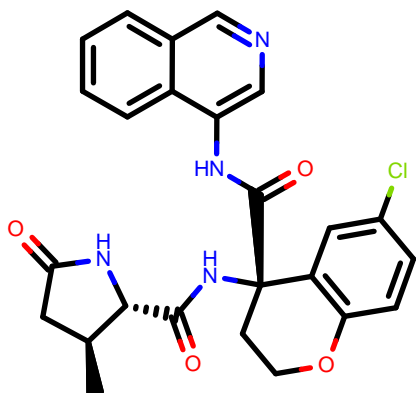
SMILES: C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)NC(=O)Cn5nnn5

RUN: RUN3929

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.37

EN300-155362_1_2_1



CID: EN300-155362_1_2_1

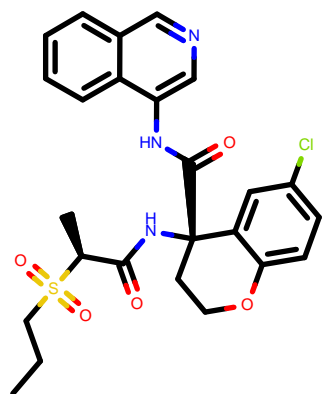
SMILES: C[C@H]1CC(=O)N[C@@]2(CO)N[C@@]3(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6709

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.21

EN300-52768_1_1_1



CID: EN300-52768_1_1_1

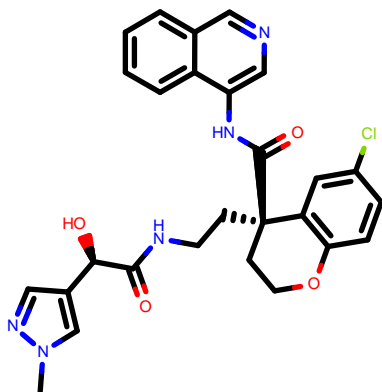
SMILES: CCCS(=O)(=O)[C@@]1(C)C(=O)N[C@@]2(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4977

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.39

EN300-198540_3_2_1



CID: EN300-198540_3_2_1

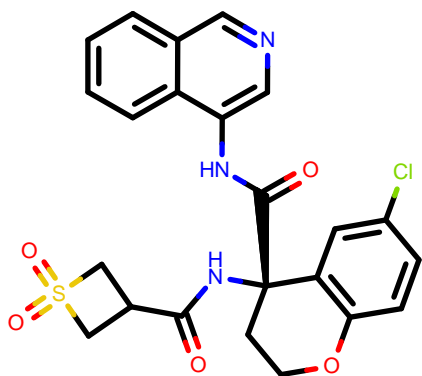
SMILES: C[n+]1cc(c[nH]1)[C@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN4636

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.46

EN300-261365_1_1_1



CID: EN300-261365_1_1_1

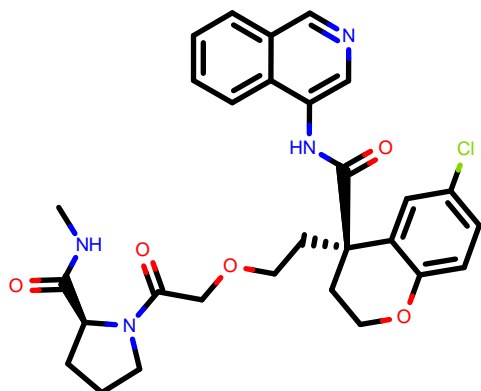
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)NC(=O)C5CS(=O)C(=O)C5

RUN: RUN4142

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.21

EN300-48902_3_1_1



CID: EN300-48902_3_1_1

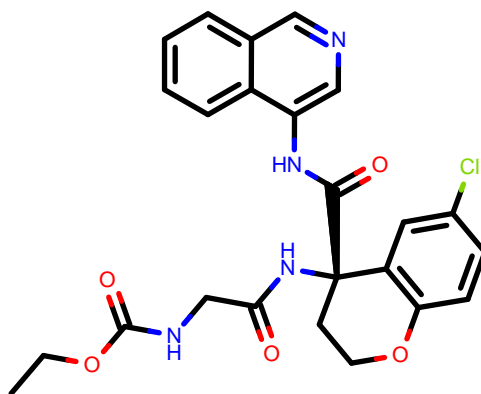
SMILES: CNC(=O)[C@@H](C@H)1CCCN1C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6513

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.40

EN300-36390_1_1_1



CID: EN300-36390_1_1_1

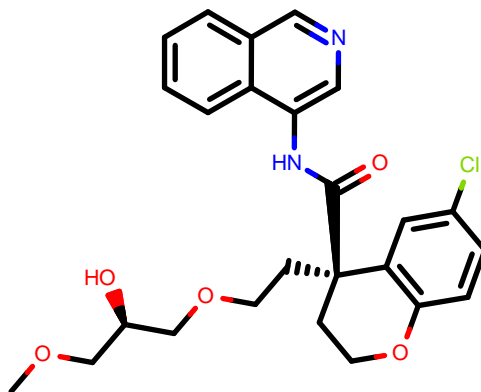
SMILES: CCOC(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN6254

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.23

EN300-1915260_3_2_1



CID: EN300-1915260_3_2_1

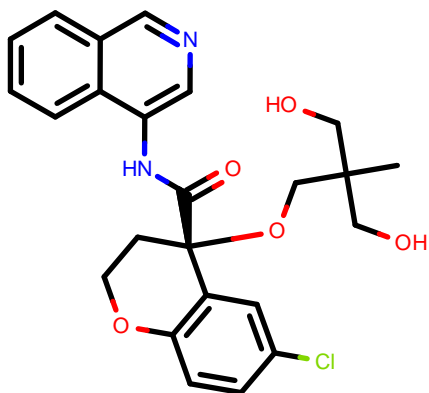
SMILES: COC[C@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O

RUN: RUN6133

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.32

EN300-218116_1_1_1



CID: EN300-218116_1_1_1

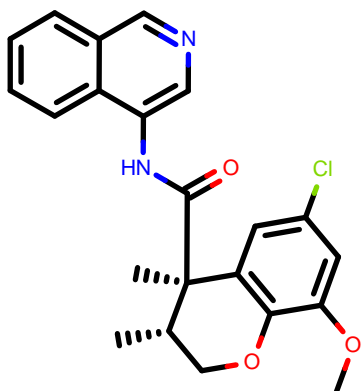
SMILES: CC(CO)(CO)CO[C@]1(C)C(CO)C(=O)Nc3cnc4c3ccc4

RUN: RUN5872

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.38

DAR-DIA-0d514e7d-25_1



CID: DAR-DIA-0d514e7d-25_1

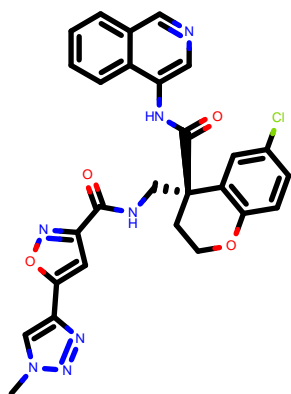
SMILES: C[C@H]1COc2c(cc2OC)Cl[C@]1(C)C(=O)Nc3cnc4c3ccc4

RUN: RUN763

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.12

ALP-UNI-0676e700-23_1



CID: ALP-UNI-0676e700-23_1

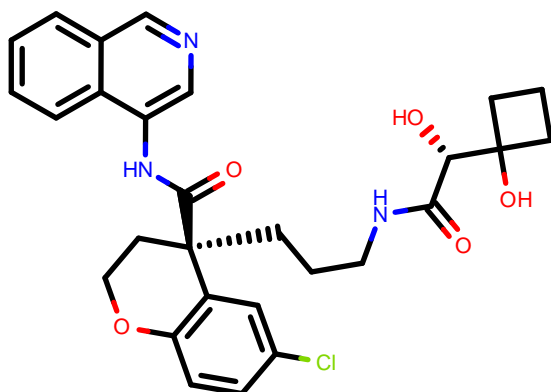
SMILES: Cn1cc(nn1)c2cc(n2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6

RUN: RUN2331

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.34

EN300-1073320_4_1_1



CID: EN300-1073320_4_1_1

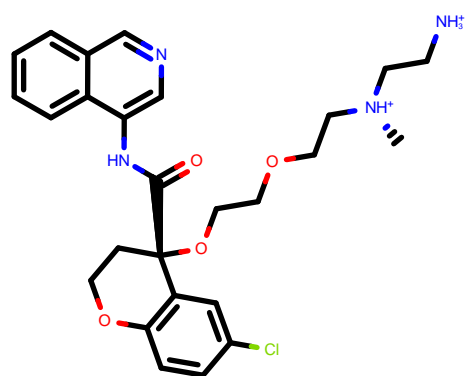
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(C)C(CCC5)O

RUN: RUN7256

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.40

ED_-GRI-5b13fbe2-15_1



CID: ED_-GRI-5b13fbe2-15_1

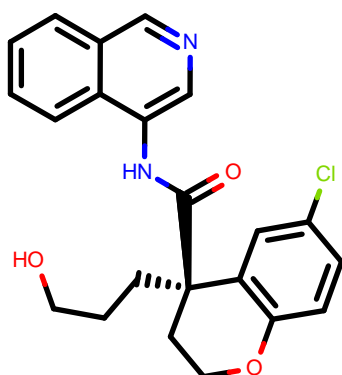
SMILES: C[N+]([C][NH3+])CCOCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN1414

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.50

EDG-MED-971238d3-8_1



CID: EDG-MED-971238d3-8_1

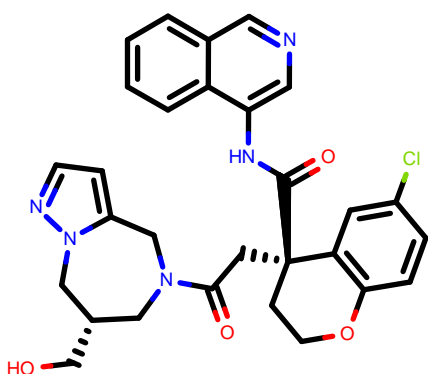
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO

RUN: RUN1306

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.20

EN300-6739414_1_2_1



CID: EN300-6739414_1_2_1

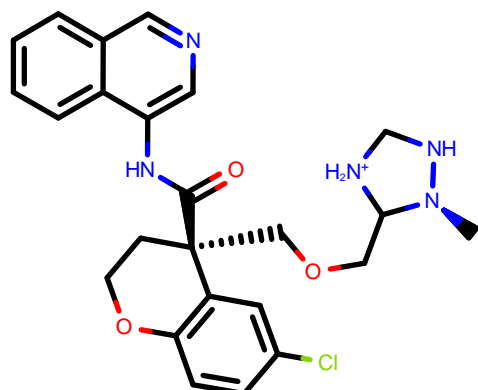
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6c6cnn6[C@H](C5)CO

RUN: RUN7553

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.28

EN300-87334_2_1_1



CID: EN300-87334_2_1_1

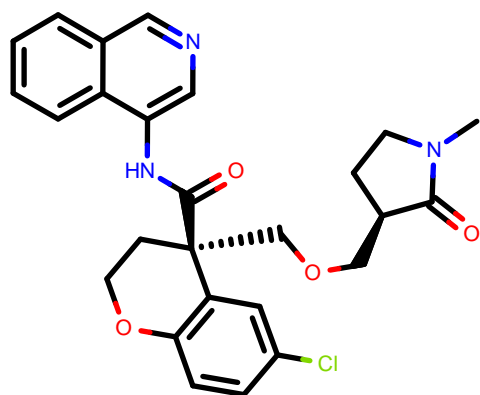
SMILES: Cn1c(ncn1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6606

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.28

EN300-260816_2_1_1



CID: EN300-260816_2_1_1

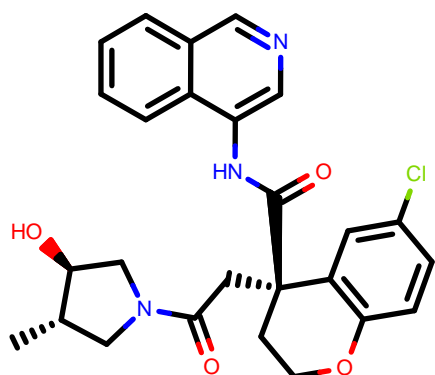
SMILES: CN1CC[C@@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4178

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.24

EN300-124052_1_2_1



CID: EN300-124052_1_2_1

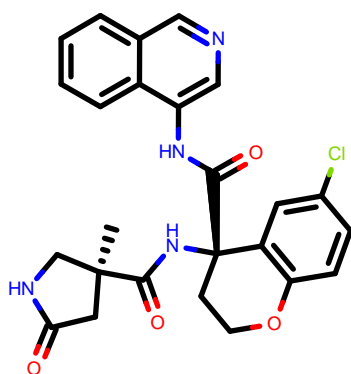
SMILES: C[C@H]1CN[C@@H](O)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4288

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.25

EN300-132157_1_1_1



CID: EN300-132157_1_1_1

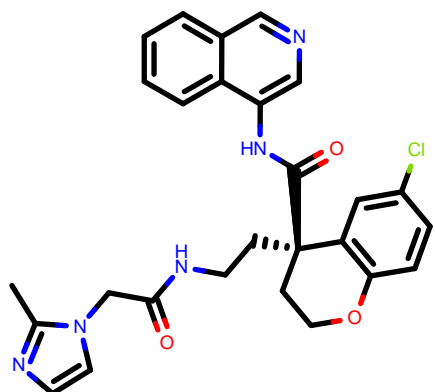
SMILES: C[C@@]1(CC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN4966

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-41507_3_1_1



CID: EN300-41507_3_1_1

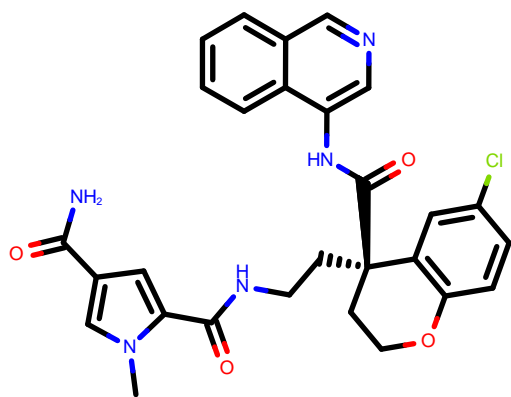
SMILES: Cc1nccn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN5753

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.31

KAD-UNI-8a629cb0-4_1



CID: KAD-UNI-8a629cb0-4_1

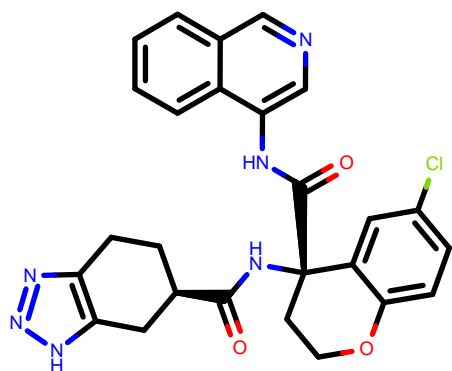
SMILES: Cn1cc(cc1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C(=O)N

RUN: RUN1946

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-185729_1_1_1



CID: EN300-185729_1_1_1

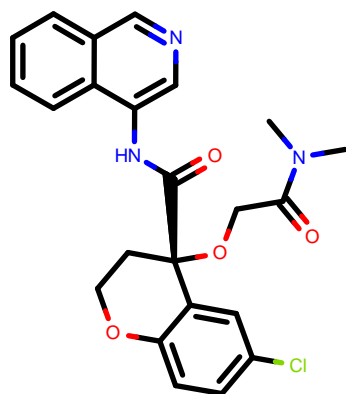
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6c6c1nHn6)C5

RUN: RUN3045

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.23

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

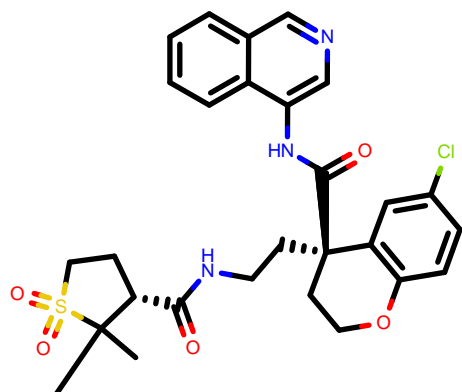
SMILES: CN(C)C(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6561

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.20

EN300-2007564_3_2_1



CID: EN300-2007564_3_2_1

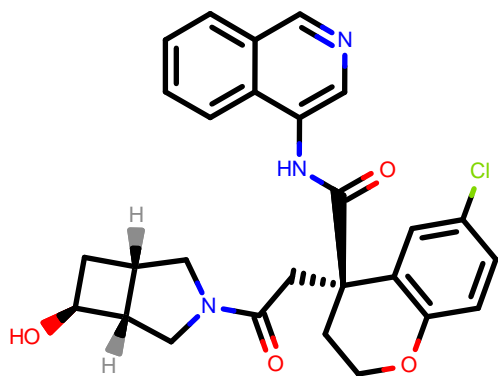
SMILES: CC1([C@H](CCS1(=O)=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C

RUN: RUN3866

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.35

EN300-305294_1_6_1



CID: EN300-305294_1_6_1

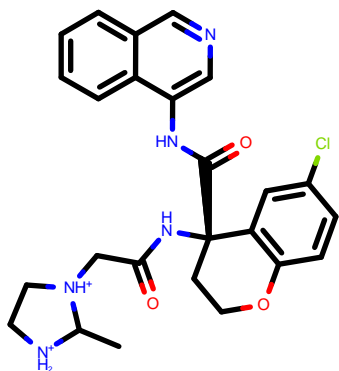
SMILES: c1ccc2c(c1)cnc2N[C@@H](C(=O)N[C@@H](C1=CC=C(C=C1)O)C(=O)N[C@@H](C1=CC=C(C=C1)O)C

RUN: RUN4981

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-41507_1_1_1



CID: EN300-41507_1_1_1

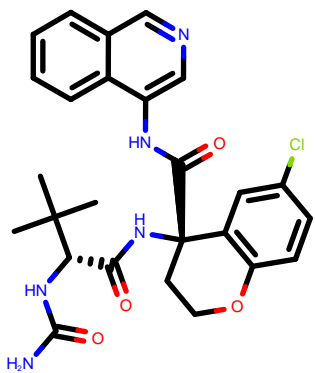
SMILES: Cc1nccn1CC(=O)N[C@@H](C(=O)N[C@@H](C1=CC=C(C=C1)O)C(=O)Nc4cnc5c4cccc5

RUN: RUN5643

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.25

EN300-201164_1_2_1



CID: EN300-201164_1_2_1

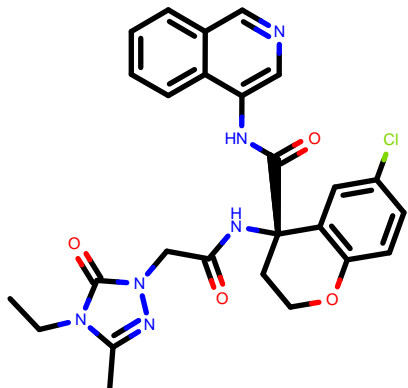
SMILES: CC(C)(C)[C@@H](C(=O)N[C@@H](C(=O)N[C@@H](C1=CC=C(C=C1)O)C(=O)Nc3ccc4c3cccc4N(C)=O)N

RUN: RUN3887

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.25

EN300-6478433_1_1_1



CID: EN300-6478433_1_1_1

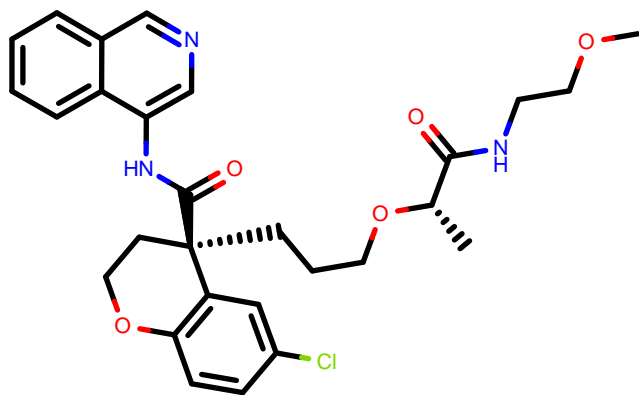
SMILES: CCn1c(nn(c1=O)CC(=O)N[C@@H](C(=O)N[C@@H](C1=CC=C(C=C1)O)C(=O)Nc4cnc5c4cccc5)C

RUN: RUN5716

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.35

EN300-23317_4_1_1



CID: EN300-23317_4_1_1

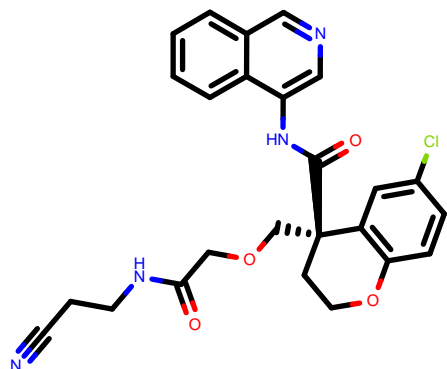
SMILES: C[C@@H](C(=O)NCCCOC)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6585

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.38

EN300-10895_2_1_1



CID: EN300-10895_2_1_1

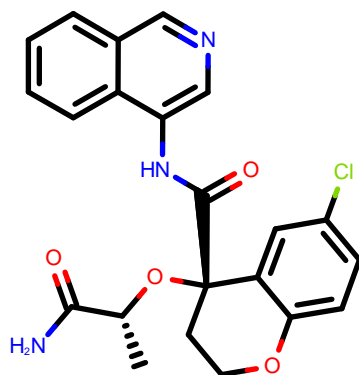
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCCC#N

RUN: RUN5767

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.30

EN300-17381_1_2_1



CID: EN300-17381_1_2_1

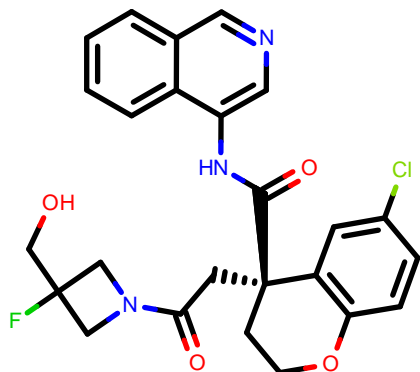
SMILES: C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN5740

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.21

EN300-204507_1_1_1



CID: EN300-204507_1_1_1

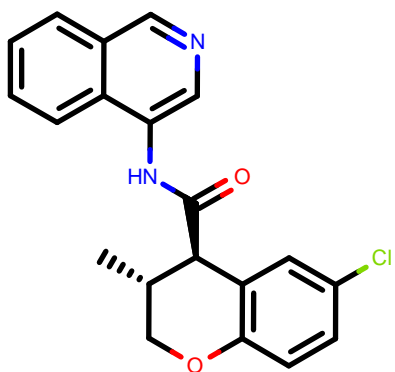
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F

RUN: RUN6947

DDG (kcal/mol): -0.83

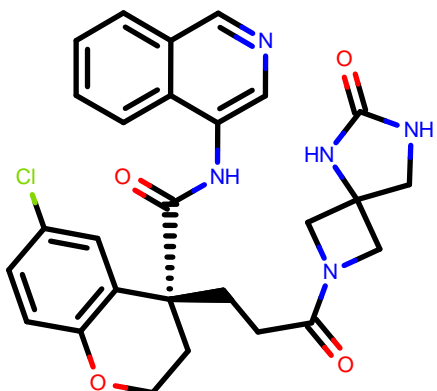
dDDG (kcal/mol): 0.35

EDJ-MED-e4b030d8-11_1_1



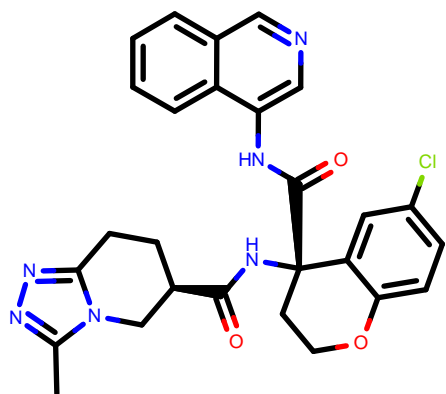
CID:	EDJ-MED-e4b030d8-11_1_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN5837
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.05

EN300-1605226_2_1_1



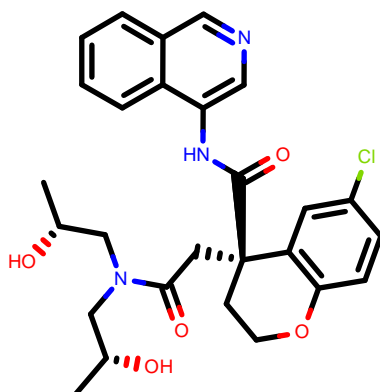
CID:	EN300-1605226_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)Cl)CCC(=O)N5CC6(C5)CNC(=O)N6</chem>
RUN:	RUN6161
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.25

EN300-50561_1_1_1



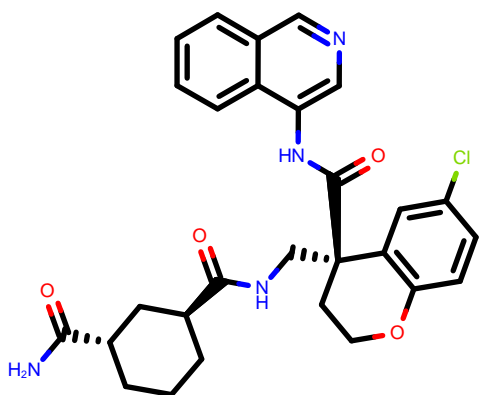
CID:	EN300-50561_1_1_1
SMILES:	<chem>Cc1nnc2n1C[C@@H](CC2)C(=O)N[C@@]3[C@@]4COCc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6</chem>
RUN:	RUN4979
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.26

EN300-722418_1_2_1



CID:	EN300-722418_1_2_1
SMILES:	<chem>C[C@H](CN(C[C@@H](C)O)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O</chem>
RUN:	RUN5522
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.44

EN300-90142_2_2_1



CID: EN300-90142_2_2_1

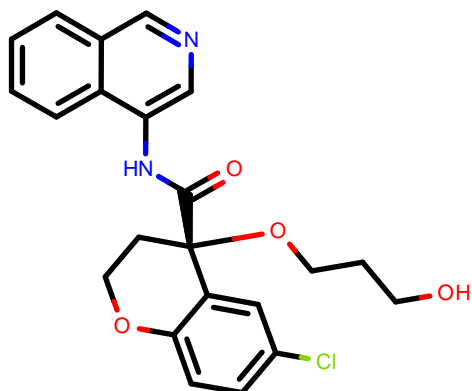
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3ccc4YCl)CNC(=O)[C@@H]5CCC[C@@H]5(C)Cl=O

RUN: RUN7181

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.33

EN300-221518_1_1_1



CID: EN300-221518_1_1_1

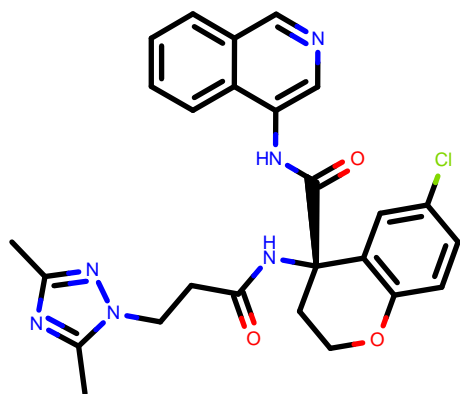
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3ccc(cc4)Cl)OCCCO

RUN: RUN5339

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.18

EN300-41366_1_1_1



CID: EN300-41366_1_1_1

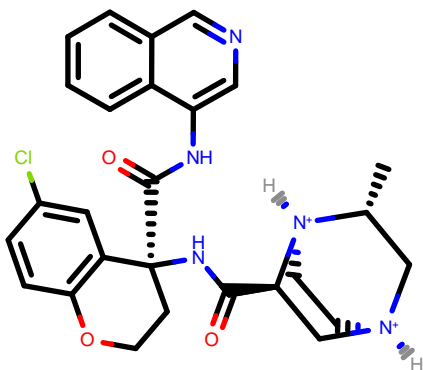
SMILES: Cc1nc(n1)CCC(=O)N[C@@]2[C@@]2(CCOc3c2ccc(cc3)Cl)C(=O)Nc4ncnc5c4ccc5C

RUN: RUN4234

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-120562_1_1_1



CID: EN300-120562_1_1_1

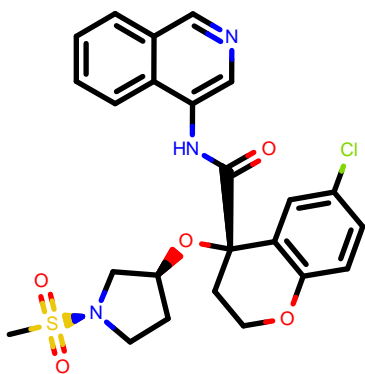
SMILES: C[C@@]1[C@@]1CN[C@@]2[C@@]2CN[C@@]3[C@@]3(CCOc4c3ccc(cc4)Cl)C(=O)Nc5ncnc6c5ccc6

RUN: RUN7502

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-301690_1_1_1



CID: EN300-301690_1_1_1

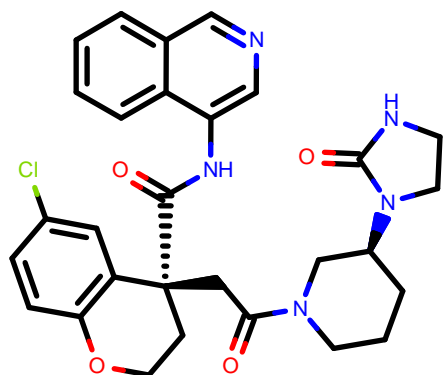
SMILES: CS(=O)(=O)[N@]1CC[C@@H](C1)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN6861

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.30

EN300-55087_1_1_1



CID: EN300-55087_1_1_1

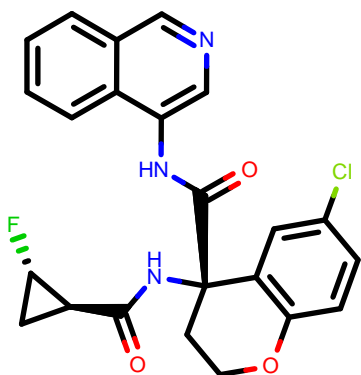
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CC[C@H]5C6NCCN6=O

RUN: RUN6042

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-97300_1_2_1



CID: EN300-97300_1_2_1

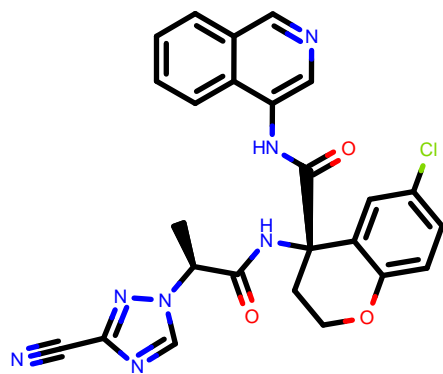
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H]5F

RUN: RUN6127

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.20

EN300-198515_1_1_1



CID: EN300-198515_1_1_1

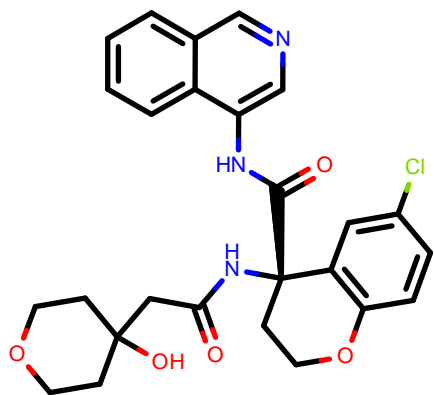
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccc4)n5ncn5)C#N

RUN: RUN2856

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.25

EN300-151423_1_1_1



CID: EN300-151423_1_1_1

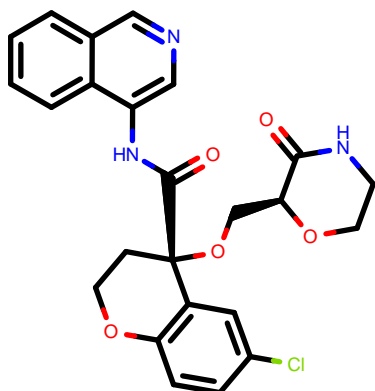
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5(CCOCC5)O

RUN: RUN4516

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.28

EN300-1706036_1_2_1



CID: EN300-1706036_1_2_1

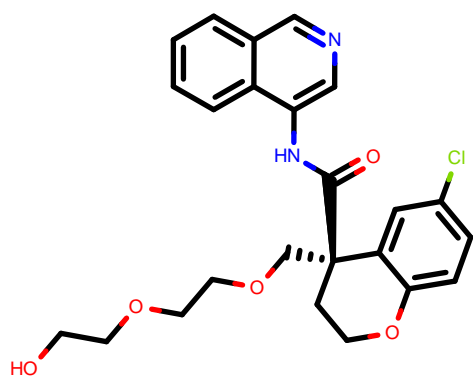
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5C(=O)NCCO5

RUN: RUN4519

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-52467_2_1_1



CID: EN300-52467_2_1_1

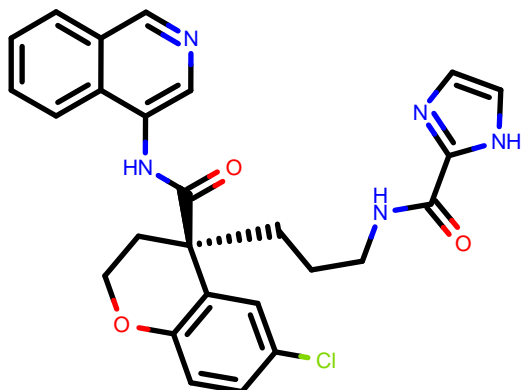
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCCOCCO

RUN: RUN6299

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.24

EN300-315836_4_1_1



CID: EN300-315836_4_1_1

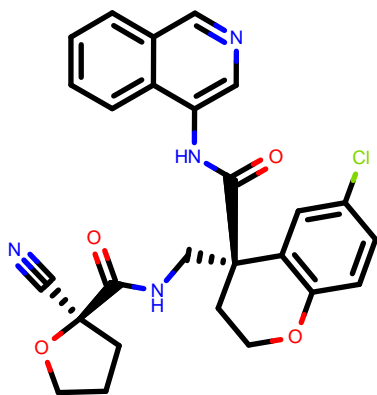
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5[nH]cnc5

RUN: RUN5610

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.29

EN300-3710141_2_2_1



CID: EN300-3710141_2_2_1

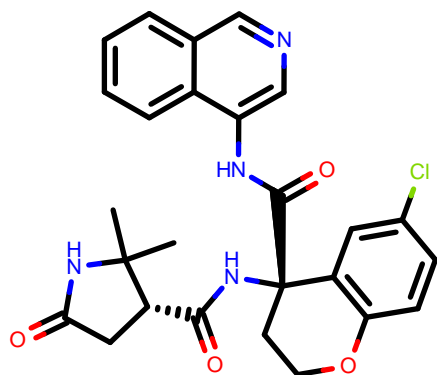
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCCO5)C#N

RUN: RUN3235

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-1694056_1_1_1



CID: EN300-1694056_1_1_1

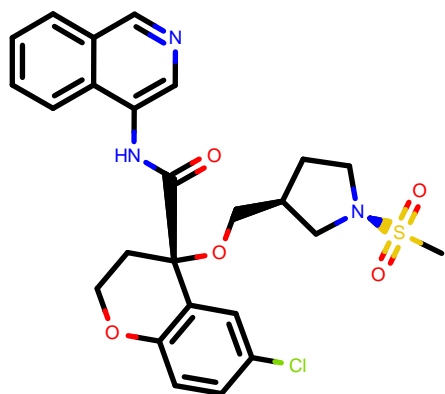
SMILES: CC1([C@@H](CC(=O)N1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)C

RUN: RUN3420

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.26

EN300-261986_1_1_1



CID: EN300-261986_1_1_1

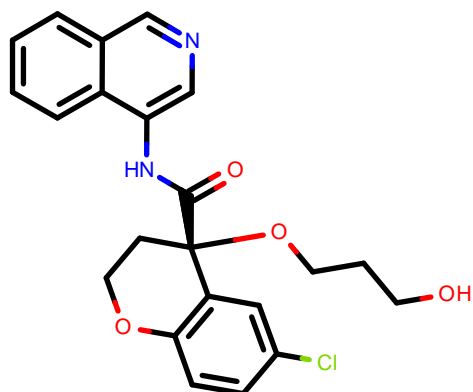
SMILES: CS(=O)(=O)[N@]1CC[C@@H](C1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3793

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.40

EN300-221518_1_1_1



CID: EN300-221518_1_1_1

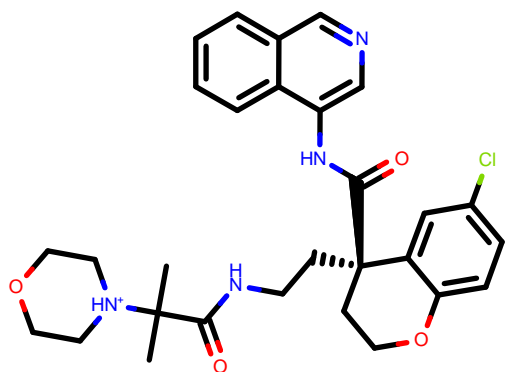
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO

RUN: RUN5155

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-64247_3_1_1



CID: EN300-64247_3_1_1

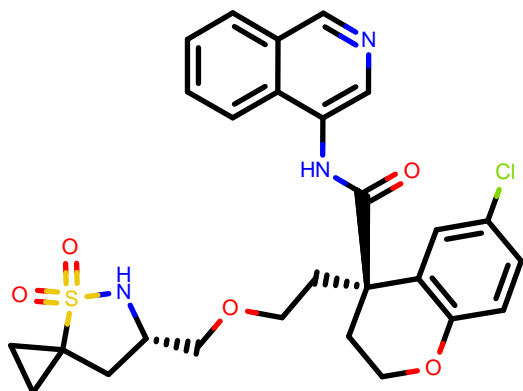
SMILES: CC(C)(C(=O)NCC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)[NH+]5CCOCC5

RUN: RUN4542

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.46

EN300-6504697_3_1_1



CID: EN300-6504697_3_1_1

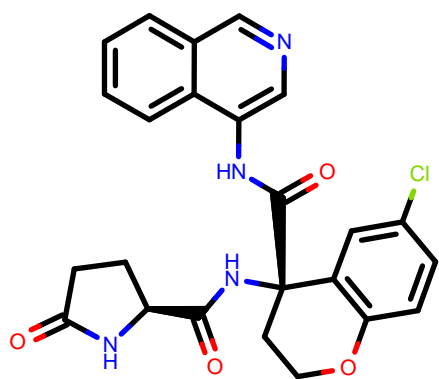
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CO6(CO6)S(=O)(=O)N5

RUN: RUN6063

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.31

EN300-72896_1_1_1



CID: EN300-72896_1_1_1

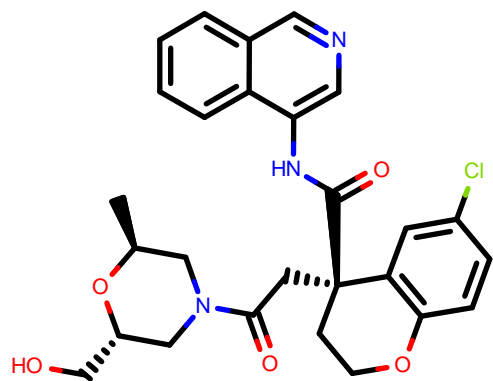
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN5397

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.21

EN300-157776_1_2_1



CID: EN300-157776_1_2_1

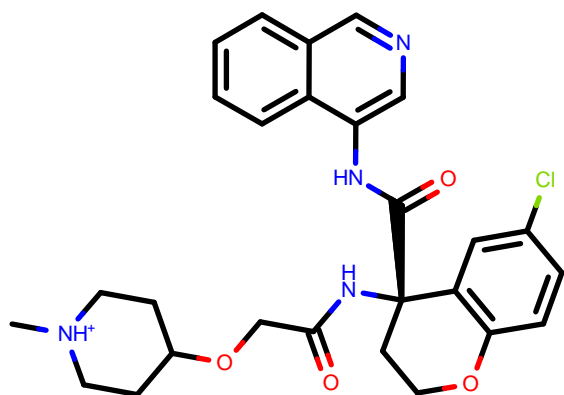
SMILES: C[C@@H]1CN[C@@H](O1)CO[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7139

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.38

EN300-237224_1_1_1



CID: EN300-237224_1_1_1

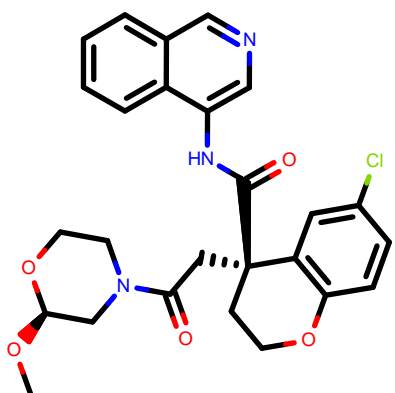
SMILES: C[NH+]1CCC(CC1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5755

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.34

EN300-108507_1_1_1



CID: EN300-108507_1_1_1

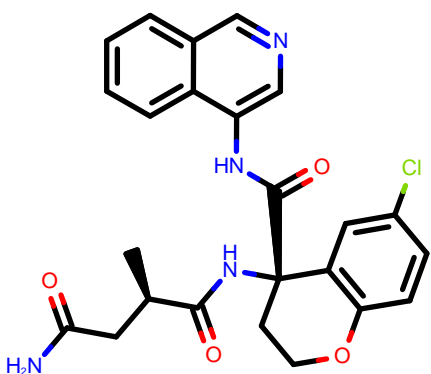
SMILES: CO[C@@H]1CN(CCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5819

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.31

EN300-202757_1_2_1



CID: EN300-202757_1_2_1

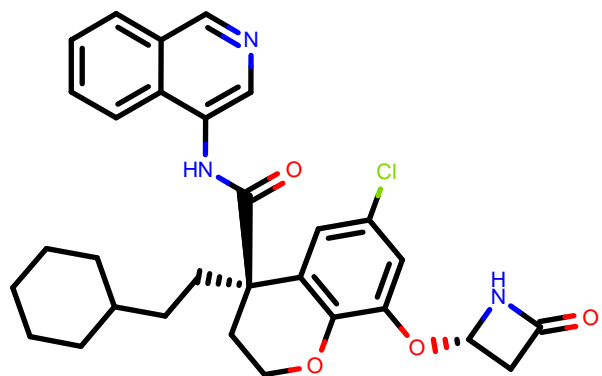
SMILES: C[C@@H](CC(=O)N)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN4604

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.32

VLA-UCB-50c39ae8-9_2



CID: VLA-UCB-50c39ae8-9_2

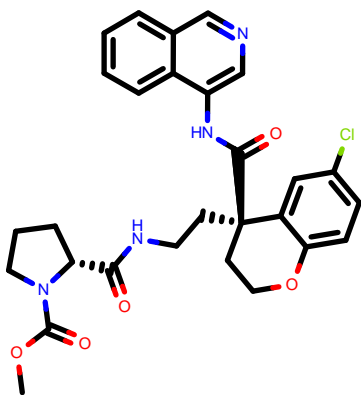
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)[C@H]5CC(=O)N5)Cl)CCc6CCCC6

RUN: RUN366

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.40

EN300-66845_3_1_1



CID: EN300-66845_3_1_1

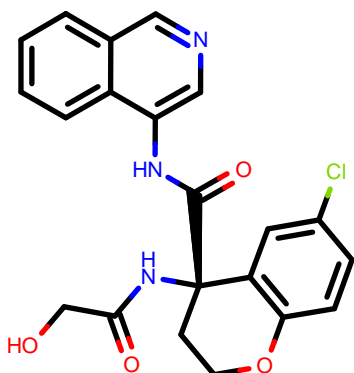
SMILES: COC(=O)N1CCC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN6534

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.32

EDG-MED-90036822-13_1



CID: EDG-MED-90036822-13_1

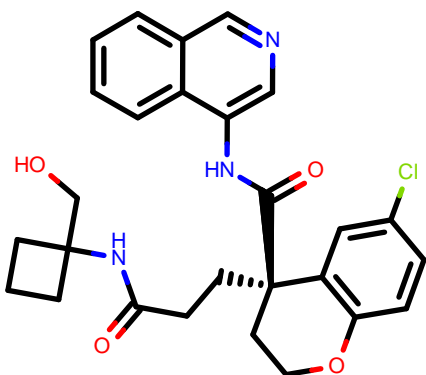
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO

RUN: RUN1522

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.16

EN300-1723511_2_1_1



CID: EN300-1723511_2_1_1

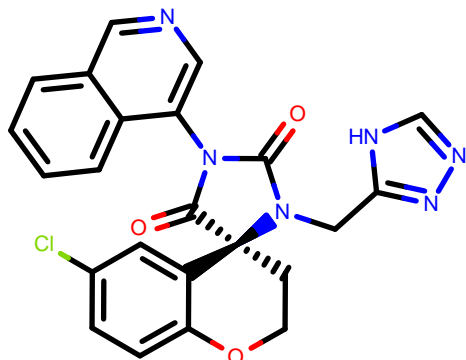
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CCC5)CO

RUN: RUN4804

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.26

VLA-UNK-f702bf1c-3_1



CID: VLA-UNK-f702bf1c-3_1

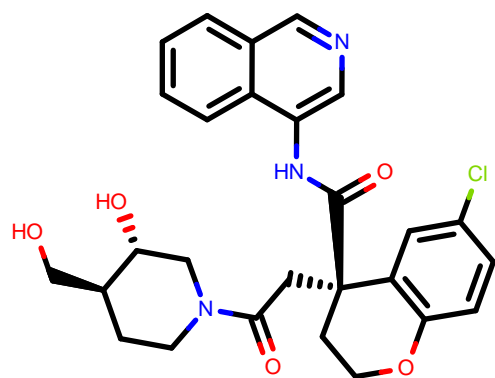
SMILES: c1ccc2c(c1)ncnc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C6([nH])n6

RUN: RUN2111

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.30

EN300-95639_1_2_1



CID: EN300-95639_1_2_1

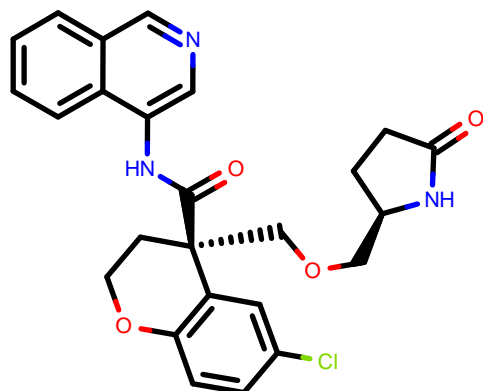
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4=C3C=CC=C4)C(=O)N5CC[C@@H]3[C@@H](C5)O/CO

RUN: RUN3763

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.34

EN300-195756_2_2_1



CID: EN300-195756_2_2_1

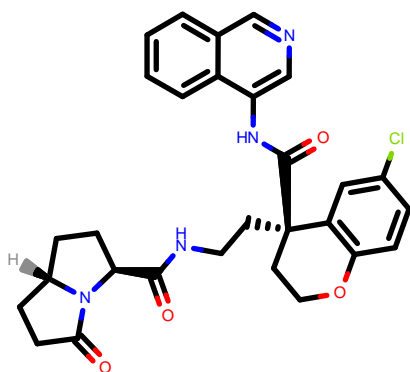
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4=C3C=CC=C4)C(=O)N5CC[C@@H]3[C@@H](C5)O

RUN: RUN5080

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.28

EN300-6479181_3_1_1



CID: EN300-6479181_3_1_1

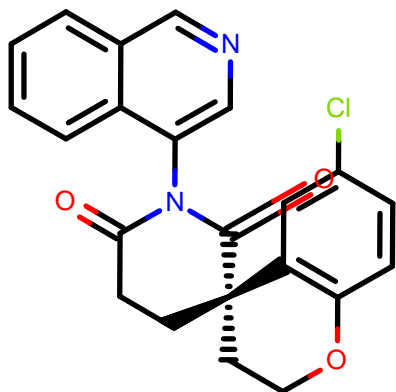
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4=C3C=CC=C4)C(=O)N5CC[C@@H]3[C@@H](C5)O

RUN: RUN6444

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.39

VLA-UCB-05e51b3f-6_1



CID: VLA-UCB-05e51b3f-6_1

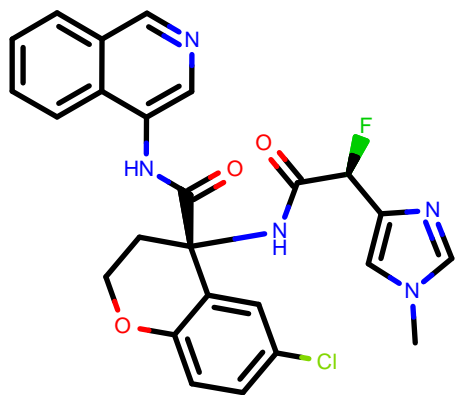
SMILES: c1ccc2c(c1)ncnc2N3C(=O)CC[C@@H]4(C3=O)CCOC5=C4C=CC=C5Cl

RUN: RUN239

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.25

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)Nc4cncc5c4cccc5)F

RUN:

RUN1580

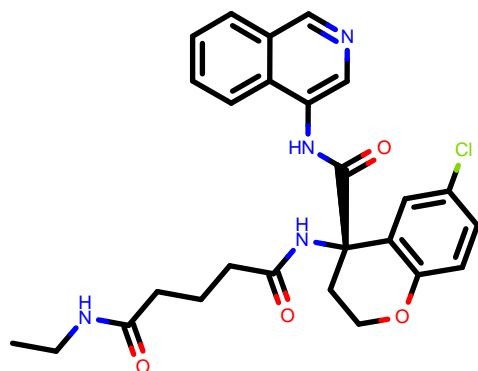
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.26

EN300-68635_1_1_1



CID: EN300-68635_1_1_1

SMILES:

CCNC(=O)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN5209

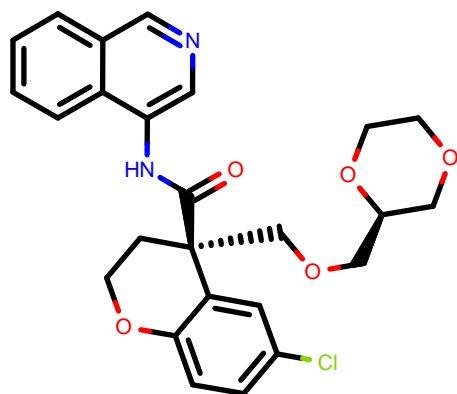
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.28

EN300-139167_2_1_1



CID: EN300-139167_2_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5H5COCCO5

RUN:

RUN4847

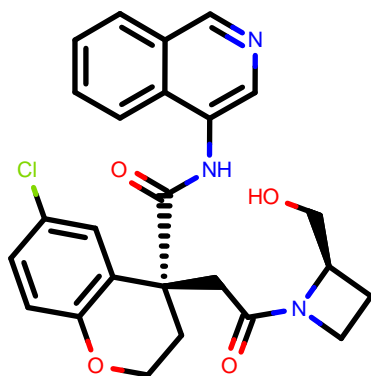
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.23

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@@]5H5CO

RUN:

RUN2464

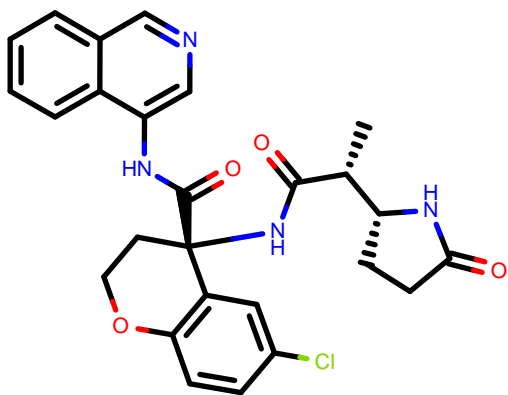
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.29

EN300-249421_1_4_1



CID: EN300-249421_1_4_1

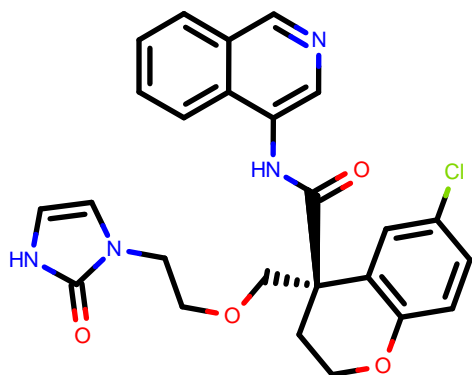
SMILES: C[C@H]([C@H]1CCC(=O)N1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3229

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.25

EN300-214800_2_1_1



CID: EN300-214800_2_1_1

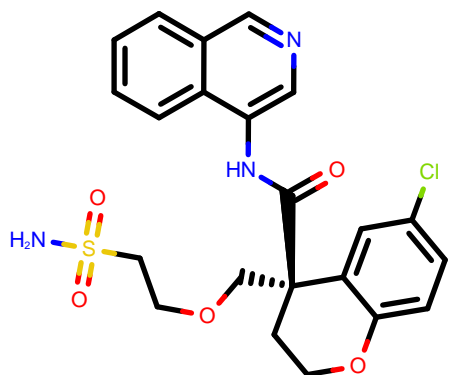
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCN5CCNC5=O

RUN: RUN4389

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.24

EN300-270710_2_1_1



CID: EN300-270710_2_1_1

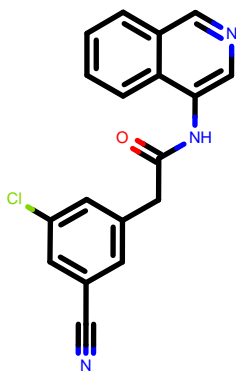
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCS(=O)(=O)N

RUN: RUN4387

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.25

MAT-POS-cc05818f-1_1



CID: MAT-POS-cc05818f-1_1

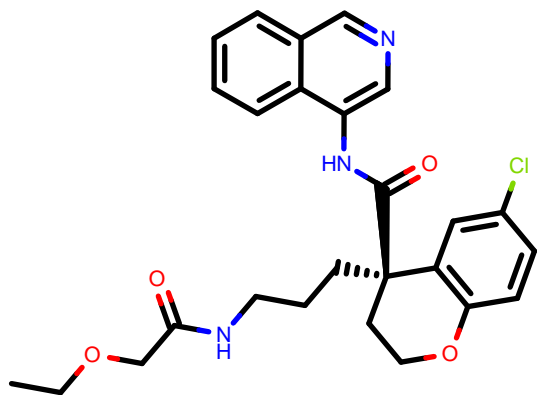
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C#N

RUN: RUN2003

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.28

EN300-21303_4_1_1



CID: EN300-21303_4_1_1

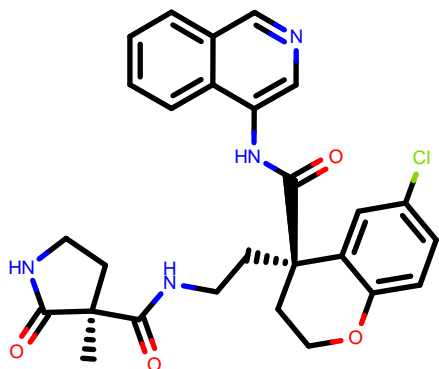
SMILES: CCOCC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN6209

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-207959_3_2_1



CID: EN300-207959_3_2_1

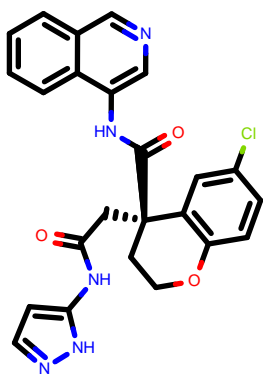
SMILES: C[C@@]1(CCN1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN4211

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.36

JAG-UCB-706446eb-6_1_1



CID: JAG-UCB-706446eb-6_1_1

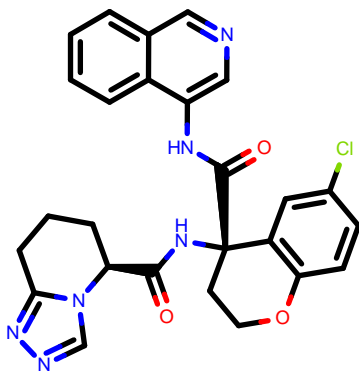
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cnc[nH]5

RUN: RUN6284

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

EN300-6478631_1_1_1



CID: EN300-6478631_1_1_1

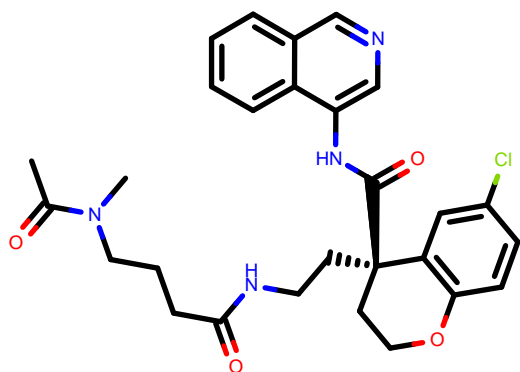
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C5CCc6n6

RUN: RUN4180

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

EN300-128750_3_1_1



CID: EN300-128750_3_1_1

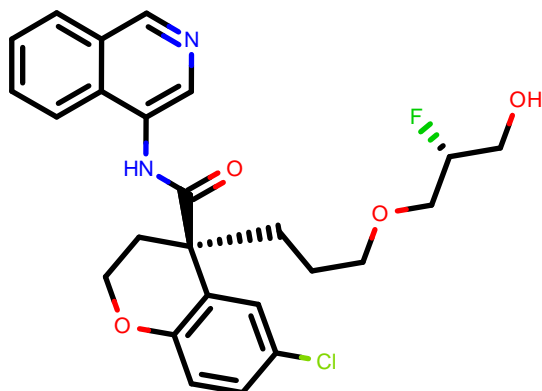
SMILES: CC(=O)N(C)CCCC(=O)NCC[C@]1(C)COCc2c1cc(cc2Cl)C(=O)Nc3ccc4c3ccccc4

RUN: RUN5299

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.31

EN300-1600517_4_1_1



CID: EN300-1600517_4_1_1

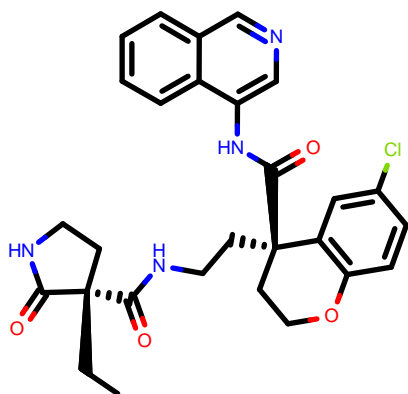
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4Cl)CCCOC[C@@]5(H)[C@](O)F

RUN: RUN7070

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.48

EN300-304135_3_1_1



CID: EN300-304135_3_1_1

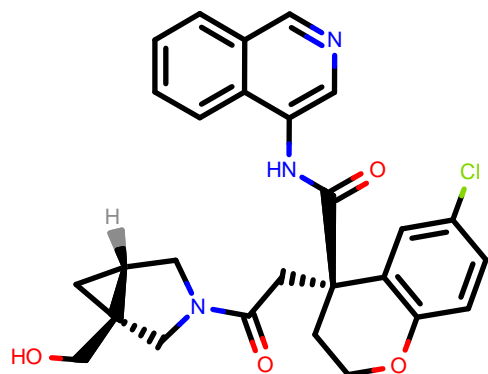
SMILES: CC[C@@]1(C)CNC1=O)C(=O)NCC[C@]2(C)COCc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN3661

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.35

EN300-154179_1_4_1



CID: EN300-154179_1_4_1

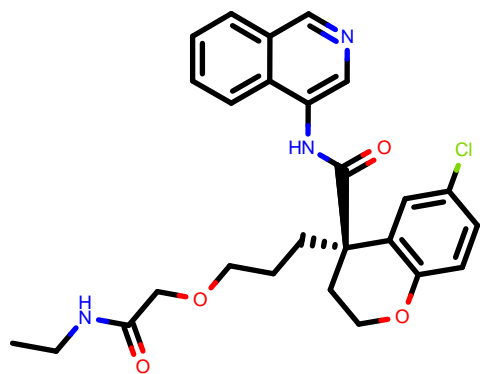
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4Cl)CC(=O)N5C[C@@]6(H)C[C@@]6(C)C5O

RUN: RUN4220

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.30

EN300-7003350_4_1_1



CID: EN300-7003350_4_1_1

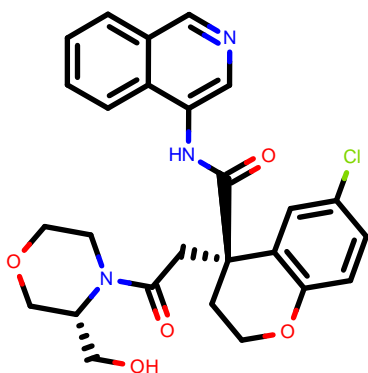
SMILES: CCNC(=O)COCCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3ccc4

RUN: RUN6944

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.26

EN300-154201_1_2_1



CID: EN300-154201_1_2_1

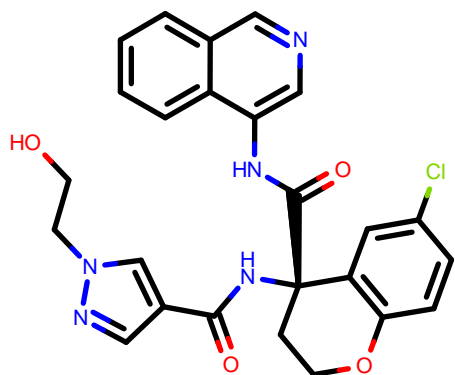
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO

RUN: RUN4859

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.36

EN300-761209_1_1_1



CID: EN300-761209_1_1_1

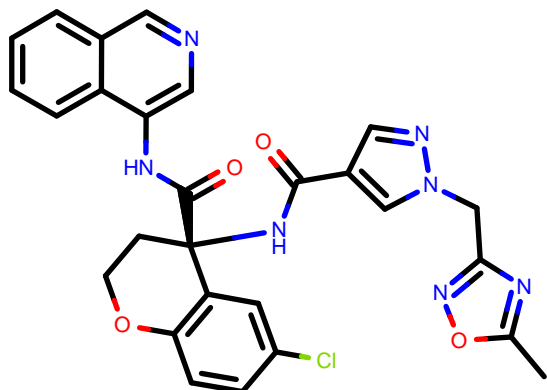
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)NC(=O)c5enn(c5)CCO

RUN: RUN5941

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.22

EN300-131219_1_1_1



CID: EN300-131219_1_1_1

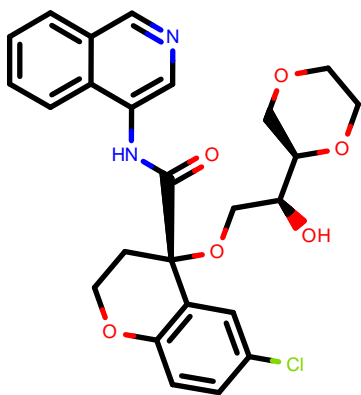
SMILES: Cc1nc(nc1)Cn2cc(cn2)C(=O)N[C@@]3(COCc4c3cc(cc4)Cl)C(=O)Nc5nc6c65ccc6

RUN: RUN4024

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.28

EN300-6238494_1_2_1



CID: EN300-6238494_1_2_1

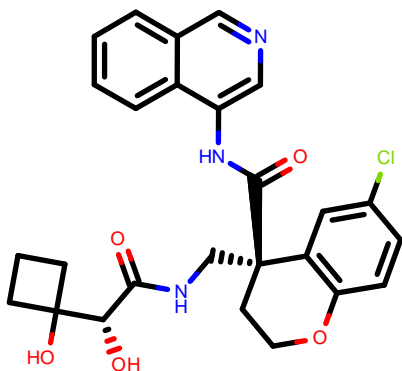
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C@H)5COCOC5O

RUN: RUN5077

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.33

EN300-1073320_2_1_1



CID: EN300-1073320_2_1_1

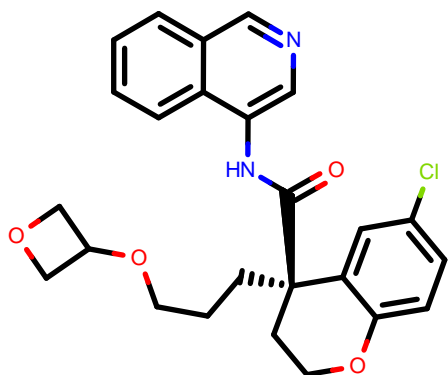
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN6663

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.39

EN300-317082_4_1_1



CID: EN300-317082_4_1_1

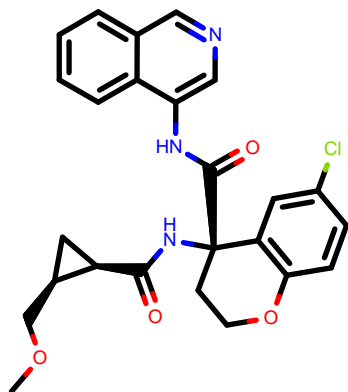
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCOC5COC5

RUN: RUN4740

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.31

EN300-705381_1_1_1



CID: EN300-705381_1_1_1

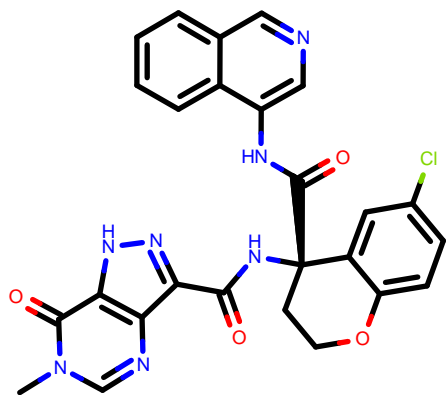
SMILES: COC[C@@H]1C[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5787

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.21

EN300-7355979_1_1_1



CID: EN300-7355979_1_1_1

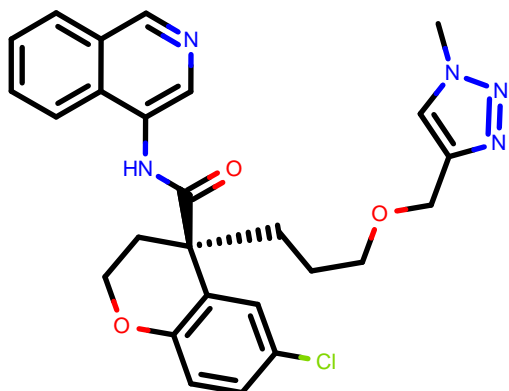
SMILES: Cn1cnc2c(c1=O)[nH]nc2C(=O)N(C@)3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nc6c5ccc6

RUN: RUN7629

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.24

EN300-120282_4_1_1



CID: EN300-120282_4_1_1

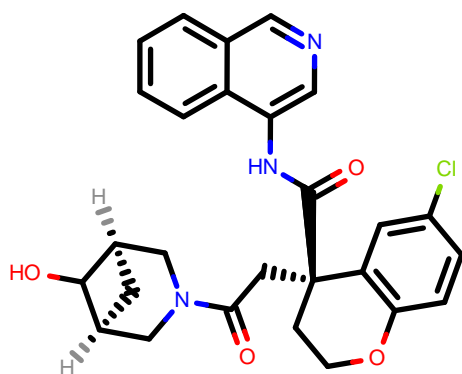
SMILES: Cn1cc(nn1)COCOC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN5527

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.33

EN300-90206_1_1_1



CID: EN300-90206_1_1_1

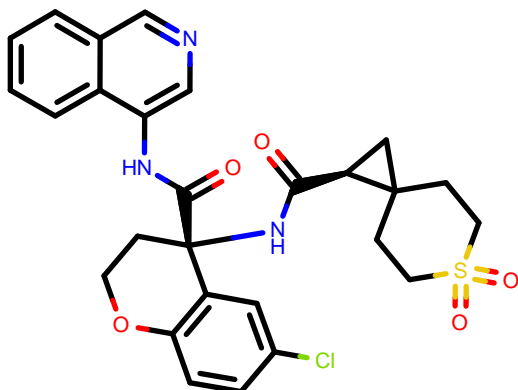
SMILES: c1ccc2c(c1)ncnc2N(C=O)C@)3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@@H](C)C5O6

RUN: RUN3861

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.25

EN300-141809_1_2_1



CID: EN300-141809_1_2_1

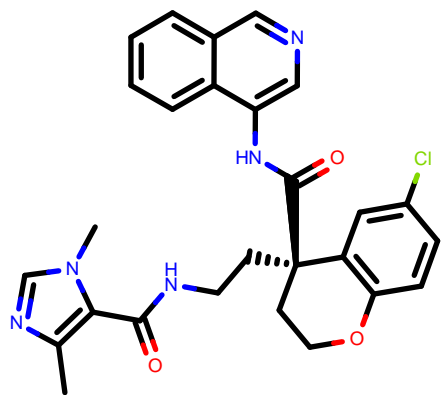
SMILES: c1ccc2c(c1)ncnc2N(C=O)C@)3(CCOc4c3cc(cc4)Cl)N(C=O)C@H5CC6CCS(=O)(=O)C6=O

RUN: RUN7591

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.34

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

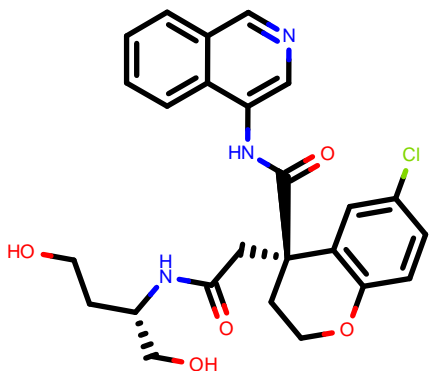
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN7355

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.36

EN300-195790_1_1_1



CID: EN300-195790_1_1_1

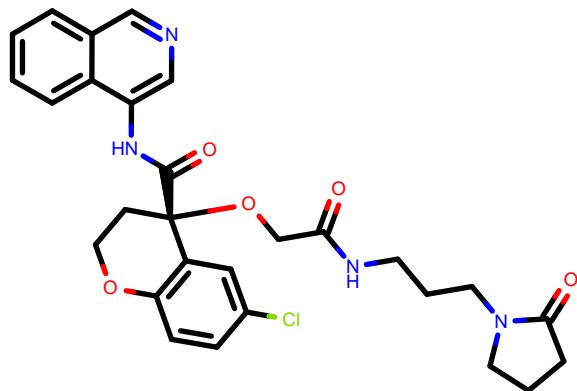
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H(CCO)CO

RUN: RUN7483

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.29

EN300-08259_1_1_1



CID: EN300-08259_1_1_1

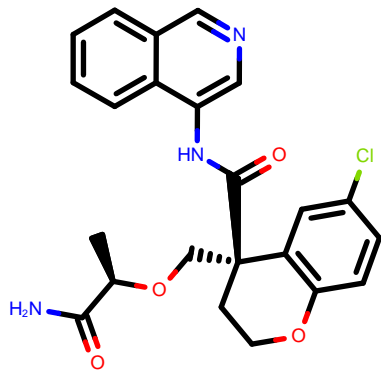
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCN5CCCC5=O

RUN: RUN5719

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.40

EN300-17381_2_2_1



CID: EN300-17381_2_2_1

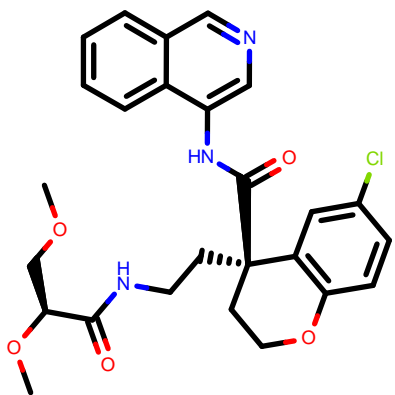
SMILES: C[C@@]H(C(=O)N)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccoc4

RUN: RUN7280

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-305282_3_1_1



CID: EN300-305282_3_1_1

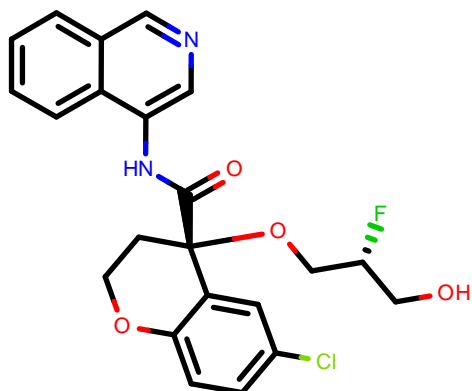
SMILES: COC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)OC

RUN: RUN7686

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.36

EN300-1600517_1_1_1



CID: EN300-1600517_1_1_1

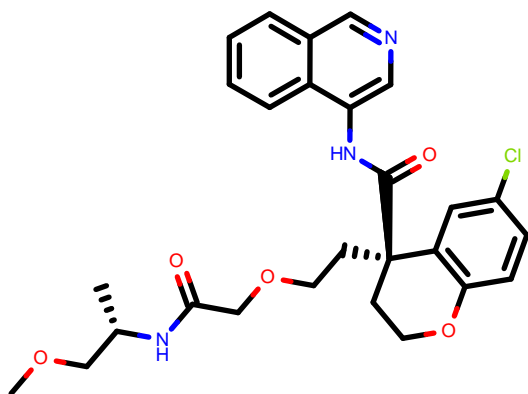
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H](CO)F

RUN: RUN5711

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

EN300-02067_3_1_1



CID: EN300-02067_3_1_1

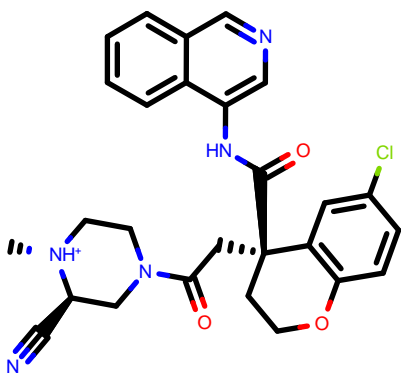
SMILES: C[C@@H](COC)NC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN6625

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.35

EDG-MED-ba1ac7b9-14_8



CID: EDG-MED-ba1ac7b9-14_8

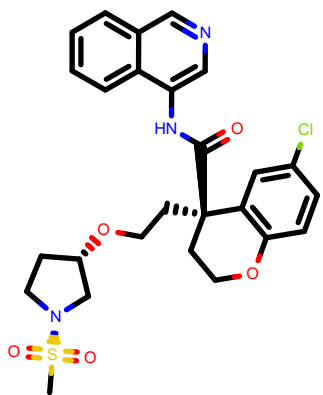
SMILES: C[N@]1CCN[C@@H]1C#N[C@@]2(C)C(=O)C[C@]3(CCOc4c3cc(cc4)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2487

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.30

KAD-UNI-8a629cb0-44_2



CID: KAD-UNI-8a629cb0-44_2

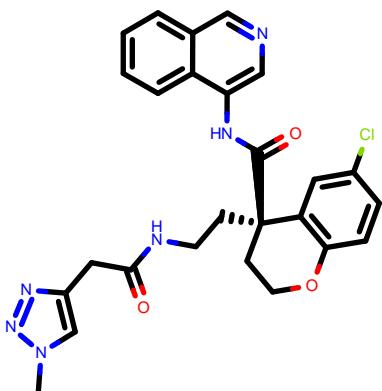
SMILES: CS(=O)(=O)[N@]1CC[C@@H](C1)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN1980

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.34

KAD-UNI-8a629cb0-47_1



CID: KAD-UNI-8a629cb0-47_1

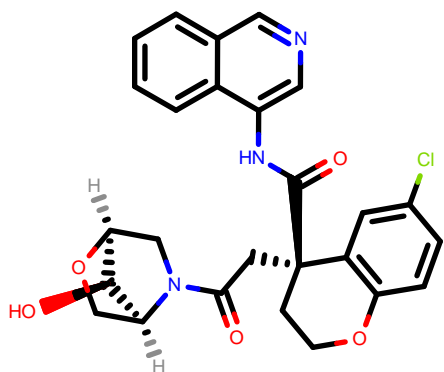
SMILES: Cn1cc(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN2028

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.32

EN300-6493060_1_1_1



CID: EN300-6493060_1_1_1

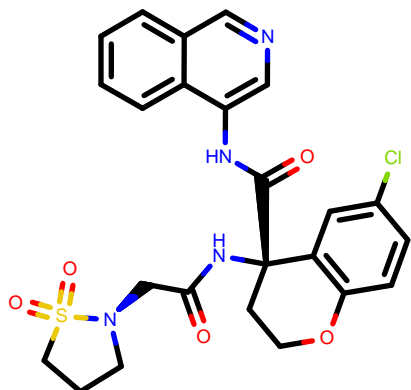
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5C[C@H]R[C@@H](C5)H5CO6/O

RUN: RUN7538

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.26

EN300-43206_1_1_1



CID: EN300-43206_1_1_1

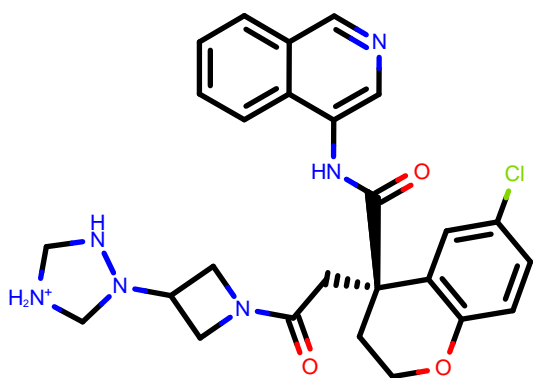
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)N@]5CCCC5(=O)=O

RUN: RUN3880

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.32

EN300-66518_1_1_1



CID: EN300-66518_1_1_1

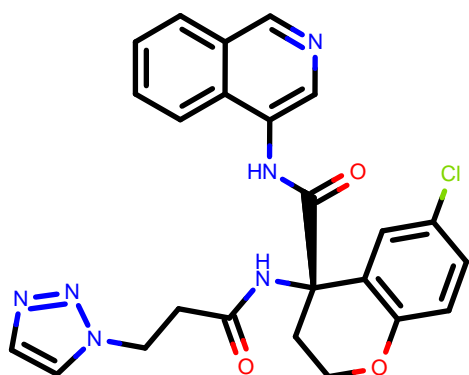
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6cnm6

RUN: RUN7541

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.27

EN300-28871_1_1_1



CID: EN300-28871_1_1_1

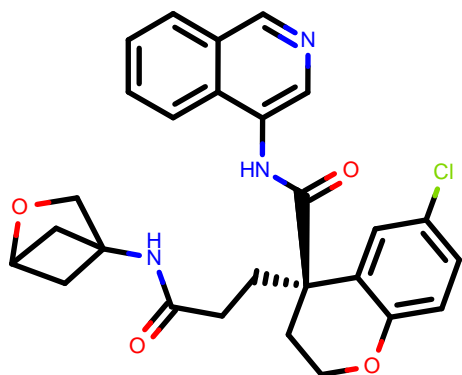
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)CCn5ccnn5

RUN: RUN4159

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

EN300-6734977_2_1_1



CID: EN300-6734977_2_1_1

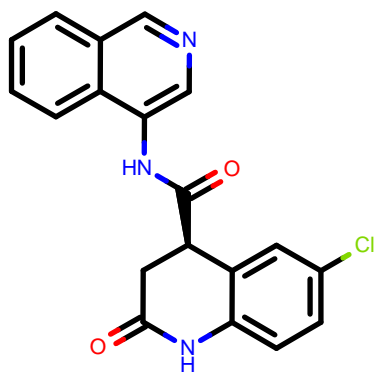
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCC(=O)NC56CC(C5)OC6

RUN: RUN5757

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.27

MIC-UNK-45817b9b-1_1



CID: MIC-UNK-45817b9b-1_1

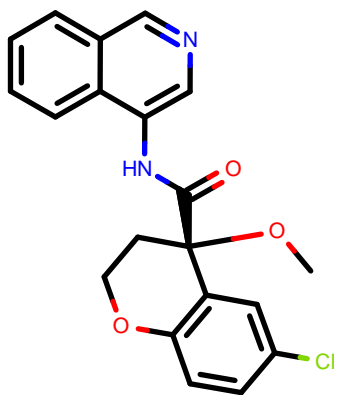
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4)Cl

RUN: RUN1166

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.29

PET-UNK-29afea89-2_1_1



CID: PET-UNK-29afea89-2_1_1

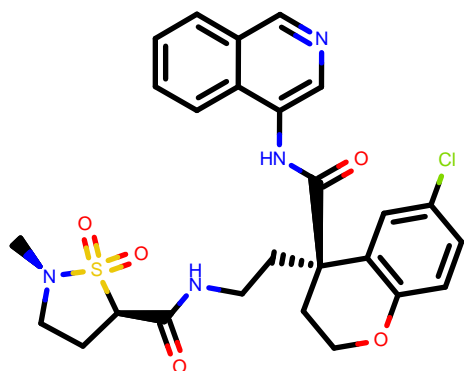
SMILES: CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6744

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.13

EN300-255496_3_1_1



CID: EN300-255496_3_1_1

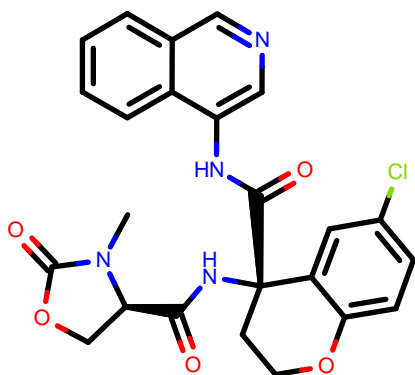
SMILES: CNc1cnc2c1cc(cc2)C(Cl)C(=O)NCC3C(=O)N(C)S(=O)(=O)C3

RUN: RUN4904

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.37

EN300-332838_1_2_1



CID: EN300-332838_1_2_1

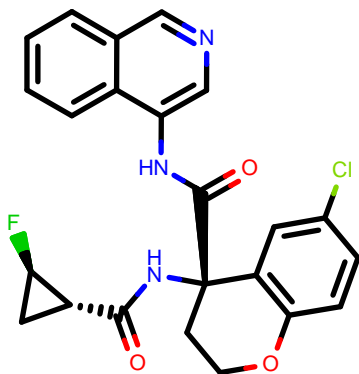
SMILES: CN1C(=O)C(C)C(=O)N1C(=O)Nc2cnc3c2cc(cc3)C(Cl)C(=O)N4cnc5c4cccc5

RUN: RUN5338

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-4698402_1_1_1



CID: EN300-4698402_1_1_1

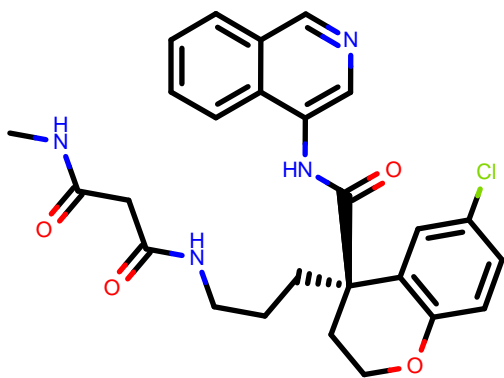
SMILES: F[C@H]1CC1C(=O)Nc2cnc3c2cc(cc3)C(Cl)C(=O)N4cnc5c4cccc5

RUN: RUN4871

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.18

EN300-128463_4_1_1



CID: EN300-128463_4_1_1

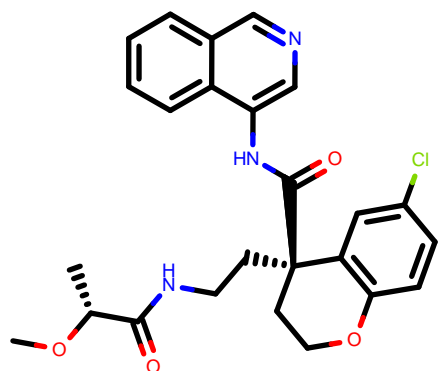
SMILES: CNC(=O)CC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3422

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.27

EN300-51257_3_2_1



CID: EN300-51257_3_2_1

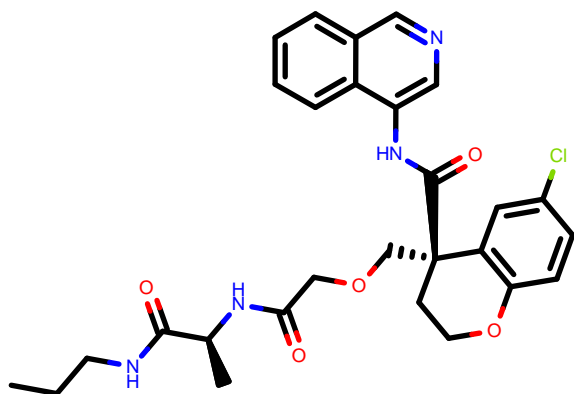
SMILES: C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC

RUN: RUN5745

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.28

EN300-23214_2_2_1



CID: EN300-23214_2_2_1

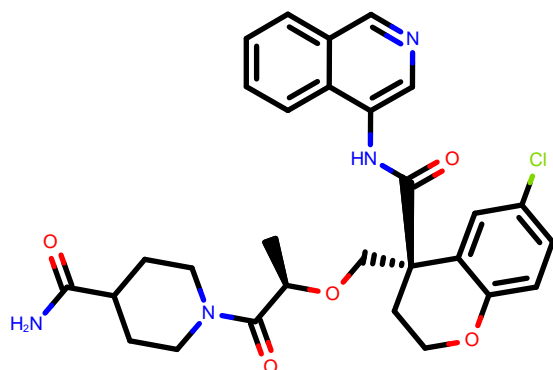
SMILES: CCCNC(=O)[C@H](C)NC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN3956

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.40

EN300-28113_2_2_1



CID: EN300-28113_2_2_1

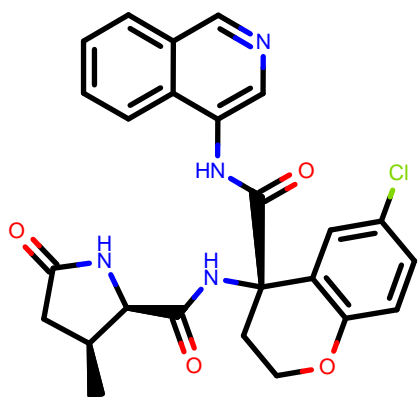
SMILES: C[C@H](C(=O)N1CCC(CC1)C(=O)N)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6745

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.34

EN300-155362_1_4_1



CID: EN300-155362_1_4_1

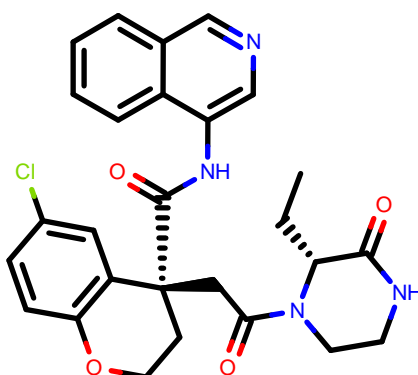
SMILES: C[C@@H]1CC(=O)N[C@@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN4432

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.26

EN300-67439_1_1_1



CID: EN300-67439_1_1_1

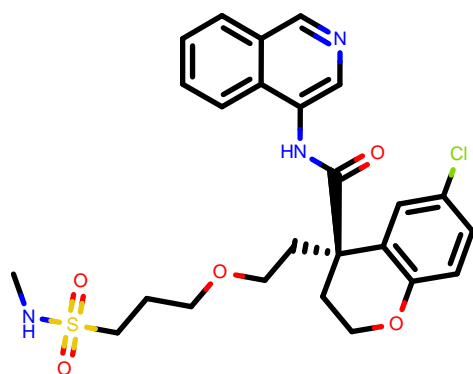
SMILES: CC[C@@]1([C@@H]1C(=O)NCCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN6067

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.27

EN300-68875_3_1_1



CID: EN300-68875_3_1_1

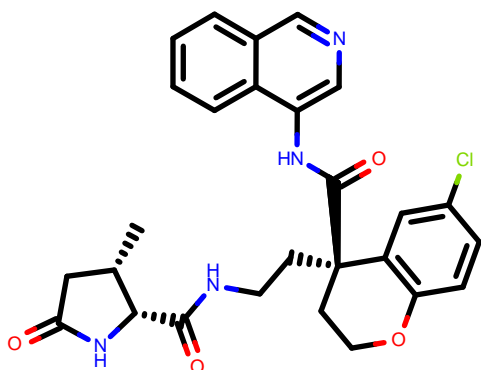
SMILES: CNS(=O)(=O)CCCOC[C@@]1([C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4

RUN: RUN6409

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.30

EN300-155362_3_4_1



CID: EN300-155362_3_4_1

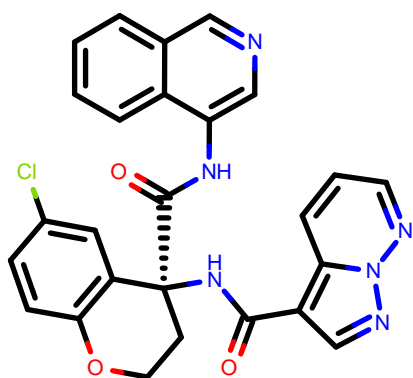
SMILES: C[C@@H]1CC(=O)N[C@@H]1C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4cccc5

RUN: RUN4891

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.31

EN300-114593_1_1_1



CID: EN300-114593_1_1_1

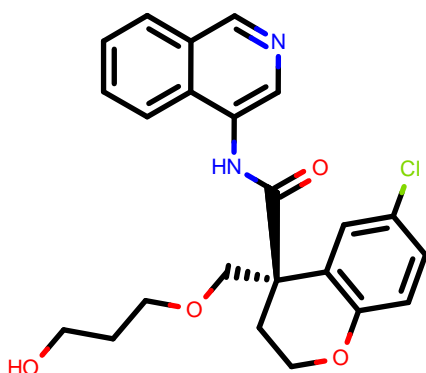
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5ccc6

RUN: RUN6036

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.22

EN300-221518_2_1_1



CID: EN300-221518_2_1_1

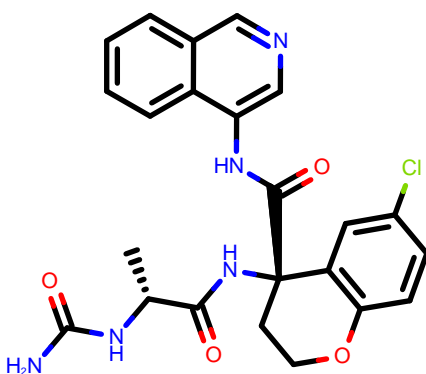
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(C)CO

RUN: RUN4390

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-00271_1_2_1



CID: EN300-00271_1_2_1

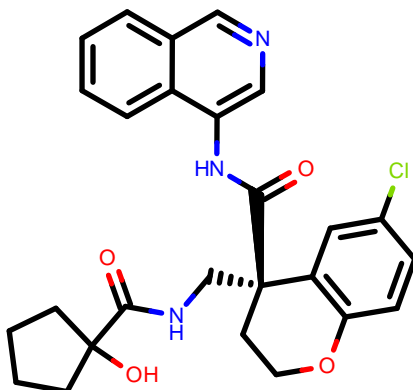
SMILES: C[C@H](C(=O)N)[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4NC(=O)N

RUN: RUN4830

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.24

EN300-25960_2_1_1



CID: EN300-25960_2_1_1

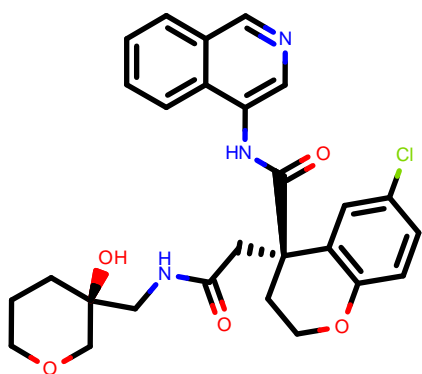
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(C)CCCC5O

RUN: RUN4139

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.41

EN300-193679_1_2_1



CID: EN300-193679_1_2_1

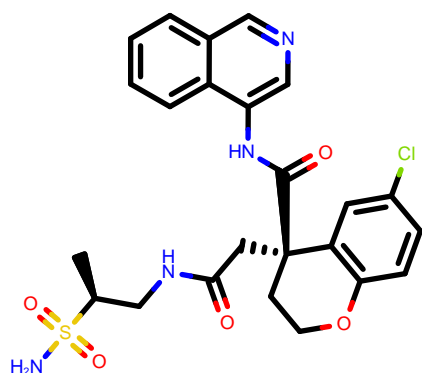
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)NC[C@]5(CCCOC5)O

RUN: RUN6173

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.39

EN300-123623_1_1_1



CID: EN300-123623_1_1_1

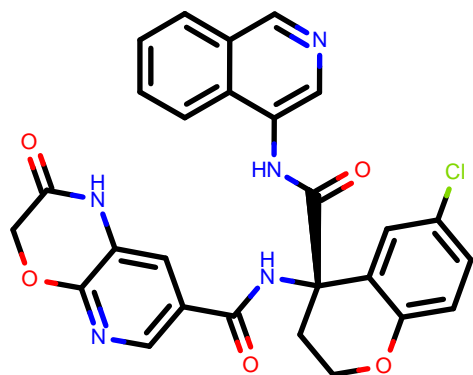
SMILES: C[C@@H](NC(=O)C[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncnc4c3ccc4)S(=O)(=O)N

RUN: RUN5871

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.30

EN300-103979_1_1_1



CID: EN300-103979_1_1_1

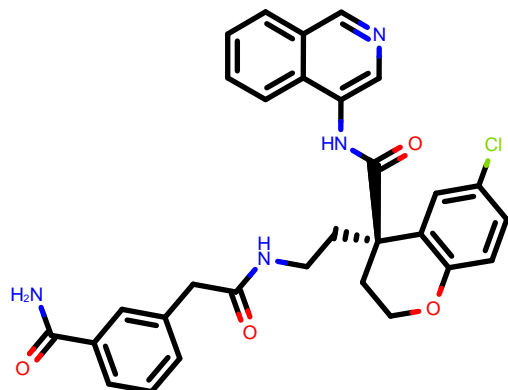
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cc6c(nc5)OCC(=O)N6

RUN: RUN6691

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.26

EN300-1179673_3_1_1



CID: EN300-1179673_3_1_1

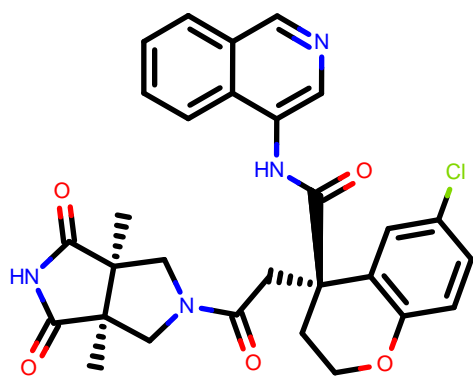
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C5c6ccc(c5)C(=O)N

RUN: RUN6147

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.29

ALP-UNI-76695c4f-10_1



CID: ALP-UNI-76695c4f-10_1

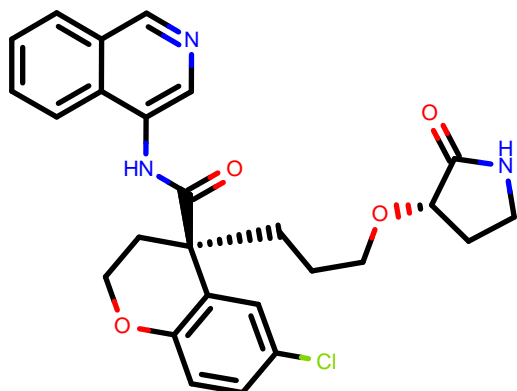
SMILES: C1C@112CN(C1@1)(Cl-O)NC2=O(C1C(-O)C1C@3)(CCOc4c3cc(cc4)Cl)C1-O)Nc5nc6c5ccc6

RUN: RUN2023

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.39

EN300-6736413_4_2_1



CID: EN300-6736413_4_2_1

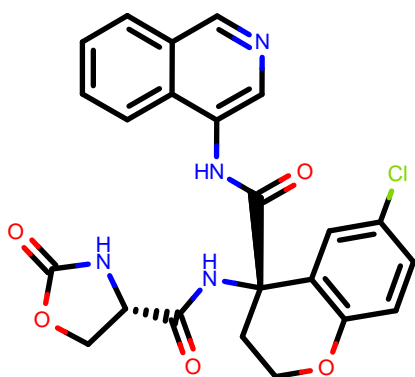
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)C(=O)C1C@H5CNC5=O

RUN: RUN4982

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.31

EN300-126389_1_1_1



CID: EN300-126389_1_1_1

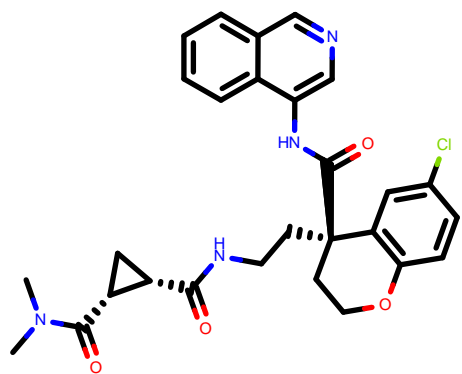
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3](CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COC(=O)N5

RUN: RUN6114

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.21

EN300-253462_3_1_1



CID: EN300-253462_3_1_1

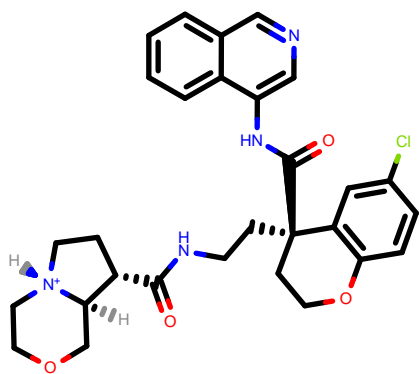
SMILES: CN(C)C(-O)[C@@H]1C[C@@H]1C1(-O)NC1C@2(CCOc3c2cc(cc3)Cl)C1-O)Nc4nc5c4ccc5

RUN: RUN3917

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.37

EN300-1588613_3_2_1



CID: EN300-1588613_3_2_1

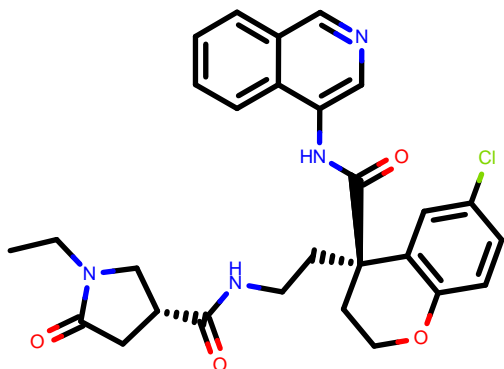
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](CCO=C4C=CC(=O)C)CCNC(=O)C@H5CC[N@@H]6C@H5COCC6

RUN: RUN6318

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.33

EN300-33478_3_1_1



CID: EN300-33478_3_1_1

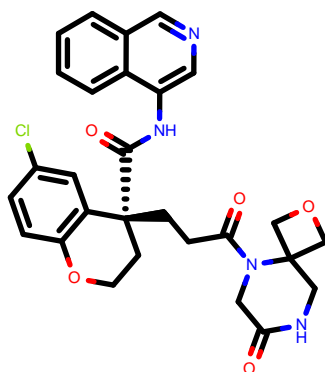
SMILES: CCN1C[C@@H](CC1=O)C(=O)NCC[C@@2](CCO=C3C=CC(=O)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7415

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.35

EN300-366278_2_1_1



CID: EN300-366278_2_1_1

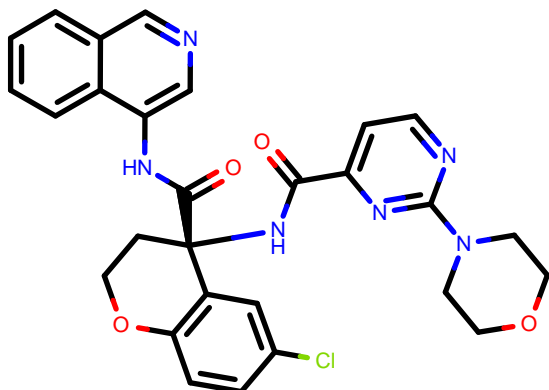
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3[C@@H](CCO=C4C=CC(=O)C)CCC(=O)N5CC(=O)NCC56COC6

RUN: RUN6500

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.27

EN300-312450_1_1_1



CID: EN300-312450_1_1_1

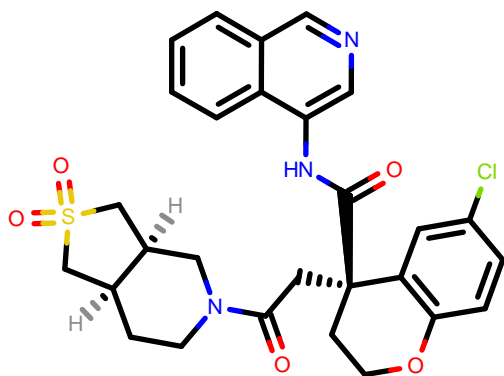
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@3[C@@H](CCO=C4C=CC(=O)C)NCC(=O)c5cnc(n5)N6COCOC6

RUN: RUN5071

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.30

EN300-365993_1_4_1



CID: EN300-365993_1_4_1

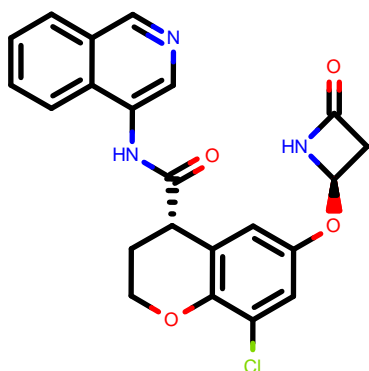
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)NSCC[C@@H]6CS(=O)(=O)C[C@@H]6C5

RUN: RUN3273

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.39

FRA-DIA-b66f7109-3_1_1



CID: FRA-DIA-b66f7109-3_1_1

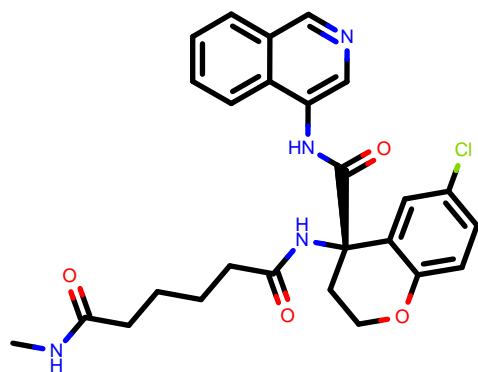
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3CCOCc4c3cc(cc4Cl)O[C@@H]5CC(=O)N5

RUN: RUN5111

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.30

EN300-154693_1_1_1



CID: EN300-154693_1_1_1

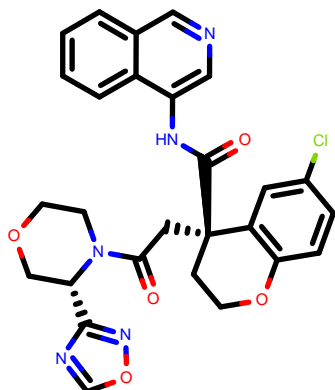
SMILES: CNC(=O)CCCCC(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5907

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.27

EN300-122849_1_2_1



CID: EN300-122849_1_2_1

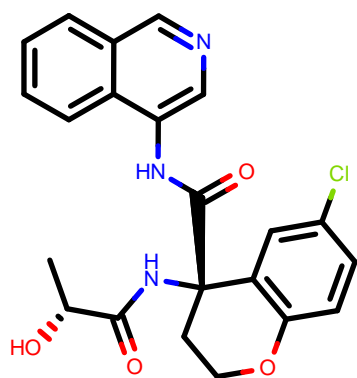
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)NSCOC[C@@H]5c6nccn6

RUN: RUN6643

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.26

EDG-MED-90036822-29_1



CID: EDG-MED-90036822-29_1

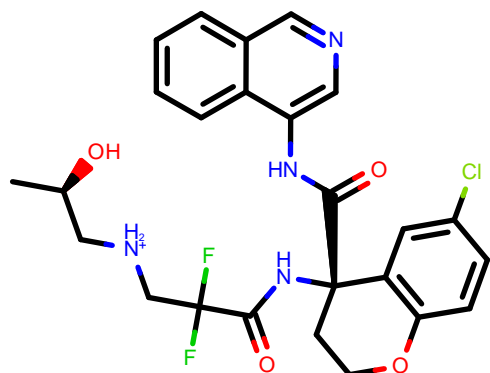
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O

RUN: RUN1536

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.21

EDG-MED-90036822-38_2



CID: EDG-MED-90036822-38_2

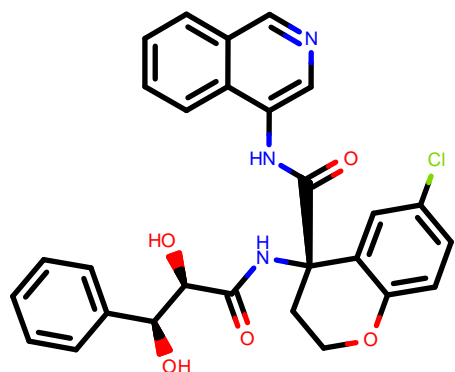
SMILES: C[C@H](CNCC(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)(F)F)O

RUN: RUN1665

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.36

EN300-2923949_1_3_1



CID: EN300-2923949_1_3_1

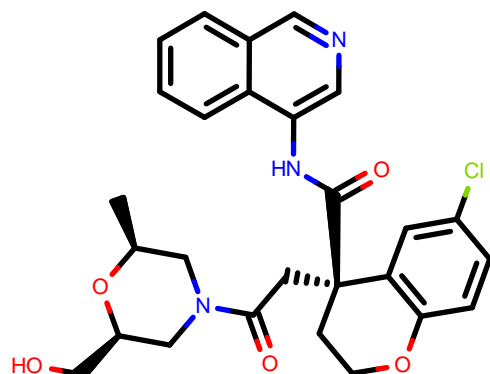
SMILES: c1ccc(cc1)C@H(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5)O

RUN: RUN6305

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.30

EN300-157776_1_4_1



CID: EN300-157776_1_4_1

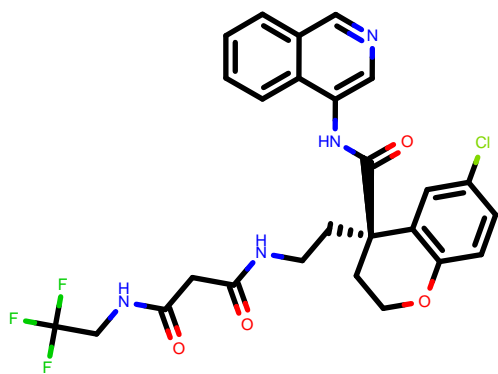
SMILES: C[C@H]1CN[C@H](O1)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4202

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.37

EN300-128715_3_1_1



CID: EN300-128715_3_1_1

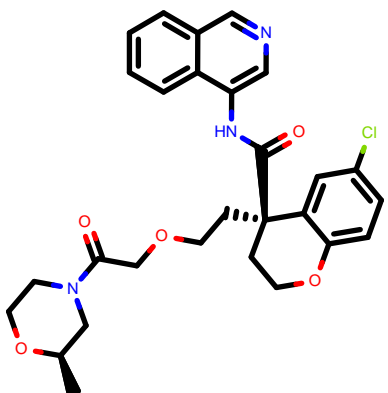
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC(F)(F)F

RUN: RUN6400

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.29

EN300-25572_3_1_1



CID: EN300-25572_3_1_1

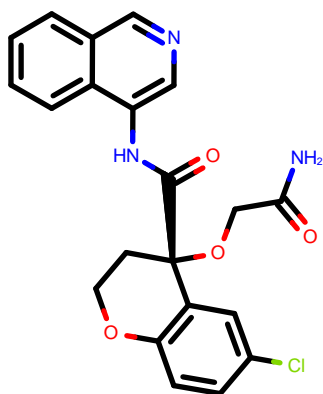
SMILES: C[C@@H]1CN(CCO1)C(=O)COCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN5292

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.31

EDG-MED-4c68219f-6_1



CID: EDG-MED-4c68219f-6_1

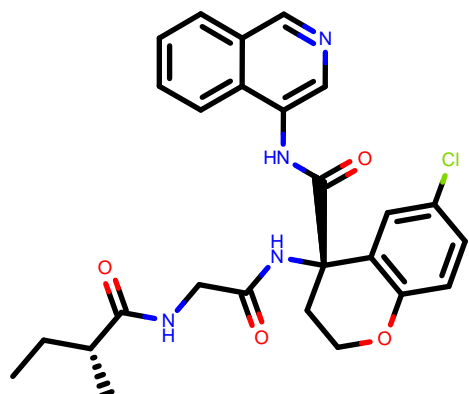
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N

RUN: RUN1498

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.17

EN300-51961_1_1_1



CID: EN300-51961_1_1_1

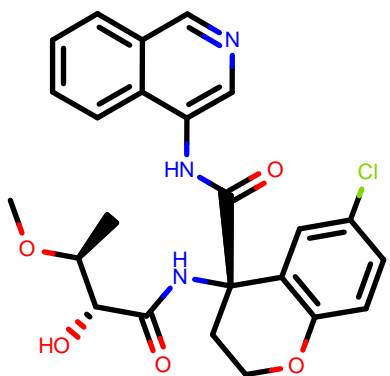
SMILES: CC[C@@H](C)C(=O)NCC(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN4188

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-220194_1_3_1



CID: EN300-220194_1_3_1

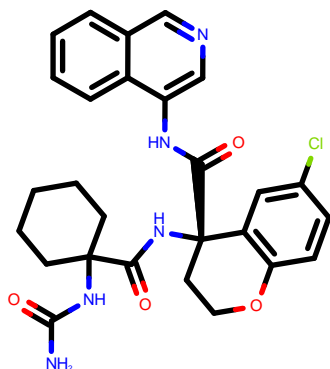
SMILES: C[C@@H]([C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN5162

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-78368_1_1_1



CID: EN300-78368_1_1_1

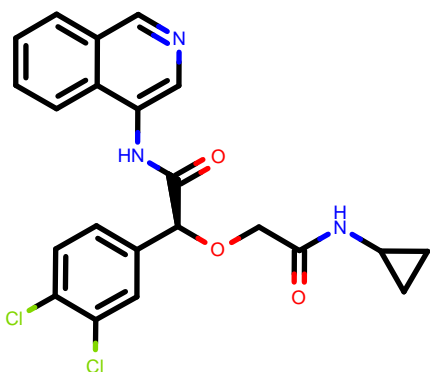
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCCC5)NC(=O)N

RUN: RUN5704

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.33

MAT-POS-de59a476-6_2



CID: MAT-POS-de59a476-6_2

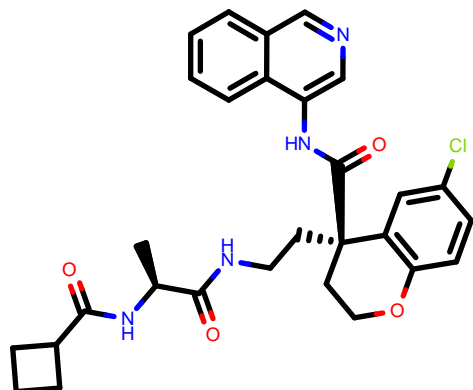
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)OCC(=O)NC4CC4

RUN: RUN2094

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.33

EN300-66082_3_1_1



CID: EN300-66082_3_1_1

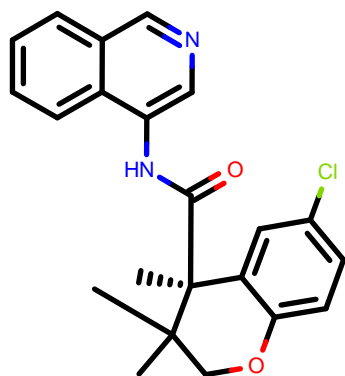
SMILES: C[C@@H]([C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)NC(=O)C5CC5

RUN: RUN5982

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.35

DAR-DIA-0d514e7d-30_1_1



CID: DAR-DIA-0d514e7d-30_1_1

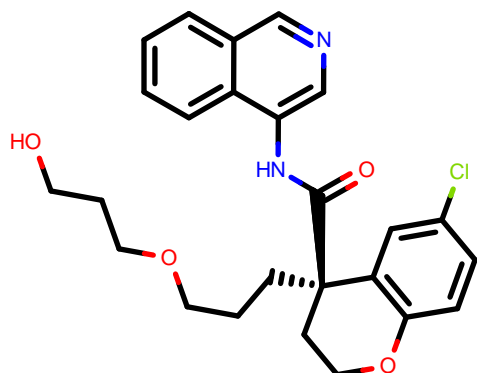
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN5116

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-221518_4_1_1



CID: EN300-221518_4_1_1

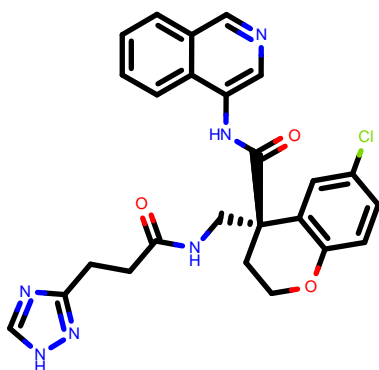
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCCO

RUN: RUN5952

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.27

EN300-101197_2_1_1



CID: EN300-101197_2_1_1

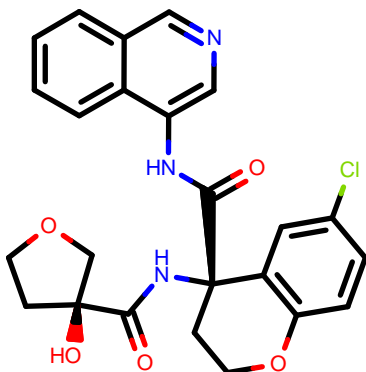
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCc5[nH]nnc5

RUN: RUN4964

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.27

EN300-148421_1_1_1



CID: EN300-148421_1_1_1

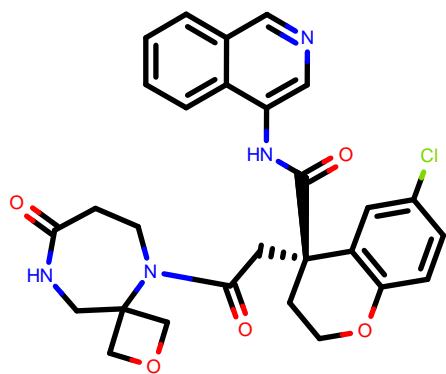
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOCC5)O

RUN: RUN6009

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.31

EN300-367589_1_1_1



CID: EN300-367589_1_1_1

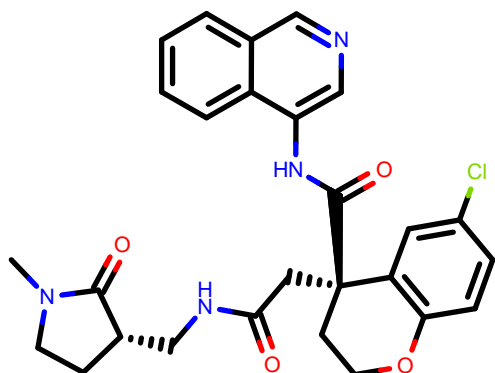
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(=O)NCC56COC6

RUN: RUN3298

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.29

EN300-1264816_1_2_1



CID: EN300-1264816_1_2_1

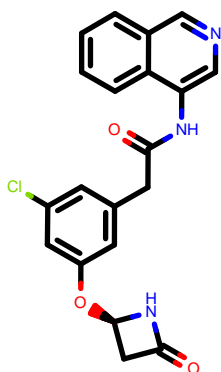
SMILES: CN1CC[C@H](C1=O)CNC(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5o4ccoc5

RUN: RUN7226

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.30

MAT-POS-3b92565d-3_1



CID: MAT-POS-3b92565d-3_1

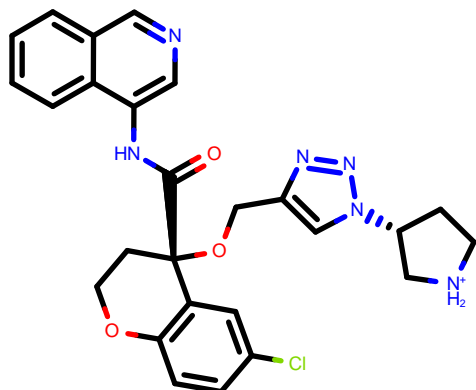
SMILES: c1ccc2c(c1)ncoc2NC(=O)Cc3cc(cc(c3)C)O[C@@H]4CC(=O)N4

RUN: RUN51

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.46

ED_-GRI-5b13fbe2-61_1



CID: ED_-GRI-5b13fbe2-61_1

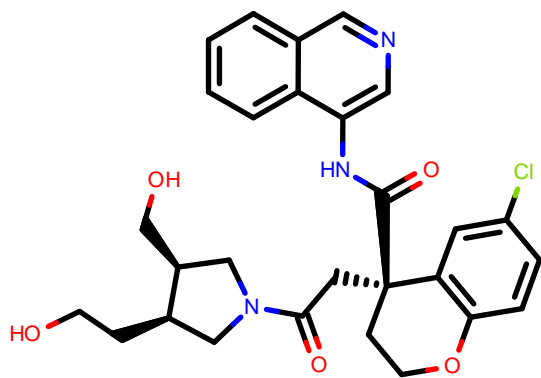
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5cn(n5)[C@@H]6CC[NH2+]C6

RUN: RUN1462

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.27

EN300-1425608_1_4_1



CID: EN300-1425608_1_4_1

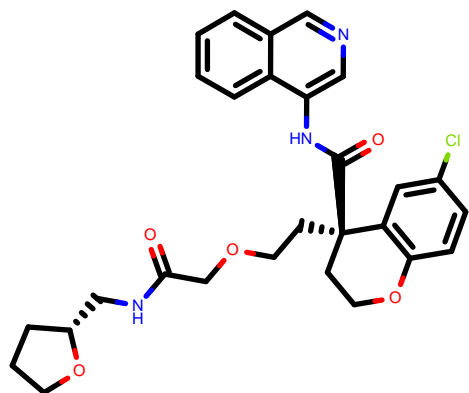
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C5)COCCO

RUN: RUN5567

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.30

EN300-01527_3_2_1



CID: EN300-01527_3_2_1

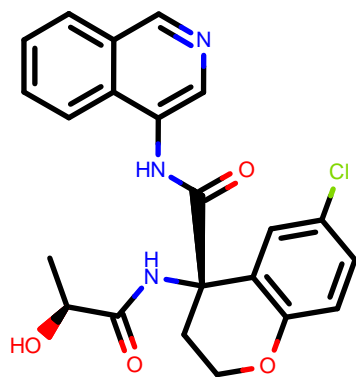
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@@H]5CCCCO5

RUN: RUN4512

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.32

EDG-MED-90036822-28_1



CID: EDG-MED-90036822-28_1

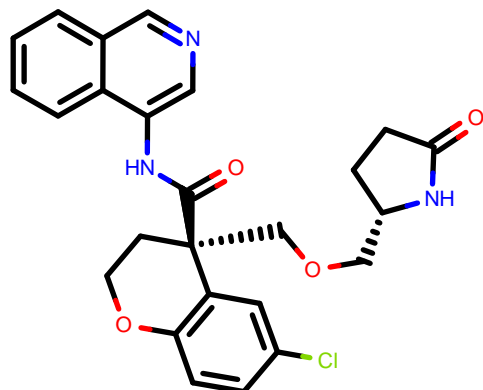
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)O

RUN: RUN1543

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.21

EN300-195756_2_1_1



CID: EN300-195756_2_1_1

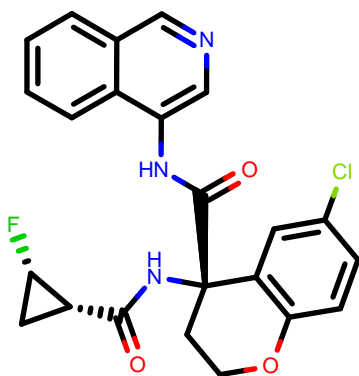
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCCC(=O)N5

RUN: RUN6049

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-97300_1_1_1



CID: EN300-97300_1_1_1

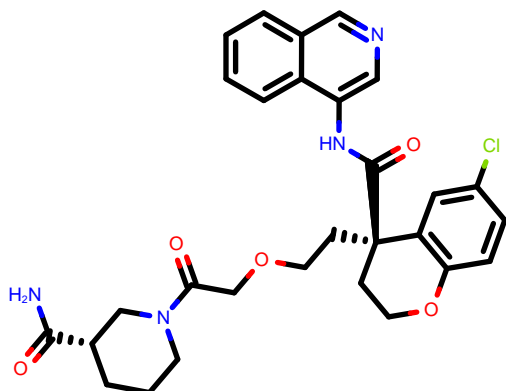
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@@H]5F

RUN: RUN5483

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.20

EN300-22880_3_1_1



CID: EN300-22880_3_1_1

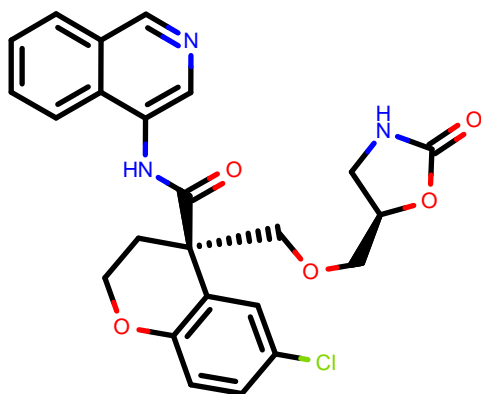
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)N5CCCC5@H]C5(C)O

RUN: RUN6417

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.40

EN300-203293_2_2_1



CID: EN300-203293_2_2_1

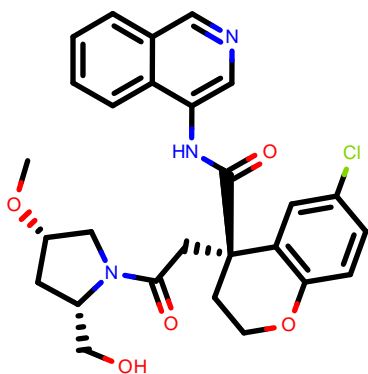
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@H]5CNC(=O)O5

RUN: RUN4794

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.30

EN300-244713_1_1_1



CID: EN300-244713_1_1_1

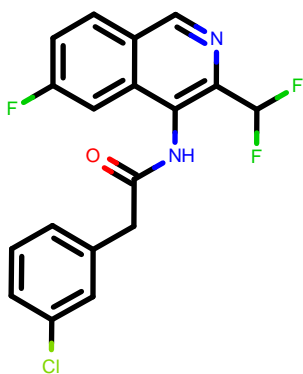
SMILES: CO[C@@H]1C[C@@H](N(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)N4cnc5c4ccc5)CO

RUN: RUN5831

DDG (kcal/mol): -0.69

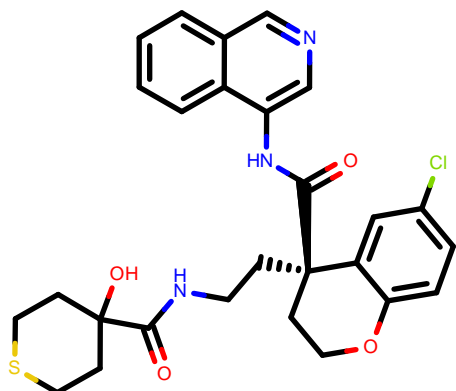
dDDG (kcal/mol): 0.31

JOH-UNI-6fede743-5_1



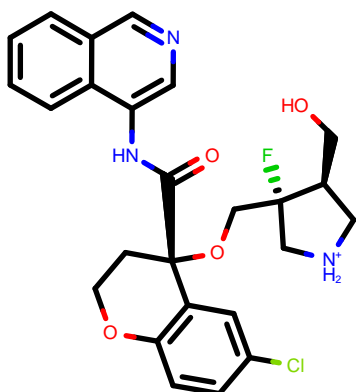
CID:	JOH-UNI-6fede743-5_1
SMILES:	<chem>c1cc(cc(c1)Cl)CC(=O)Nc2c3cc(ccc3cnc2C(F)F)F</chem>
RUN:	RUN1071
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.39

EN300-122340_3_1_1



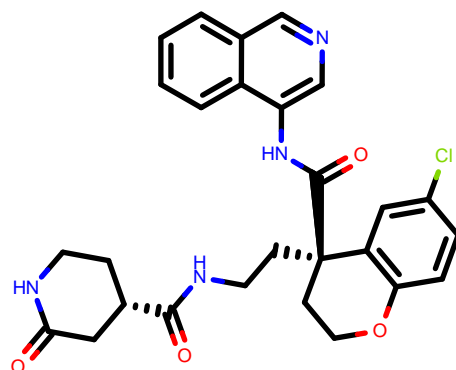
CID:	EN300-122340_3_1_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCSC5)O</chem>
RUN:	RUN7050
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.34

ED_-GRI-5b13fbe2-55_1



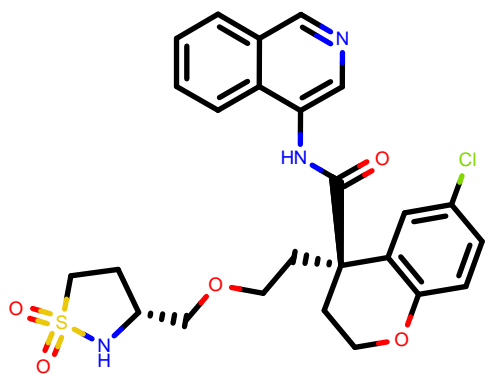
CID:	ED_-GRI-5b13fbe2-55_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5(C[NH2+])C[C@@]H5COF</chem>
RUN:	RUN1482
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.37

EN300-107493_3_2_1



CID:	EN300-107493_3_2_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]H5CCNC(=O)C5</chem>
RUN:	RUN6343
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.27

EN300-1699871_3_2_1



CID: EN300-1699871_3_2_1

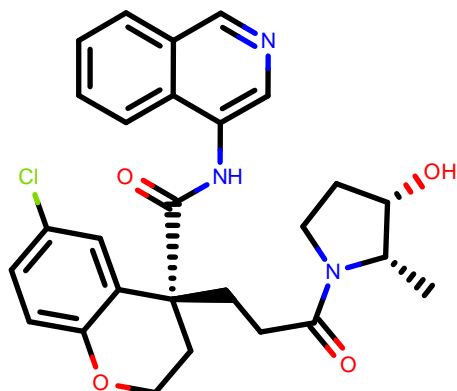
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5CCS(=O)(=O)N5

RUN: RUN6321

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-2008120_2_1_1



CID: EN300-2008120_2_1_1

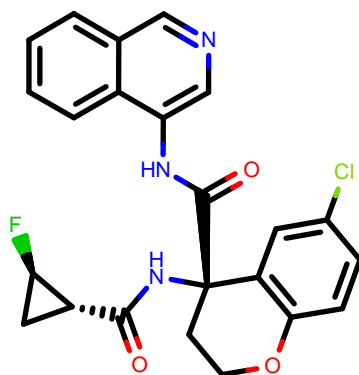
SMILES: C[C@H]1[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5)O

RUN: RUN6647

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-97300_1_3_1



CID: EN300-97300_1_3_1

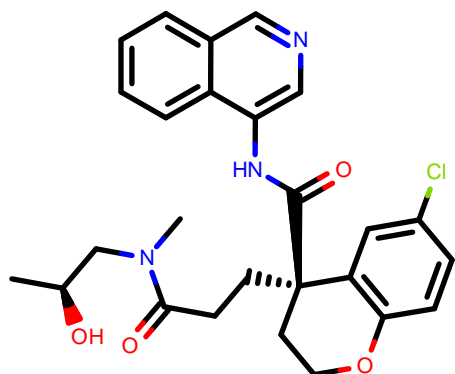
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[C@H]5F

RUN: RUN4800

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.17

EN300-210254_2_1_1



CID: EN300-210254_2_1_1

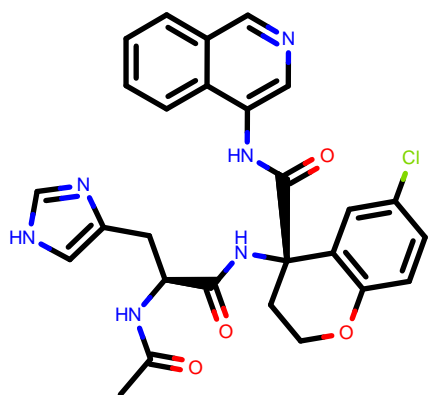
SMILES: C[C@H](CN(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4)O

RUN: RUN5574

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.26

EN300-196320_1_1_1



CID: EN300-196320_1_1_1

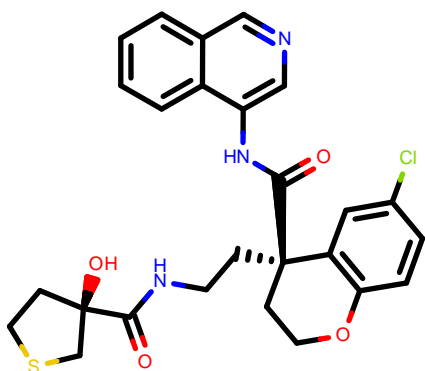
SMILES: CC(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN6611

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-122656_3_2_1



CID: EN300-122656_3_2_1

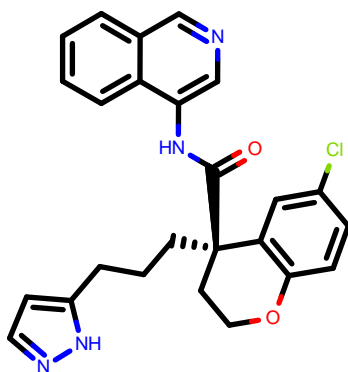
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCSC5)O

RUN: RUN4125

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.43

VLA-UCB-34f3ed0c-10_1



CID: VLA-UCB-34f3ed0c-10_1

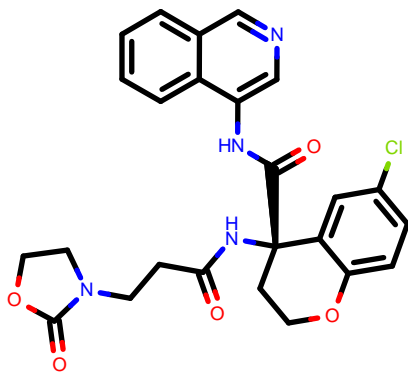
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5c[nH]5

RUN: RUN570

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.28

EN300-53918_1_1_1



CID: EN300-53918_1_1_1

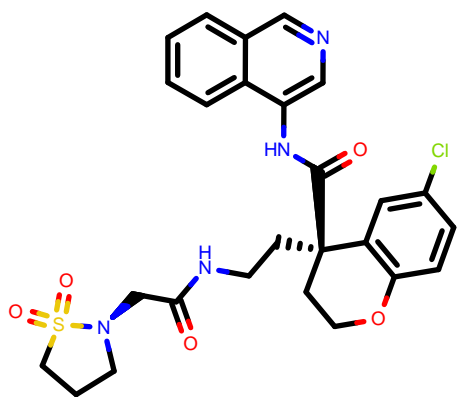
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCN5COC5=O

RUN: RUN6001

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.25

EN300-43206_3_1_1



CID: EN300-43206_3_1_1

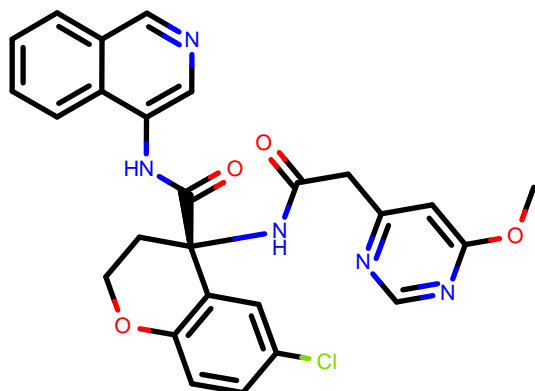
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)c4cc3(cc4)C)CCNC(=O)C[N@]5CCCS5(=O)=O

RUN: RUN5472

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.34

EN300-7444950_1_1_1



CID: EN300-7444950_1_1_1

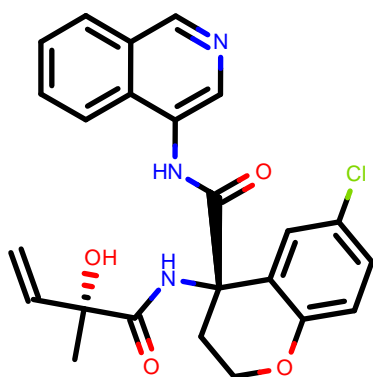
SMILES: COc1cc(ncn1)CC(=O)N[C@@]2(C)C(CO)c3cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN: RUN4311

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.34

EN300-248888_1_1_1



CID: EN300-248888_1_1_1

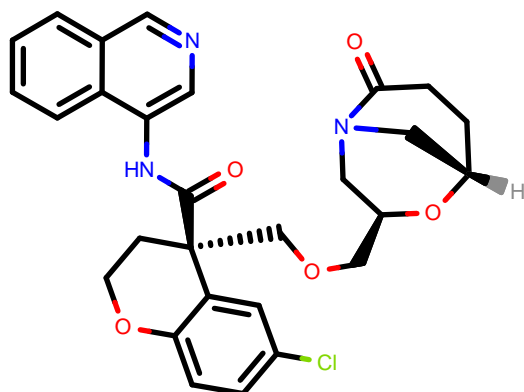
SMILES: C[C@@](C)(C(=O)N[C@@]1(C)C(CO)c2cc(cc2)C)C(=O)Nc3ncoc4c3cccc4)O

RUN: RUN5908

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

LEE-CAM-7ab9b158-4_3



CID: LEE-CAM-7ab9b158-4_3

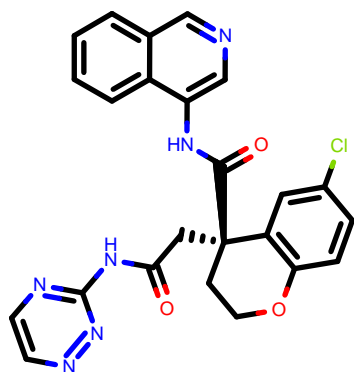
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)c4cc3(cc4)C)COC[C@@]5(C)N6C[C@@]7(H)O5CCCC7=O

RUN: RUN2079

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.46

CHO-MSK-a31cca77-3_1



CID: CHO-MSK-a31cca77-3_1

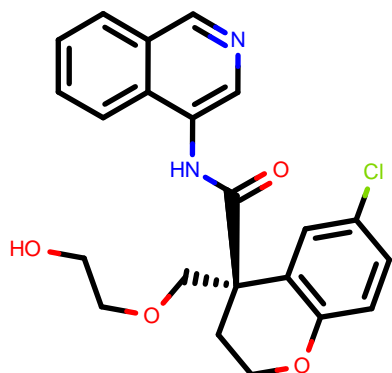
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nccnn5

RUN: RUN2054

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.25

EN300-21258_2_1_1



CID: EN300-21258_2_1_1

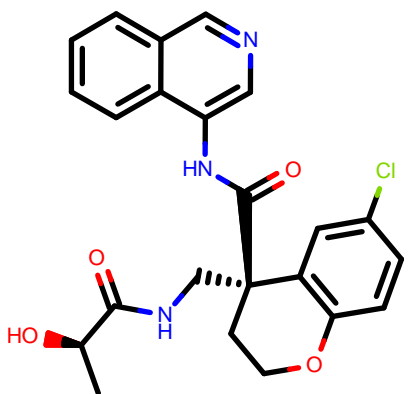
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCO

RUN: RUN6798

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.18

EN300-19542_2_2_1



CID: EN300-19542_2_2_1

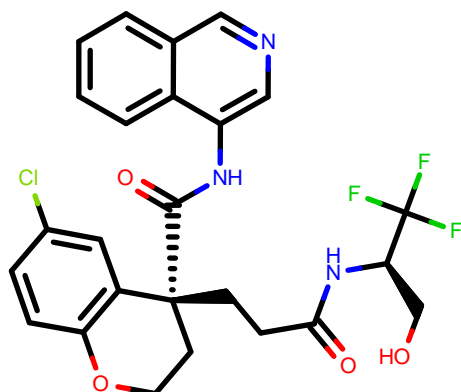
SMILES: C[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6504

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.25

EN300-296237_2_2_1



CID: EN300-296237_2_2_1

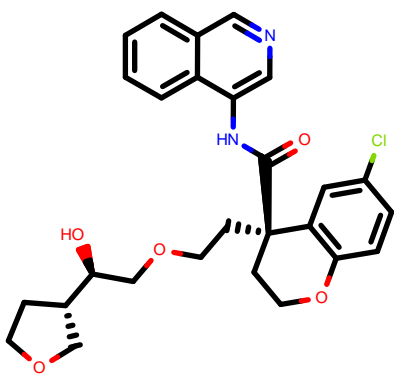
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H](CO)(F)F

RUN: RUN7068

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.50

EN300-1911992_3_3_1



CID: EN300-1911992_3_3_1

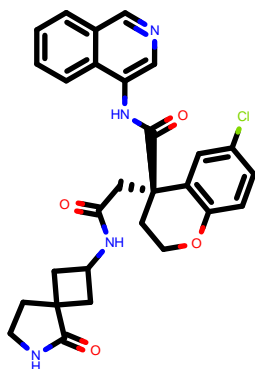
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(Cc4cc4c3cc(cc4)Cl)CCOC[C@@H](C@H)5CCOC5O

RUN: RUN6212

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.36

EN300-743350_1_1_1



CID: EN300-743350_1_1_1

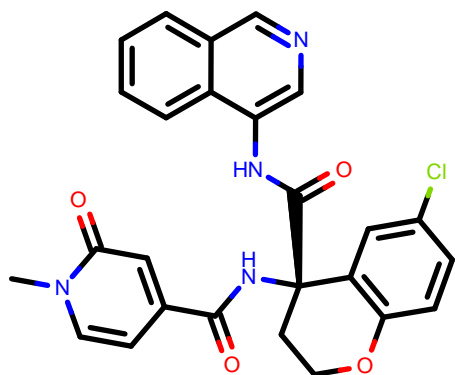
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(Cc4cc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CCN6=O

RUN: RUN6111

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.28

EN300-30480_1_1_1



CID: EN300-30480_1_1_1

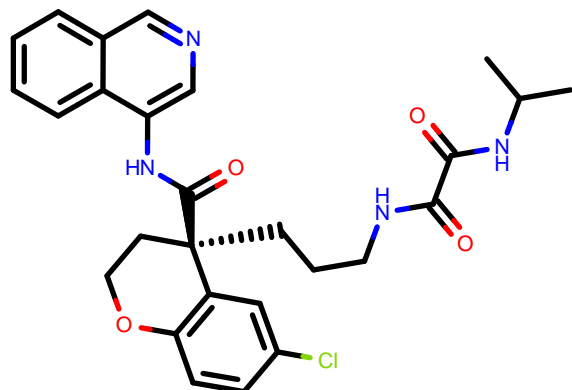
SMILES: Cn1ccc(cc1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN6061

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.24

EN300-1262640_4_1_1



CID: EN300-1262640_4_1_1

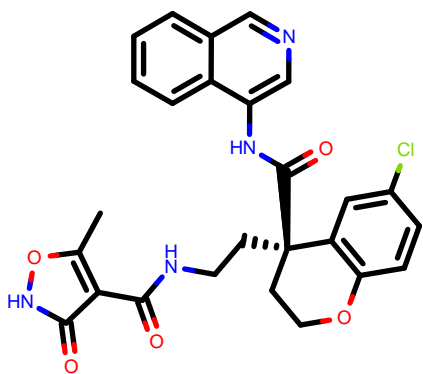
SMILES: CC(C)NC(=O)C(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4

RUN: RUN5427

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.31

EN300-110423_3_1_1



CID: EN300-110423_3_1_1

SMILES:

Cc1c(cc(=O)[nH]o1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN:

RUN4893

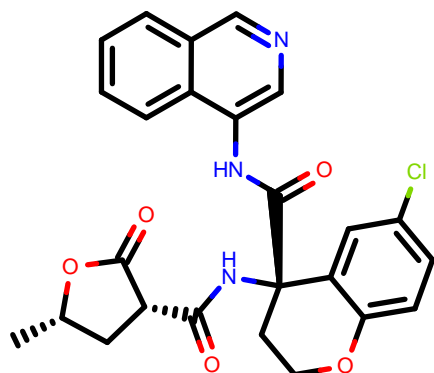
DDG (kcal/mol):

-0.66

dDDG (kcal/mol):

0.30

EN300-7444533_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

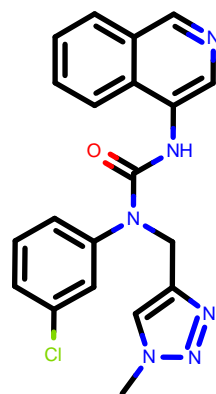
DDG (kcal/mol):

-0.66

dDDG (kcal/mol):

0.21

MIC-UNK-bcd487e9-9_1



CID: MIC-UNK-bcd487e9-9_1

SMILES:

Cn1cc(nn1)CN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN498

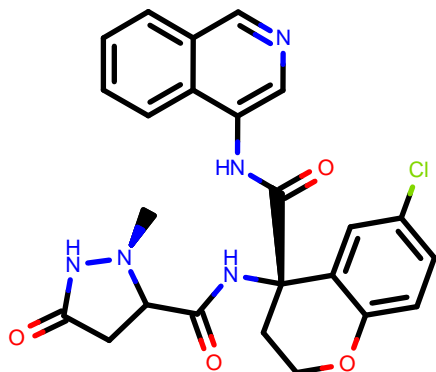
DDG (kcal/mol):

-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)Cl)C(=O)Nc4ccc5c4ccc5

RUN:

RUN3668

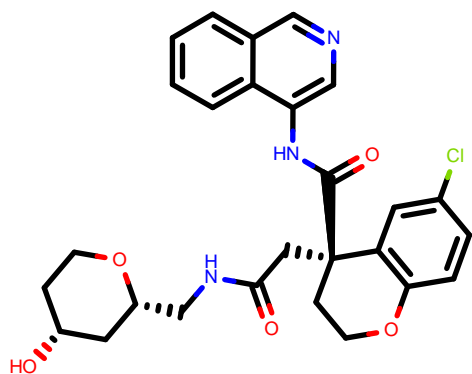
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.21

EN300-1708899_1_1_1



CID: EN300-1708899_1_1_1

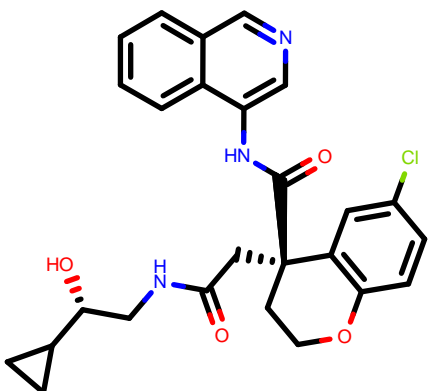
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H]3[C@@O]c4c3ccc(cc4)C1CC(=O)NC1C[C@@H]5[C@@H](C)CO5O

RUN: RUN7638

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.28

EN300-67533_1_2_1



CID: EN300-67533_1_2_1

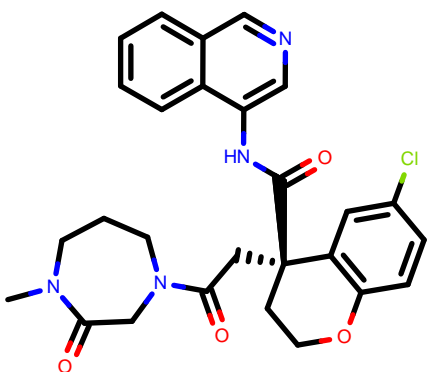
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H]3[C@@O]c4c3ccc(cc4)C1CC(=O)NC1C[C@@H](C5CC5)O

RUN: RUN4009

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

EN300-160143_1_1_1



CID: EN300-160143_1_1_1

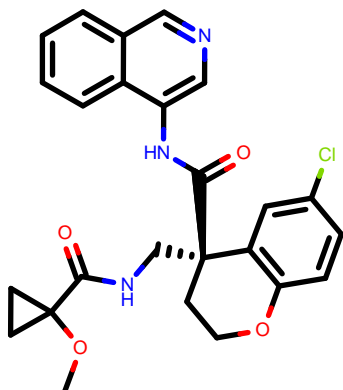
SMILES: CN1CCCN(CC1=O)C(=O)C[C@@H]2[C@@O]c3c2ccc(cc3)C1C(=O)Nc4ccc5c4ccc5

RUN: RUN3975

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

EN300-182124_2_1_1



CID: EN300-182124_2_1_1

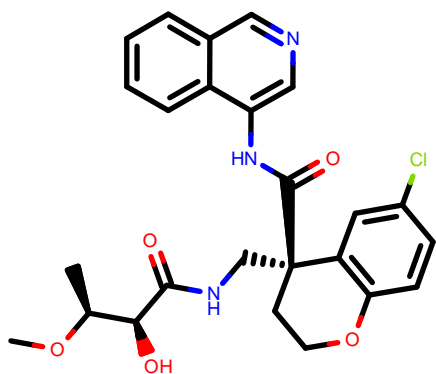
SMILES: COC1(CC1)C(=O)NC[C@@H]2[C@@O]c3c2ccc(cc3)C1C(=O)Nc4ccc5c4ccc5

RUN: RUN4843

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.26

EN300-220194_2_1_1



CID: EN300-220194_2_1_1

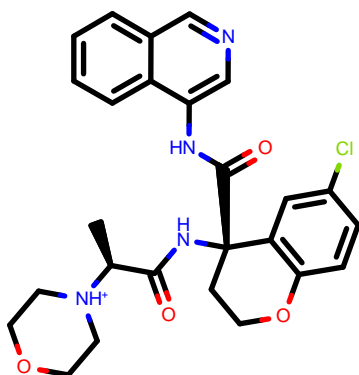
SMILES: C[C@@H][C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN6556

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.32

EN300-41473_1_1_1



CID: EN300-41473_1_1_1

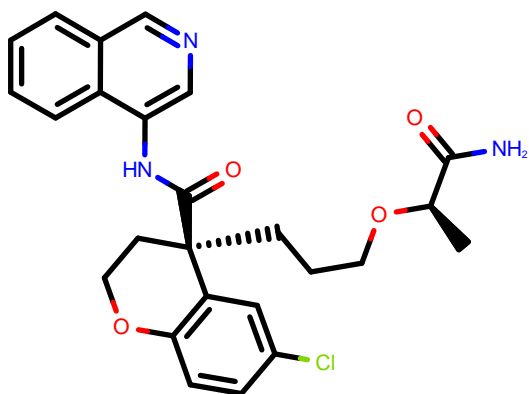
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)[NH+]5CCOCC5

RUN: RUN4444

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.35

EN300-17381_4_2_1



CID: EN300-17381_4_2_1

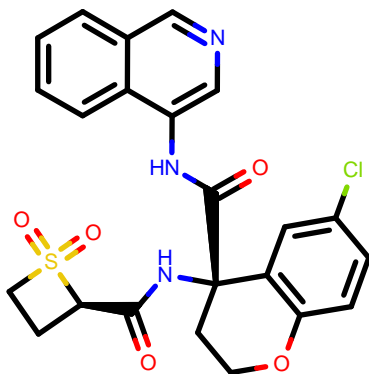
SMILES: C[C@@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN4840

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.30

EN300-1387104_1_2_1



CID: EN300-1387104_1_2_1

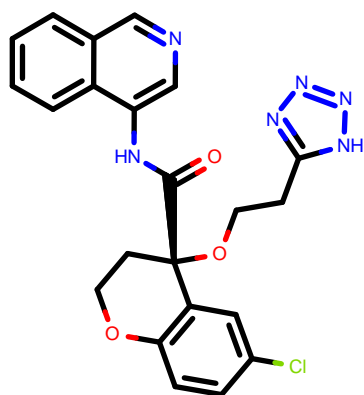
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCS5(=O)=O

RUN: RUN3053

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.29

ED_-GRI-5b13fbe2-56_1



CID: ED_-GRI-5b13fbe2-56_1

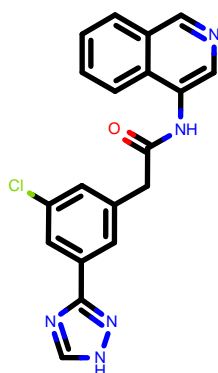
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5n[n-]nn5

RUN: RUN1427

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.25

MAT-POS-281d2ee9-2_1



CID: MAT-POS-281d2ee9-2_1

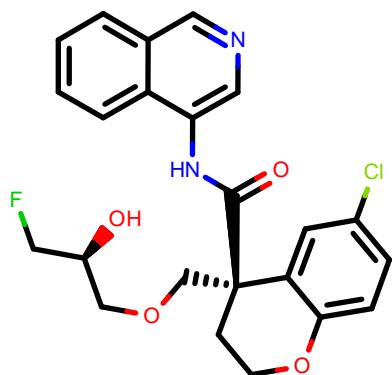
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)c4[nH]ncn4

RUN: RUN1721

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.31

EDJ-MED-fcba3f31-4_1



CID: EDJ-MED-fcba3f31-4_1

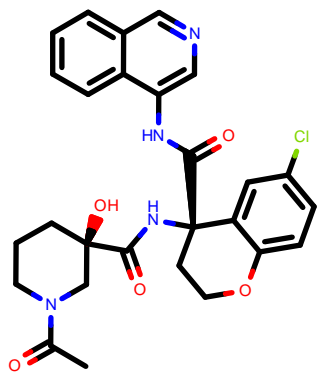
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O

RUN: RUN2384

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.31

EN300-210552_1_1_1



CID: EN300-210552_1_1_1

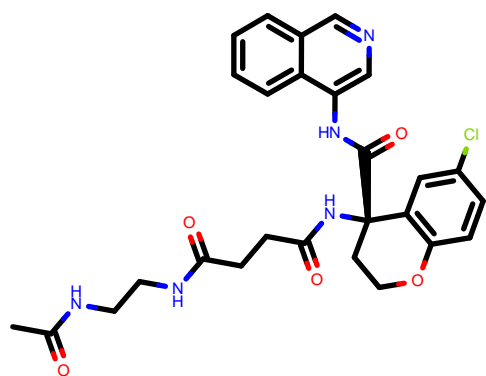
SMILES: CC(=O)N1CCC[C@@]1(C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4CCCC5O4CCCC5O

RUN: RUN5879

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.31

EN300-73507_1_1_1



CID: EN300-73507_1_1_1

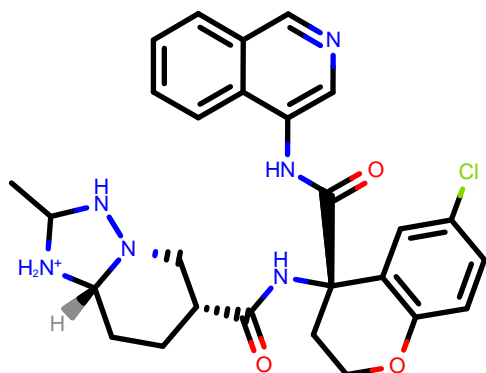
SMILES: CC(=O)NCCNC(=O)CCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN5896

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.30

ALP-UNI-dbbfd3db-4_1



CID: ALP-UNI-dbbfd3db-4_1

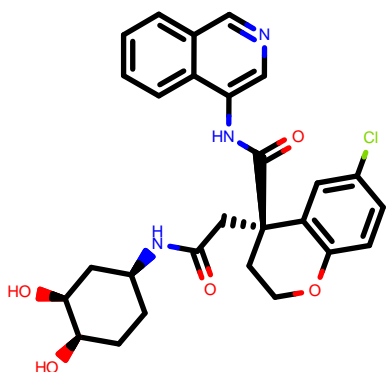
SMILES: Cc1nc2n(m1)C[C@@H](CC2)C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nccc6c5cccc6

RUN: RUN2600

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.26

EN300-741822_1_2_1



CID: EN300-741822_1_2_1

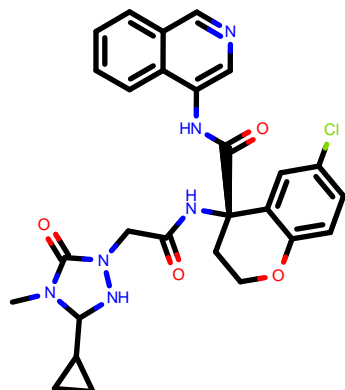
SMILES: c1ccc2c(c1)nccc2N(C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CC[C@@H]6[C@@H](C)C5)O

RUN: RUN5507

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.24

EN300-6478432_1_1_1



CID: EN300-6478432_1_1_1

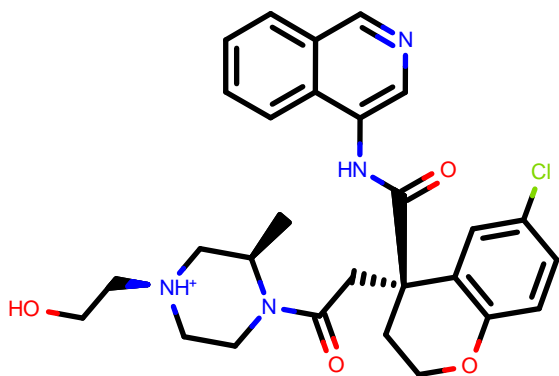
SMILES: Cn1c(mn(c1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C6CC6

RUN: RUN5158

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.42

EDG-MED-ba1ac7b9-27_5



CID: EDG-MED-ba1ac7b9-27_5

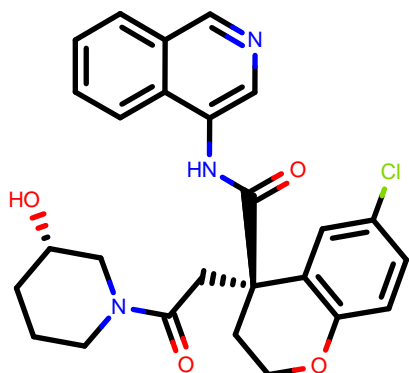
SMILES: C[C@@H]1CN[C@@H+]2CCN1C(=O)C[C@@]3(CCOc4cc2cc3)C1=O)N4cnc5c4ccc5)CCO

RUN: RUN2553

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.63

EN300-188582_1_1_1



CID: EN300-188582_1_1_1

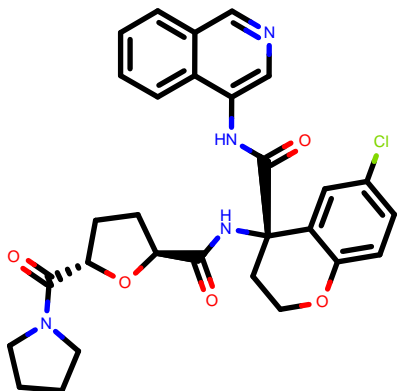
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(c4)C)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN4759

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

ALP-UNI-dbbfd3db-6_3



CID: ALP-UNI-dbbfd3db-6_3

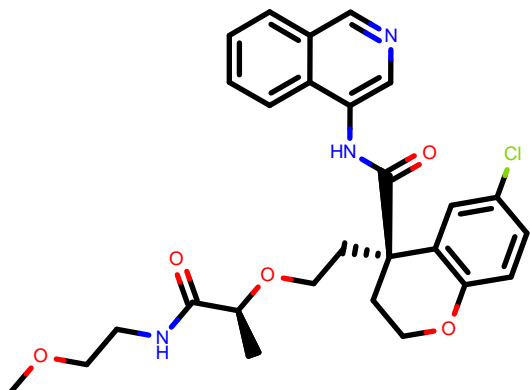
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(c4)C)N1=O)C@@H5CC[C@@H](O5)C1=O)N6CCCC6

RUN: RUN2616

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-23317_3_1_1



CID: EN300-23317_3_1_1

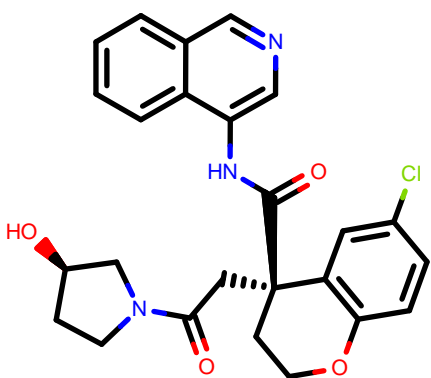
SMILES: C[C@@H](C(=O)NCCOC)OCC[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncoc4c3ccc4

RUN: RUN5994

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.41

EN300-295515_1_2_1



CID: EN300-295515_1_2_1

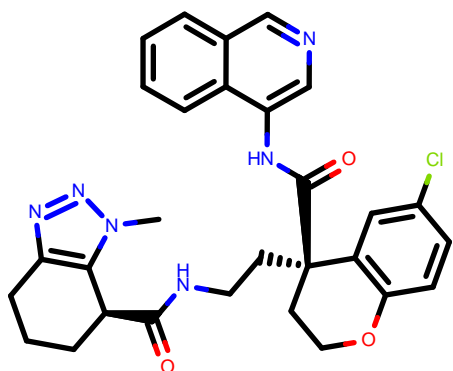
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N5CC[C@H](C5)O

RUN: RUN6156

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.28

EN300-1664865_3_1_1



CID: EN300-1664865_3_1_1

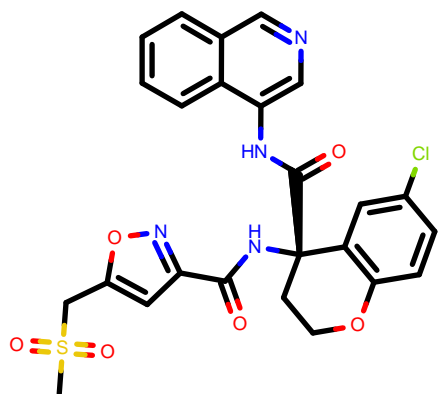
SMILES: Cn1c2c(nn1)CCC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ncc6c5ccccc6

RUN: RUN3479

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.35

EN300-1987964_1_1_1



CID: EN300-1987964_1_1_1

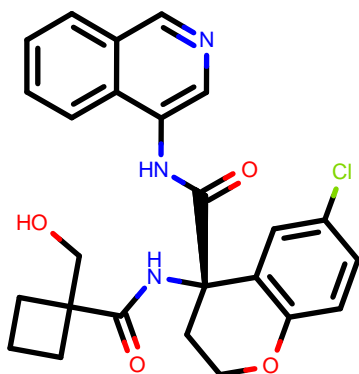
SMILES: CS(=O)(=O)Cc1cc(n1)C(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN5749

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.37

EN300-149975_1_1_1



CID: EN300-149975_1_1_1

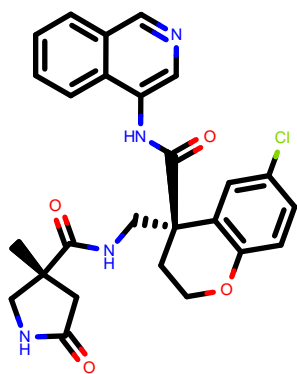
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)CO

RUN: RUN3549

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.25

EN300-132157_2_2_1



CID: EN300-132157_2_2_1

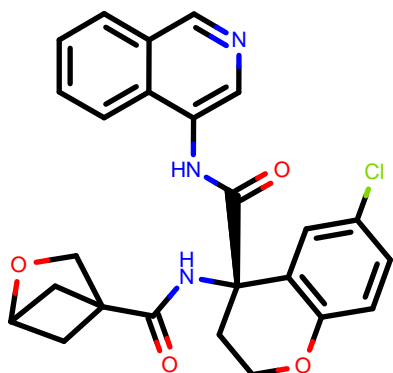
SMILES: C[C@@]1(C(=O)NC1C(=O)NC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN4111

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-1604607_1_1_1



CID: EN300-1604607_1_1_1

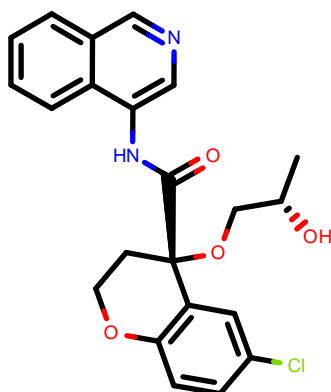
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C56CC(C5)OC6

RUN: RUN3837

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.27

EN300-185378_1_1_1



CID: EN300-185378_1_1_1

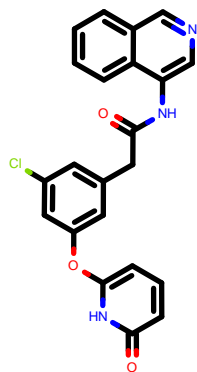
SMILES: C[C@@@H](CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN7459

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.31

MAT-POS-9ff17035-2_1



CID: MAT-POS-9ff17035-2_1

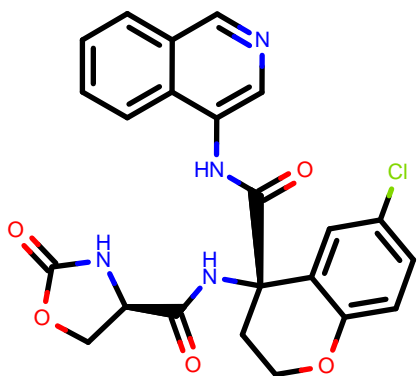
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Oc4cccc(=O)[nH]4

RUN: RUN101

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.40

EN300-305996_1_1_1



CID: EN300-305996_1_1_1

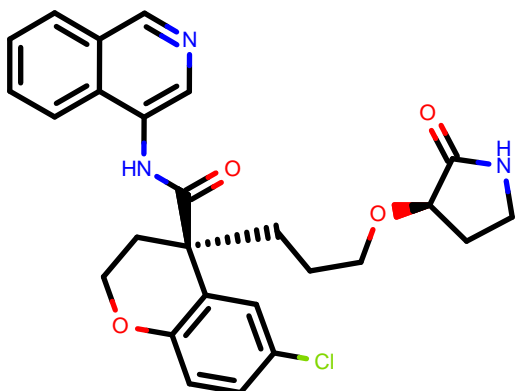
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5COC(=O)N5

RUN: RUN6808

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.22

EN300-6736413_4_1_1



CID: EN300-6736413_4_1_1

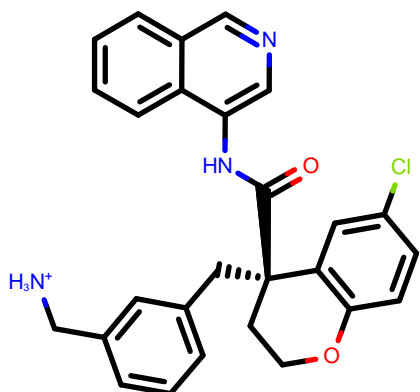
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5COCNC5=O

RUN: RUN3792

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.32

JAG-UCB-706446eb-8_1



CID: JAG-UCB-706446eb-8_1

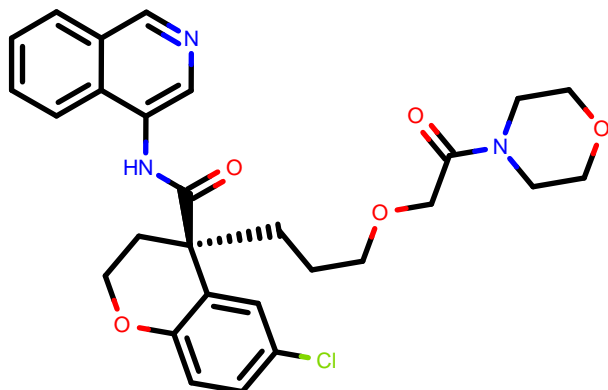
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)Cc5ccccc(c5)[NH3+]

RUN: RUN563

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.30

EN300-1241327_4_1_1



CID: EN300-1241327_4_1_1

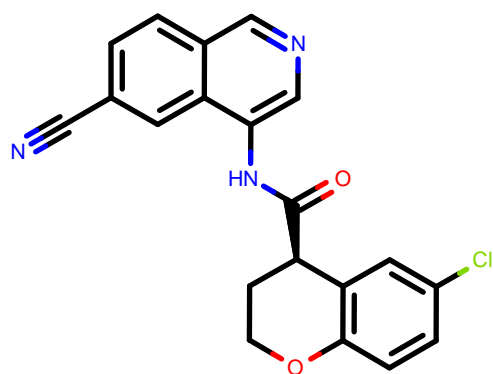
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCCOCC(=O)N5CCOCC5

RUN: RUN5509

DDG (kcal/mol): -0.61

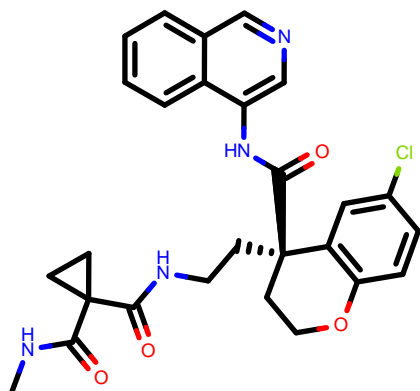
dDDG (kcal/mol): 0.31

BEN-DND-c852c98b-1_1



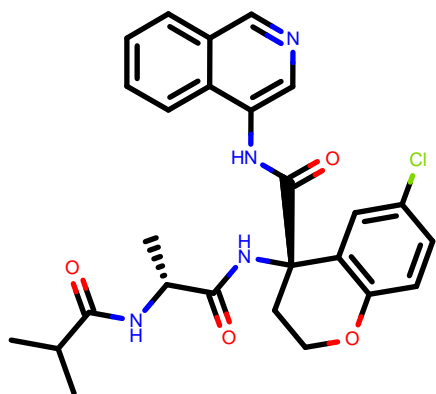
CID:	BEN-DND-c852c98b-1_1
SMILES:	<chem>c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN1086
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.05

EN300-66770_3_1_1



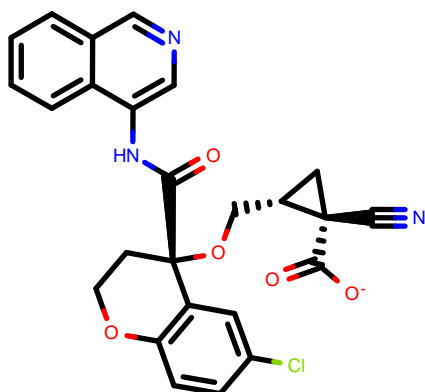
CID:	EN300-66770_3_1_1
SMILES:	<chem>CNC(=O)C1(CC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN5453
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.27

EN300-31184_1_2_1



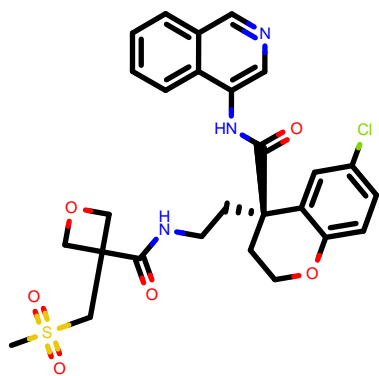
CID:	EN300-31184_1_2_1
SMILES:	<chem>C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)C(C)C</chem>
RUN:	RUN3759
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.29

ED_-GRI-5b13fbe2-50_3



CID:	ED_-GRI-5b13fbe2-50_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5H5C[C@@]5(C#N)C(=O)[O-]</chem>
RUN:	RUN1447
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.41

EN300-262204_3_1_1



CID: EN300-262204_3_1_1

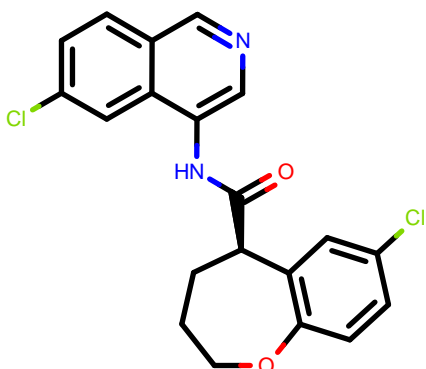
SMILES: CS(=O)(=O)CC1(COC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3050

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.48

ALF-EVA-5b152d2f-3_1



CID: ALF-EVA-5b152d2f-3_1

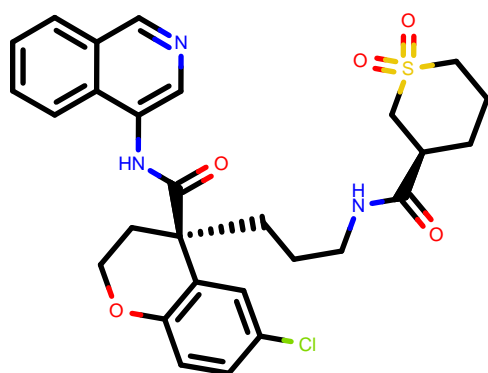
SMILES: c1cc2cncc(c2cc1Cl)NC(=O)[C@@H]3CCCOc4c3cc(cc4)Cl

RUN: RUN2174

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.20

EN300-77778_4_1_1



CID: EN300-77778_4_1_1

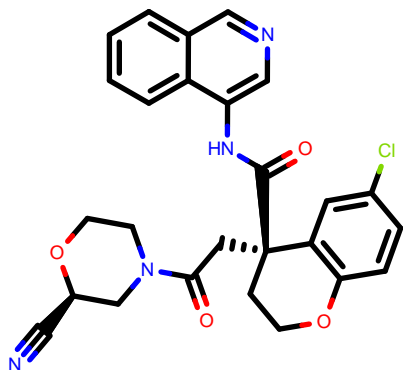
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@]4(CO)C(=O)NCC[C@@]5(CCOc6c4ccccc6)C(=O)Nc7ncoc8c7ccoc8

RUN: RUN7562

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.42

EDJ-MED-d203f206-25_1



CID: EDJ-MED-d203f206-25_1

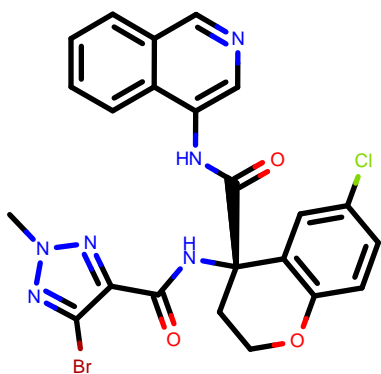
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@]4(CO)C(=O)NCC[C@@]5(CCOc6c4ccccc6)C(=O)Nc7ncoc8c7ccoc8

RUN: RUN2408

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.25

EN300-1439991_1_1_1



CID: EN300-1439991_1_1_1

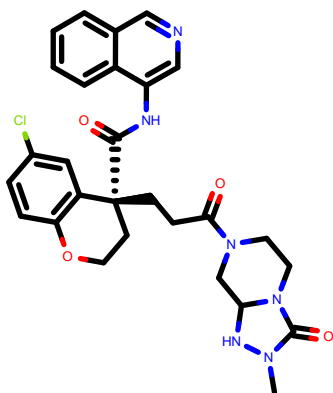
SMILES: Cn1nc(c(n1)Br)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3414

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.25

EN300-814032_2_1_1



CID: EN300-814032_2_1_1

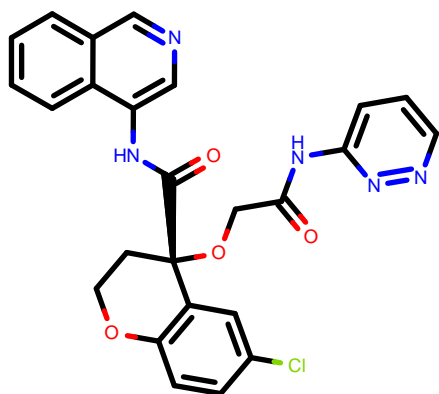
SMILES: Cn1c(=O)n2c(n1)CN(CC2)C(=O)CC[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6

RUN: RUN6840

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-761618_1_1_1



CID: EN300-761618_1_1_1

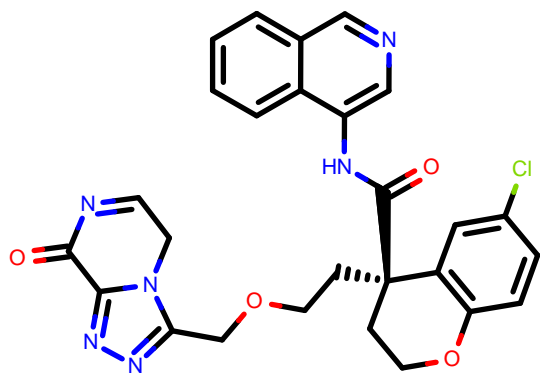
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)Nc5ccnnc5

RUN: RUN6037

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

EN300-378316_3_1_1



CID: EN300-378316_3_1_1

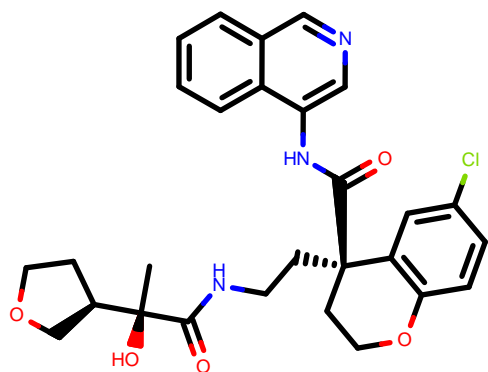
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOCc5[nH]nc6[n+][5c]c[nH]6=O

RUN: RUN4789

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.37

EN300-217494_3_1_1



CID: EN300-217494_3_1_1

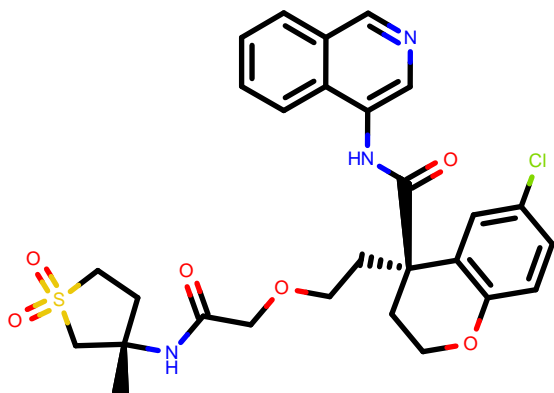
SMILES: C[C@@]1([C@@H]1CCOC1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5O

RUN: RUN4074

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.24

EN300-10414_3_1_1



CID: EN300-10414_3_1_1

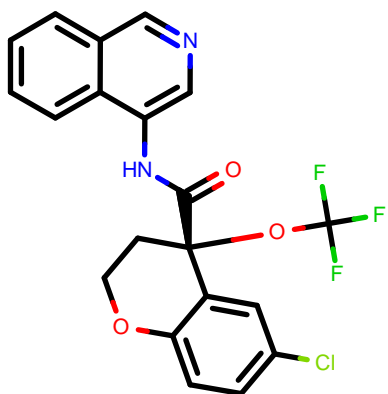
SMILES: C[C@@]1(CC(=O)C(=O)C1)NC(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5S

RUN: RUN5456

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.40

DAR-DIA-e7614d05-1_1



CID: DAR-DIA-e7614d05-1_1

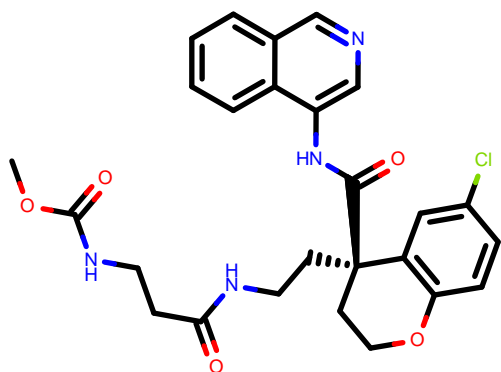
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC(F)(F)F

RUN: RUN2310

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.15

EN300-71558_3_1_1



CID: EN300-71558_3_1_1

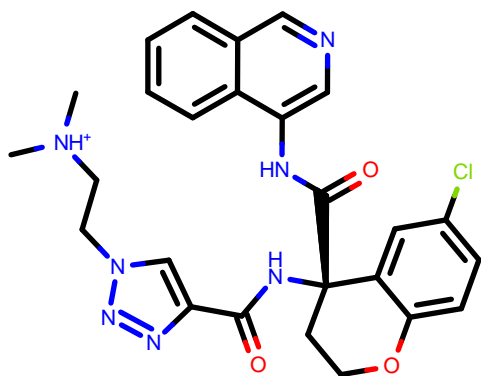
SMILES: COC(=O)NCCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN4452

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-7543132_1_1_1



CID: EN300-7543132_1_1_1

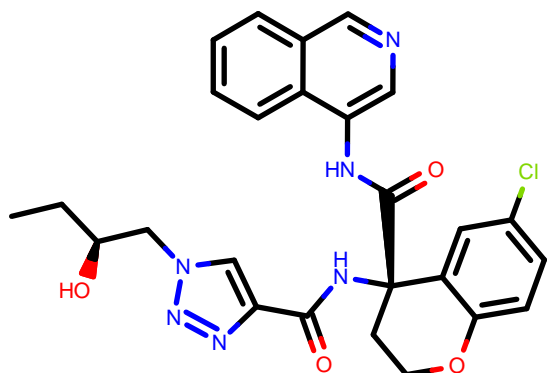
SMILES: C[NH+](C)CCn1cc(mn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7062

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.37

EN300-366050_1_1_1



CID: EN300-366050_1_1_1

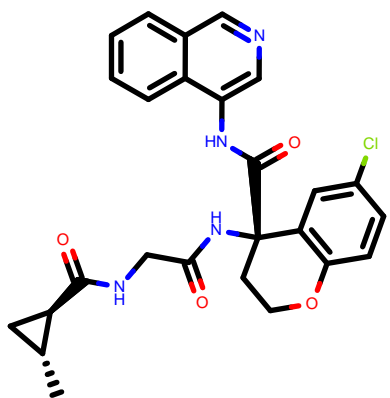
SMILES: CC[C@H](O)CCn1cc(mn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5O

RUN: RUN5177

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.24

EN300-30768_1_3_1



CID: EN300-30768_1_3_1

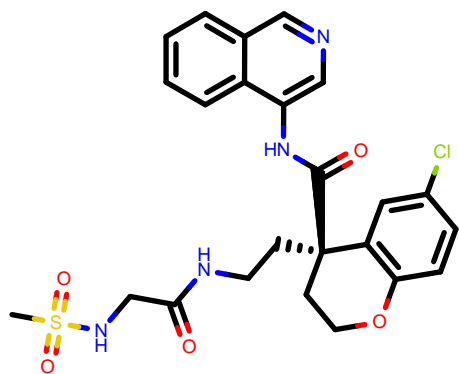
SMILES: C[C@H]1C[C@H]1C(=O)NCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5174

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-30419_3_1_1



CID: EN300-30419_3_1_1

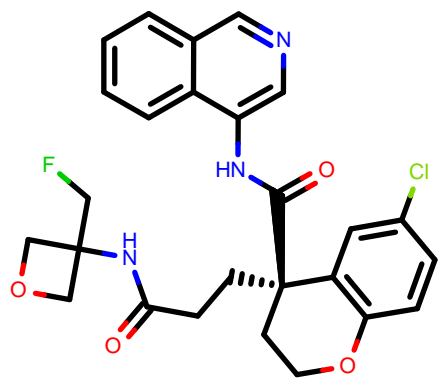
SMILES: CS(=O)(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN5360

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.39

EN300-6970573_2_1_1



CID: EN300-6970573_2_1_1

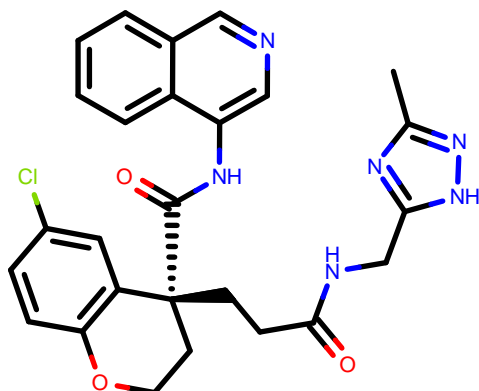
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(COC5)CF

RUN: RUN4132

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-70487_2_1_1



CID: EN300-70487_2_1_1

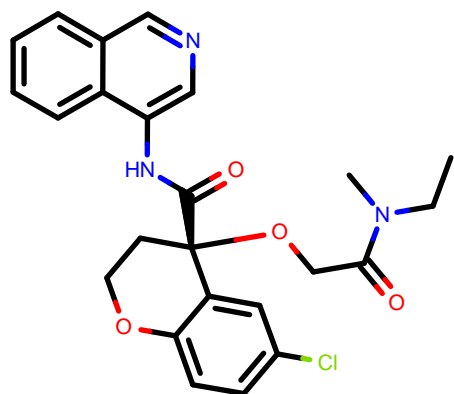
SMILES: Cc1[nH]nc(n1)CNC(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN5412

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

EN300-1253122_1_1_1



CID: EN300-1253122_1_1_1

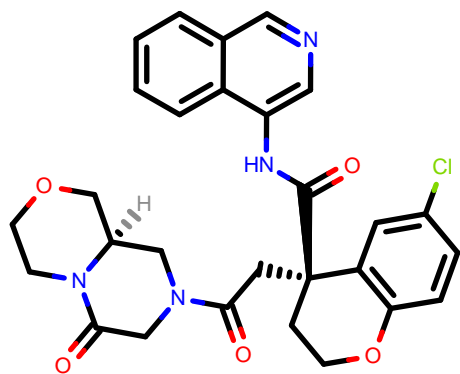
SMILES: CCN(C)C(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN4763

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.23

EDJ-MED-d203f206-32_1



CID: EDJ-MED-d203f206-32_1

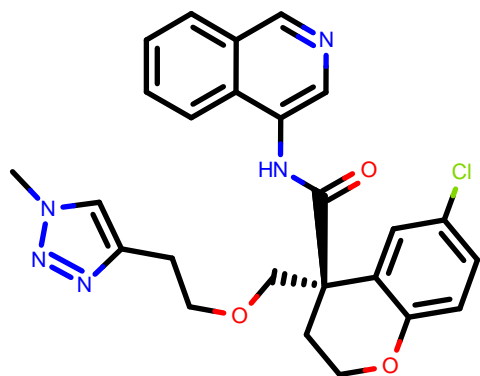
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]6H6COCNC6C1=O)C5

RUN: RUN2453

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-1600786_2_1_1



CID: EN300-1600786_2_1_1

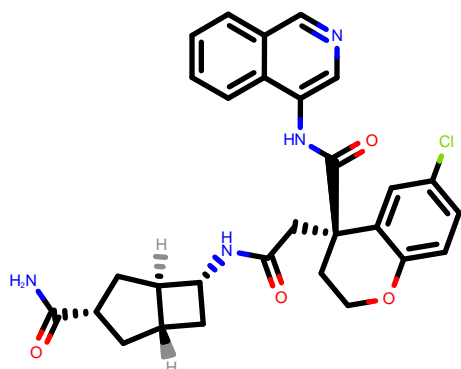
SMILES: Cn1cc(nn1)CCOC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5164

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.28

ALP-UNI-3496895b-15_7



CID: ALP-UNI-3496895b-15_7

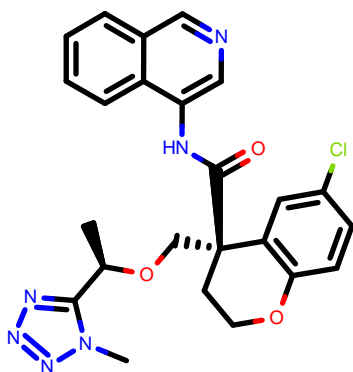
SMILES: c1ccc2c(e1)cncc2N(C(=O)C@)3(CCOc4c3cc(cc4)C)C(=O)N[C@@H]5[C@@H]6[C@H]5[C@@H]6[C@H]5C(=O)N

RUN: RUN2347

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-173006_2_2_1



CID: EN300-173006_2_2_1

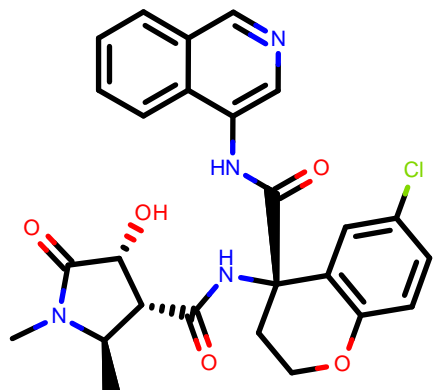
SMILES: C[C@H]([c1n[n]n1C])OC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3911

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.29

EN300-378828_1_1_1



CID: EN300-378828_1_1_1

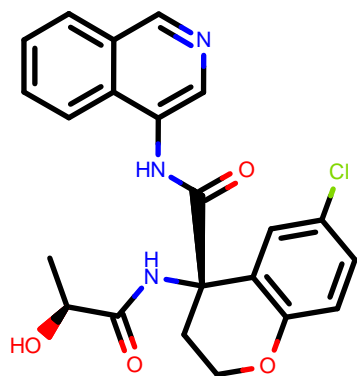
SMILES: C[C@@H]1[C@@H]2[C@H]1[C@@H]3[C@@H]2[C@@H]3C(=O)N[C@@H]4[C@@H]5[C@@H]4[C@@H]5C(=O)Nc6cncc7c6cccc7

RUN: RUN7725

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.27

EN300-91905_1_1_1



CID: EN300-91905_1_1_1

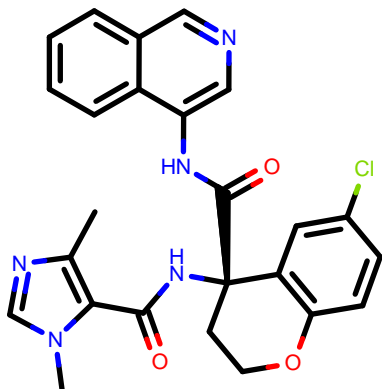
SMILES: C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN6583

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.20

EN300-6498351_1_1_1



CID: EN300-6498351_1_1_1

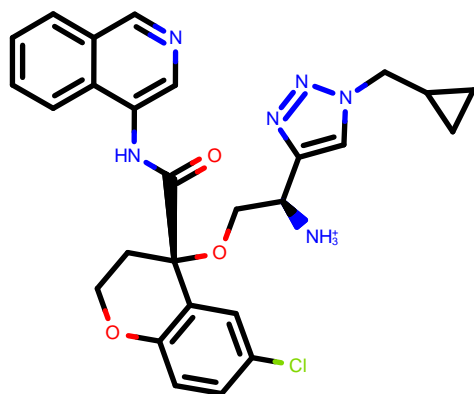
SMILES: Cc1c(n(en1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN3979

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-16_1



CID: ED_-GRI-5b13fbe2-16_1

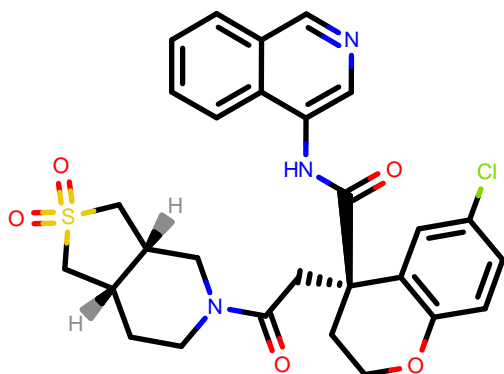
SMILES: c1ccc2c(c1)ncnc2N[C@@](Cl)(COCc3cc4c(c3)cc(O)cc4)Nc5cnc6c5cnc6

RUN: RUN1458

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.34

EN300-365993_1_1_1



CID: EN300-365993_1_1_1

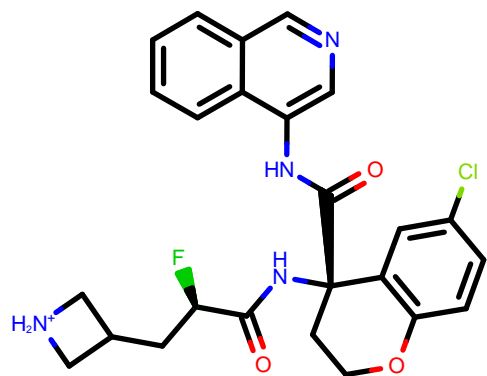
SMILES: c1ccc2c(c1)ncnc2N[C@@](Cl)(COCc3cc4c(c3)cc(O)cc4)Nc5cnc6c5cnc6S(=O)(=O)N7CCNCC7

RUN: RUN6242

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.42

EDG-MED-90036822-81_1



CID: EDG-MED-90036822-81_1

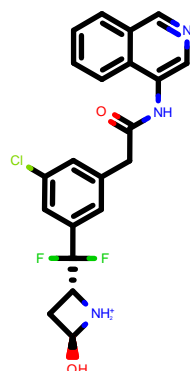
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](C)C5C[NH2+][C5]F

RUN: RUN1644

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.51

ALP-POS-fab80cf2-1_2



CID: ALP-POS-fab80cf2-1_2

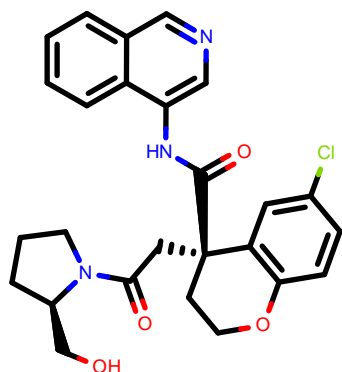
SMILES: c1ccc2c(c1)cncc2NC(=O)C(c3cc(cc3)Cl)C(C@H)4CC(=O)N4(F)F

RUN: RUN1365

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.47

EN300-378343_1_1_1



CID: EN300-378343_1_1_1

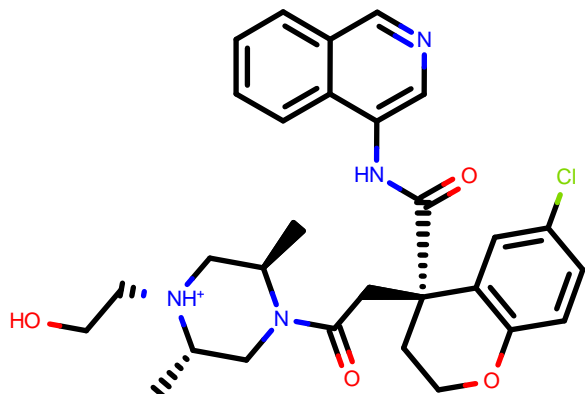
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC=C[C@@H]5CO

RUN: RUN5959

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.23

EDG-MED-ba1ac7b9-26_2



CID: EDG-MED-ba1ac7b9-26_2

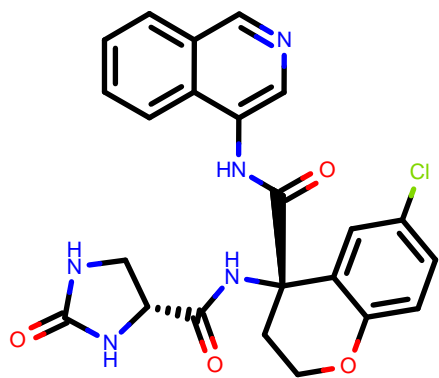
SMILES: C[C@@H]1[C@H]([C@@H]2[C@H](CN1C)C)C[C@@]3(CCOc4c3cc(cc4)Cl)C(C)N4C5C6C(=O)C(C)C5

RUN: RUN2592

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.43

EN300-222145_1_1_1



CID: EN300-222145_1_1_1

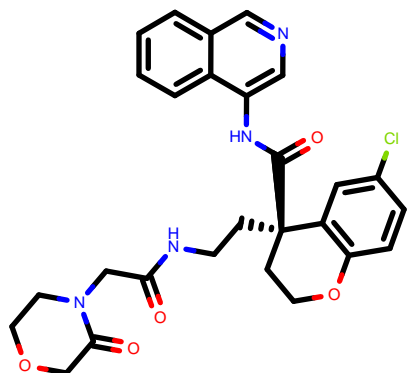
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CNC(=O)N5

RUN: RUN3854

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.24

EN300-186943_3_1_1



CID: EN300-186943_3_1_1

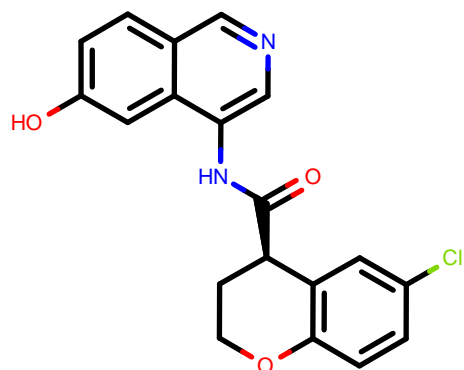
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5COCOC5=O

RUN: RUN5349

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.32

BEN-DND-c852c98b-4_1



CID: BEN-DND-c852c98b-4_1

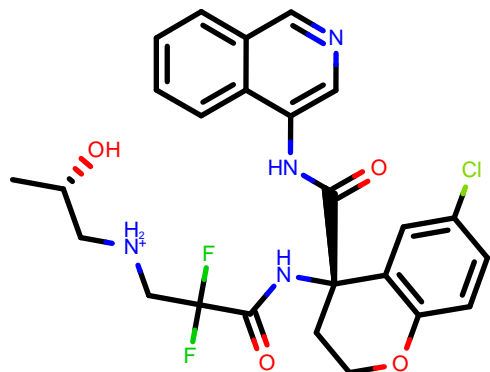
SMILES: c1cc2cnccc(c2cc1O)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1097

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.04

EDG-MED-90036822-38_1



CID: EDG-MED-90036822-38_1

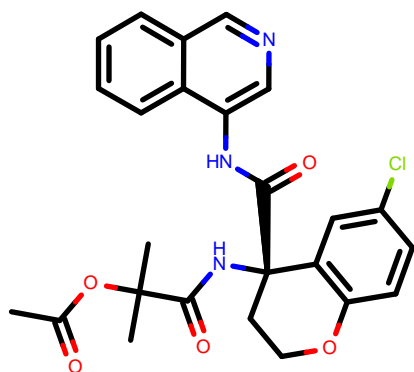
SMILES: C[C@@H](CNCC(C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3ccc4(F)F)O

RUN: RUN1664

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.41

EN300-155589_1_1_1



CID: EN300-155589_1_1_1

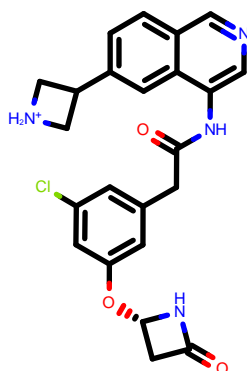
SMILES: CC(=O)OC(C)(C)C(=O)N[C@@H](CCOCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6175

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.26

ALF-EVA-0b412456-8_2



CID: ALF-EVA-0b412456-8_2

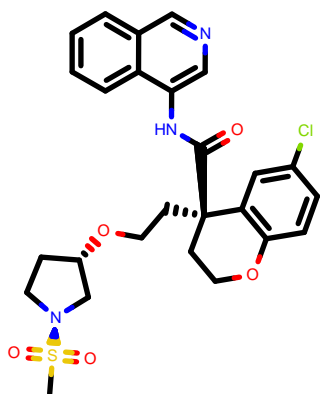
SMILES: c1cc2nccc(c2c1C3C[NH2+])C3)NC(=O)Cc4cc(ccc4)Cl)O[C@@H]5CC(=O)N5

RUN: RUN2568

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.43

EN300-301690_3_1_1



CID: EN300-301690_3_1_1

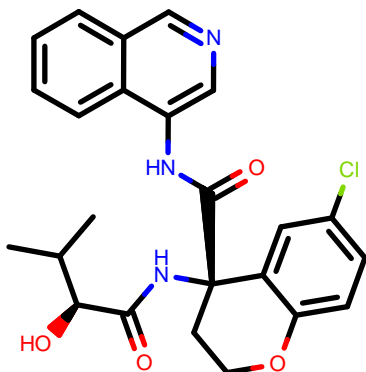
SMILES: CS(=O)(=O)[N@@H]1CC[C@@H](C1)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5198

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.35

EN300-199359_1_1_1



CID: EN300-199359_1_1_1

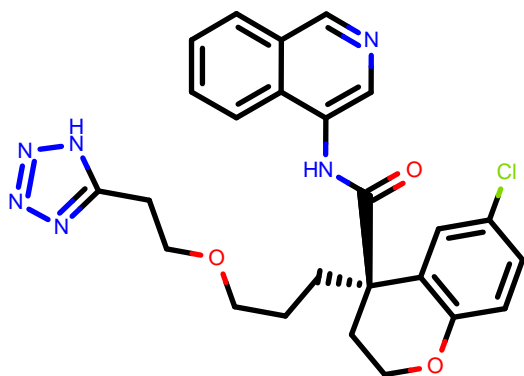
SMILES: CC(C)[C@@H](C(=O)N[C@@H](CCOCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6139

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.24

EN300-183231_4_1_1



CID: EN300-183231_4_1_1

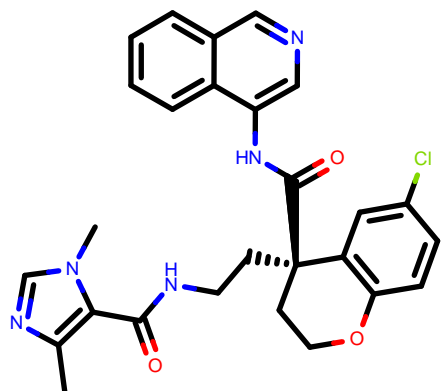
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)CCOCCc5n[nH]n5

RUN: RUN5203

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.63

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

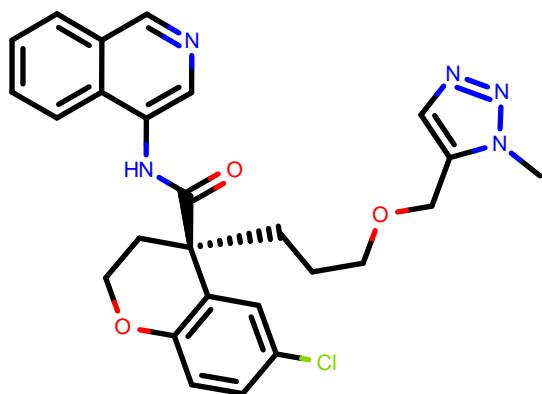
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN4476

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.30

EN300-216673_4_1_1



CID: EN300-216673_4_1_1

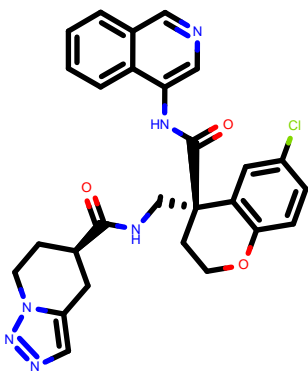
SMILES: Cn1c(cnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccc5

RUN: RUN5223

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.32

EN300-7430501_2_1_1



CID: EN300-7430501_2_1_1

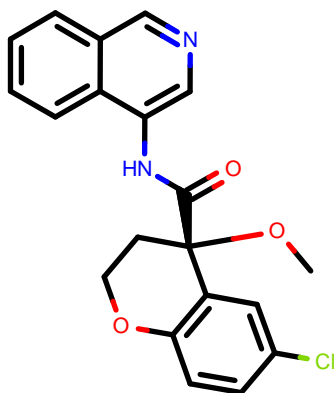
SMILES: c1ccc2c(c1)cnc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)CNC(=O)C@@@5Cn6c(cnn6)C5

RUN: RUN6843

DDG (kcal/mol): -0.58

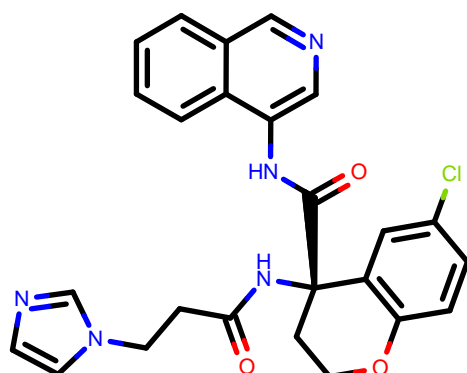
dDDG (kcal/mol): 0.29

EDG-MED-0e5afe9d-3_2



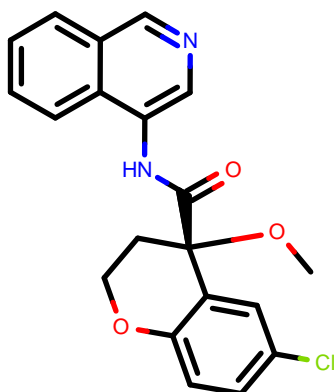
CID:	EDG-MED-0e5afe9d-3_2
SMILES:	<chem>CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN2185
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.11

EN300-75342_1_1_1



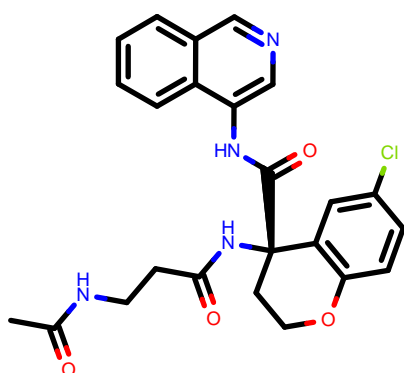
CID:	EN300-75342_1_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnc5</chem>
RUN:	RUN4990
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.21

PET-UNK-29afea89-2_1



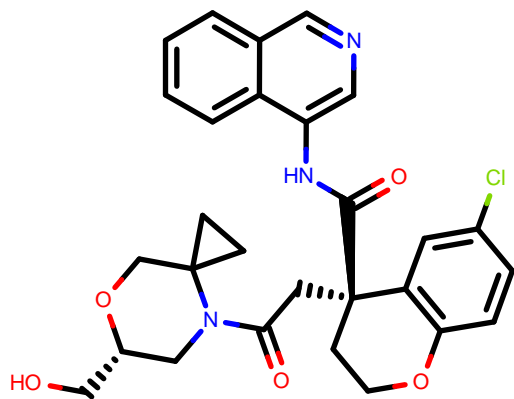
CID:	PET-UNK-29afea89-2_1
SMILES:	<chem>CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN564
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.12

EN300-04073_1_1_1



CID:	EN300-04073_1_1_1
SMILES:	<chem>CC(=O)NCCC(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN6694
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.28

EN300-7493255_1_1_1



CID: EN300-7493255_1_1_1

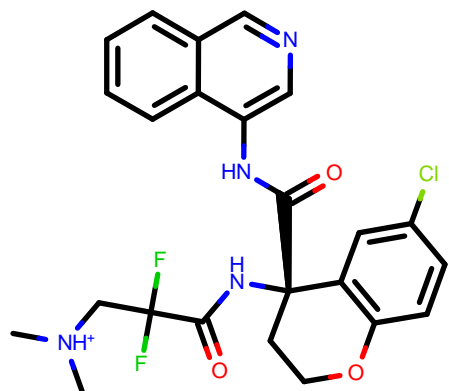
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](OCC56CC6)CO

RUN: RUN4946

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.38

EDG-MED-90036822-87_1



CID: EDG-MED-90036822-87_1

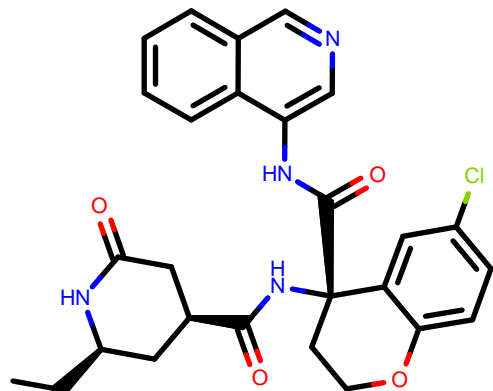
SMILES: CN(C)CC(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)(F)F

RUN: RUN1687

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.24

EN300-7439980_1_1_1



CID: EN300-7439980_1_1_1

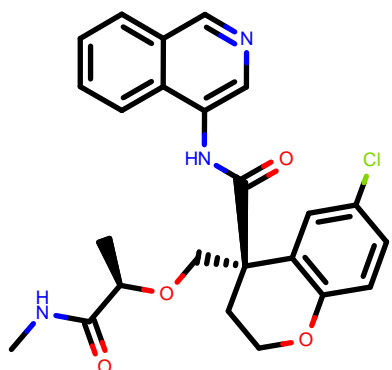
SMILES: CC[C@@H]1C[C@@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)N

RUN: RUN5180

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EN300-211482_2_2_1



CID: EN300-211482_2_2_1

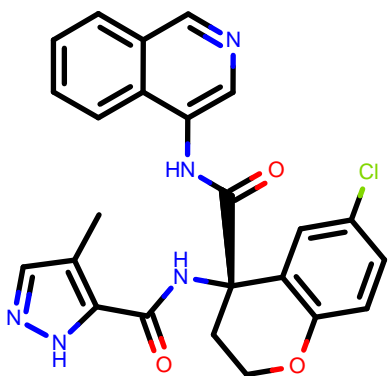
SMILES: C[C@H](C(=O)NC)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4

RUN: RUN5546

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.27

EN300-248178_1_1_1



CID: EN300-248178_1_1_1

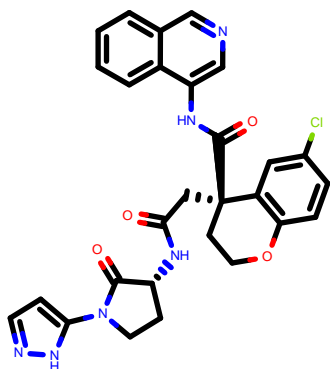
SMILES: Cc1cn[nH]c1C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN3697

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

ALP-UNI-3496895b-4_1



CID: ALP-UNI-3496895b-4_1

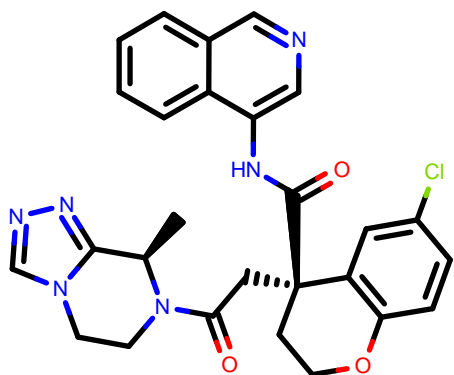
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3ccc4YCl)CC(=O)N[C@@]5H5CCN(CS=O)S6ccc[nH]6

RUN: RUN2368

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.29

EDG-MED-ba1ac7b9-19_3



CID: EDG-MED-ba1ac7b9-19_3

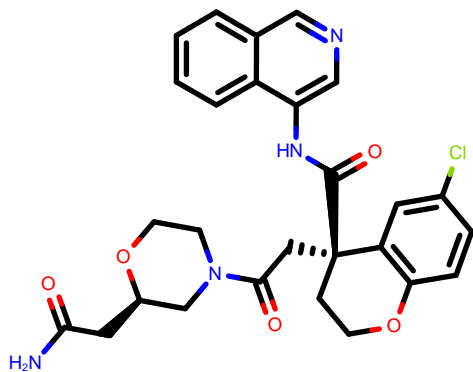
SMILES: C[C@@]([H])1c2nncn2CCN1C(=O)C[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)Nc5cncc6c5cccc6

RUN: RUN2525

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.40

EN300-321558_1_1_1



CID: EN300-321558_1_1_1

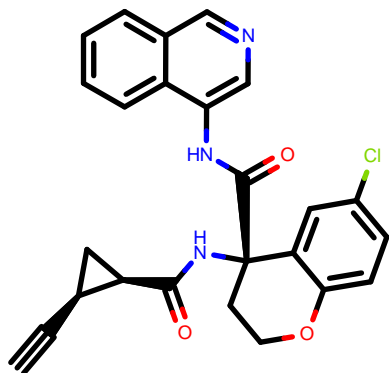
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]([H])(C5)CC(=O)N

RUN: RUN6253

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EN300-254137_1_1_1



CID: EN300-254137_1_1_1

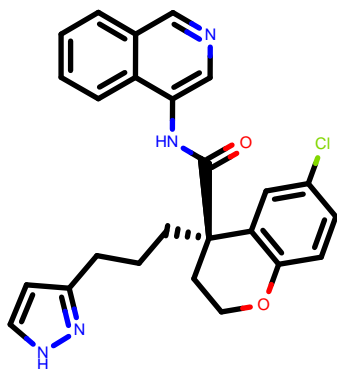
SMILES: C#C[C@H]1C[C@H]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN3977

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.21

VLA-UCB-34f3ed0c-10_1_1



CID: VLA-UCB-34f3ed0c-10_1_1

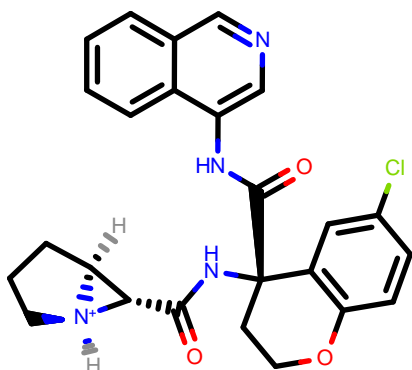
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5cn[nH]5

RUN: RUN4862

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.25

EDG-MED-90036822-73_4



CID: EDG-MED-90036822-73_4

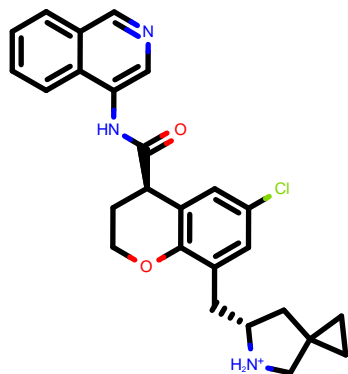
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)NCl)C[C@H]3C@H]N[C@@H]5CCCC5

RUN: RUN1595

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.35

DAR-DIA-23e5a6a0-9_1



CID: DAR-DIA-23e5a6a0-9_1

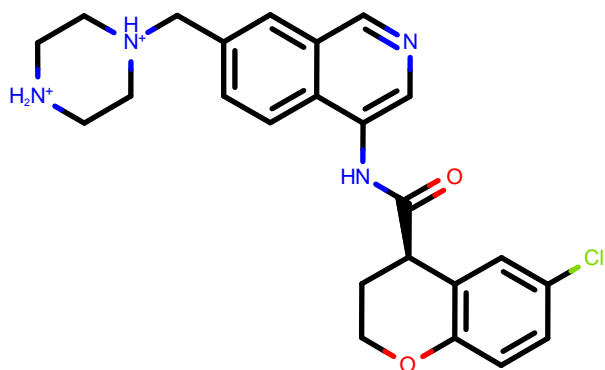
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[C@]5(C)C(C)N[C@@H]5Cl

RUN: RUN406

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.40

MAK-UNK-8be7dca9-1_1



CID: MAK-UNK-8be7dca9-1_1

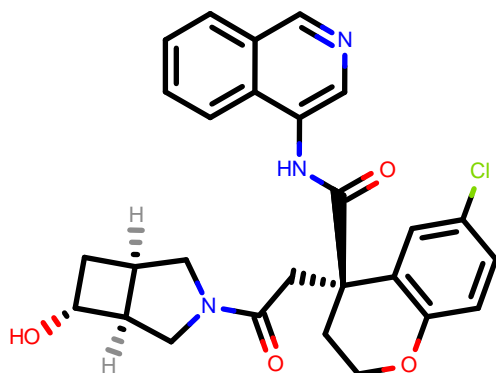
SMILES: c1cc2c(cc1CN3CC[NH2+][CC3])ncc2NC(=O)[C@@H]4CCOC5c4cc(cc5)Cl

RUN: RUN439

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.14

EN300-305294_1_3_1



CID: EN300-305294_1_3_1

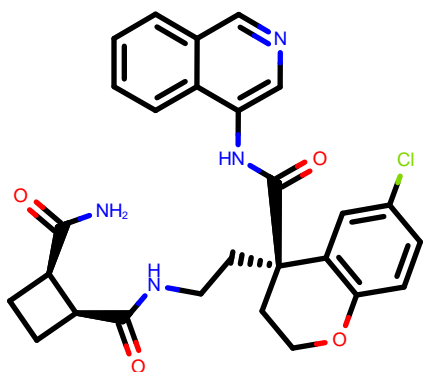
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)O[C@@]3O[C@@]5[C@H](C)[C@@H]6C5O

RUN: RUN7143

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.22

EN300-217107_3_4_1



CID: EN300-217107_3_4_1

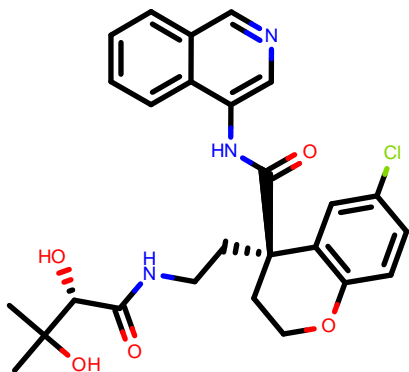
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)O[C@@]3O[C@@]5[C@H](C)[C@@H]5C(=O)N

RUN: RUN4083

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.29

EN300-299532_3_1_1



CID: EN300-299532_3_1_1

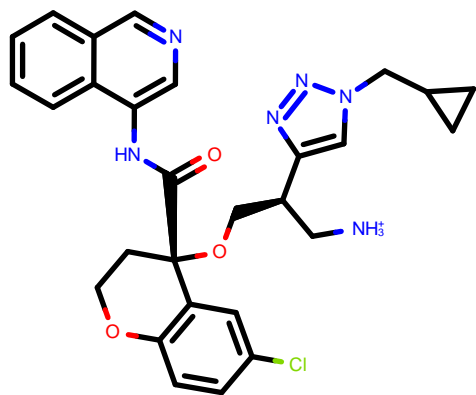
SMILES: CC(C)(C)[C@@H](C(=O)NCC[C@@]1(C)COC2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4O)O

RUN: RUN5305

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-49_2



CID: ED_-GRI-5b13fbe2-49_2

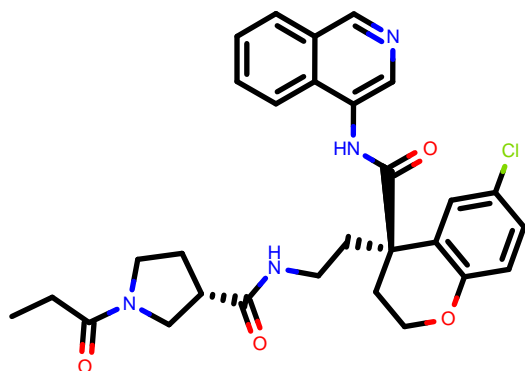
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](C[NH3+])c5cn(m5)CC6CC6

RUN: RUN1533

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.39

EN300-114133_3_1_1



CID: EN300-114133_3_1_1

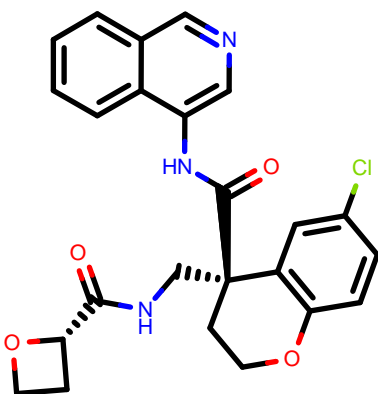
SMILES: CCC(=O)N1CC[C@H](C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN: RUN5353

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.45

EN300-85760_2_1_1



CID: EN300-85760_2_1_1

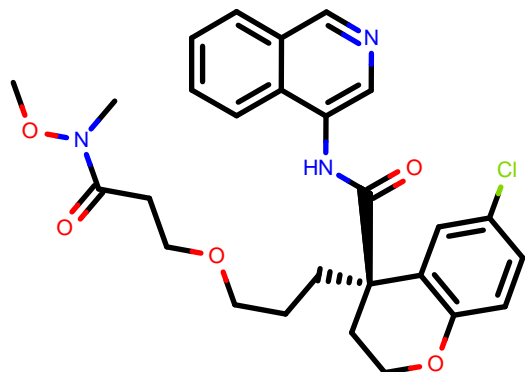
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5H5CCO5

RUN: RUN4378

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-174603_4_1_1



CID: EN300-174603_4_1_1

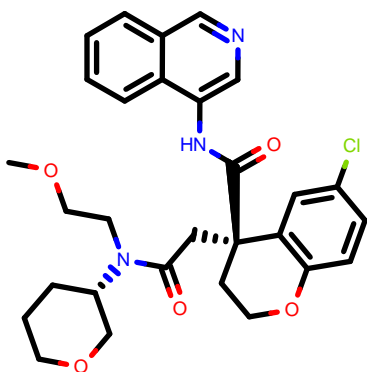
SMILES: CN(C(=O)CCOCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4)OC

RUN: RUN6029

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.40

JAG-UCB-706446eb-5_2_1



CID: JAG-UCB-706446eb-5_2_1

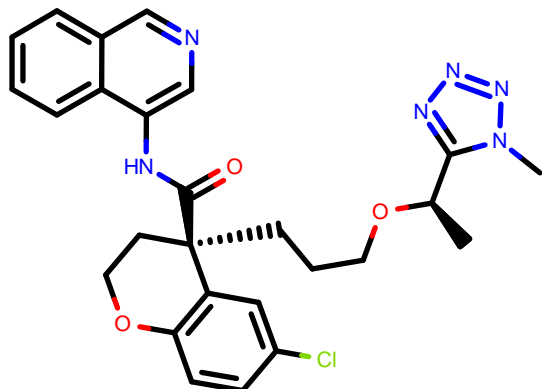
SMILES: COCNC([C@H]1CCCOC1)C(=O)C[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5

RUN: RUN5511

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.45

EN300-173006_4_2_1



CID: EN300-173006_4_2_1

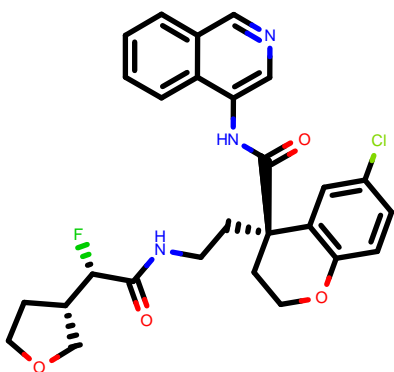
SMILES: C[C@H](c1nncn1)OCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4ccc5

RUN: RUN7763

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.35

EN300-783124_3_4_1



CID: EN300-783124_3_4_1

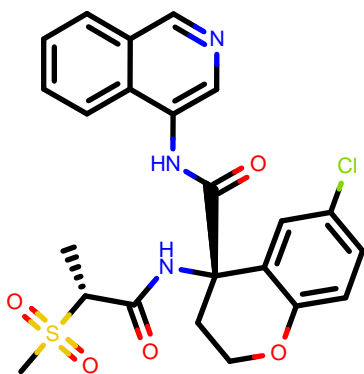
SMILES: c1ccc2c(c1)nc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]([C@H]5CCOC5)F

RUN: RUN3278

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.27

EN300-39405_1_2_1



CID: EN300-39405_1_2_1

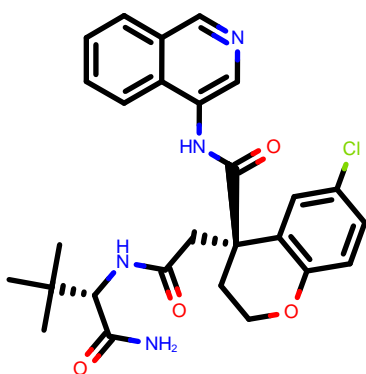
SMILES: C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nc4c3ccc4)S(=O)(=O)C

RUN: RUN6453

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.29

EN300-96001_1_1_1



CID: EN300-96001_1_1_1

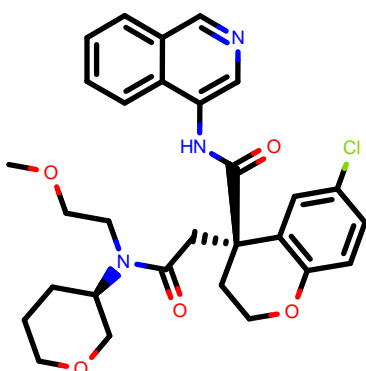
SMILES: CC(C)(C)[C@@H](C(=O)N)NC(=O)C[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6353

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.27

JAG-UCB-706446eb-5_1



CID: JAG-UCB-706446eb-5_1

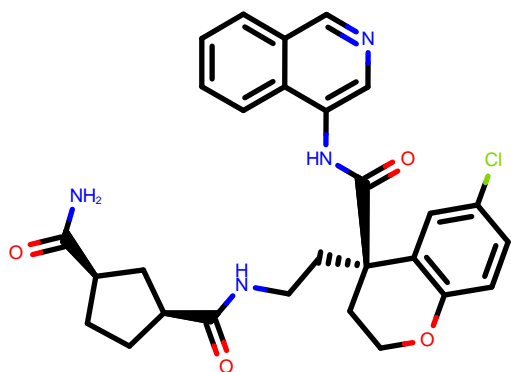
SMILES: COCCN([C@@H]1CCCOC1)C(=O)C[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN651

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.36

EN300-370753_3_1_1



CID: EN300-370753_3_1_1

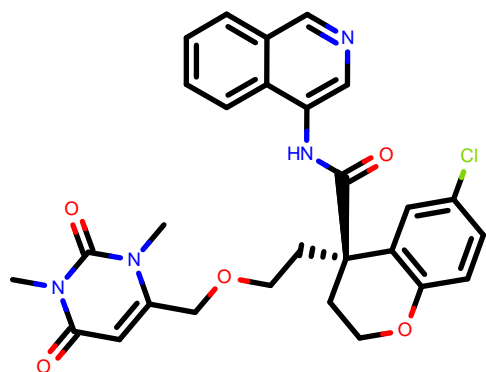
SMILES: c1ccc2c(c1)cnc2N[C@@H](C(=O)C[C@H]3(CCOc4c3cc(cc4)Cl)CNC1=O)C(=O)Nc5cnc6c5cccc6N

RUN: RUN5860

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.31

EN300-25386_3_1_1



CID: EN300-25386_3_1_1

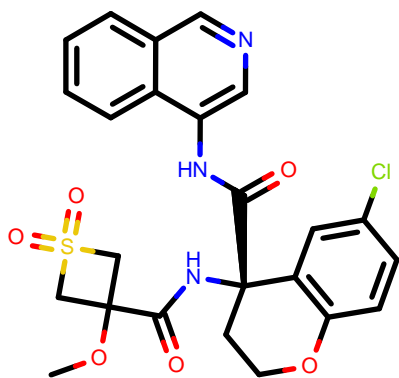
SMILES: Cn1c(cc(=O)n1=O)C(=O)C[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5214

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.31

EN300-704025_1_1_1



CID: EN300-704025_1_1_1

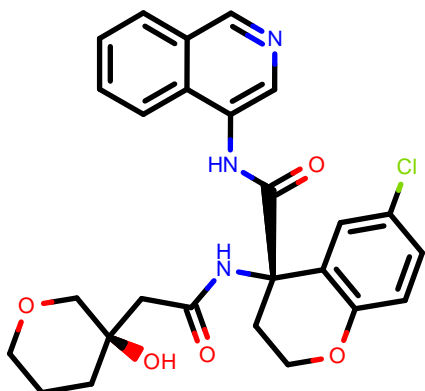
SMILES: COC1(CS(=O)(=O)C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN5267

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.33

EN300-1071940_1_1_1



CID: EN300-1071940_1_1_1

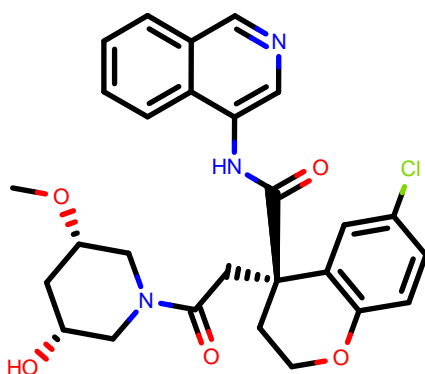
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCCOC5)O

RUN: RUN6219

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-6763507_1_4_1



CID: EN300-6763507_1_4_1

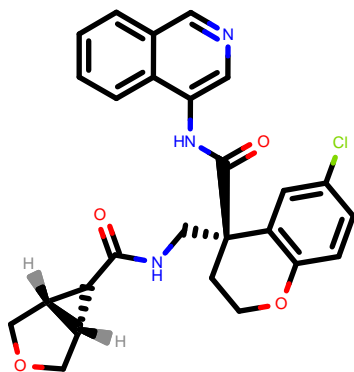
SMILES: CO[C@@H]1[C]C@H[C@@H]2(CN(C1)C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN: RUN5699

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.30

EN300-257945_2_1_1



CID: EN300-257945_2_1_1

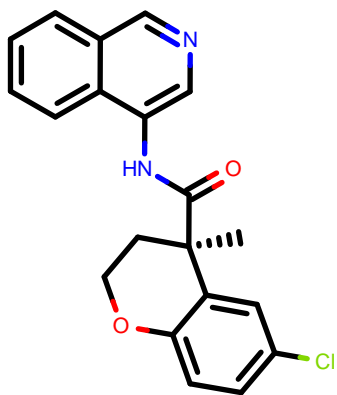
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5[C@@H]6[C@@H]5COC6

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

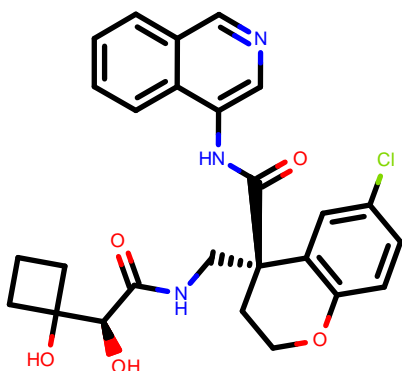
SMILES: C[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN6122

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.10

EN300-1073320_2_2_1



CID: EN300-1073320_2_2_1

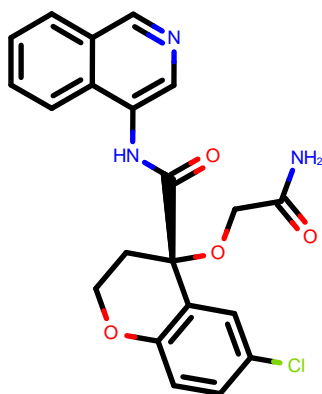
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CNC(=O)[C@H](C5(CC5)O)O

RUN: RUN6314

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-18249_1_1_1



CID: EN300-18249_1_1_1

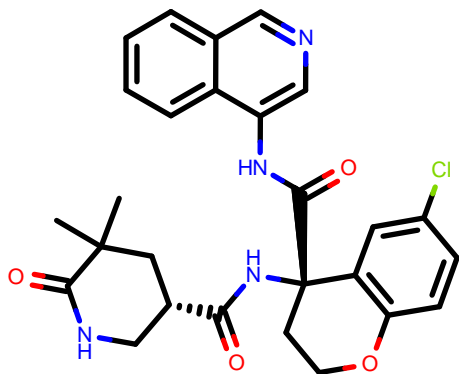
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)N

RUN: RUN5798

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.19

EN300-7351945_1_1_1



CID: EN300-7351945_1_1_1

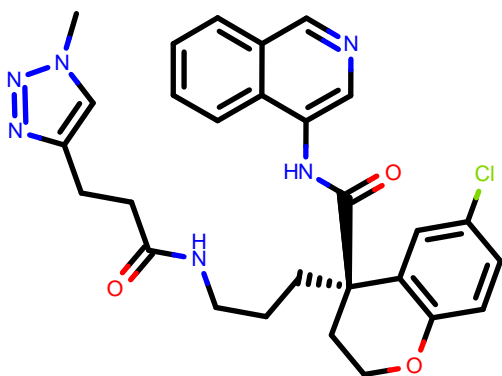
SMILES: CC1(C[C@@H](CNC1=O)C(=O)N[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN2693

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.21

EN300-306047_4_1_1



CID: EN300-306047_4_1_1

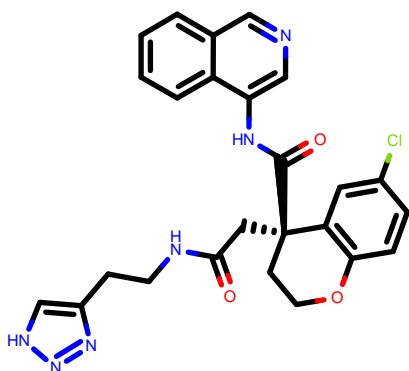
SMILES: Cn1cc(nn1)CCC(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN5081

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.35

EN300-1178209_1_1_1



CID: EN300-1178209_1_1_1

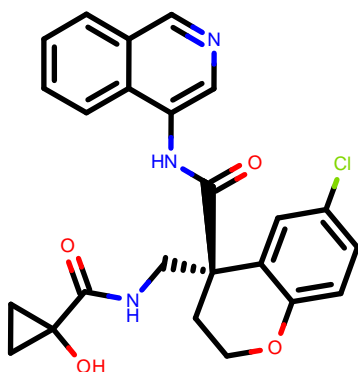
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCc5cn[nH]n5

RUN: RUN6413

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-25702_2_1_1



CID: EN300-25702_2_1_1

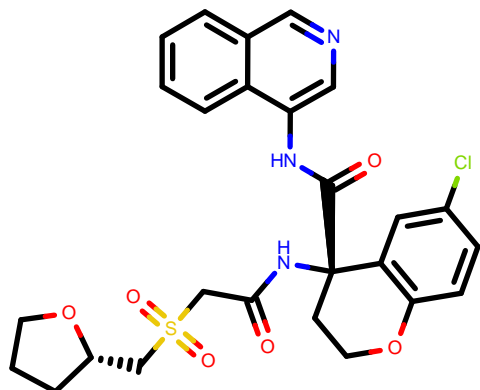
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)O

RUN: RUN4128

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-67023_1_1_1



CID: EN300-67023_1_1_1

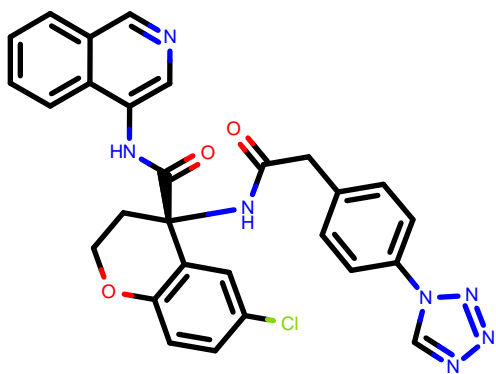
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS(=O)(=O)C[C@@]5H5CC5O5

RUN: RUN6657

DDG (kcal/mol): -0.54

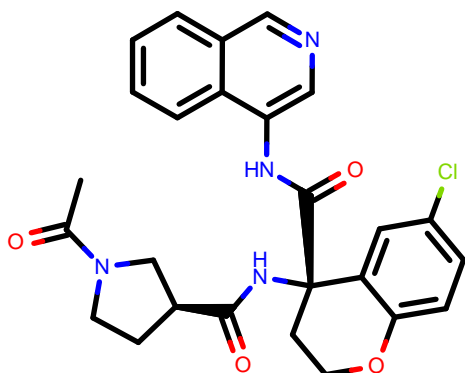
dDDG (kcal/mol): 0.37

ALP-UNI-dbbfd3db-1_1



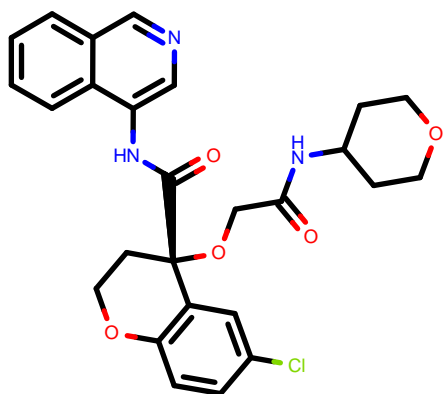
CID:	ALP-UNI-dbbfd3db-1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)C4=CC=CC=C4)C(=O)C5=CC=CC=C5N6C=NN=N6</chem>
RUN:	RUN2628
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.32

EN300-100180_1_1_1



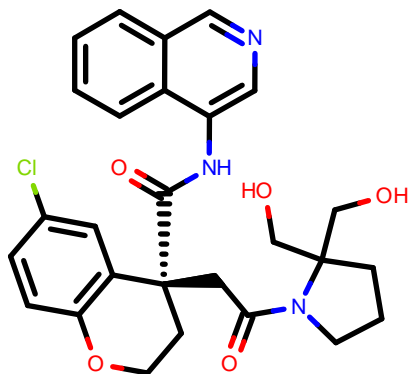
CID:	EN300-100180_1_1_1
SMILES:	<chem>CC(=O)N1CC[C@H](C1)C(=O)N[C@@]2(C(=O)C3=CC=CC=C3)C(=O)Nc4ccc(Cl)cc4</chem>
RUN:	RUN7034
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.45

EN300-67573_1_1_1



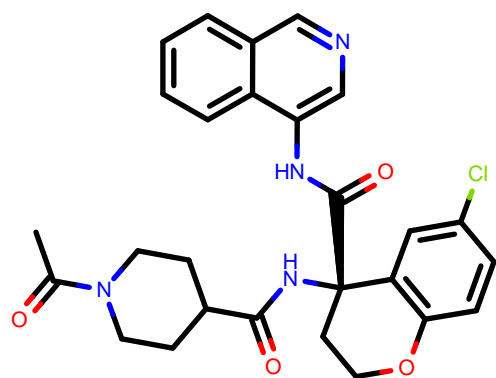
CID:	EN300-67573_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)C4=CC=CC=C4)C(=O)OCC(=O)N5CCOCC5</chem>
RUN:	RUN5637
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.27

EN300-1091448_1_1_1



CID:	EN300-1091448_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)C4=CC=CC=C4)C(=O)N5CCCC5(CO)CO</chem>
RUN:	RUN3434
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.33

EN300-18557_1_1_1



CID: EN300-18557_1_1_1

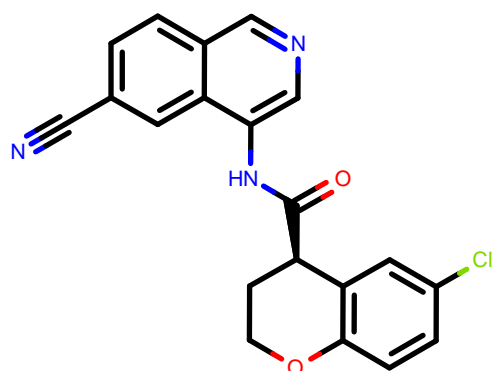
SMILES: CC(=O)N1CCC(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6814

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.32

BEN-DND-c852c98b-1_1_1



CID: BEN-DND-c852c98b-1_1_1

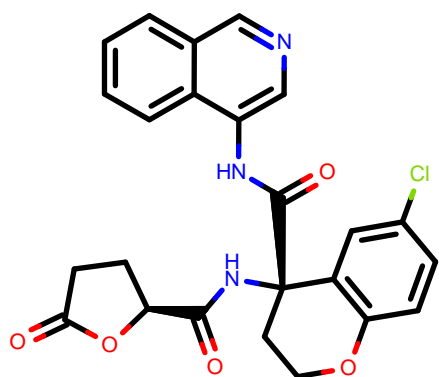
SMILES: c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN6707

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.13

EN300-359750_1_1_1



CID: EN300-359750_1_1_1

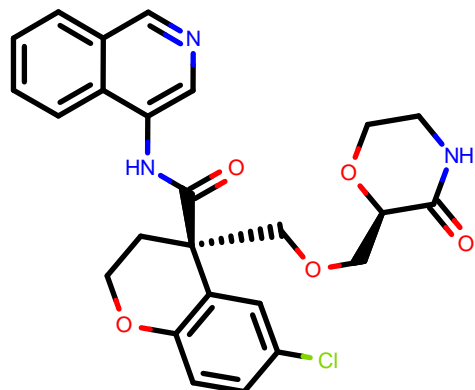
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)O5

RUN: RUN6817

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.23

EN300-1706036_2_1_1



CID: EN300-1706036_2_1_1

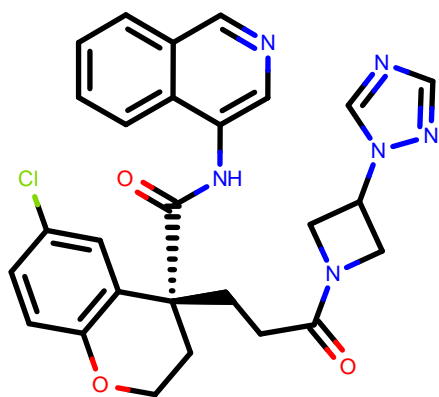
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C(=O)NCCO5

RUN: RUN6540

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.27

KAD-UNI-8a629cb0-48_1



CID: KAD-UNI-8a629cb0-48_1

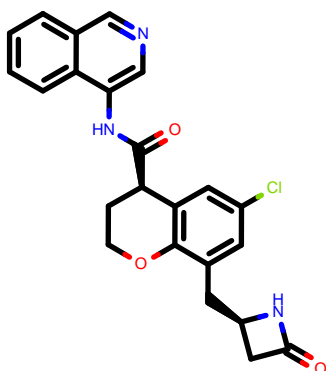
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCC(=O)N5CC(C5)n6cncn6

RUN: RUN2040

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.27

DAR-DIA-6a508060-5_1



CID: DAR-DIA-6a508060-5_1

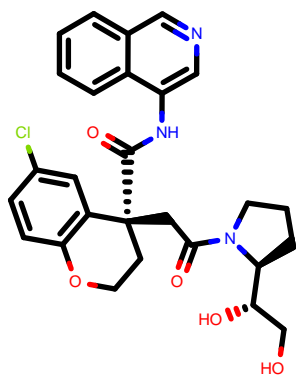
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@H3(CCOc4c3cc(cc4)C)CC(=O)N5CC(=O)N5Cl

RUN: RUN280

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.17

EDJ-MED-d203f206-15_1



CID: EDJ-MED-d203f206-15_1

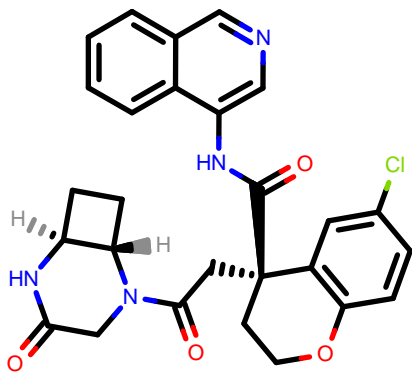
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CC(=O)N5CCC(C@H)5C@H(CO)O

RUN: RUN2399

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.41

EN300-6499164_1_1_1



CID: EN300-6499164_1_1_1

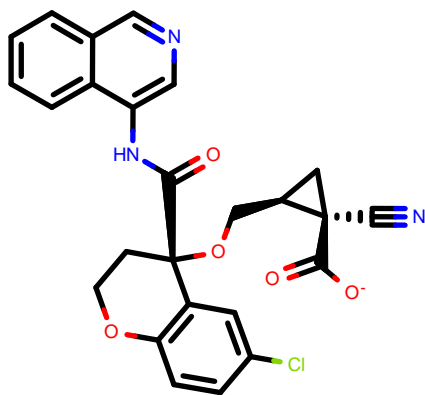
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CC(=O)N5CC(=O)N5C@@H(C)C@H5CO6

RUN: RUN5053

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-50_2



CID: ED_-GRI-5b13fbe2-50_2

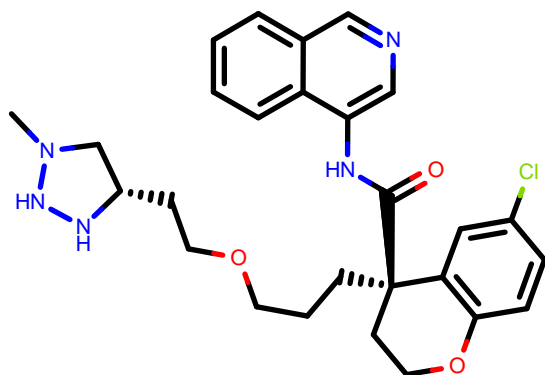
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5C[C@@]5(C#N)C(=O)[O-]

RUN: RUN1439

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

EN300-1600786_4_1_1



CID: EN300-1600786_4_1_1

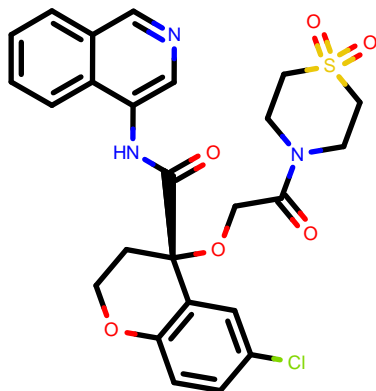
SMILES: Cn1cc(nn1)CCOCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN6877

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.39

EN300-1265948_1_1_1



CID: EN300-1265948_1_1_1

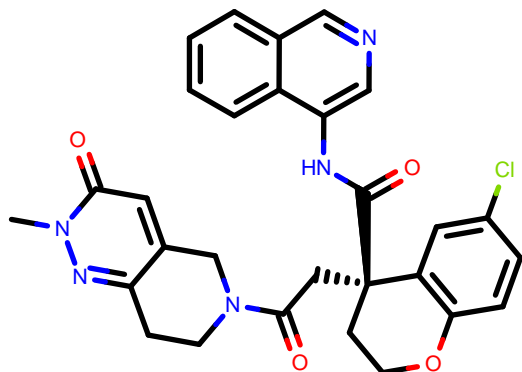
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN6065

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

ALP-UNI-3496895b-13_1



CID: ALP-UNI-3496895b-13_1

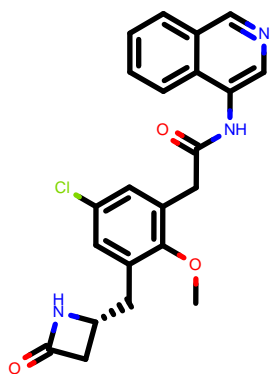
SMILES: Cn1c(=O)cc2c(n1)CCN(C2)C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6

RUN: RUN2364

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.28

EDJ-MED-50011917-3_1



CID: EDJ-MED-50011917-3_1

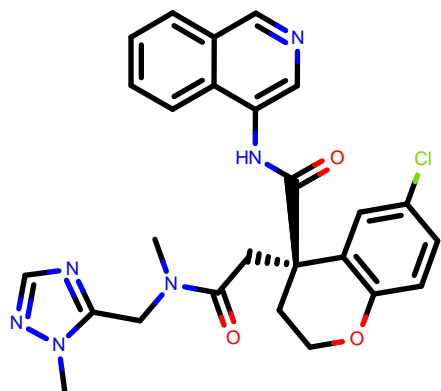
SMILES: COc1c(cc(cc1CC(=O)Nc2ncc3c2ccc3)C)C[C@@H]4CC(=O)N4

RUN: RUN333

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.34

EN300-7444635_1_1_1



CID: EN300-7444635_1_1_1

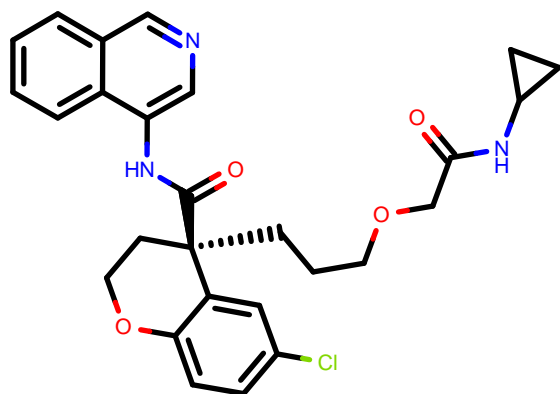
SMILES: Cn1c(nen1)CN(C)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN: RUN7742

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.33

EN300-1253178_4_1_1



CID: EN300-1253178_4_1_1

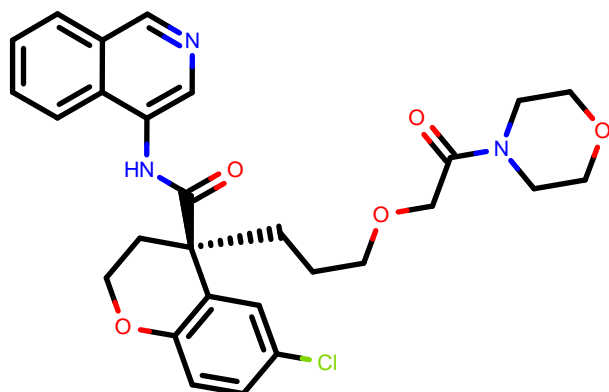
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)NC5CC5

RUN: RUN7104

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.36

EN300-1241327_4_1_1



CID: EN300-1241327_4_1_1

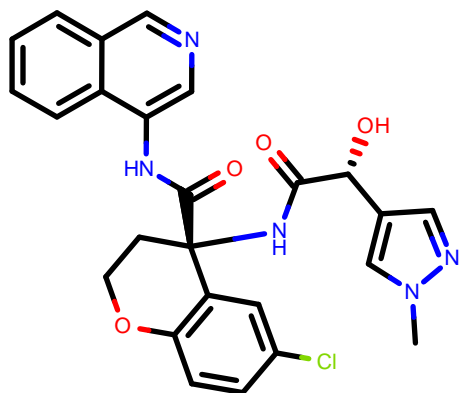
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)N5CCOCC5

RUN: RUN7673

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.32

EN300-198540_1_2_1



CID: EN300-198540_1_2_1

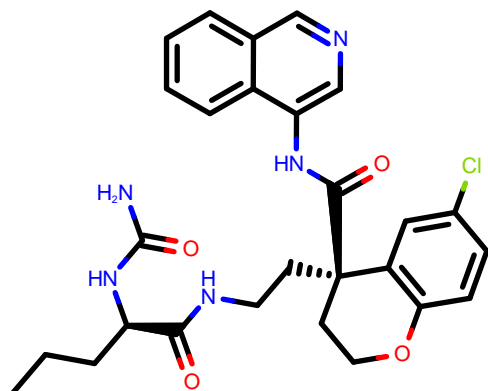
SMILES: Cn1cc(en1)[C@H](C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5o4cccc5)O

RUN: RUN7145

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.29

EN300-102901_3_1_1



CID: EN300-102901_3_1_1

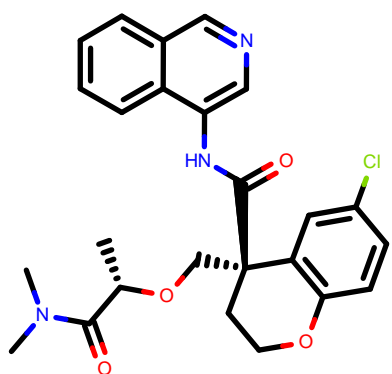
SMILES: CCC[C@H](C(=O)NCC)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N

RUN: RUN4375

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.46

EN300-14458_2_1_1



CID: EN300-14458_2_1_1

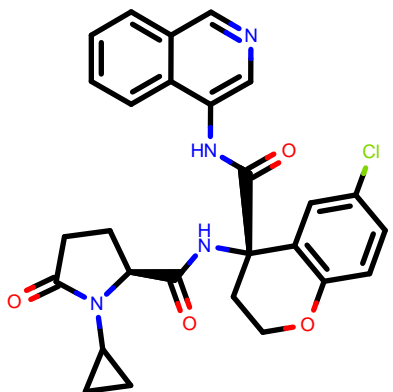
SMILES: C[C@@]([H])(C(=O)N(C)C)OC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN6275

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.25

EN300-3044054_1_1_1



CID: EN300-3044054_1_1_1

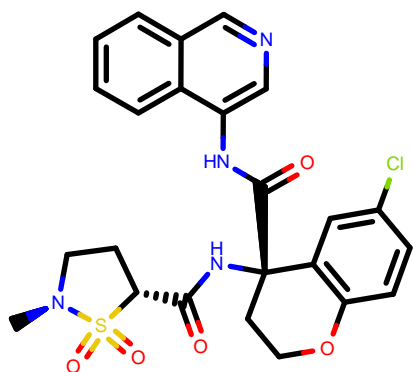
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]([H])5CCCC(=O)N5C6CC6

RUN: RUN7120

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.29

EN300-255496_1_1_1



CID: EN300-255496_1_1_1

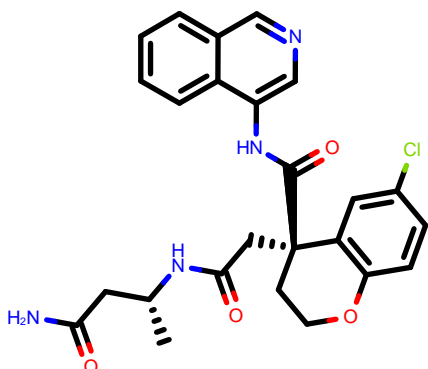
SMILES: C[N@@]1CC[C@@H](S1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4097

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.30

EN300-84785_1_2_1



CID: EN300-84785_1_2_1

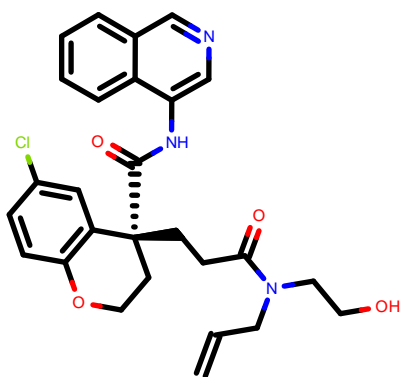
SMILES: C[C@H](CC(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN3093

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.25

EN300-79536_2_1_1



CID: EN300-79536_2_1_1

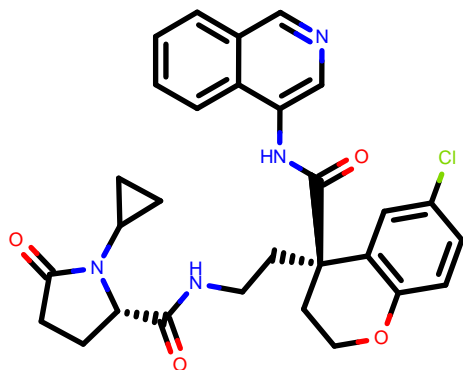
SMILES: C=CCN(CCO)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN6320

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.27

EN300-3044054_3_1_1



CID: EN300-3044054_3_1_1

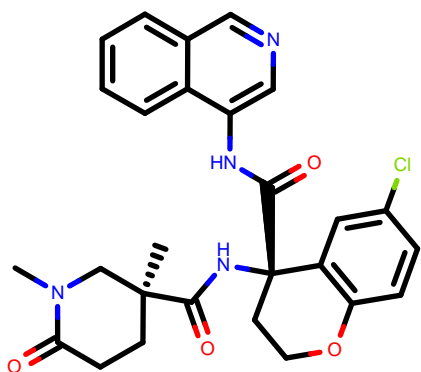
SMILES: c1cc2c(c1)nc2N(C)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(NC1C)C(=O)Nc5ncoc6c5ccoc6

RUN: RUN7060

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.27

EN300-6734171_1_1_1



CID: EN300-6734171_1_1_1

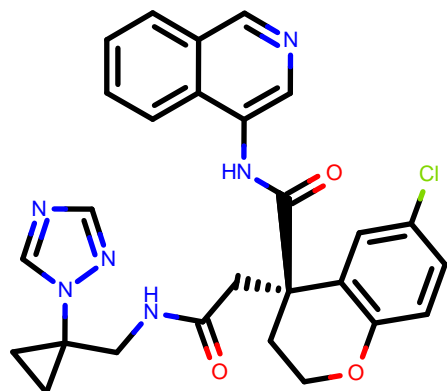
SMILES: C[C@@]1(CCC(=O)N(C)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3675

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.33

EN300-6733137_1_1_1



CID: EN300-6733137_1_1_1

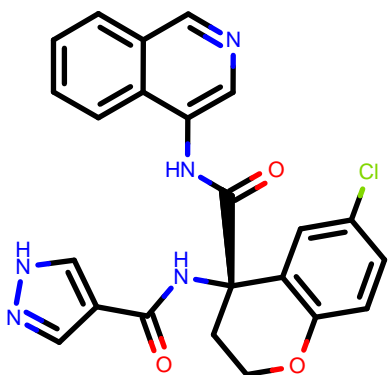
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CC5)n6ncn6

RUN: RUN7313

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.33

EN300-41863_1_1_1



CID: EN300-41863_1_1_1

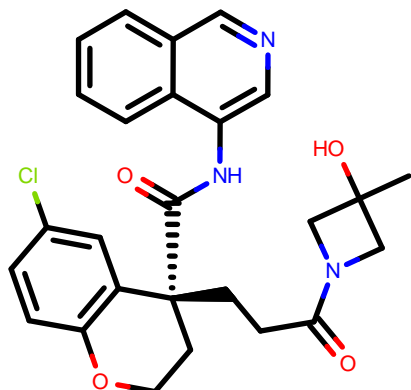
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]nc5

RUN: RUN5935

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.17

EN300-176587_2_1_1



CID: EN300-176587_2_1_1

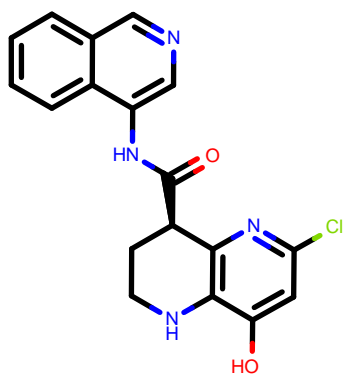
SMILES: CC1(CN(C)C(=O)CC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7765

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.24

BEN-BAS-c2bc0d80-4_1



CID: BEN-BAS-c2bc0d80-4_1

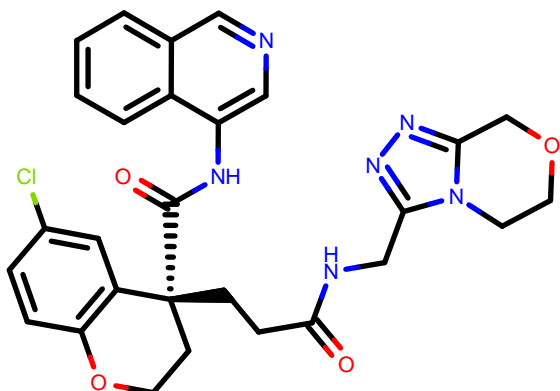
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC=Nc4c3[nH]c(cc4=O)Cl

RUN: RUN1012

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.31

EN300-155447_2_1_1



CID: EN300-155447_2_1_1

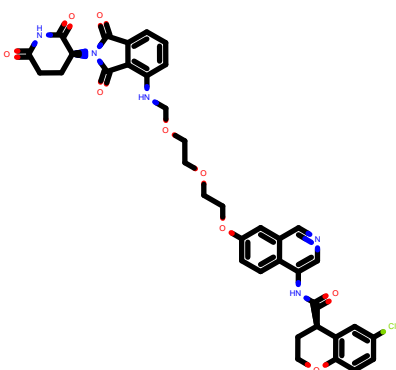
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5nc6n5CCOC6

RUN: RUN6213

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.23

DAR-DIA-9e4459de-11_6



CID: DAR-DIA-9e4459de-11_6

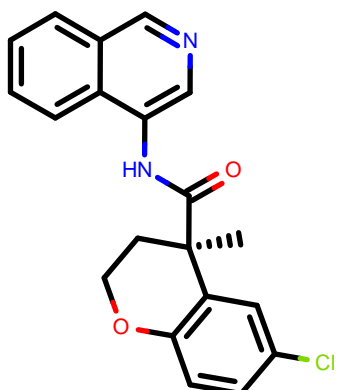
SMILES: c1cc2c(c1)NCOC3CCOC3ccc4c(c3)cncc4NC(=O)[C@@]5(CCOc6c3cc(cc6)Cl)c(n(c2O)[C@@H]7CCCl=O)NC7=O)O

RUN: RUN1390

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.43

DAR-DIA-6a508060-10_2



CID: DAR-DIA-6a508060-10_2

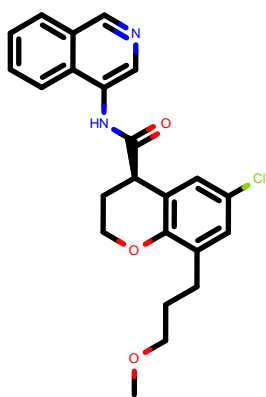
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN294

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.10

LAU-MED-88a3970a-13_1



CID: LAU-MED-88a3970a-13_1

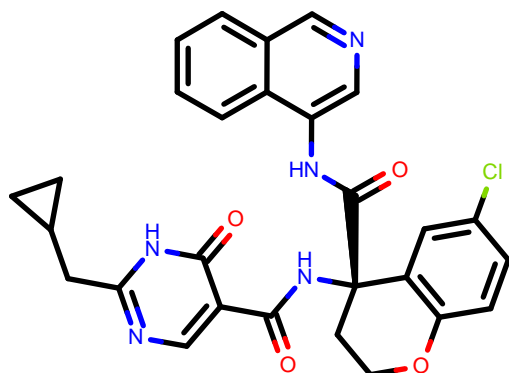
SMILES: COCCc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN1360

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.18

EN300-363154_1_1_1



CID: EN300-363154_1_1_1

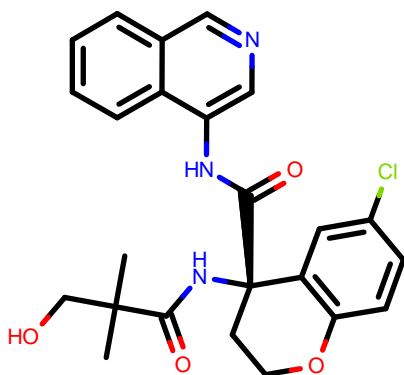
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncn([nH]5=O)C6CC6

RUN: RUN6007

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.42

EN300-65050_1_1_1



CID: EN300-65050_1_1_1

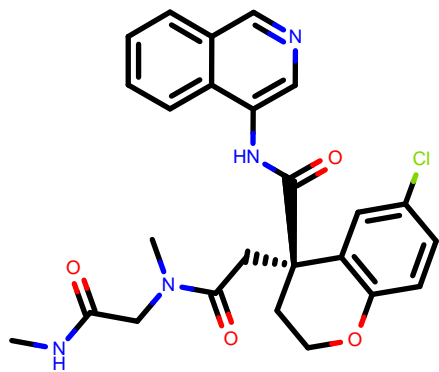
SMILES: CC(C)(CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5003

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.32

EN300-34491_1_1_1



CID: EN300-34491_1_1_1

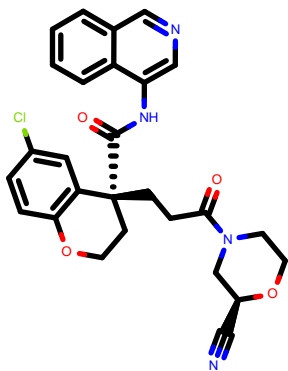
SMILES: CNC(=O)CN(C)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5515

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

EN300-70489_2_2_1



CID: EN300-70489_2_2_1

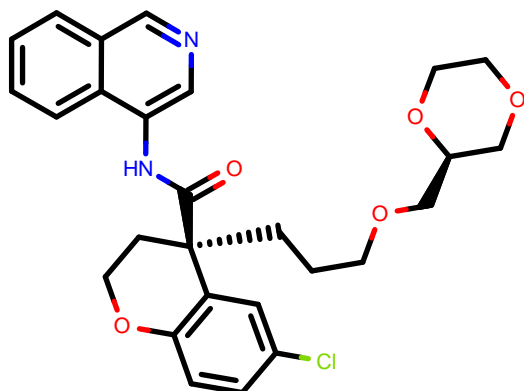
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCO[C@H](C5)C#N

RUN: RUN4993

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.31

EN300-139167_4_1_1



CID: EN300-139167_4_1_1

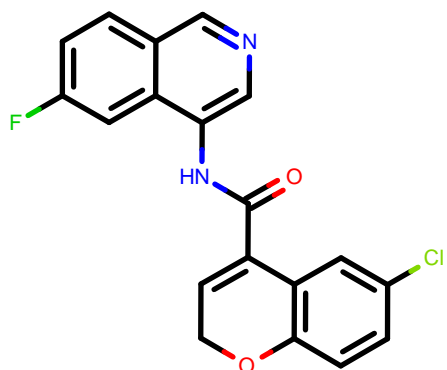
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]4H5COCOC5

RUN: RUN4895

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

ALP-POS-ce760d3f-5_1



CID: ALP-POS-ce760d3f-5_1

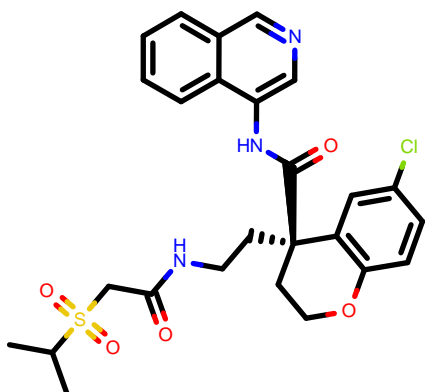
SMILES: c1cc2cncc(c2cc1F)NC(=O)C3=CCOc4c3cc(cc4)Cl

RUN: RUN1279

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.29

EN300-51028_3_1_1



CID: EN300-51028_3_1_1

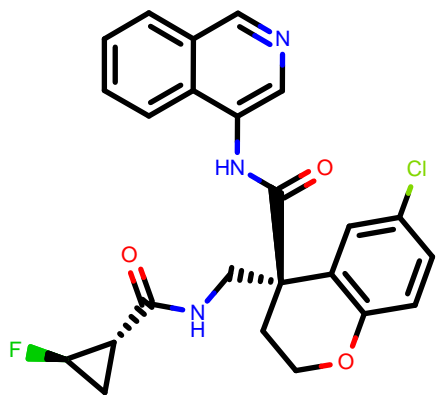
SMILES: CC(C)S(=O)(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN7278

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.34

EN300-97300_2_3_1



CID: EN300-97300_2_3_1

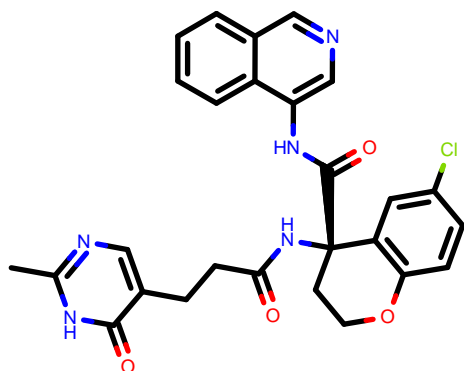
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@@H]5C[C@H]5F

RUN: RUN5268

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.15

EN300-6734334_1_1_1



CID: EN300-6734334_1_1_1

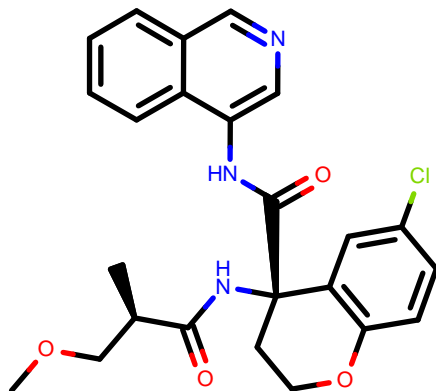
SMILES: Cc1[nH]c(=O)c(en1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN7379

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.23

EN300-69162_1_2_1



CID: EN300-69162_1_2_1

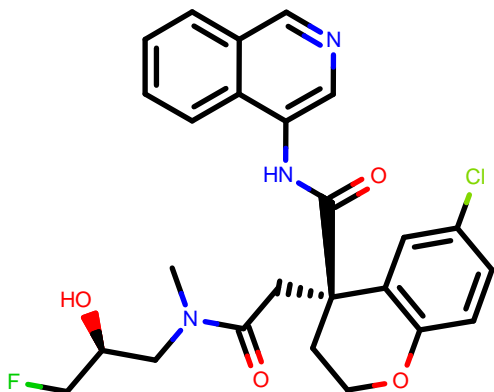
SMILES: C[C@H](COC)C(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN6508

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.22

EN300-1651623_1_1_1



CID: EN300-1651623_1_1_1

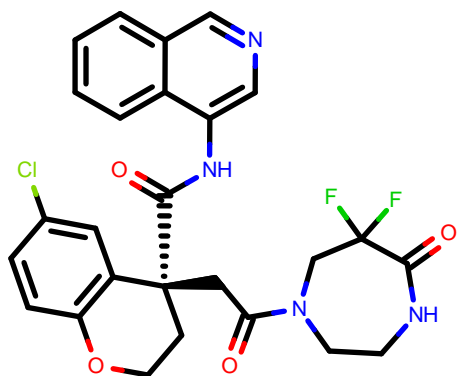
SMILES: CN(C[C@@H](CF)O)C(=O)C[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN7258

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

EN300-1083988_1_1_1



CID: EN300-1083988_1_1_1

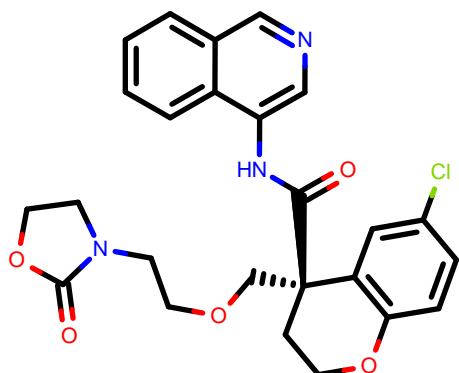
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)C(C5)F)F

RUN: RUN7436

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.30

EN300-370967_2_1_1



CID: EN300-370967_2_1_1

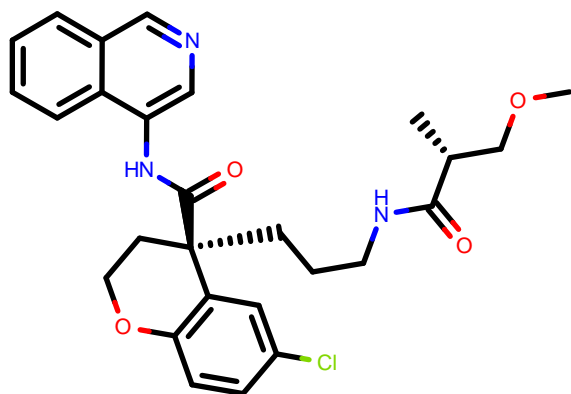
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCOC5=O

RUN: RUN4616

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.28

EN300-69162_4_2_1



CID: EN300-69162_4_2_1

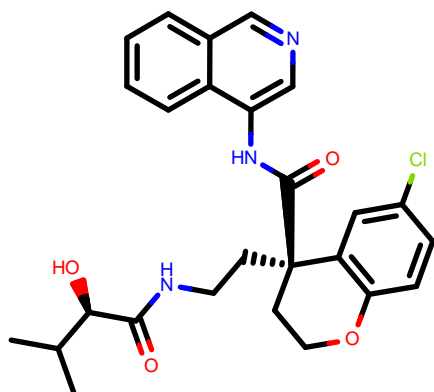
SMILES: C[C@H](COC)C(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN6622

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.31

EN300-115017_3_1_1



CID: EN300-115017_3_1_1

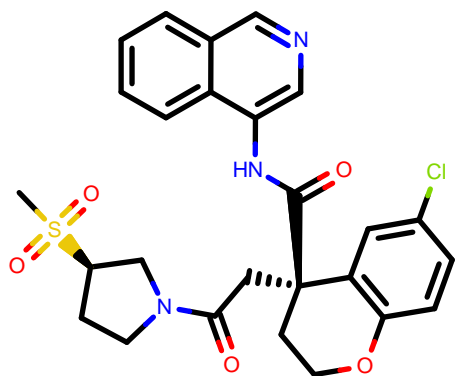
SMILES: CC(C)[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)O

RUN: RUN5824

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

EN300-200609_1_1_1



CID: EN300-200609_1_1_1

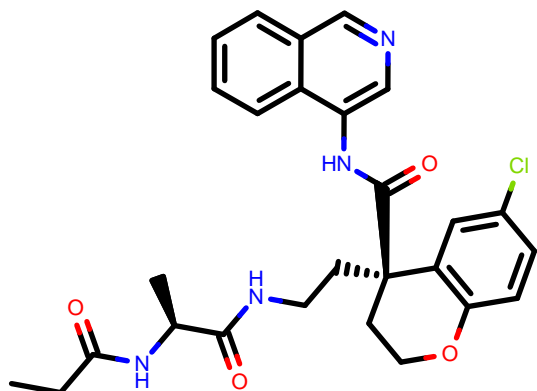
SMILES: CS(=O)(=O)[C@@H]1CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN5910

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.42

EN300-31148_3_1_1



CID: EN300-31148_3_1_1

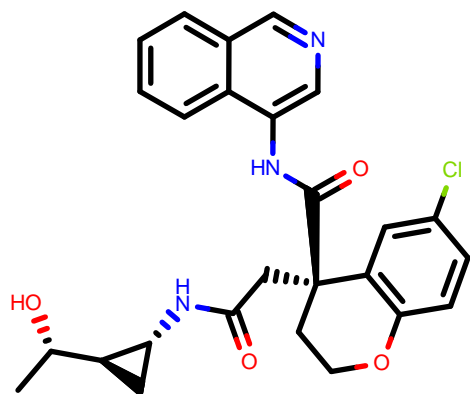
SMILES: CCC(=O)N[C@@H](C)[C@H]1CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5455

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.34

EN300-7463275_1_1_1



CID: EN300-7463275_1_1_1

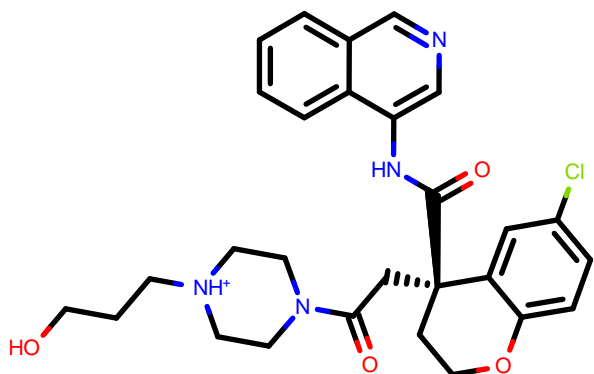
SMILES: C[C@]@@H]([C@@H]1[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN6406

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.25

ALP-UNI-3496895b-8_1



CID: ALP-UNI-3496895b-8_1

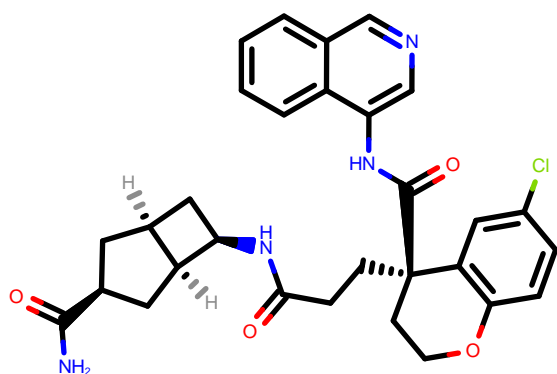
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+]([CC5])CCCO

RUN: RUN2348

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.31

EN300-1268016_2_11_1



CID: EN300-1268016_2_11_1

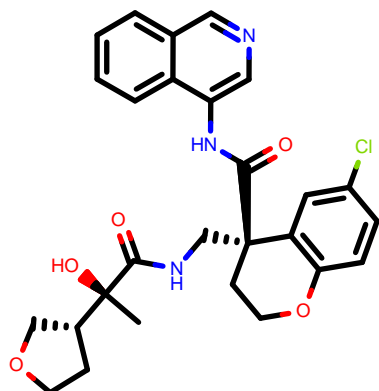
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCCOc4ccc(cc4)C)C(=O)N[C@@H]5C[C@@H]6C[C@@H]5C6Cl=O

RUN: RUN7190

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.35

EN300-217494_2_2_1



CID: EN300-217494_2_2_1

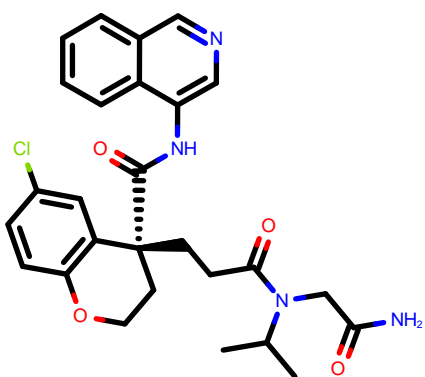
SMILES: CC@@H1CCOC1)(C(=O)N[C@@H]2(CCOc3ccc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN3919

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.33

EN300-35450_2_1_1



CID: EN300-35450_2_1_1

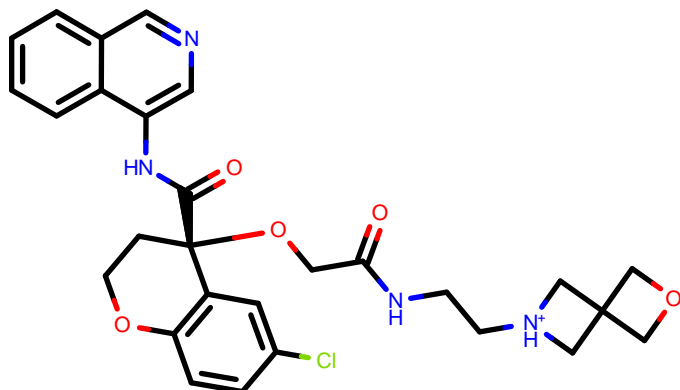
SMILES: CC(C)N(CC(=O)N)C(=O)CC[C@@H]1(CCOc2ccc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5579

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.26

EDG-MED-4c68219f-5_1



CID: EDG-MED-4c68219f-5_1

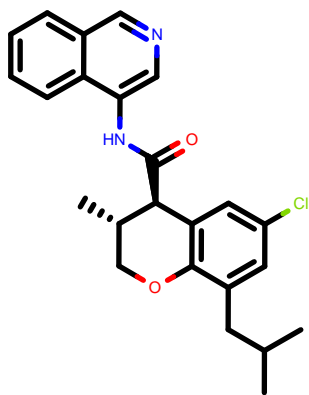
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4ccc(cc4)C)OCC(=O)NCC[NH+]5CC6(C5)COC6

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

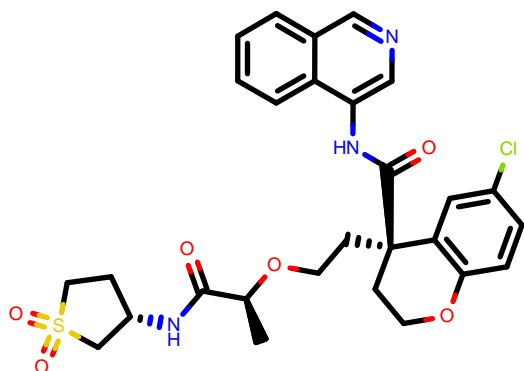
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C)CC(C)C

RUN: RUN7219

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.17

EN300-23318_3_3_1



CID: EN300-23318_3_3_1

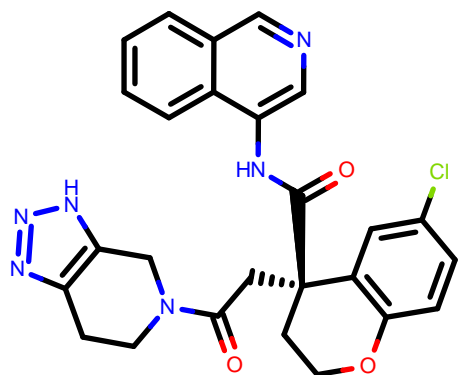
SMILES: C[C@@H](Cl)C(=O)N[C@@H](CCS(=O)(=O)O)C[C@@H]2[C@@H](COc3c2cc(c(c3)C)C)Nc4cncc5c4cccc5

RUN: RUN4433

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.39

EN300-90293_1_1_1



CID: EN300-90293_1_1_1

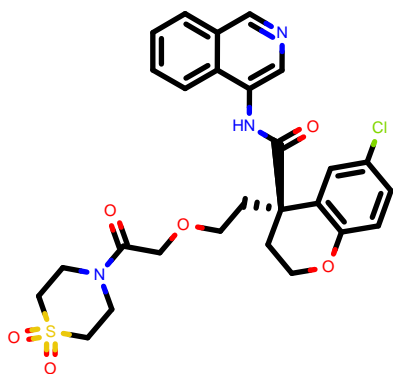
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](COc4c3cc(c(c4)C)C)CC(=O)N5CCc6c(n[nH]6)C5

RUN: RUN4634

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-1265948_3_1_1



CID: EN300-1265948_3_1_1

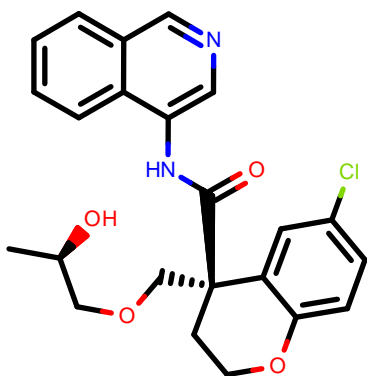
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(c(c4)C)C)COC(=O)N5CCS(=O)(=O)CC5

RUN: RUN3783

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.37

EN300-185378_2_2_1



CID: EN300-185378_2_2_1

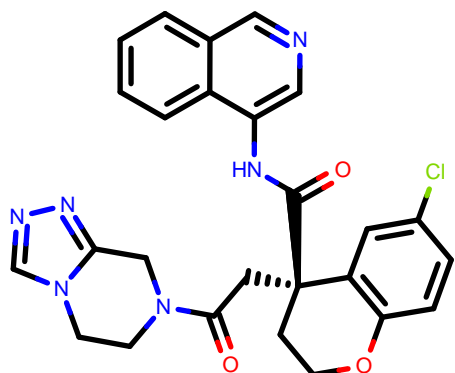
SMILES: C[C@H](COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)O

RUN: RUN4995

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.24

EN300-71125_1_1_1



CID: EN300-71125_1_1_1

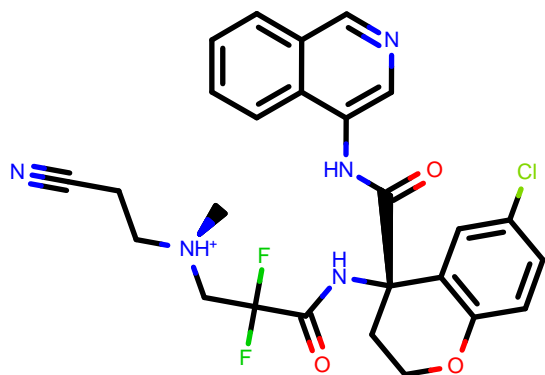
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cn6cnc6C5

RUN: RUN7023

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.31

EDG-MED-90036822-92_2



CID: EDG-MED-90036822-92_2

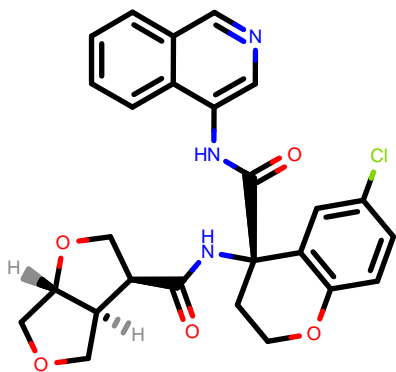
SMILES: C[N+](CCC#N)CC(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)(F)F

RUN: RUN1688

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.30

EN300-6482296_1_1_1



CID: EN300-6482296_1_1_1

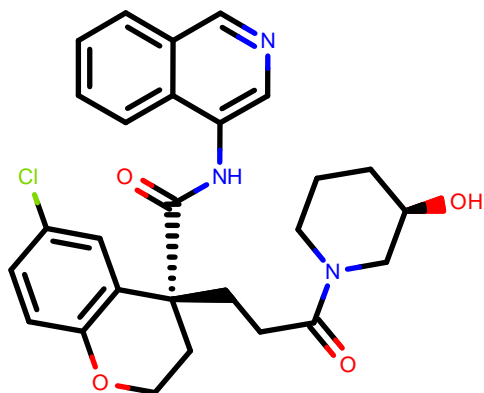
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H5C[C@@]6H5COC6

RUN: RUN7669

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.26

EN300-266117_2_1_1



CID: EN300-266117_2_1_1

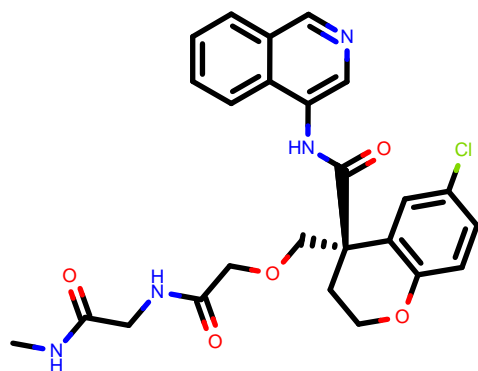
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCC[C@H](C5)O

RUN: RUN5090

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.34

EN300-23223_2_1_1



CID: EN300-23223_2_1_1

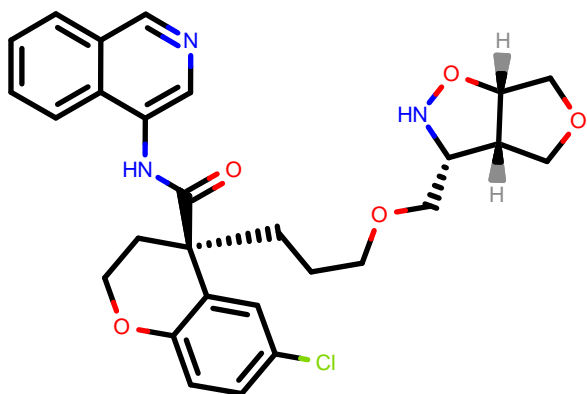
SMILES: CNC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4

RUN: RUN4327

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-7436306_4_1_2



CID: EN300-7436306_4_1_2

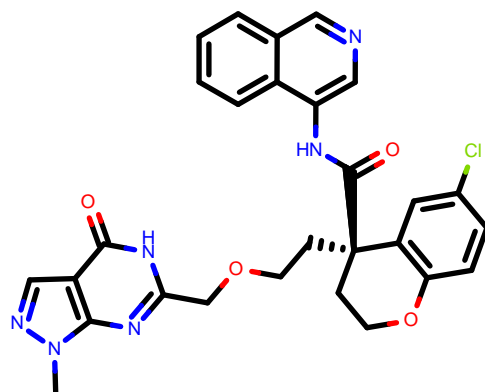
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCOC[C@H]5C@H(C)OCC5

RUN: RUN5462

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.37

EN300-44149_3_1_1



CID: EN300-44149_3_1_1

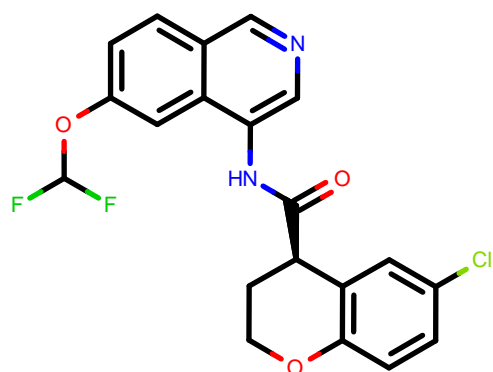
SMILES: Cn1c2c(en1)c(=O)[nH]c(n2)COC[C@]3(CCOc4c3cc(cc4)C)C(=O)Nc5ncoc6c5ccc6

RUN: RUN4772

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.34

BEN-DND-c852c98b-6_1_1



CID: BEN-DND-c852c98b-6_1_1

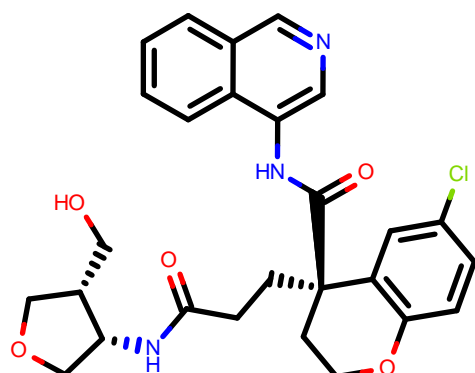
SMILES: c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN7570

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.06

EN300-1663228_2_1_1



CID: EN300-1663228_2_1_1

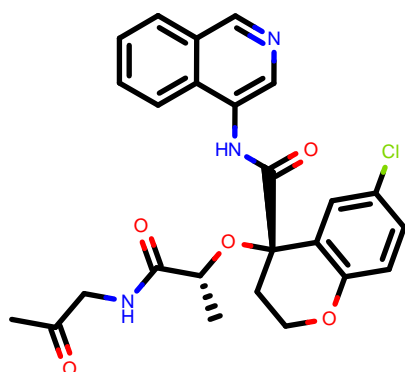
SMILES: c1ccc2c(c1)ncnc2NC(=O)CC[C@@H]3(CCOc4cc(Cl)ccc4O)NC(=O)C[C@@H]5COC[C@H]5CO

RUN: RUN7264

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

EN300-131093_1_2_1



CID: EN300-131093_1_2_1

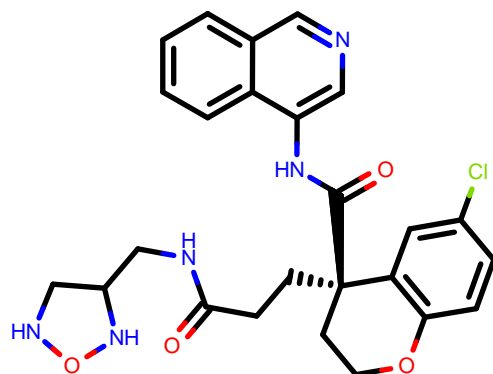
SMILES: CC(=O)CCNC(=O)O[C@@H]1(CCOc2c1cc(Cl)cc2)C(=O)Nc3nccc4c3ccc4

RUN: RUN5340

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

EN300-1068239_2_1_1



CID: EN300-1068239_2_1_1

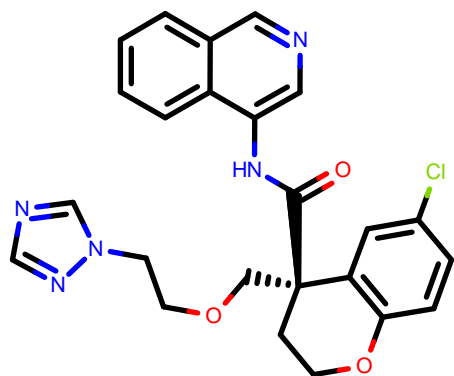
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(Cl)ccc4O)NC(=O)Nc5non5

RUN: RUN7020

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.26

EN300-6255179_2_1_1



CID: EN300-6255179_2_1_1

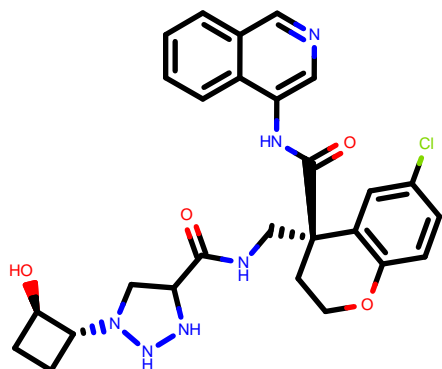
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cncn5

RUN: RUN6440

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.24

EN300-316196_2_1_1



CID: EN300-316196_2_1_1

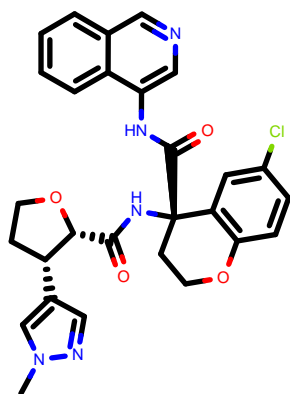
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncn5[C@@]6H9CC[C@]6H9O

RUN: RUN7221

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.35

EN300-305454_1_1_1



CID: EN300-305454_1_1_1

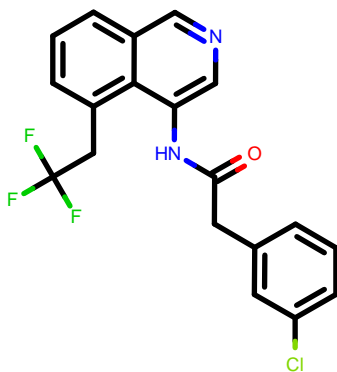
SMILES: Cn1cc(en1)[C@@]2H9CC[C@]2H9[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncn5

RUN: RUN3882

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

JOH-UNI-ee5ed7c8-3_1



CID: JOH-UNI-ee5ed7c8-3_1

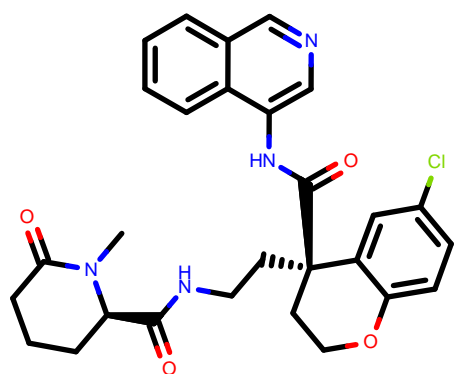
SMILES: c1cc(cc(c1)Cl)CC(=O)Nc2cnc3c2c(ccc3)CC(F)(F)F

RUN: RUN1727

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.25

EN300-325738_3_2_1



CID: EN300-325738_3_2_1

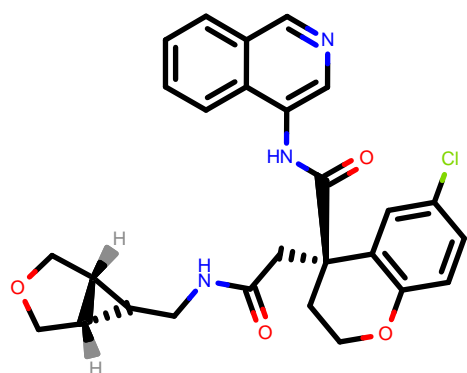
SMILES: CN1C@H](CCCC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN4708

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

EN300-210089_1_1_1



CID: EN300-210089_1_1_1

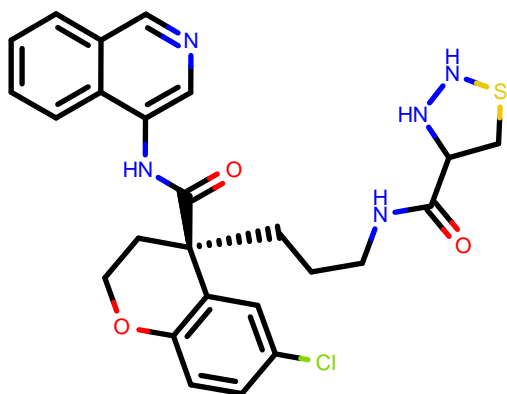
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)NCC5[C@@H]6[C@@H]5COc6

RUN: RUN7367

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-24297_4_1_1



CID: EN300-24297_4_1_1

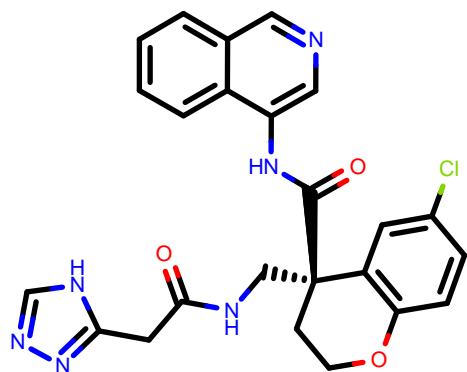
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCCNC(=O)c5csnns5

RUN: RUN3680

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.37

EN300-96159_2_1_1



CID: EN300-96159_2_1_1

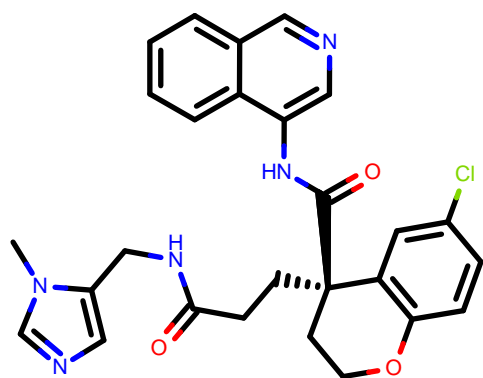
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)Cc5[nH]nns5

RUN: RUN7660

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-216594_2_1_1



CID: EN300-216594_2_1_1

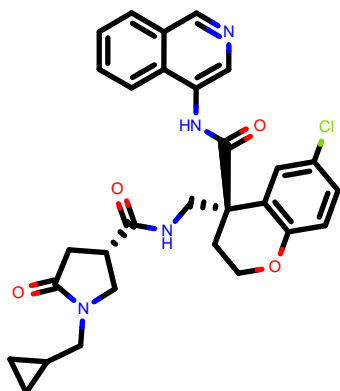
SMILES: Cn1cncc1CNC(=O)CC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6648

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-31969_2_2_1



CID: EN300-31969_2_2_1

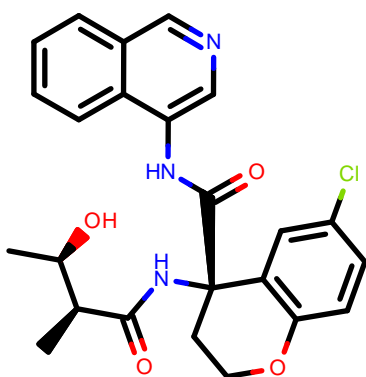
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(COCOC4c3cc(c4)Cl)CNC(=O)[C@@H]5CC1=O[N]C5)COC6C6

RUN: RUN7192

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.31

EN300-7089802_1_1_1



CID: EN300-7089802_1_1_1

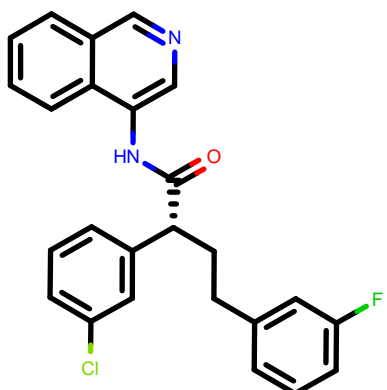
SMILES: C[C@@H]([C@@H](C)O)C(=O)N[C@@]1(COCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5097

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.28

MIC-UNK-c66144cb-1_2



CID: MIC-UNK-c66144cb-1_2

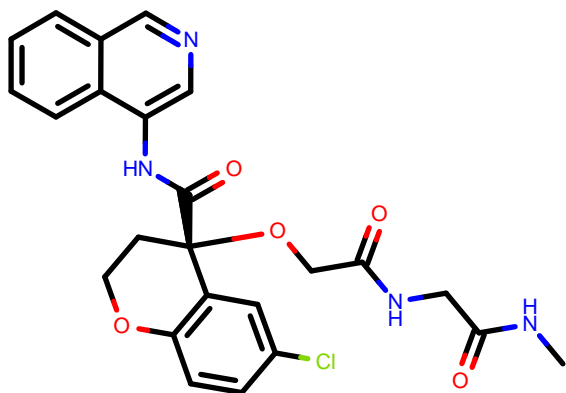
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](CCc3cccc(c3)F)c4cccc(c4)Cl

RUN: RUN122

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.31

EN300-23223_1_1_1



CID: EN300-23223_1_1_1

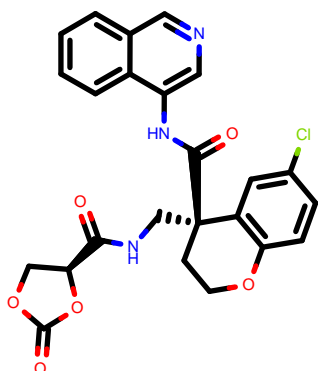
SMILES: CNC(=O)CNC(=O)CO[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4

RUN: RUN5079

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.25

EN300-5253939_2_1_1



CID: EN300-5253939_2_1_1

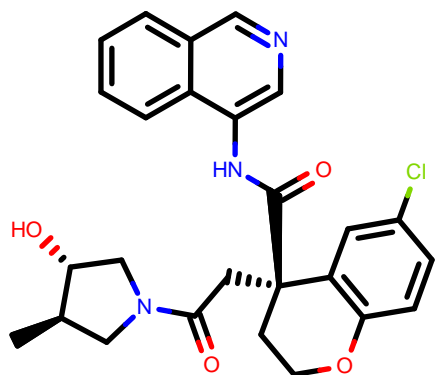
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5OC(=O)O5

RUN: RUN4222

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.26

EN300-6497226_1_1_1



CID: EN300-6497226_1_1_1

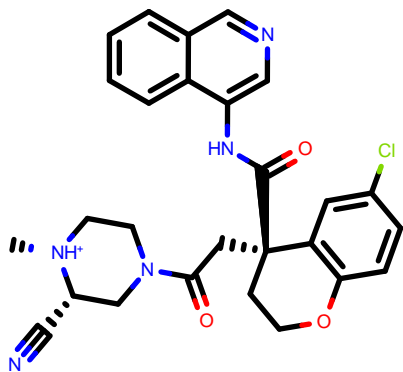
SMILES: C[C@@H]1CN(C[C@H]1O)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN7026

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.20

EDG-MED-ba1ac7b9-14_5



CID: EDG-MED-ba1ac7b9-14_5

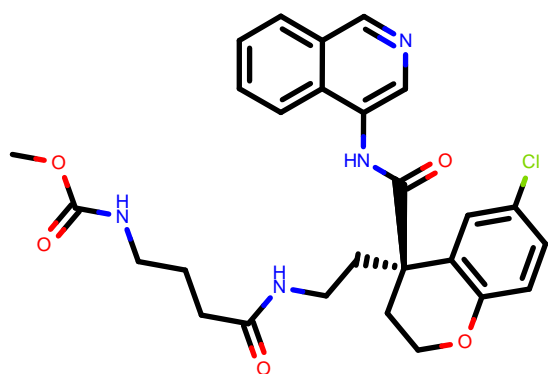
SMILES: C[N@@]1CCN(C[C@@H]1C#N)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5

RUN: RUN2506

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-71560_3_1_1



CID: EN300-71560_3_1_1

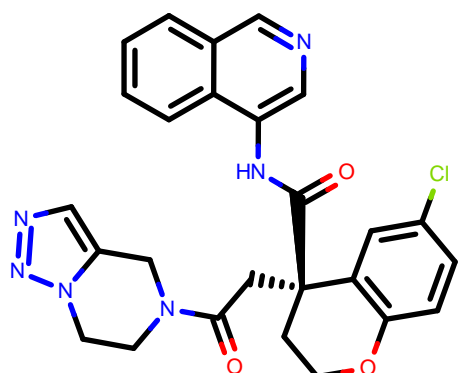
SMILES: COC(=O)NCCCC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccoc4

RUN: RUN5496

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.37

EN300-29228_1_1_1



CID: EN300-29228_1_1_1

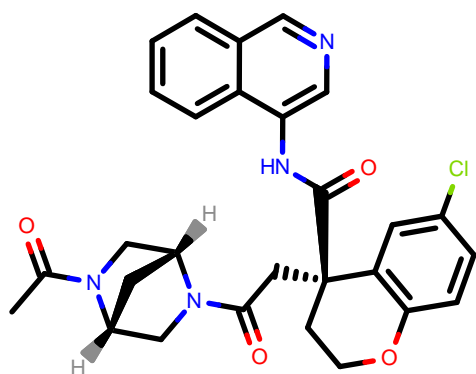
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CNC6c(cnn6)C5

RUN: RUN6205

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.29

ALP-UNI-76695c4f-6_1



CID: ALP-UNI-76695c4f-6_1

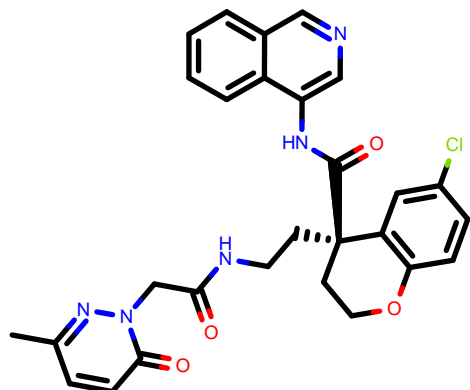
SMILES: CC(=O)N1C[C@@H]2[C@@H]1CN2C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccoc6

RUN: RUN2061

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.25

EN300-69556_3_1_1



CID: EN300-69556_3_1_1

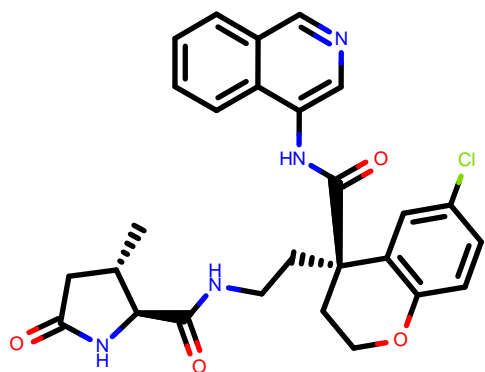
SMILES: Cc1ccc(=O)n(n1)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccoc5

RUN: RUN5138

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.38

EN300-155362_3_2_1



CID: EN300-155362_3_2_1

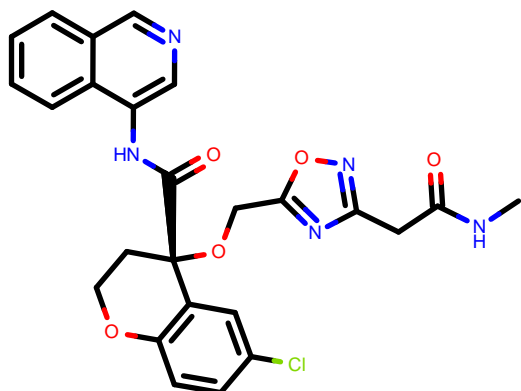
SMILES: C[C@H]1CC(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7769

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.30

EN300-99983_1_1_1



CID: EN300-99983_1_1_1

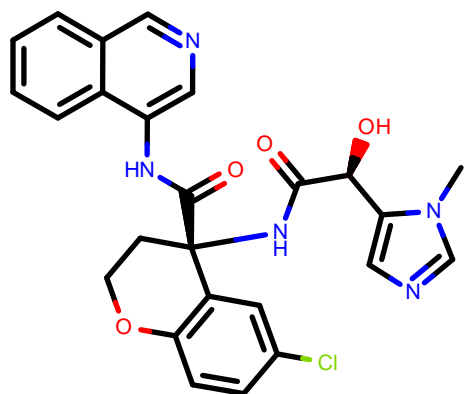
SMILES: CNC(=O)Cc1nc(on1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3644

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-190283_1_1_1



CID: EN300-190283_1_1_1

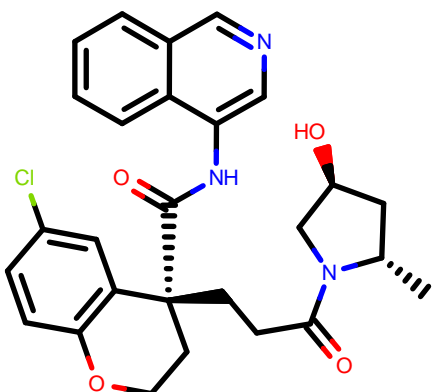
SMILES: Cn1cnc1[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7787

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.39

EN300-173562_2_2_1



CID: EN300-173562_2_2_1

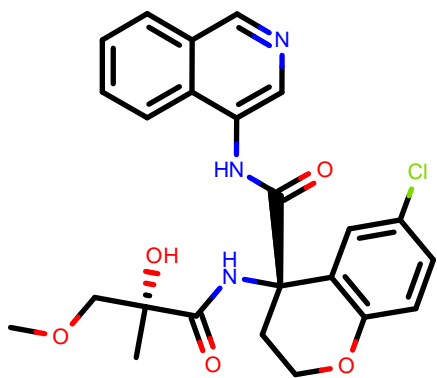
SMILES: C[C@H]1C[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7312

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.26

EN300-76841_1_1_1



CID: EN300-76841_1_1_1

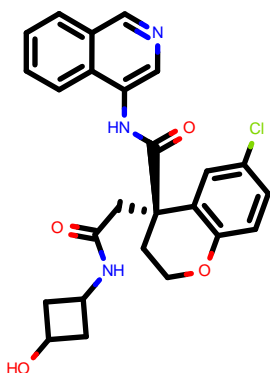
SMILES: C[C@@](COC)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4)O

RUN: RUN4164

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.31

EN300-100583_1_1_1



CID: EN300-100583_1_1_1

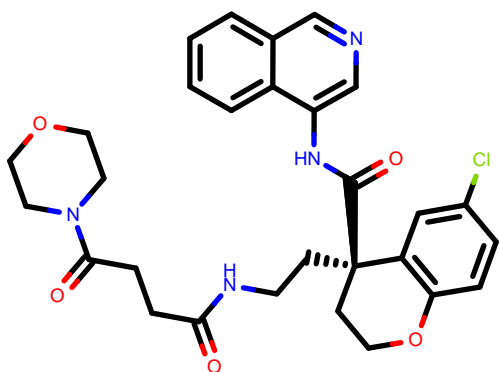
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CC(=O)NC5CC(C5)O

RUN: RUN4885

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.23

EN300-05277_3_1_1



CID: EN300-05277_3_1_1

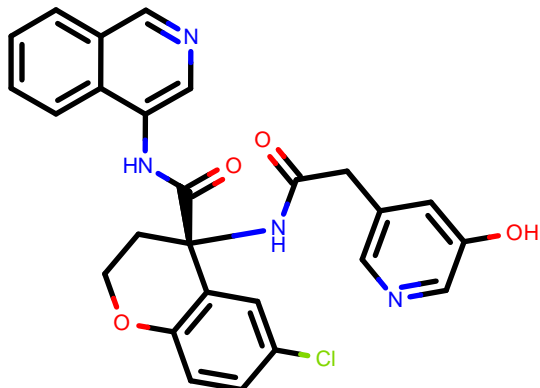
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCC(=O)N5CCOC5

RUN: RUN5856

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-222620_1_1_1



CID: EN300-222620_1_1_1

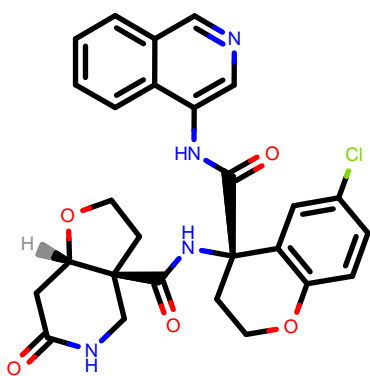
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccncc5)O

RUN: RUN3814

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.27

EN300-6731226_1_1_1



CID: EN300-6731226_1_1_1

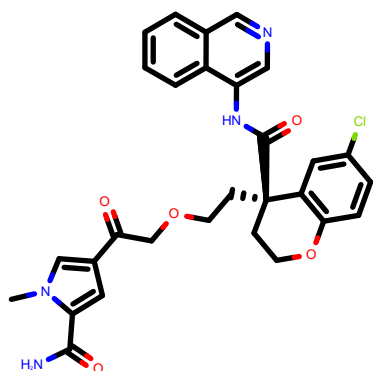
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCO4C3cc(c4)C)NC(=O)[C@@H]5C[C@@H](H)SCC(=O)N6

RUN: RUN4194

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.41

EN300-35592_3_1_1



CID: EN300-35592_3_1_1

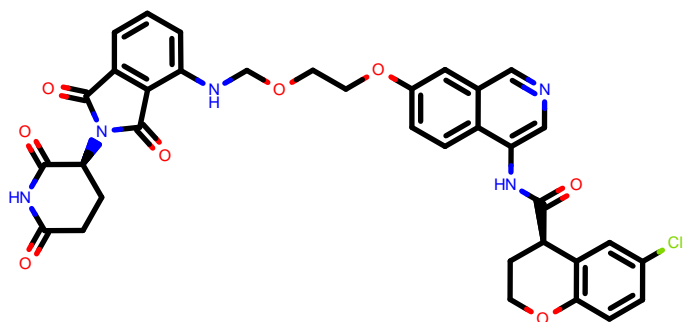
SMILES: Cn1cc(cc1C(=O)N)C(=O)COCC[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4cccc5c4cccc5

RUN: RUN6956

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.25

DAR-DIA-9e4459de-13_6



CID: DAR-DIA-9e4459de-13_6

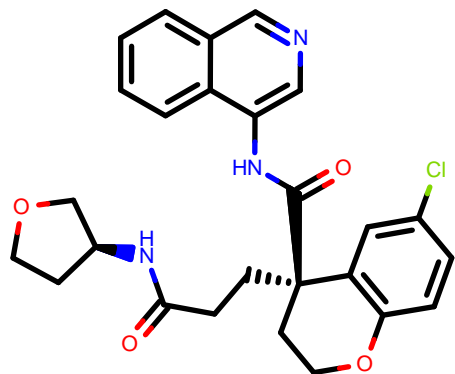
SMILES: c1cc2c(c1)NC(=O)C3=CC=CC=C3C(=O)N[C@@H]4[C@@H](CCO5C4cc(c5)C)C(=O)Nc6cccc7c6cccc7

RUN: RUN1332

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.46

EN300-171752_2_2_1



CID: EN300-171752_2_2_1

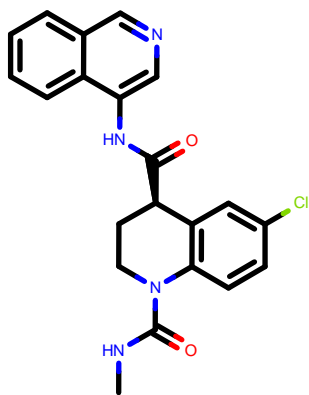
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCO4C3cc(c4)C)C(=O)N[C@@H]5CCOC5

RUN: RUN7456

DDG (kcal/mol): -0.43

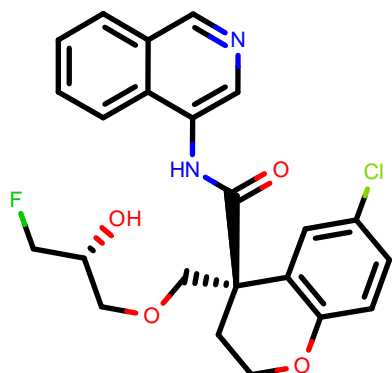
dDDG (kcal/mol): 0.29

RAL-THA-4aa06b95-3_2



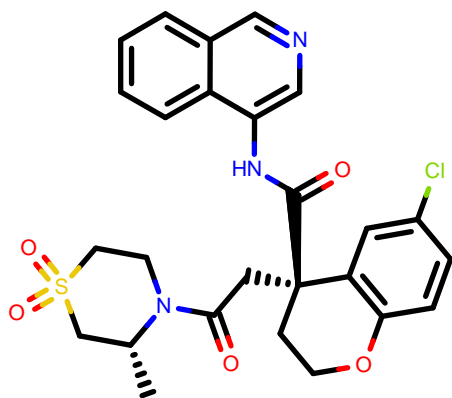
CID:	RAL-THA-4aa06b95-3_2
SMILES:	<chem>CNC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN1123
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.28

EN300-1968342_2_2_1



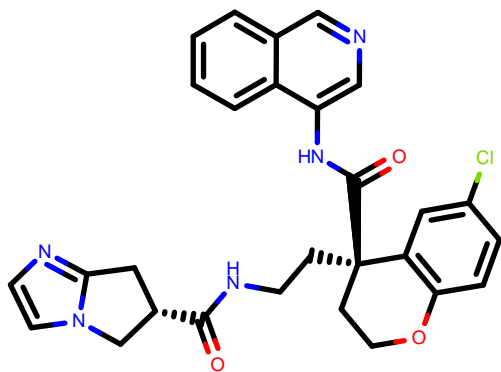
CID:	EN300-1968342_2_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O</chem>
RUN:	RUN4289
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.28

EN300-171215_1_1_1



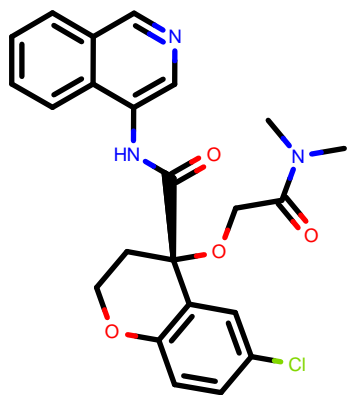
CID:	EN300-171215_1_1_1
SMILES:	<chem>C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN5445
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.26

KAD-UNI-8a629cb0-12_1



CID:	KAD-UNI-8a629cb0-12_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5Cn6[nH+]cn6C5</chem>
RUN:	RUN1996
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.38

EN300-216063_1_1_1



CID: EN300-216063_1_1_1

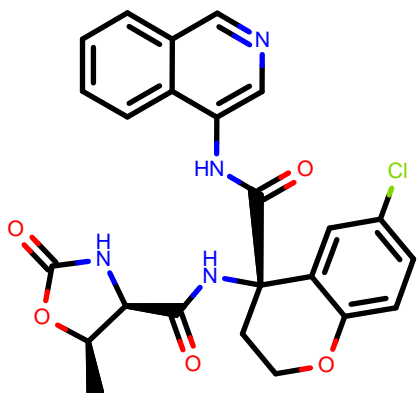
SMILES: CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5519

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.22

EN300-172640_1_1_1



CID: EN300-172640_1_1_1

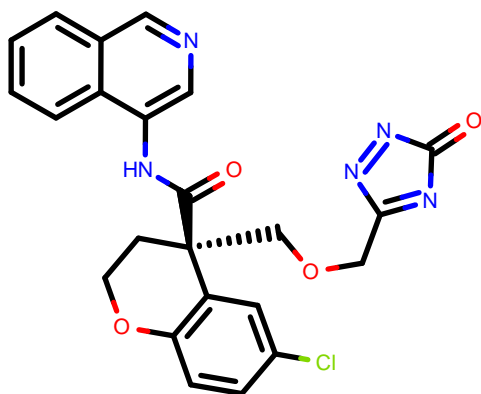
SMILES: C[C@@H]1[C@@H](NC(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4373

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EDJ-MED-fcba3f31-10_1



CID: EDJ-MED-fcba3f31-10_1

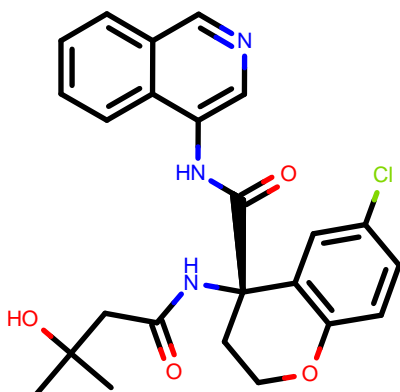
SMILES: c1ccc2c(c1)ncnc2N[C(=O)]C@@3(CCOc4c3cc(cc4)Cl)COCc5[nH]c(=O)[nH]n5

RUN: RUN2350

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.22

EN300-117931_1_1_1



CID: EN300-117931_1_1_1

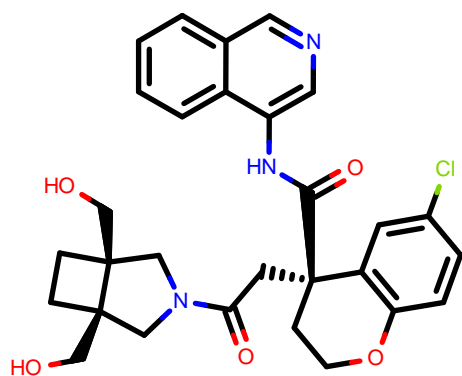
SMILES: CC(C)(CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN5137

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.24

EN300-1272865_1_1_1



CID: EN300-1272865_1_1_1

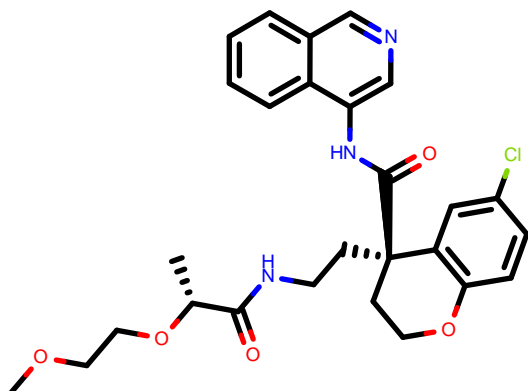
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(C)C(=O)N5C[C@@]6(C)C[C@@]7(C)C5(C)CO

RUN: RUN4607

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.34

EN300-77359_3_2_1



CID: EN300-77359_3_2_1

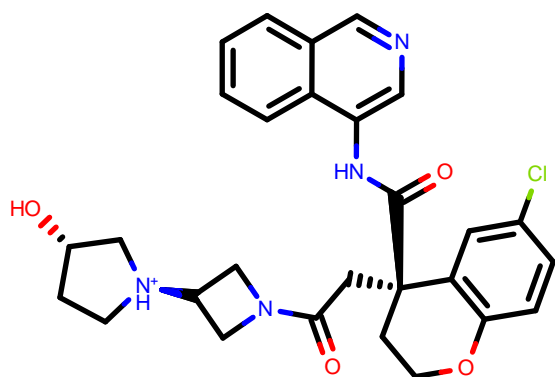
SMILES: C[C@H](C(=O)NCC[C@@]1(C)CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3ccc4)OCCOC

RUN: RUN3800

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.27

EDG-MED-ba1ac7b9-4_3



CID: EDG-MED-ba1ac7b9-4_3

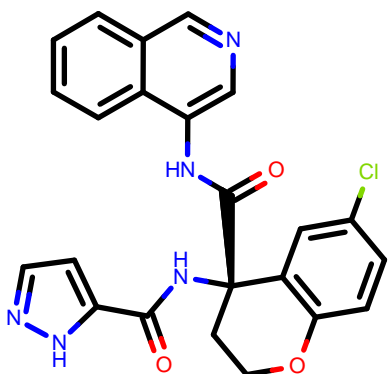
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C(C)C(=O)N5C(C)C5(N)H+8CC[C@@]6(C)C@H]C6)O

RUN: RUN2479

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.39

EN300-37077_1_1_1



CID: EN300-37077_1_1_1

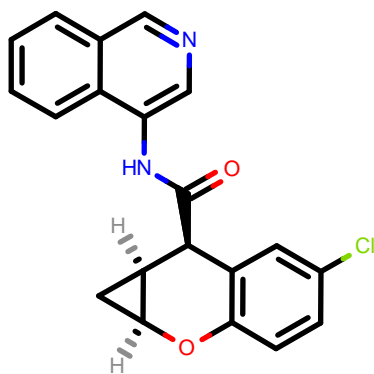
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)c5cc[nH]5

RUN: RUN6229

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.20

DAR-DIA-0d514e7d-33_3



CID: DAR-DIA-0d514e7d-33_3

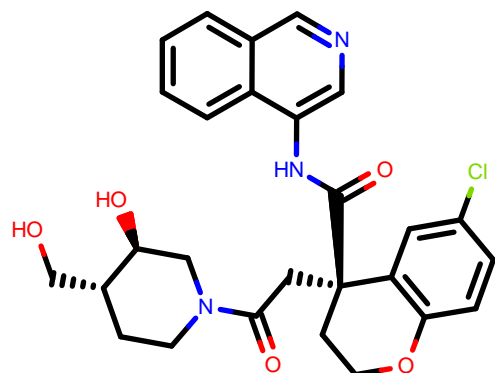
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4O)[C@@H]5[C@H]3C5)Cl

RUN: RUN809

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.22

EN300-95639_1_3_1



CID: EN300-95639_1_3_1

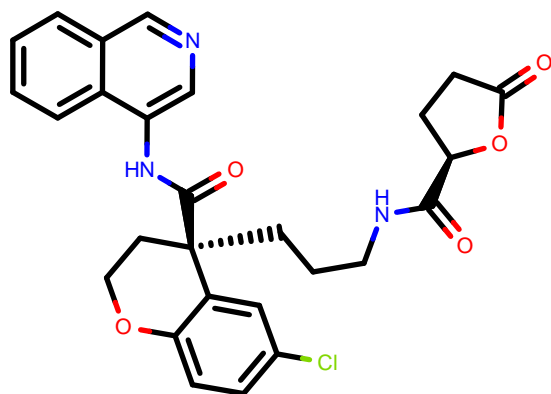
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@]4(O)C(O)C(O)C(C1=O)N5CC[C@@H]3[C@H]5)O)CO

RUN: RUN6108

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.39

EN300-332606_4_1_1



CID: EN300-332606_4_1_1

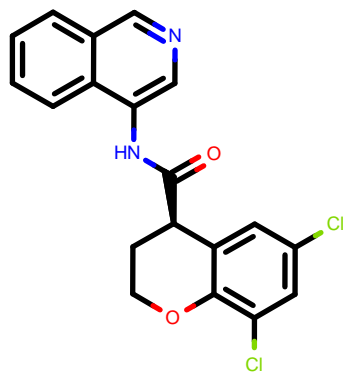
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@]4(O)C(O)C(O)C(C1=O)N5CC[C@@H]3[C@H]5)O)O5

RUN: RUN6368

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.34

RAL-THA-05e671eb-16_1



CID: RAL-THA-05e671eb-16_1

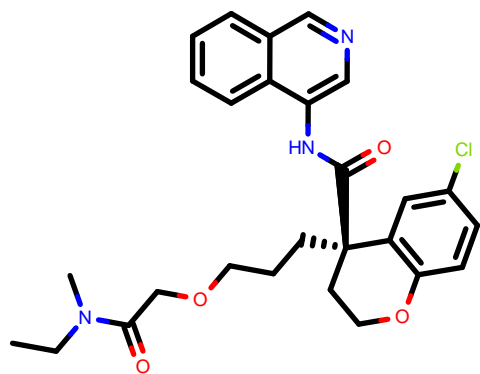
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4Cl)Cl

RUN: RUN1894

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.08

EN300-1253122_4_1_1



CID: EN300-1253122_4_1_1

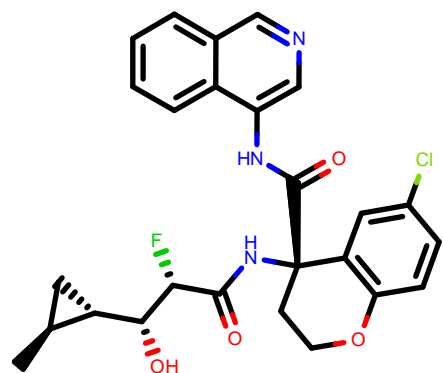
SMILES: CCN(C)C(=O)COC[C@@]1(C)C(=O)C2=CC(=O)C=C2C1C(=O)Nc3cnc4c3ccc4

RUN: RUN7450

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EDG-MED-90036822-94_6



CID: EDG-MED-90036822-94_6

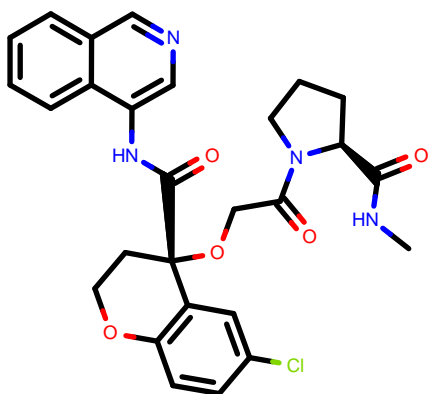
SMILES: C[C@@H](C)C(F)C(O)C(=O)N[C@@]1(C)C(=O)Nc2cnc3c2ccc3F

RUN: RUN1674

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.28

EN300-48902_1_1_1



CID: EN300-48902_1_1_1

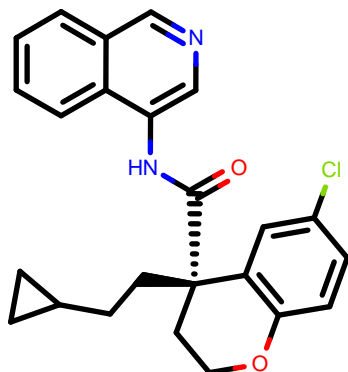
SMILES: CNC(=O)[C@@]1(C)C(=O)Nc2cnc3c2ccc3C1C(=O)O[C@@]2(C)C(=O)C3=CC(=O)C=C3

RUN: RUN5568

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.34

ALP-POS-477dc5b7-3_2_1



CID: ALP-POS-477dc5b7-3_2_1

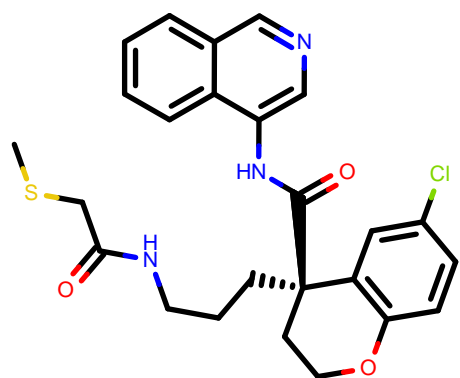
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]1(C)C(=O)Nc3cnc4c3ccc4

RUN: RUN6547

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.32

EN300-07879_4_1_1



CID: EN300-07879_4_1_1

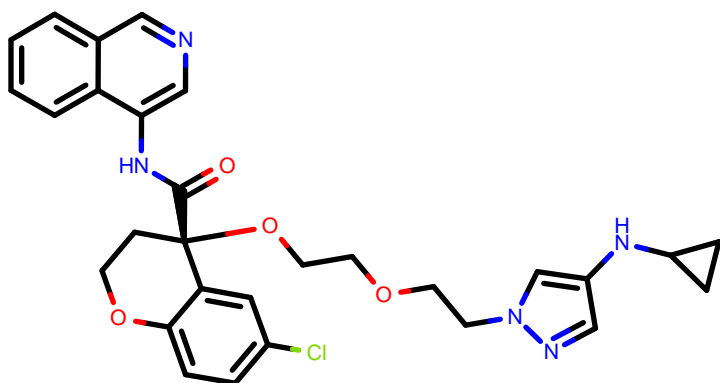
SMILES: CSCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN6332

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

ED_-GRI-5b13fbe2-75_1



CID: ED_-GRI-5b13fbe2-75_1

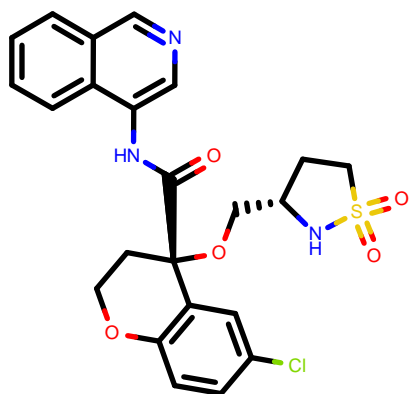
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCc5ccn5NC6CC6

RUN: RUN1529

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.31

EN300-1699871_1_1_1



CID: EN300-1699871_1_1_1

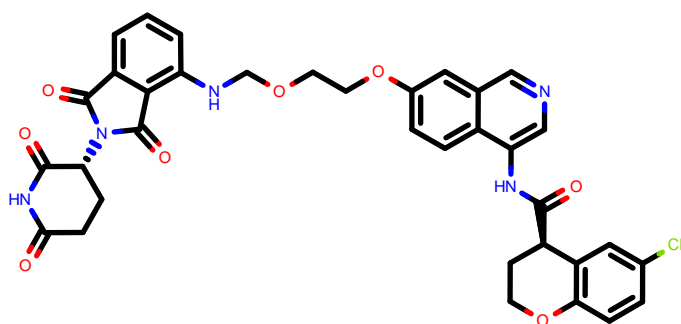
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5(S(=O)(=O)N)N5

RUN: RUN6582

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.26

DAR-DIA-9e4459de-13_3



CID: DAR-DIA-9e4459de-13_3

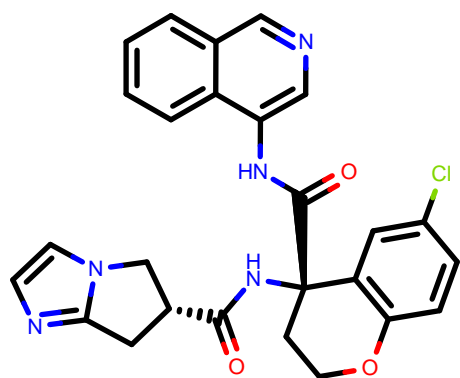
SMILES: c1cc2c(c1)NC(=O)OCC3C(=O)N(C3)C(=O)Nc4ccc5c4ccn5C(=O)Nc6ccc7c6ccn7

RUN: RUN1340

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.36

EN300-7385329_1_1_1



CID: EN300-7385329_1_1_1

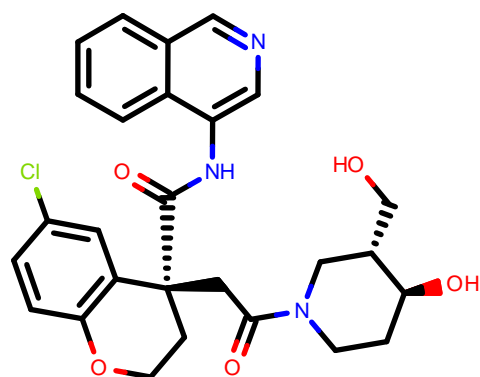
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C6c[nH]c[n+]6C5

RUN: RUN3802

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.23

EN300-233678_1_3_1



CID: EN300-233678_1_3_1

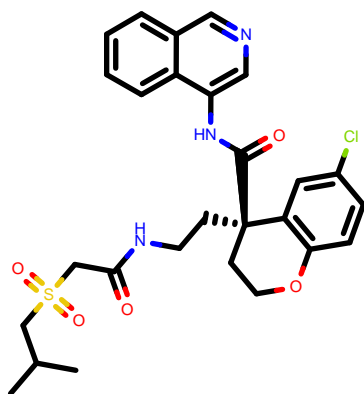
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N5CC(O)C@H]C@H]5CO5

RUN: RUN5454

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

EN300-42243_3_1_1



CID: EN300-42243_3_1_1

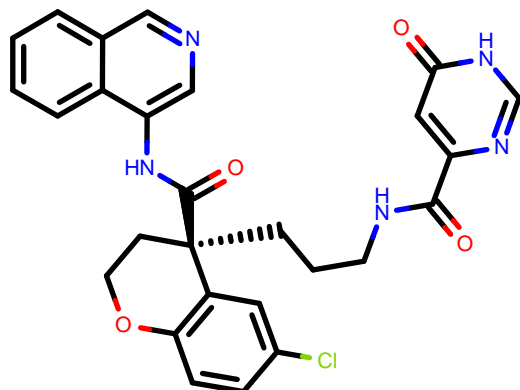
SMILES: CC(C)CS(=O)(=O)CC(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5356

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.43

EN300-817811_4_1_1



CID: EN300-817811_4_1_1

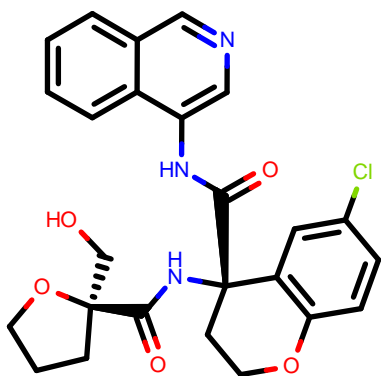
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc(=O)[nH]c[n5]

RUN: RUN7293

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.26

EN300-1425677_1_2_1



CID: EN300-1425677_1_2_1

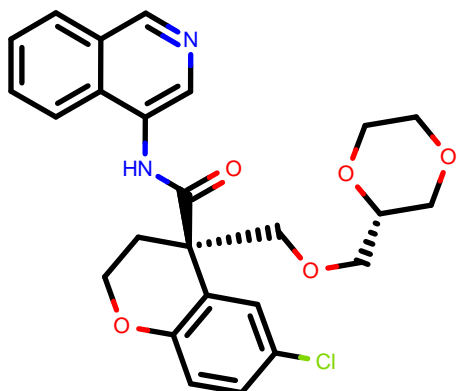
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@]5(CCCO5)CO

RUN: RUN5695

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.31

EN300-139167_2_2_1



CID: EN300-139167_2_2_1

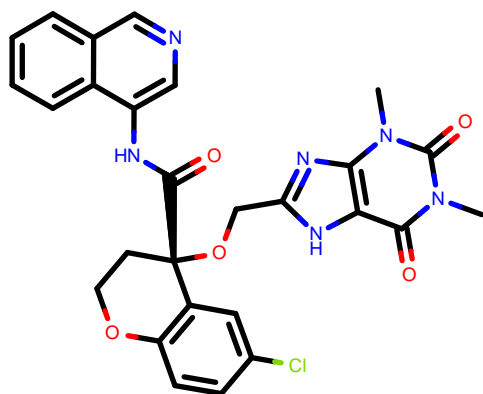
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@]5H5COCCO5

RUN: RUN4396

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

EN300-31037_1_1_1



CID: EN300-31037_1_1_1

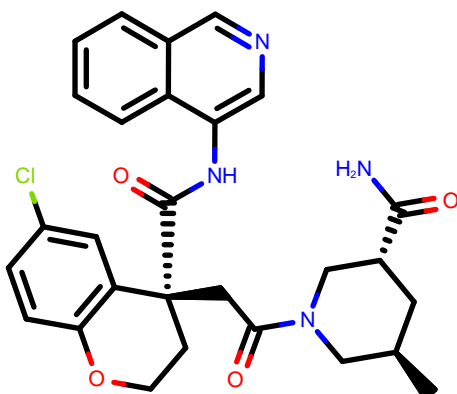
SMILES: Cn1c2c(c(=O)n(c1=O)C)[nH]c(n2)COC[C@@]3(CCOc4c3cc(cc4)C)C(=O)Nc5nc6c5ccc6

RUN: RUN6632

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.29

EN300-1724086_1_3_1



CID: EN300-1724086_1_3_1

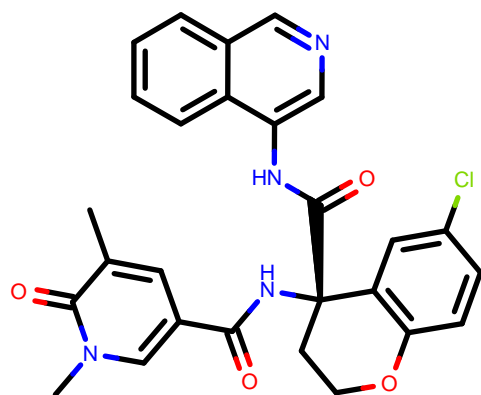
SMILES: C[C@]1(C[C@H]1)CNC(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nc5c4cccc5Cl=ON

RUN: RUN2917

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.34

EN300-1703340_1_1_1



CID: EN300-1703340_1_1_1

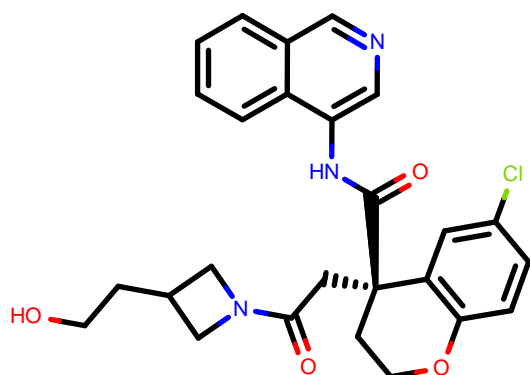
SMILES: Cc1ccn(c1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccoc5

RUN: RUN5653

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.32

EN300-7413100_1_1_1



CID: EN300-7413100_1_1_1

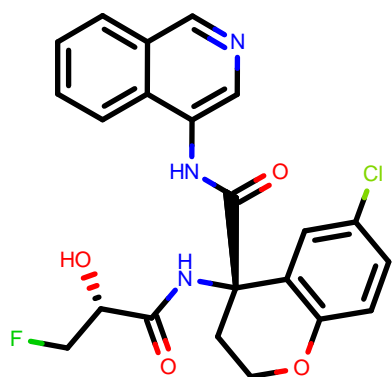
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CCO

RUN: RUN5199

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.26

EDG-MED-90036822-17_2



CID: EDG-MED-90036822-17_2

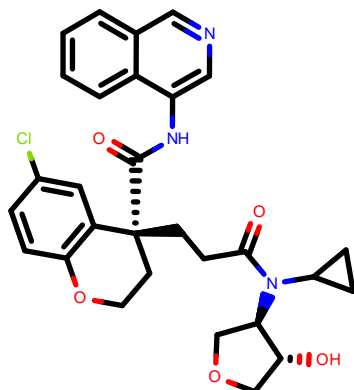
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](CF)O

RUN: RUN1521

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.29

EN300-1214616_2_1_1



CID: EN300-1214616_2_1_1

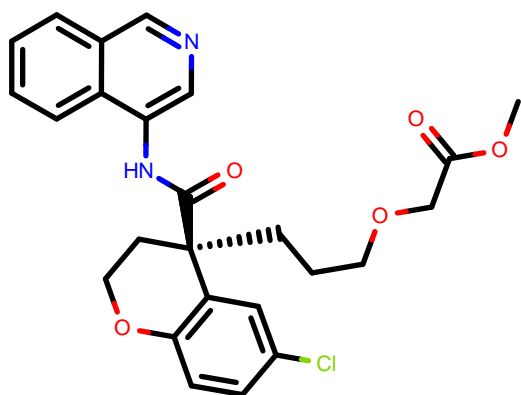
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4(C)CCO[C@H]5COCC[C@H]5O

RUN: RUN6190

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.23

EN300-19700_4_1_1



CID: EN300-19700_4_1_1

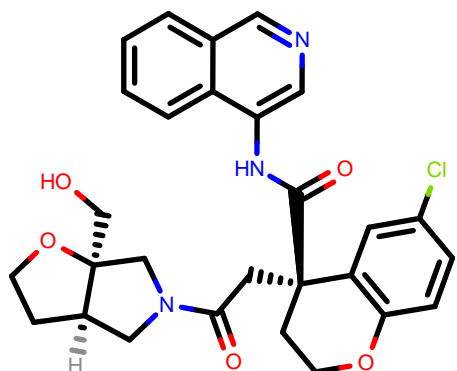
SMILES: COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN4379

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.35

EN300-7466671_1_1_1



CID: EN300-7466671_1_1_1

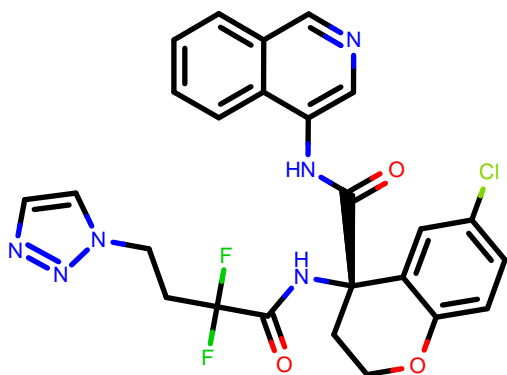
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5[C@@H]6CCO[C@]6(C)C5

RUN: RUN7486

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.35

EN300-6474220_1_1_1



CID: EN300-6474220_1_1_1

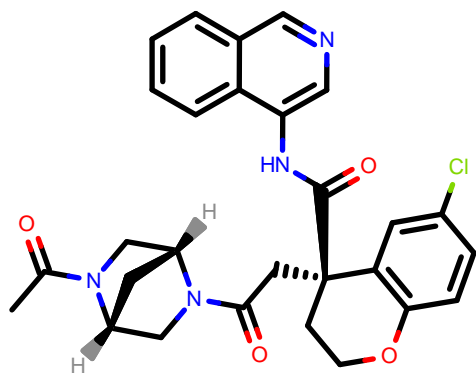
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(Cn5cnn5)F

RUN: RUN4059

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

ALP-UNI-3496895b-3_1



CID: ALP-UNI-3496895b-3_1

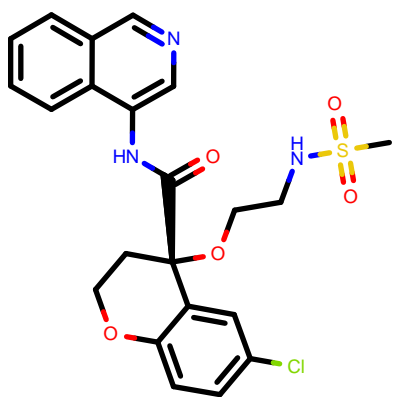
SMILES: CC(=O)N1[C@@H]2[C@@H]1CN2C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6

RUN: RUN2334

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

EN300-1238839_1_1_1



CID: EN300-1238839_1_1_1

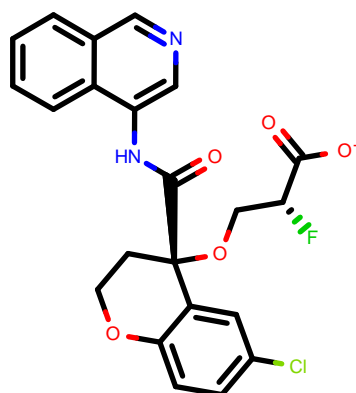
SMILES: CS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN7588

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

ED_-GRI-5b13fbe2-47_2



CID: ED_-GRI-5b13fbe2-47_2

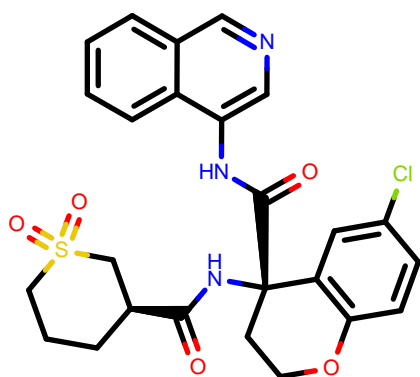
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C(=O)[O-])F

RUN: RUN1420

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-77778_1_2_1



CID: EN300-77778_1_2_1

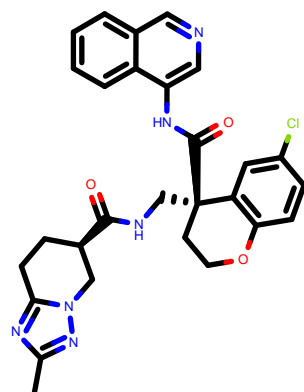
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5OCCS(=O)(=O)C5

RUN: RUN3249

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.25

EN300-746187_2_1_1



CID: EN300-746187_2_1_1

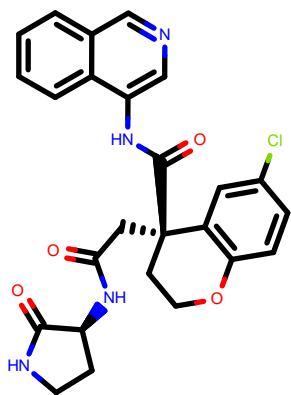
SMILES: Cc1nc2n(n1)C[C@@H](CC2)C(=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5cccc6

RUN: RUN7664

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

EN300-307333_1_1_1



CID: EN300-307333_1_1_1

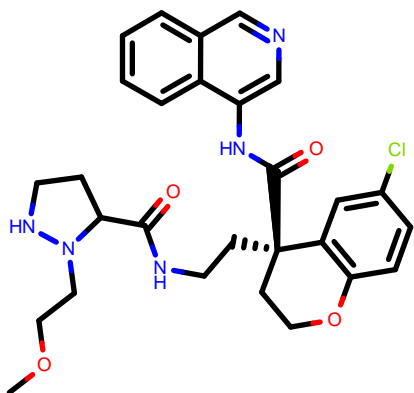
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCNC5=O

RUN: RUN7818

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-92664_3_1_1



CID: EN300-92664_3_1_1

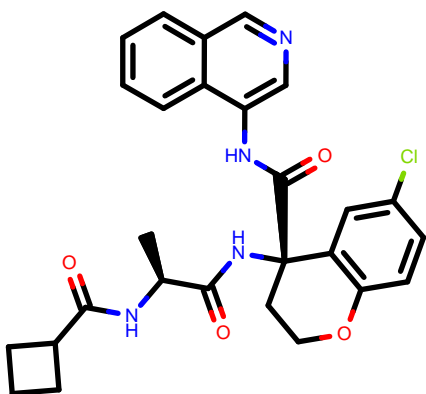
SMILES: COCCn1c(ccn1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5

RUN: RUN5710

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

ALP-UNI-dbbfd3db-15_1



CID: ALP-UNI-dbbfd3db-15_1

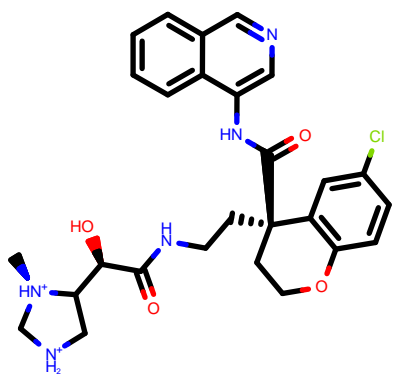
SMILES: C[C@@]@H[C@@]N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3nccc4c3cccc4)NC(=O)C5CC5

RUN: RUN2627

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.32

EN300-190283_3_2_1



CID: EN300-190283_3_2_1

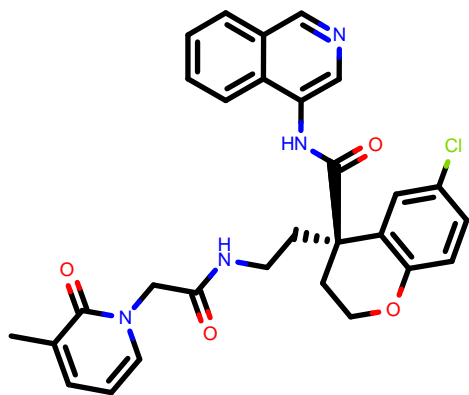
SMILES: C[n+](c[nH]cc1[C@@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4ccc5)O

RUN: RUN5399

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.46

EN300-126104_3_1_1



CID: EN300-126104_3_1_1

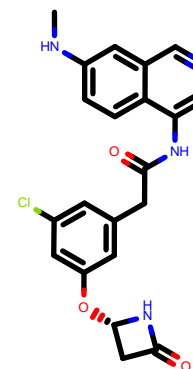
SMILES: Cc1cccn(c1=O)CC(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN5086

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.31

ALF-EVA-0b412456-6_2



CID: ALF-EVA-0b412456-6_2

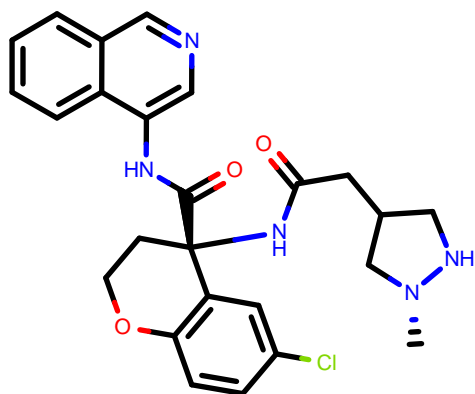
SMILES: CNc1ccc2c(c1)cncc2NC(=O)Cc3ccc(cc3)Cl)O[C@H]4CC(=O)N4

RUN: RUN2572

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.38

EN300-63872_1_1_1



CID: EN300-63872_1_1_1

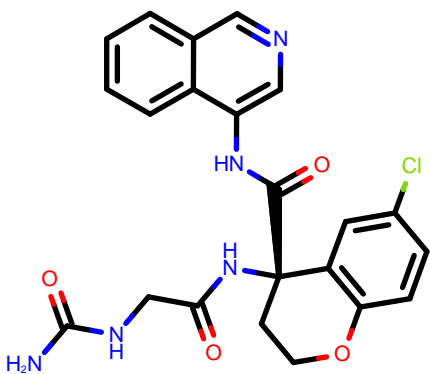
SMILES: Cn1cc(en1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4878

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.27

EN300-10397_1_1_1



CID: EN300-10397_1_1_1

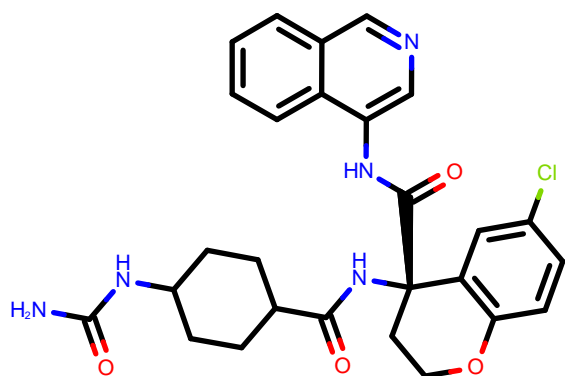
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N

RUN: RUN6565

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.21

EN300-53591_1_1_1



CID: EN300-53591_1_1_1

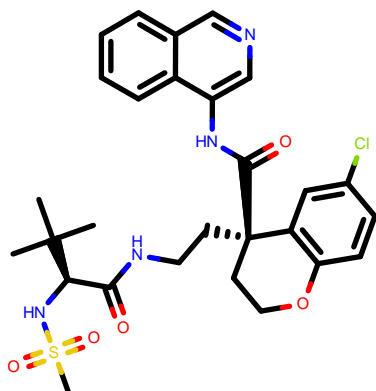
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CCC(CCS)NC(=O)N

RUN: RUN3397

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.28

EN300-112872_3_1_1



CID: EN300-112872_3_1_1

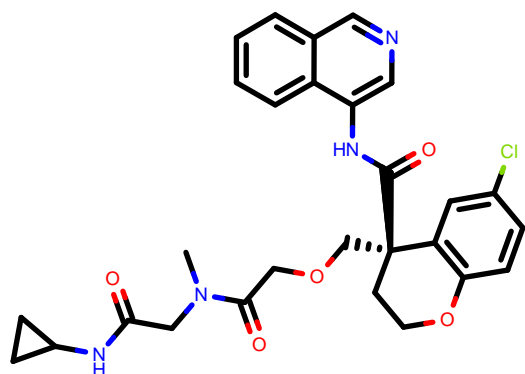
SMILES: CC(C)C(C)[C@@H](Cl)C(=O)NC(C)C1(CCOc2c1ccccc2)C(C)C(=O)Nc3ccc4c3ccccc4NS(=O)(=O)C

RUN: RUN7574

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.44

EN300-13668_2_1_1



CID: EN300-13668_2_1_1

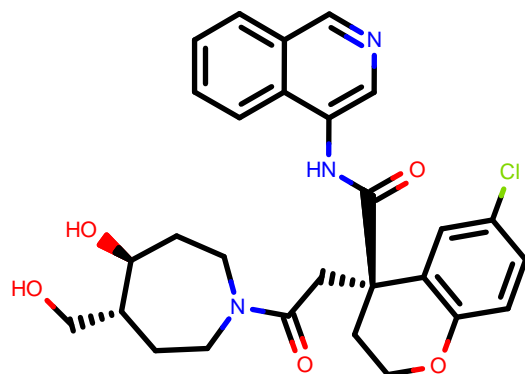
SMILES: CN(CC(=O)NC1CC1)C(=O)COC(C)C2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccccc5

RUN: RUN5296

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

EN300-7353672_1_3_1



CID: EN300-7353672_1_3_1

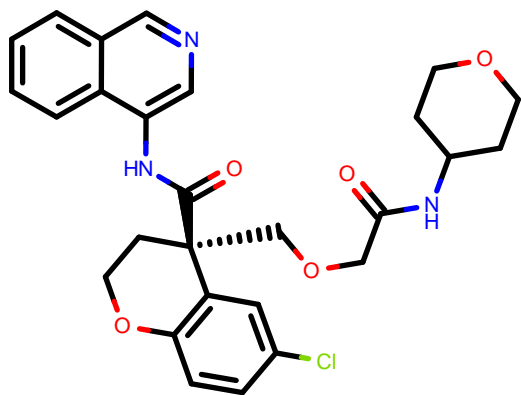
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(C)C(=O)N(C)C5(C)C(O)C(O)C5

RUN: RUN4505

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.32

EN300-67573_2_1_1



CID: EN300-67573_2_1_1

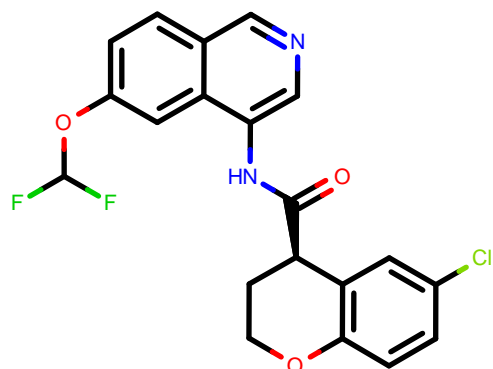
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)NC5CCOCC5

RUN: RUN6333

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

BEN-DND-c852c98b-6_1



CID: BEN-DND-c852c98b-6_1

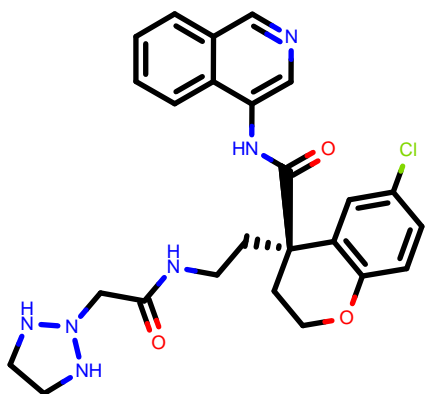
SMILES: c1cc2cnc(c2cc1OC(F)F)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl

RUN: RUN1135

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.06

EN300-100916_3_1_1



CID: EN300-100916_3_1_1

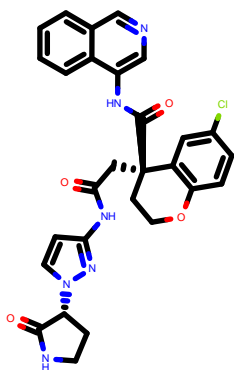
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[N@@]5NCC=N5

RUN: RUN4935

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.30

ALP-UNI-3496895b-12_1



CID: ALP-UNI-3496895b-12_1

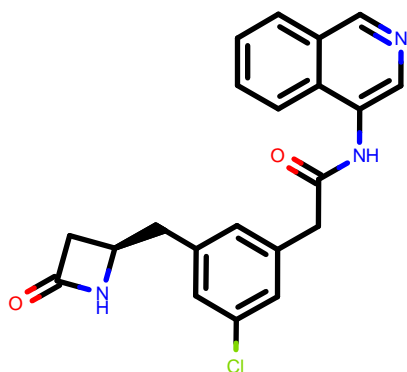
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5cncn5[C@@]6NCCN6=O

RUN: RUN2344

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.31

EDJ-MED-50011917-1_1



CID: EDJ-MED-50011917-1_1

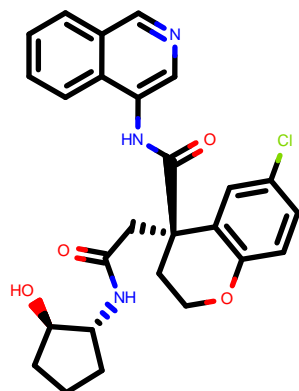
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@@H]4CC(=O)N4

RUN: RUN305

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.39

EN300-60314_1_1_1



CID: EN300-60314_1_1_1

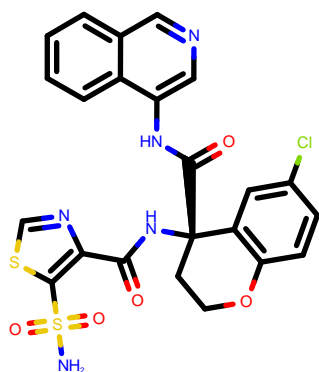
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@H]5O

RUN: RUN4549

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

EN300-132613_1_1_1



CID: EN300-132613_1_1_1

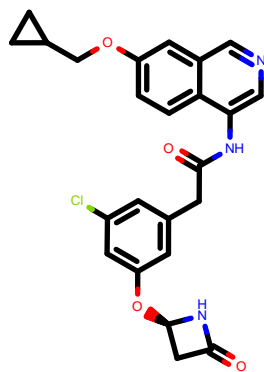
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(scn5)S(=O)(=O)N

RUN: RUN4582

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.25

ALF-EVA-0b412456-7_1



CID: ALF-EVA-0b412456-7_1

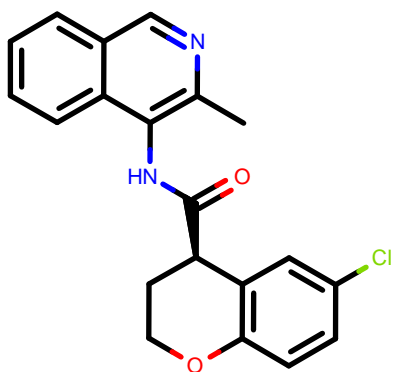
SMILES: c1cc2c(cc1OCC3CC3)cncc2NC(=O)Cc4cc(cc(c4)Cl)O[C@@H]5CC(=O)N5

RUN: RUN2597

DDG (kcal/mol): -0.38

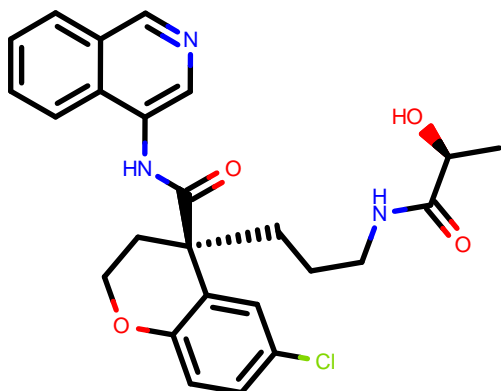
dDDG (kcal/mol): 0.35

ADA-UCB-dc2b944c-10_1



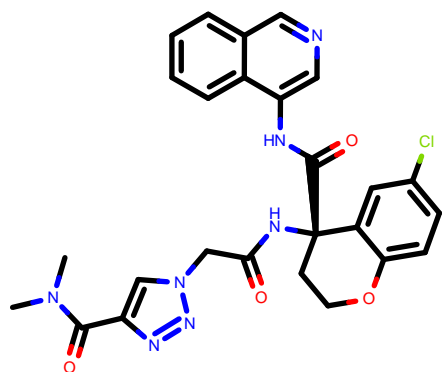
CID:	ADA-UCB-dc2b944c-10_1
SMILES:	<chem>Cc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN497
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.09

EN300-91905_4_1_1



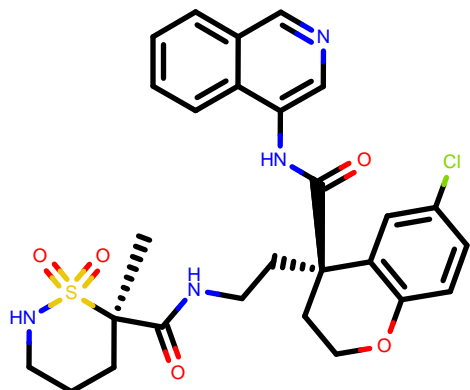
CID:	EN300-91905_4_1_1
SMILES:	<chem>C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O</chem>
RUN:	RUN6128
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.38

EN300-2853791_1_1_1



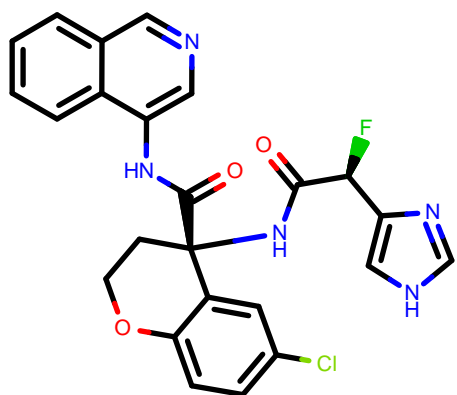
CID:	EN300-2853791_1_1_1
SMILES:	<chem>CN(C)C(=O)c1cn(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5</chem>
RUN:	RUN7252
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.27

EN300-1709315_3_1_1



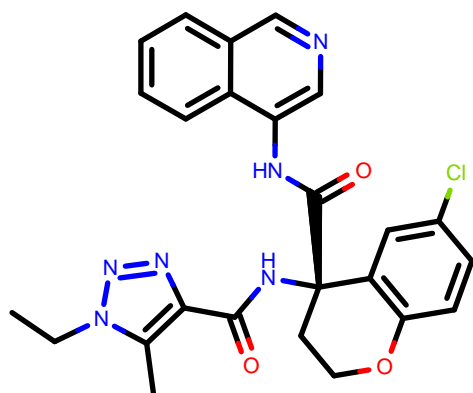
CID:	EN300-1709315_3_1_1
SMILES:	<chem>C[C@@]1(CCCNS1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5</chem>
RUN:	RUN6460
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.34

EDG-MED-90036822-20_2



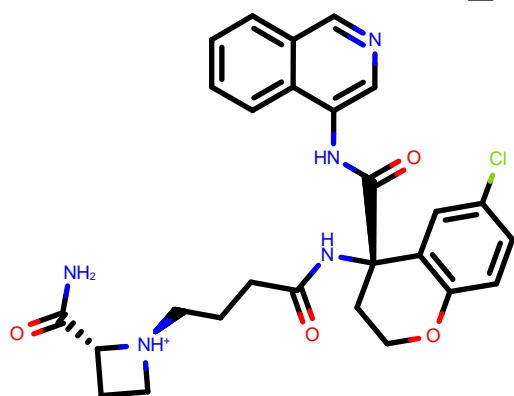
CID:	EDG-MED-90036822-20_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)NC(=O)[C@H](c5cnc[nH]5)F</chem>
RUN:	RUN1560
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.23

EN300-151411_1_1_1



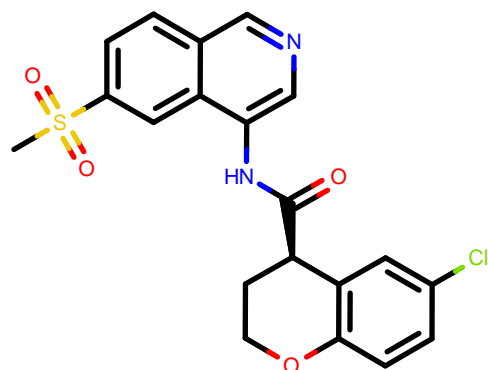
CID:	EN300-151411_1_1_1
SMILES:	<chem>CCn1c(c(nn1)C(=O)N[C@@]2(CCOCc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)Cl</chem>
RUN:	RUN7053
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.29

EDG-MED-90036822-12_2



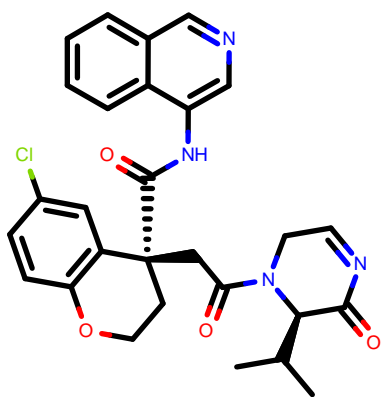
CID:	EDG-MED-90036822-12_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)NC(=O)[C@H](c5cnc[nH]5)CCc6[nH]c6c[nH]n</chem>
RUN:	RUN1570
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.32

BEN-DND-c852c98b-5_1



CID:	BEN-DND-c852c98b-5_1
SMILES:	<chem>CS(=O)(=O)c1ccc2ncnc(c2c1)NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)C</chem>
RUN:	RUN1104
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.08

EN300-67791_1_1_1



CID: EN300-67791_1_1_1

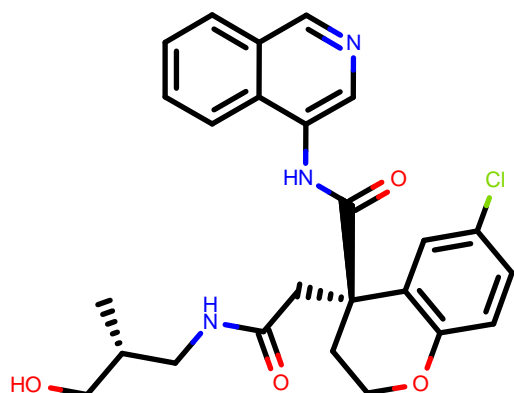
SMILES: CC(C)[C@@H]1C(=O)NCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN6602

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.38

EN300-53656_1_2_1



CID: EN300-53656_1_2_1

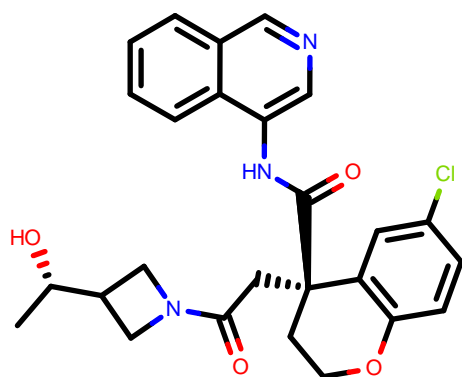
SMILES: C[C@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4)CO

RUN: RUN6718

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-365650_1_1_1



CID: EN300-365650_1_1_1

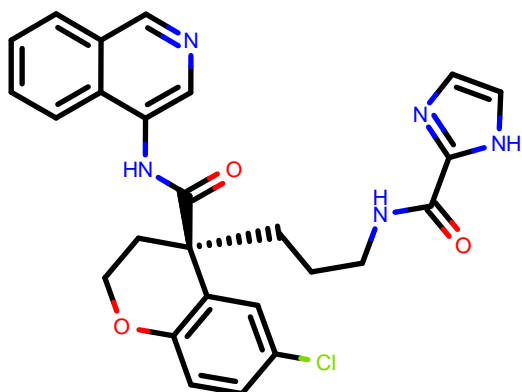
SMILES: C[C@H](C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)O

RUN: RUN7639

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-315836_4_1_1



CID: EN300-315836_4_1_1

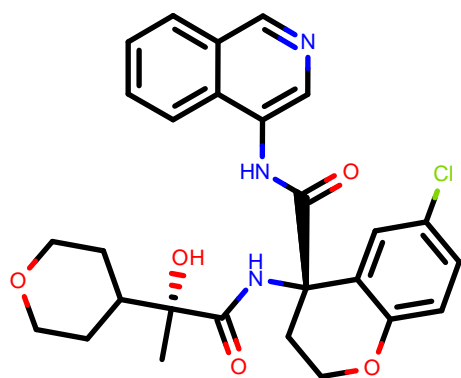
SMILES: c1ccc2c(c1)cncc2N[C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5[nH]cn5

RUN: RUN6304

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.31

EN300-217499_1_1_1



CID: EN300-217499_1_1_1

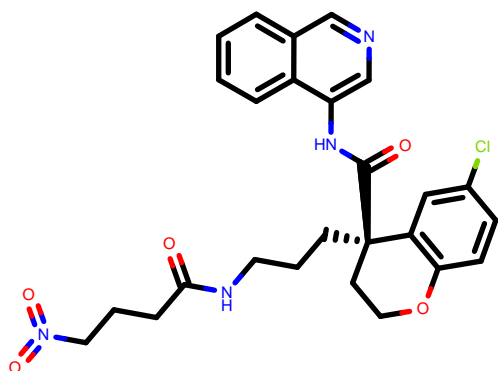
SMILES: C[C@@](C1CCOCC1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)O

RUN: RUN7647

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.22

EN300-143449_4_1_1



CID: EN300-143449_4_1_1

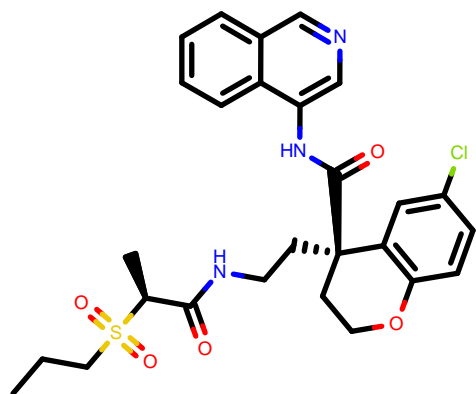
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCN(=O)=O

RUN: RUN5467

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.31

EN300-52768_3_1_1



CID: EN300-52768_3_1_1

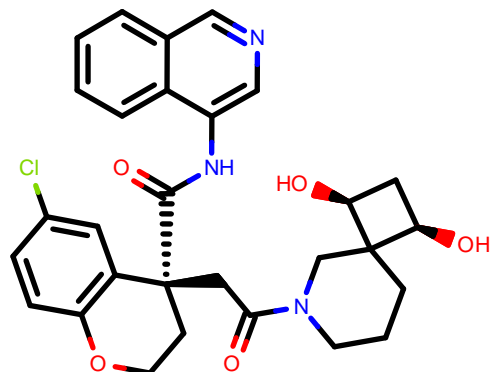
SMILES: CCCS(=O)(=O)[C@@H](C)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN6141

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.44

EDJ-MED-d203f206-10_1



CID: EDJ-MED-d203f206-10_1

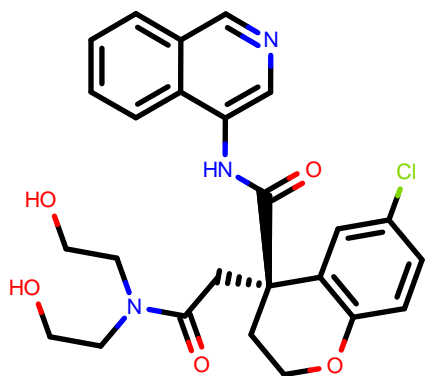
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC5(C)[C@@H](C)[C@@H](O)O

RUN: RUN2425

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.39

EN300-19762_1_1_1



CID: EN300-19762_1_1_1

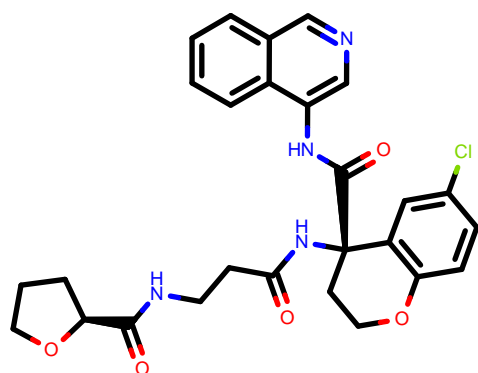
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(=O)N(CCO)CCO

RUN: RUN3000

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.39

EN300-86732_1_1_1



CID: EN300-86732_1_1_1

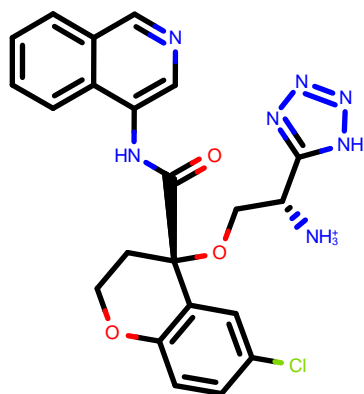
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)CCNC(=O)[C@@H]5OCCCO5

RUN: RUN5488

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-4_1



CID: ED_-GRI-5b13fbe2-4_1

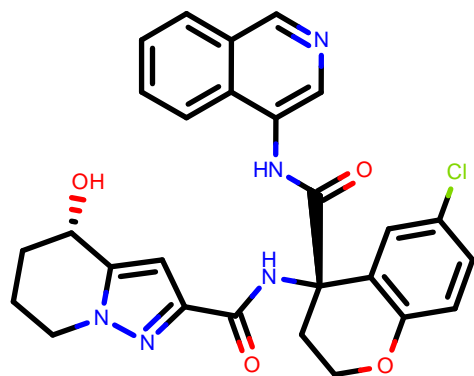
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)OC[C@H](c5[nH]n5)[NH3+]

RUN: RUN1386

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.30

EN300-399606_1_1_1



CID: EN300-399606_1_1_1

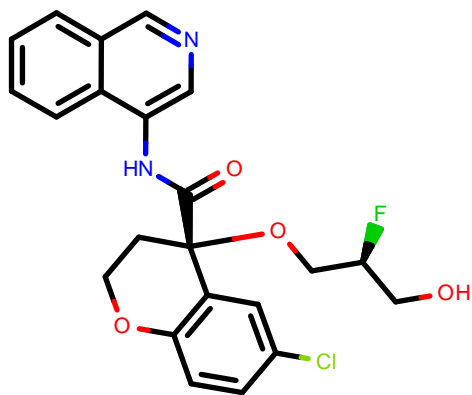
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)c5cc6n(n5)C[C@]3@H6O

RUN: RUN3538

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.24

EN300-1600517_1_2_1



CID: EN300-1600517_1_2_1

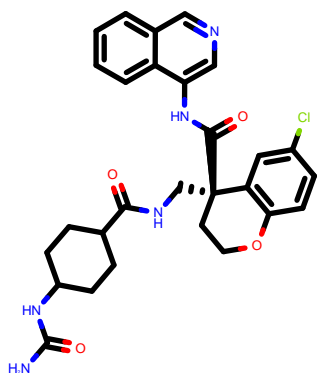
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CO)F

RUN: RUN7795

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-53591_2_1_1



CID: EN300-53591_2_1_1

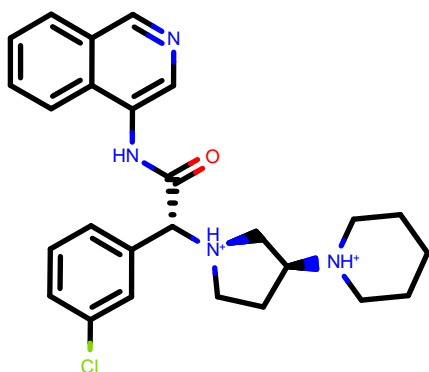
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CCCC(C5)NC(=O)N

RUN: RUN7449

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.29

MIC-UNK-5a93dd5f-12_3



CID: MIC-UNK-5a93dd5f-12_3

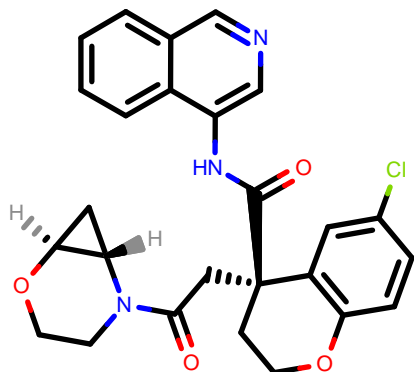
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCCc4c3cc(c4)Cl)N@]4CC[C@@]3(C4)[NH+]5CCCCC5

RUN: RUN701

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.37

EN300-91609_1_1_1



CID: EN300-91609_1_1_1

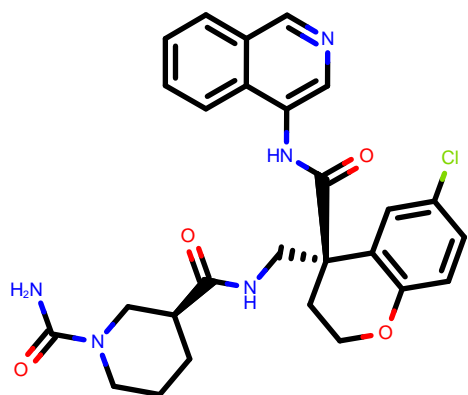
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]3(C)N5C

RUN: RUN6411

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.27

EN300-14767_2_2_1



CID: EN300-14767_2_2_1

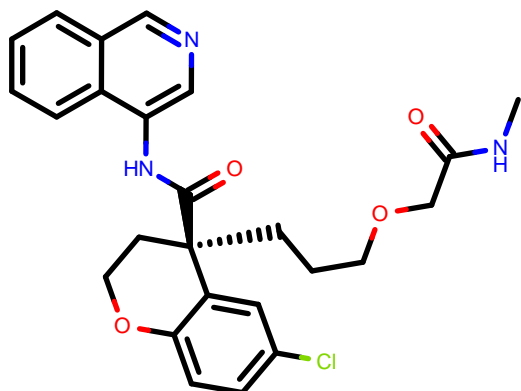
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCN(C5)C(=O)N

RUN: RUN5298

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.27

EN300-2977549_4_1_1



CID: EN300-2977549_4_1_1

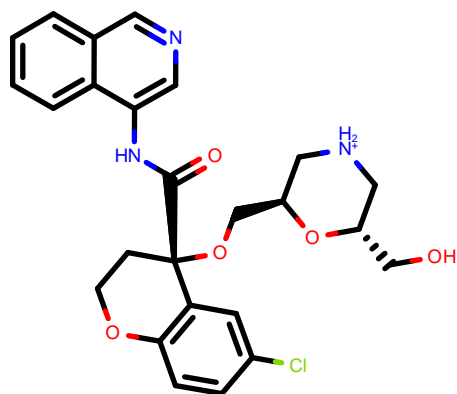
SMILES: CNC(=O)COCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN4392

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-20_1



CID: ED_-GRI-5b13fbe2-20_1

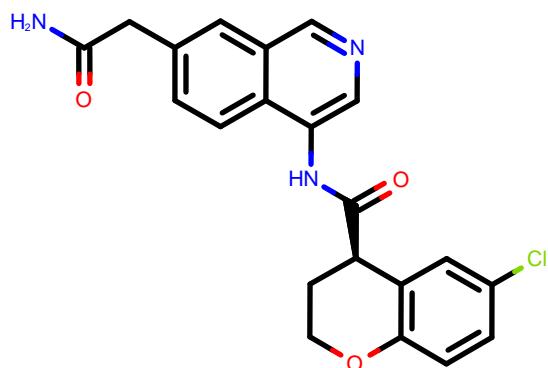
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[NH2+]C[C@@H](O5)CO

RUN: RUN1431

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.41

MAK-UNK-8be7dca9-2_1



CID: MAK-UNK-8be7dca9-2_1

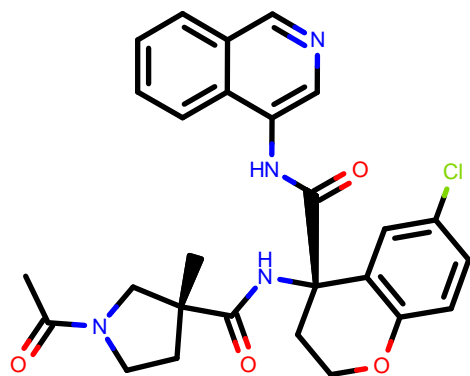
SMILES: c1cc2c(cc1CC(=O)N)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN429

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.07

EN300-98018_1_1_1



CID: EN300-98018_1_1_1

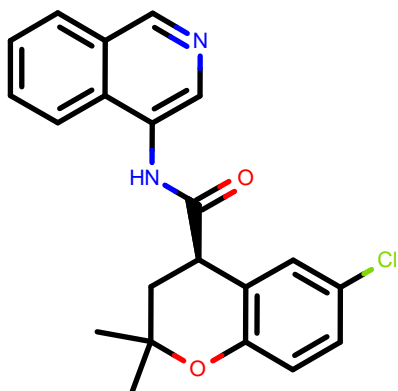
SMILES: CC(=O)N1CC[C@@](C1)(C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN3666

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.36

ADA-UCB-dc2b944c-16_1_1



CID: ADA-UCB-dc2b944c-16_1_1

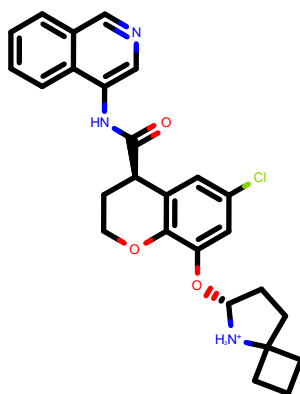
SMILES: CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ccc4c3cccc4)C

RUN: RUN5395

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.10

DAR-DIA-23e5a6a0-1_1_1



CID: DAR-DIA-23e5a6a0-1_1_1

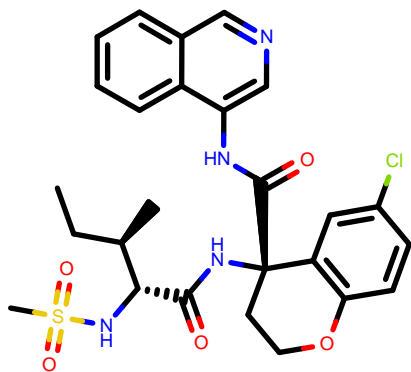
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@H]3COCc4c3cc(cc4O)[C@@H]5CCCC6([NH2+][5])OCC6)Cl

RUN: RUN6217

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.36

EN300-76541_1_3_1



CID: EN300-76541_1_3_1

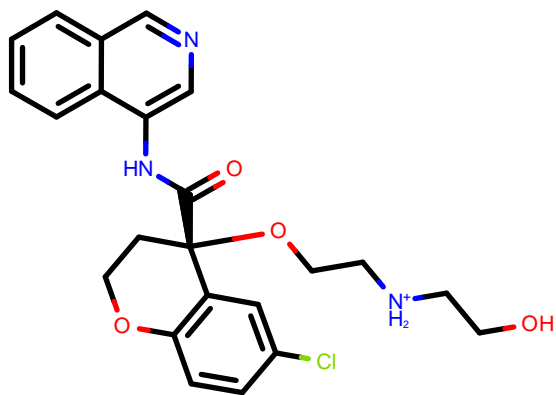
SMILES: CC(C)C[C@@H](C)[C@@H](Cl)C(=O)N[C@@]1(CCOc2c1ccc2)C(=O)Nc3ccc4c3cccc4NS(=O)(=O)C

RUN: RUN2743

DDG (kcal/mol): -0.35

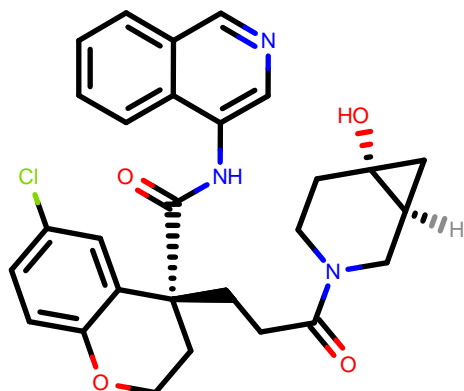
dDDG (kcal/mol): 0.47

ED_-GRI-5b13fbe2-30_1



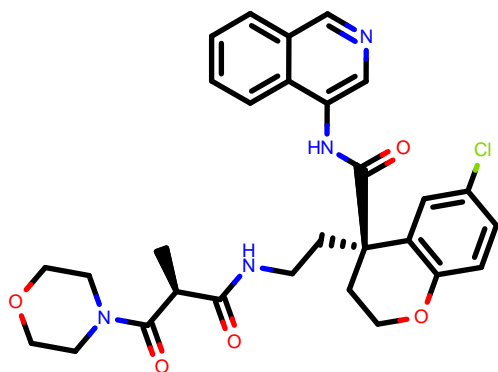
CID:	ED_-GRI-5b13fbe2-30_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+][C]O</chem>
RUN:	RUN1410
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.58

EN300-303908_2_1_1



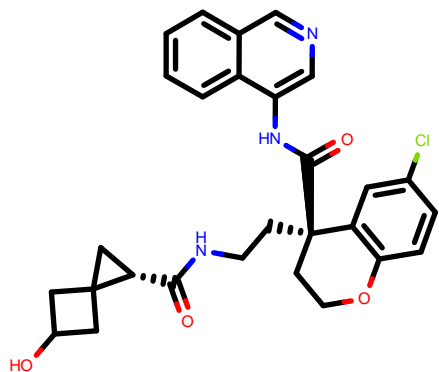
CID:	EN300-303908_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@]6(C)[C@@H]6CSO</chem>
RUN:	RUN5811
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.26

EN300-2855057_3_1_1



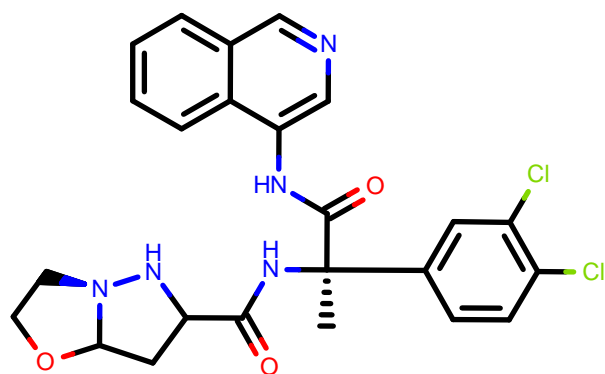
CID:	EN300-2855057_3_1_1
SMILES:	<chem>[C]C@@H[C@@]1(C=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)C(=O)N5CCOCC5</chem>
RUN:	RUN7775
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.45

EN300-1717166_3_2_1



CID:	EN300-1717166_3_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC56C(C)O</chem>
RUN:	RUN4831
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.31

MAT-POS-e9e99895-5_1



CID: MAT-POS-e9e99895-5_1

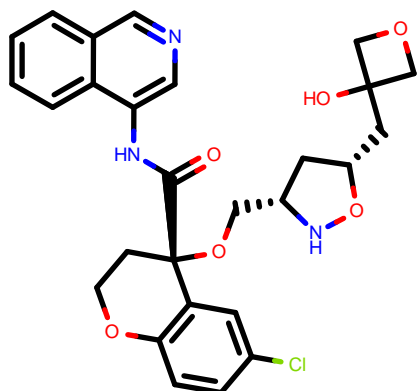
SMILES: C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2nc3c2ccc3)NC(=O)c4cc5n(n4)CCO5

RUN: RUN2074

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.33

EN300-7457160_1_2_1



CID: EN300-7457160_1_2_1

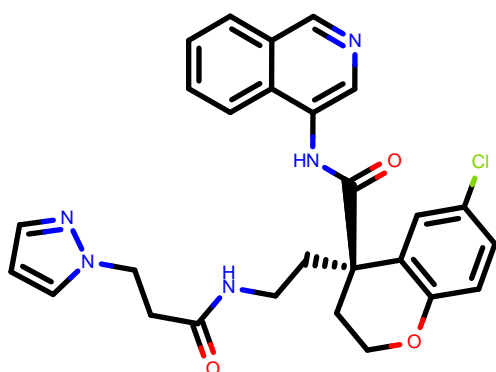
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4OCOC4C3OC[C@@]5[H]5[C@@]6[H]O[N]5C[C@@]6COC6O

RUN: RUN5703

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.32

EN300-25986_3_1_1



CID: EN300-25986_3_1_1

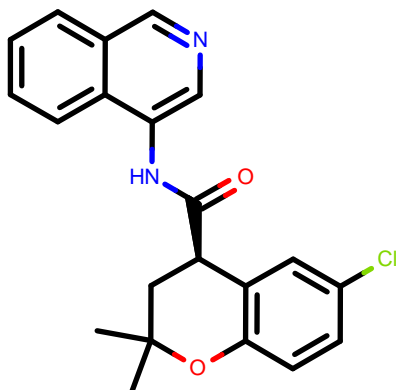
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn5

RUN: RUN3710

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.29

ADA-UCB-dc2b944c-16_1



CID: ADA-UCB-dc2b944c-16_1

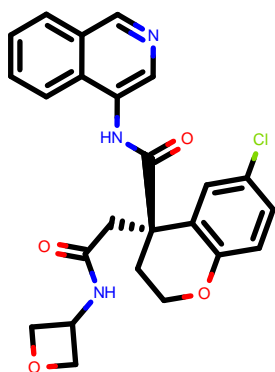
SMILES: CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3ccc4)C

RUN: RUN557

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.09

EN300-49064_1_1_1



CID: EN300-49064_1_1_1

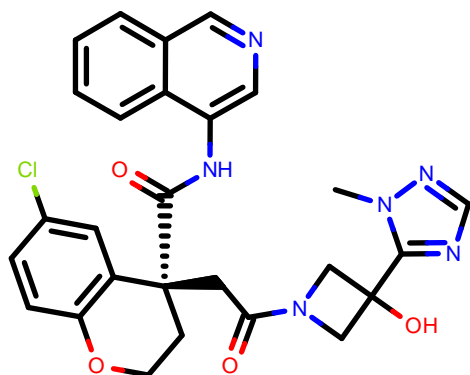
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5COC5

RUN: RUN7265

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.24

EN300-381149_1_1_1



CID: EN300-381149_1_1_1

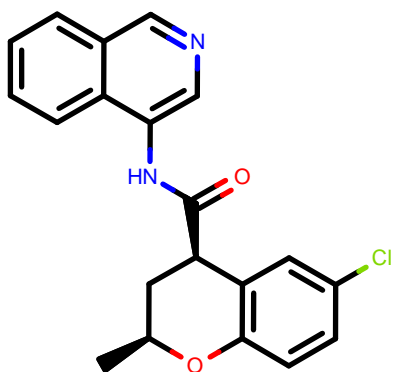
SMILES: Cn1c(ncn1)C2(CN(C2)C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cnc6c5ccc6)O

RUN: RUN5963

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.32

EDJ-MED-e4b030d8-3_1



CID: EDJ-MED-e4b030d8-3_1

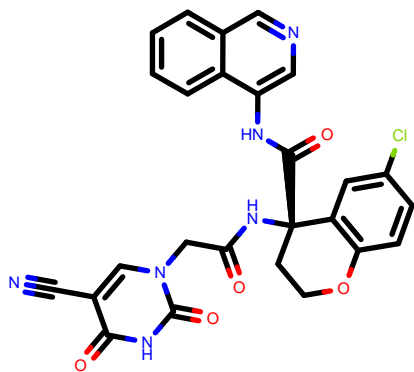
SMILES: C[C@H]1C[C@H](c2cc(c3c2O1)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN241

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.09

ALP-UNI-dbbfd3db-11_1



CID: ALP-UNI-dbbfd3db-11_1

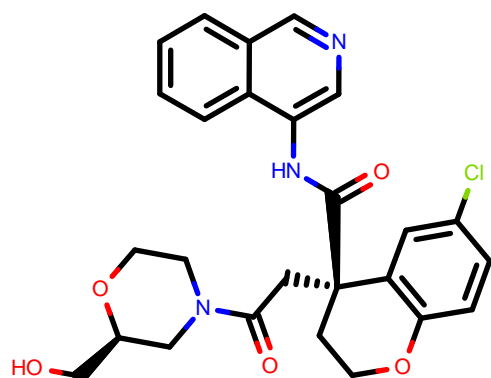
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc(c(=O)[nH]c5=O)C#N

RUN: RUN2615

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.35

EN300-175487_1_1_1



CID: EN300-175487_1_1_1

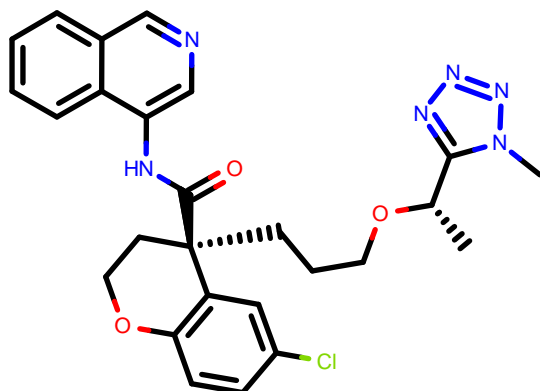
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@@H](C5)CO

RUN: RUN4256

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.40

EN300-173006_4_1_1



CID: EN300-173006_4_1_1

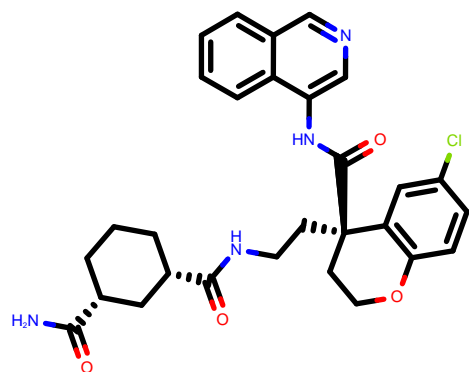
SMILES: C[C@@H](c1nncn1)OCC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN6306

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.36

EN300-90142_3_4_1



CID: EN300-90142_3_4_1

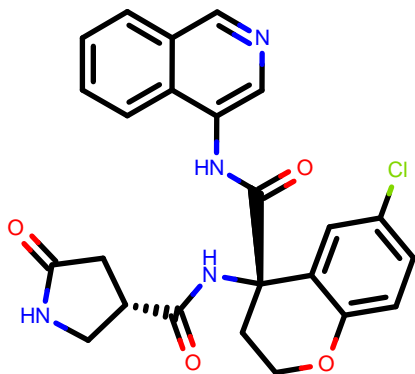
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CN(C)O[C@@H]5CC[C@@H](C5)Cl=O

RUN: RUN4037

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.31

EN300-59487_1_2_1



CID: EN300-59487_1_2_1

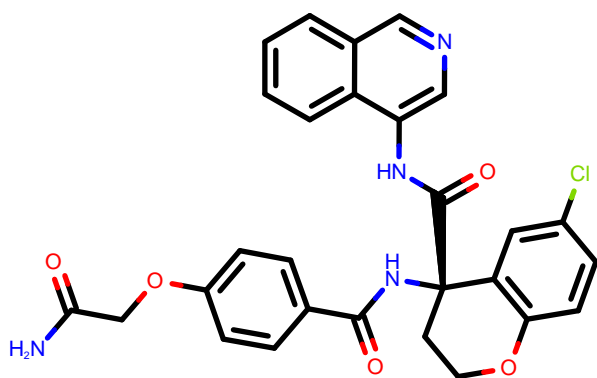
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC(=O)N5

RUN: RUN5796

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.26

EN300-14949_1_1_1



CID: EN300-14949_1_1_1

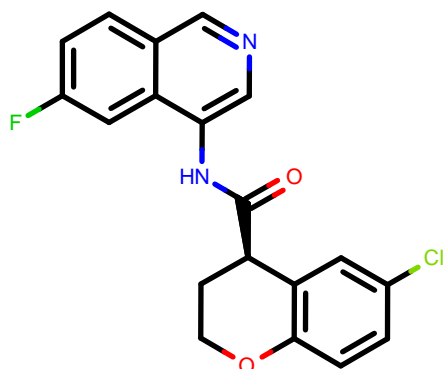
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)OCC(=O)N

RUN: RUN6182

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.31

EDG-MED-5d232de5-1_1



CID: EDG-MED-5d232de5-1_1

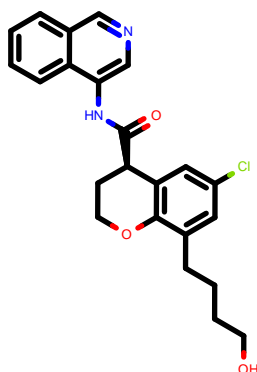
SMILES: c1cc2cnc(c2cc1F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2191

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.04

LAU-MED-88a3970a-7_1



CID: LAU-MED-88a3970a-7_1

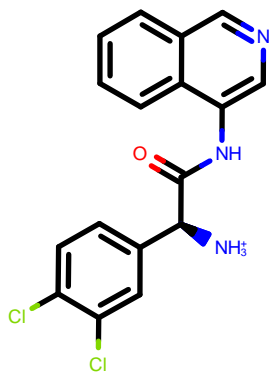
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOC4c3cc(cc4CCCCO)Cl

RUN: RUN1351

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.18

MAT-POS-1f3f1a6f-1_2



CID: MAT-POS-1f3f1a6f-1_2

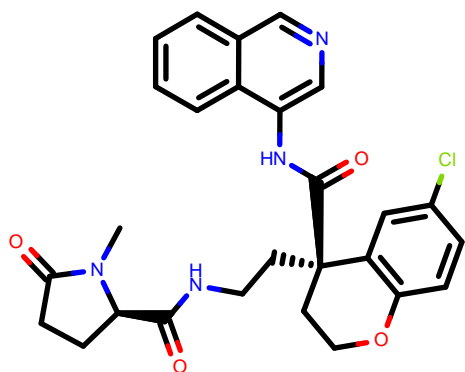
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)[NH3+]

RUN: RUN2091

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.36

EN300-132963_3_2_1



CID: EN300-132963_3_2_1

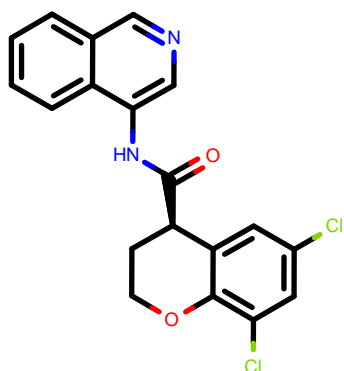
SMILES: CN1[C@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN5920

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.30

ALP-UNI-3735e77e-2_1



CID: ALP-UNI-3735e77e-2_1

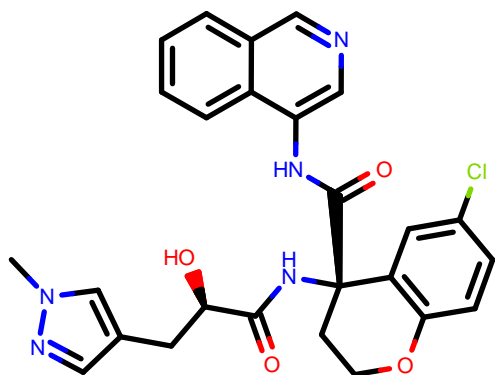
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN1781

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.08

EN300-172020_1_2_1



CID: EN300-172020_1_2_1

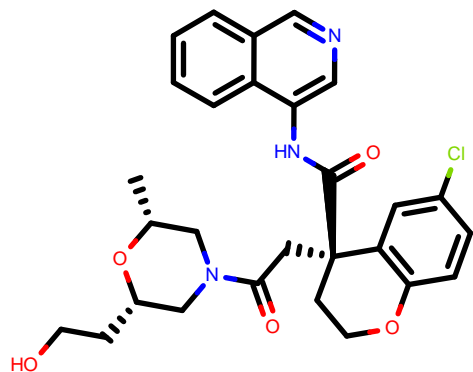
SMILES: Cn1cc(en1)C[C@H](C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5)O

RUN: RUN6385

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.29

EN300-212814_1_1_1



CID: EN300-212814_1_1_1

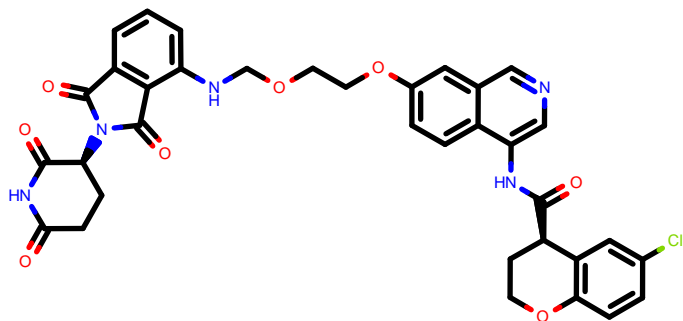
SMILES: C[C@@H](CN1C[C@@H](O1)CCOC)C(=O)N[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN6068

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.32

DAR-DIA-9e4459de-13_7



CID:

DAR-DIA-9e4459de-13_7

SMILES:

c1cc2c(c1)NC(OCCOC3=CC=CC=C3N=C4C(=O)NCC4)C=C5C(=O)NCC5

RUN:

RUN1325

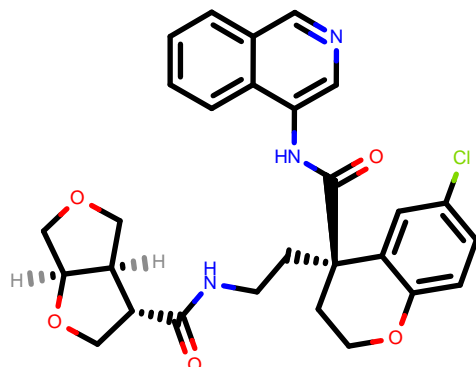
DDG (kcal/mol):

-0.33

dDDG (kcal/mol):

0.33

EN300-6482296_3_5_1



CID:

EN300-6482296_3_5_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H](Cl)C3=CC=CC=C3N=C4C(=O)NCC4

RUN:

RUN6050

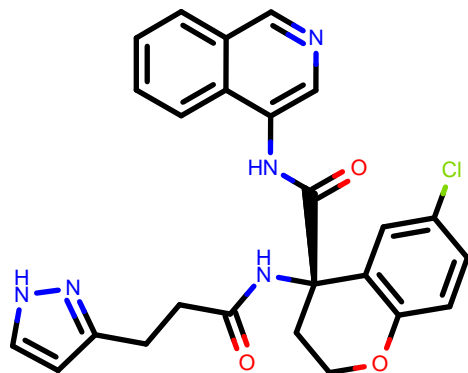
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

0.31

EN300-1664603_1_1_1



CID:

EN300-1664603_1_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H](Cl)C3=CC=CC=C3N=C4C(=O)NCC4

RUN:

RUN4540

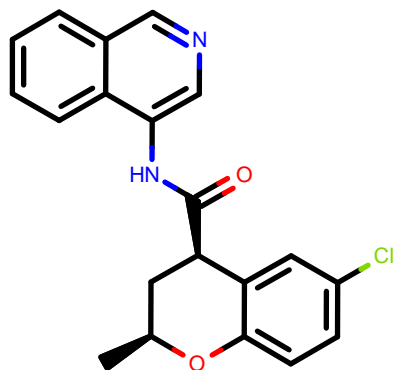
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

0.21

EDJ-MED-e4b030d8-3_1_1



CID:

EDJ-MED-e4b030d8-3_1_1

SMILES:

C[C@H]1C[C@H](c2cc(c3c(O)C)C(=O)Nc3ncc4c3cccc4

RUN:

RUN5751

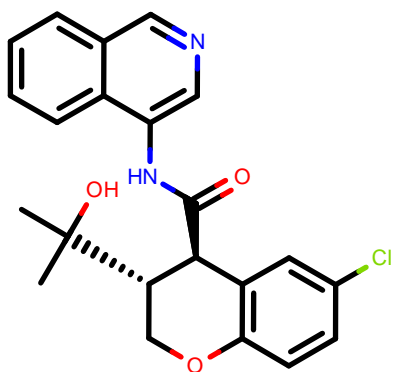
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

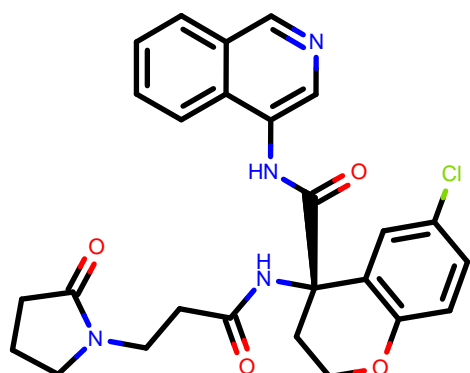
0.09

BEN-BAS-5c03e89e-1_2



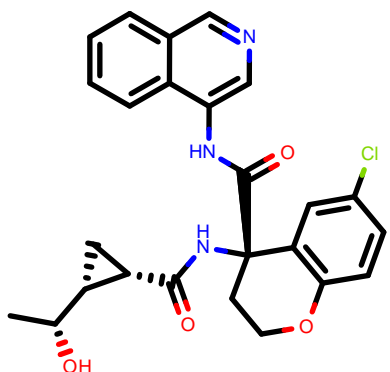
CID:	BEN-BAS-5c03e89e-1_2
SMILES:	<chem>CC(C)(C@H)1COc2ccc(cc2[C@@H]1C(=O)Nc3cnc4c3ccc4)Cl</chem> O
RUN:	RUN1073
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.11

EN300-67191_1_1_1



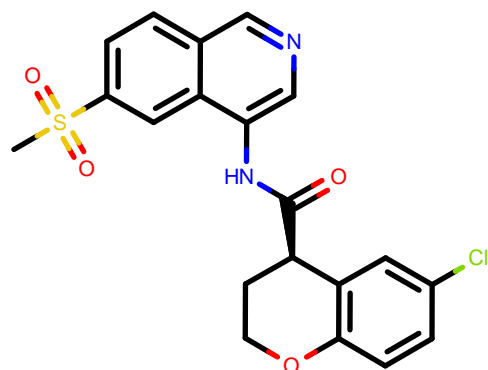
CID:	EN300-67191_1_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O</chem>
RUN:	RUN7721
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.27

EN300-6729572_1_2_1



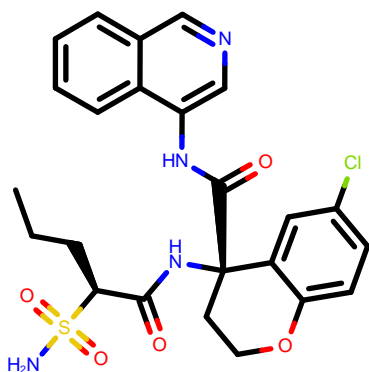
CID:	EN300-6729572_1_2_1
SMILES:	<chem>C[C@@H]([C@@H]1C[C@@H]1C(=O)N)C@2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)O</chem>
RUN:	RUN4528
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.22

BEN-DND-c852c98b-5_1_1



CID:	BEN-DND-c852c98b-5_1_1
SMILES:	<chem>CS(=O)(=O)c1ccc2ncnc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN7628
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.09

EN300-206592_1_1_1



CID: EN300-206592_1_1_1

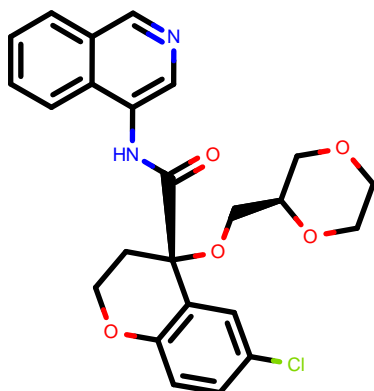
SMILES: CCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)S(=O)(=O)N

RUN: RUN7065

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.23

EN300-139167_1_2_1



CID: EN300-139167_1_2_1

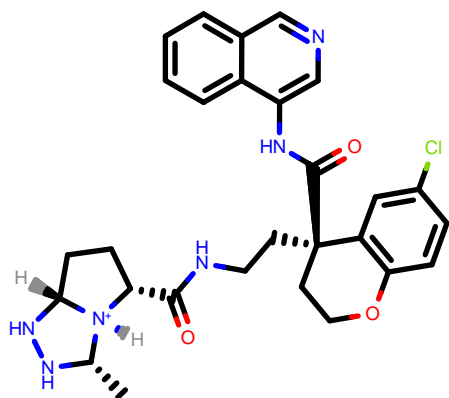
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCCO5

RUN: RUN4574

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.23

EN300-6489289_3_2_3



CID: EN300-6489289_3_2_3

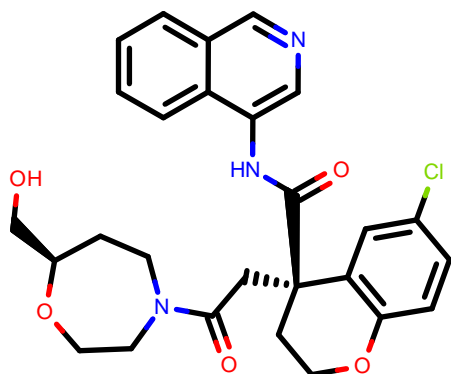
SMILES: C[C@@H]1NN[C@@H]2[N@@H]1[C@@H](C2)Cl=O)NC[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccc6c5ccc6

RUN: RUN4661

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.42

EN300-2007620_1_1_1



CID: EN300-2007620_1_1_1

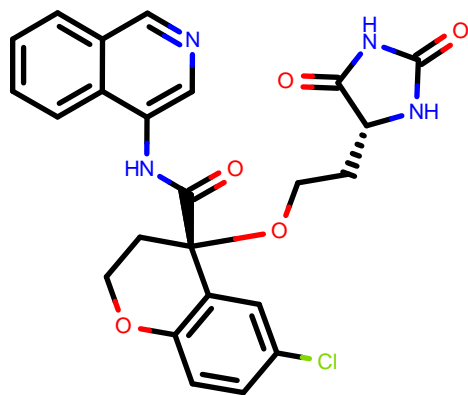
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]1(O)CC5)CO

RUN: RUN6142

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.29

EN300-6498856_1_1_1



CID: EN300-6498856_1_1_1

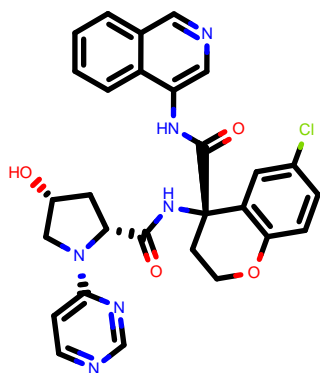
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4ccc(cc4)Cl)OCC[C@@H]5C(=O)NC(=O)N5

RUN: RUN6316

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.24

EN300-310022_1_4_1



CID: EN300-310022_1_4_1

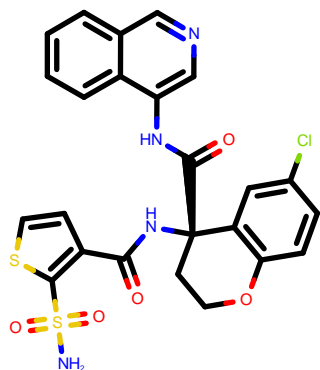
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4ccc(cc4)Cl)NC(=O)[C@@H]5C[C@H](CN5c6ccccc6)O

RUN: RUN4463

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.30

EN300-294602_1_1_1



CID: EN300-294602_1_1_1

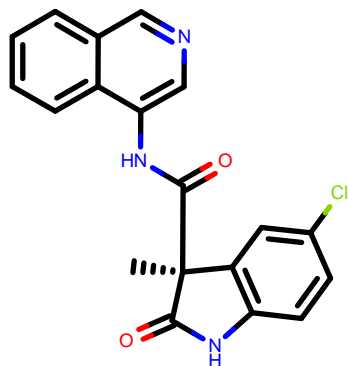
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4ccc(cc4)Cl)NC(=O)c5ccc(s5S(=O)(=O)N

RUN: RUN3264

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.26

EDJ-MED-9e38fd34-1_1



CID: EDJ-MED-9e38fd34-1_1

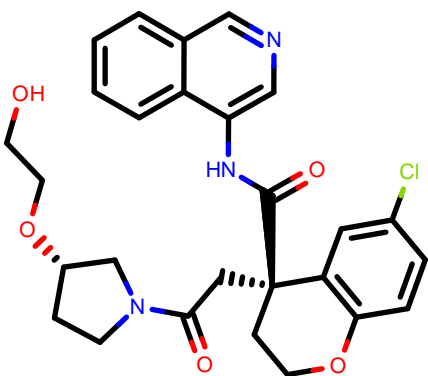
SMILES: C[C@@]1(c2ccc(ccc2NC1=O)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN2179

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

EN300-6764893_1_1_1



CID: EN300-6764893_1_1_1

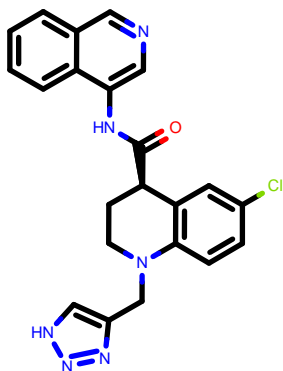
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)OCCO

RUN: RUN7288

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.32

RAL-THA-8416115c-14_3



CID: RAL-THA-8416115c-14_3

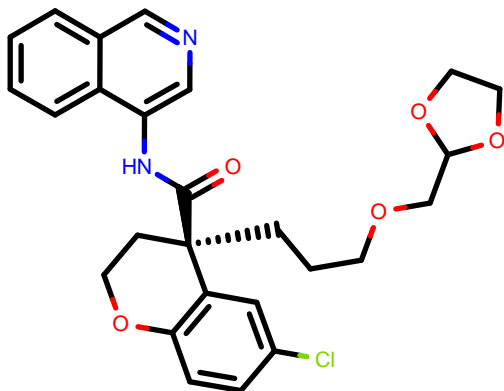
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCN(c4c3cc(cc4)Cl)Cc5cn[nH]n5

RUN: RUN1201

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.29

EN300-77092_4_1_1



CID: EN300-77092_4_1_1

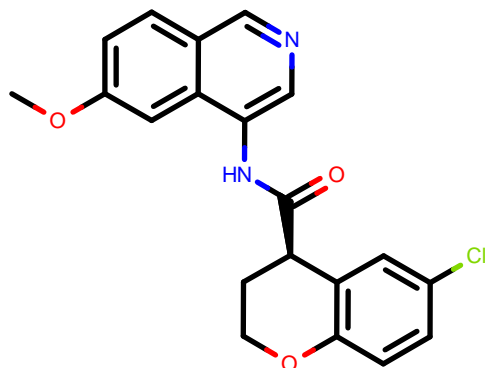
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5

RUN: RUN6019

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.36

MAT-POS-f9802937-7_1



CID: MAT-POS-f9802937-7_1

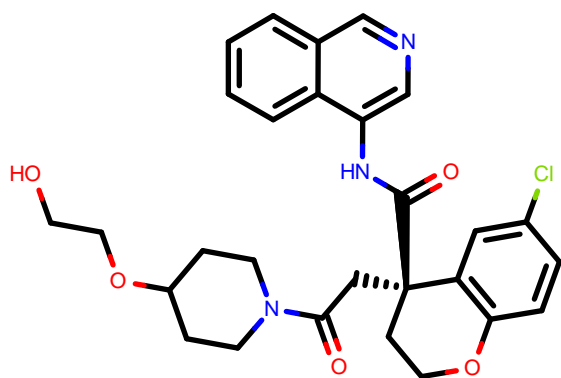
SMILES: COc1ccc2cncc(c2c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5

RUN: RUN2231

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.06

EN300-104088_1_1_1



CID: EN300-104088_1_1_1

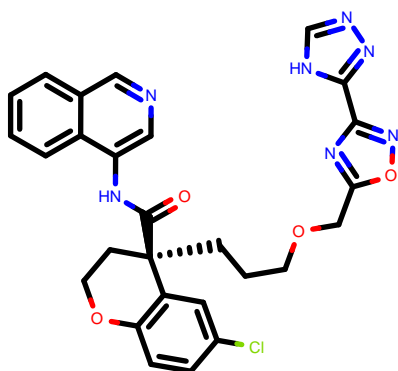
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)OCCO

RUN: RUN6447

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.30

EN300-92031_4_1_1



CID: EN300-92031_4_1_1

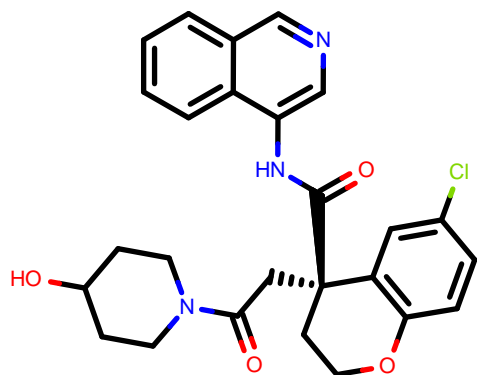
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5nc(n5)c6[nH]nnc6

RUN: RUN7263

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-379533_1_1_1



CID: EN300-379533_1_1_1

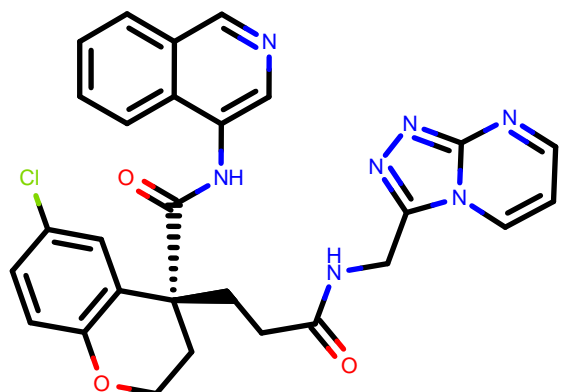
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)O

RUN: RUN6248

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-61021_2_1_1



CID: EN300-61021_2_1_1

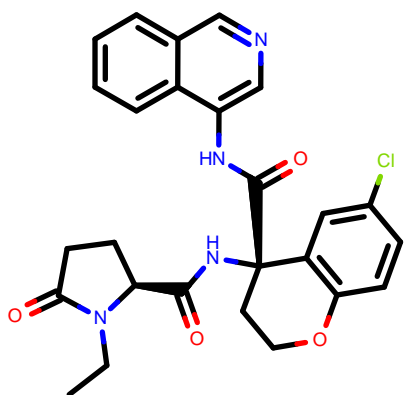
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5nn6n5ccc6

RUN: RUN6236

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.27

EN300-718785_1_1_1



CID: EN300-718785_1_1_1

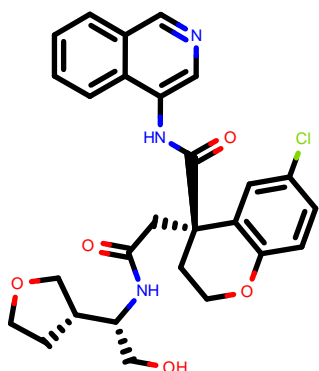
SMILES: CCN1[C@@H](CCC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4484

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.26

EN300-104493_1_2_1



CID: EN300-104493_1_2_1

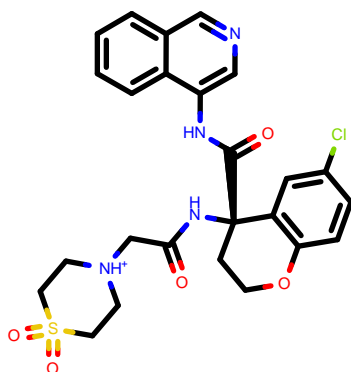
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)[C@@H]5CCOC5

RUN: RUN6177

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.35

EN300-39305_1_1_1



CID: EN300-39305_1_1_1

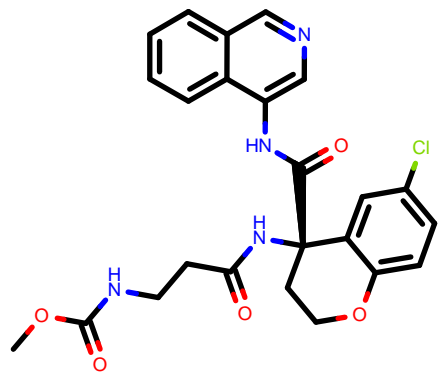
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)NS5CCS(=O)(=O)CC5

RUN: RUN6636

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.30

EN300-71558_1_1_1



CID: EN300-71558_1_1_1

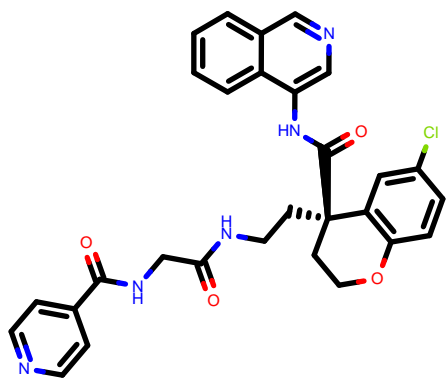
SMILES: COC(=O)NCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN5520

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.23

EN300-36089_3_1_1



CID: EN300-36089_3_1_1

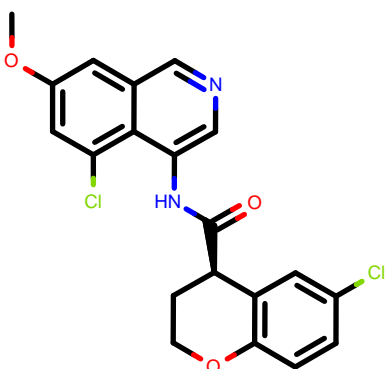
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)c5cccnc5

RUN: RUN4988

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.39

ALF-EVA-ced740bd-2_1



CID: ALF-EVA-ced740bd-2_1

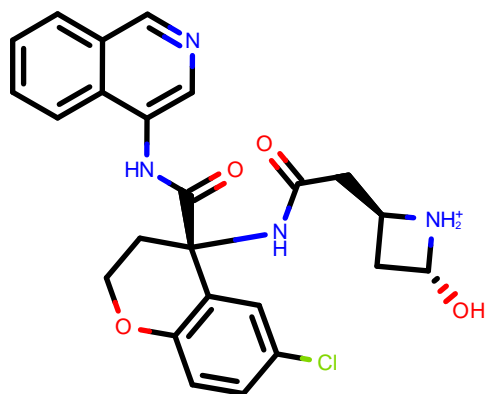
SMILES: COc1cc2cnccc(c2c(c1)Cl)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN2611

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.21

EN300-250593_1_1_1



CID: EN300-250593_1_1_1

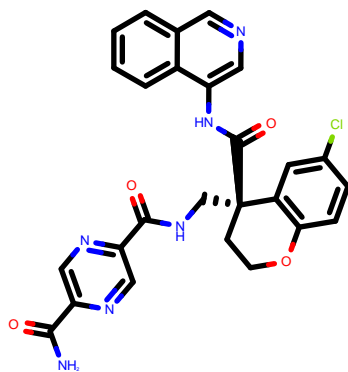
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(O)N5

RUN: RUN6247

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-1273172_2_1_1



CID: EN300-1273172_2_1_1

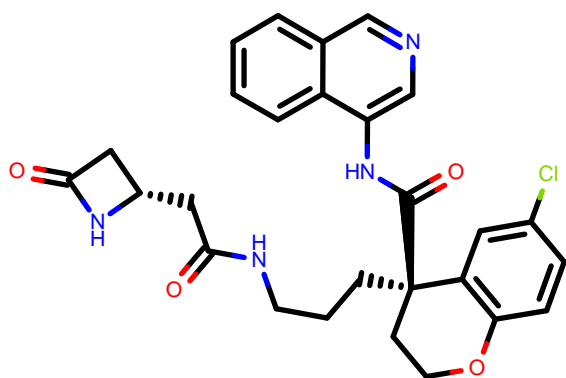
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ncnc(c5)C(=O)N

RUN: RUN7668

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-250593_4_2_1



CID: EN300-250593_4_2_1

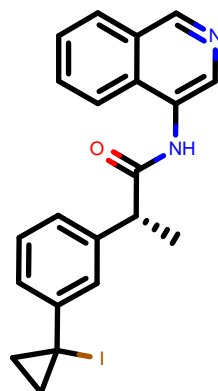
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCNC(=O)C[C@H]5CC(=O)N5

RUN: RUN6102

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.26

DAR-DIA-0cde14eb-58_2



CID: DAR-DIA-0cde14eb-58_2

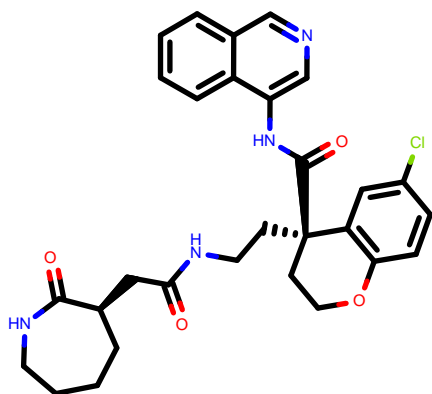
SMILES: C[C@H](c1cccc(c1)C2(CC2)I)C(=O)Nc3cnc4c3cccc4

RUN: RUN27

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.38

EN300-198633_3_2_1



CID: EN300-198633_3_2_1

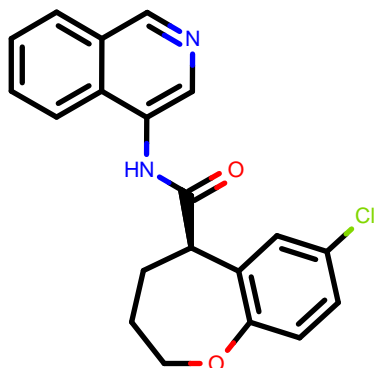
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCNC(=O)C[C@H]5CCOCCN5=O

RUN: RUN6633

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.32

ALF-EVA-5b152d2f-1_1



CID: ALF-EVA-5b152d2f-1_1

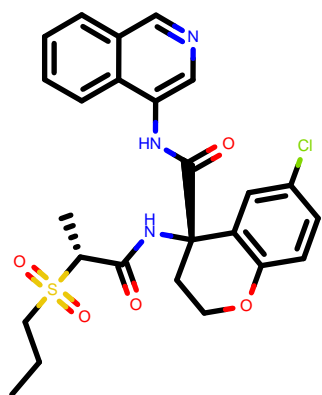
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CCNC(=O)C[C@H]5CCOCCN5=O

RUN: RUN2167

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.19

EN300-52768_1_2_1



CID: EN300-52768_1_2_1

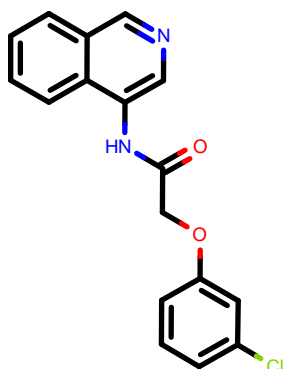
SMILES: CCCS(=O)(=O)[C@H](C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6392

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.35

ALP-POS-f13221e1-2_1



CID: ALP-POS-f13221e1-2_1

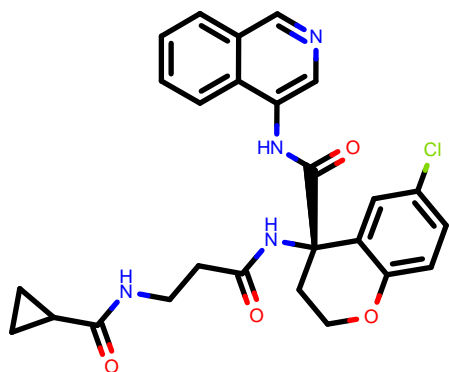
SMILES: c1ccc2c(c1)cncc2NC(=O)COc3cccc(c3)Cl

RUN: RUN147

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.31

EN300-31147_1_1_1



CID: EN300-31147_1_1_1

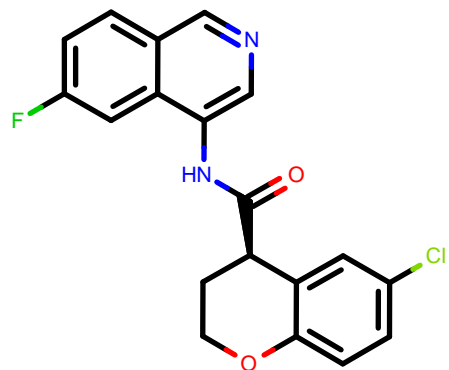
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5OC5

RUN: RUN7113

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.27

ALP-POS-696356e4-1_1



CID: ALP-POS-696356e4-1_1

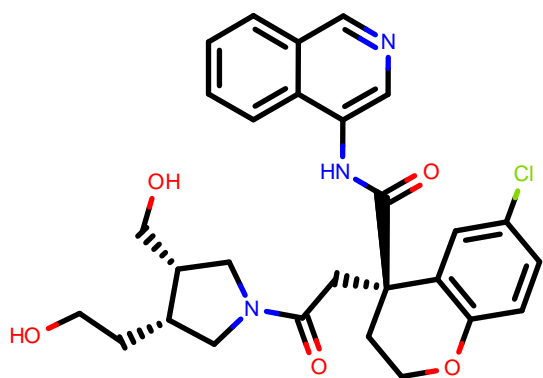
SMILES: c1cc2cncc(c2cc1F)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C

RUN: RUN1198

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.04

EN300-1425608_1_1_1



CID: EN300-1425608_1_1_1

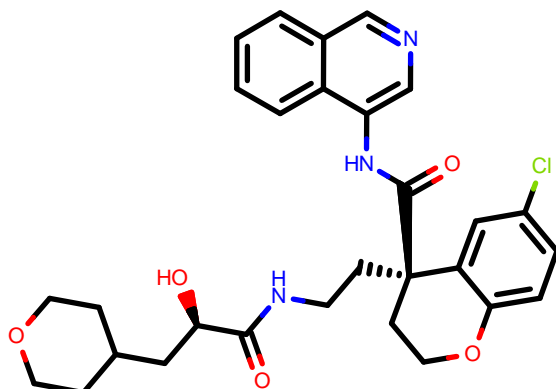
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)c3ccc(Cl)cc3C(=O)N5C[C@H](C)C5OCCO

RUN: RUN6429

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.33

EN300-1452069_3_1_1



CID: EN300-1452069_3_1_1

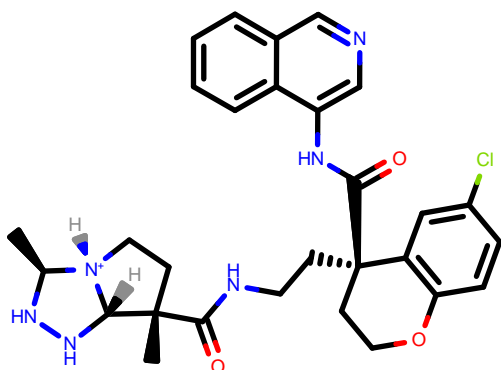
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)c3ccc(Cl)cc3C(=O)N[C@@H](CC)C4OCCO4

RUN: RUN5889

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.43

EN300-7431629_3_2_1



CID: EN300-7431629_3_2_1

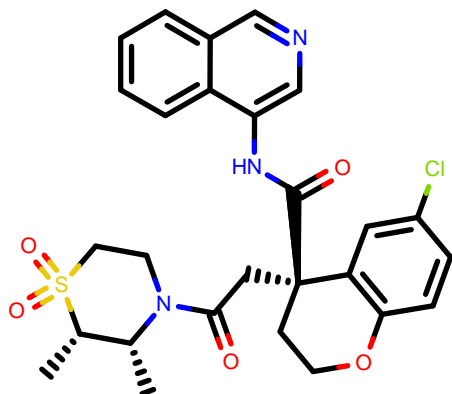
SMILES: C[C@@H]1N[C@@H]2N[C@@H]1CC[C@@H]2C(=O)N[C@@H](C)C(=O)c3ccc(Cl)cc3C(=O)N4C5CCNCC5

RUN: RUN3205

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.69

EN300-80940_1_1_1



CID: EN300-80940_1_1_1

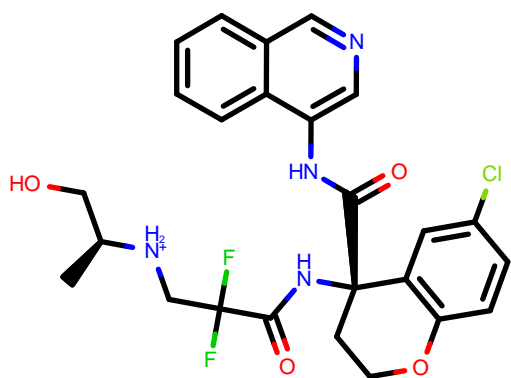
SMILES: C[C@@H]1[C@@H](C)N[C@@H](S(=O)(=O)C)C1N[C@@H](C)C(=O)N[C@@H](C)C(=O)c2ccc(Cl)cc2

RUN: RUN3490

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.31

EDG-MED-90036822-39_1



CID: EDG-MED-90036822-39_1

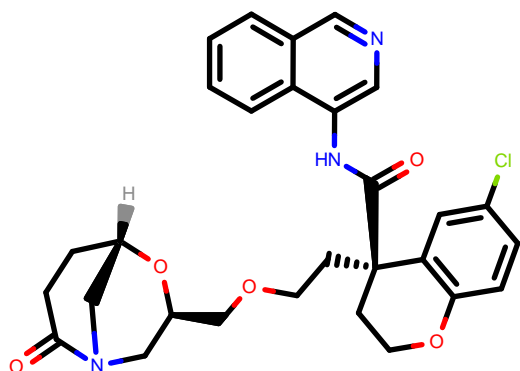
SMILES: C[C@@H](CO)NCC(C(=O)N[C@@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)F

RUN: RUN1621

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.32

EN300-2008102_3_2_1



CID: EN300-2008102_3_2_1

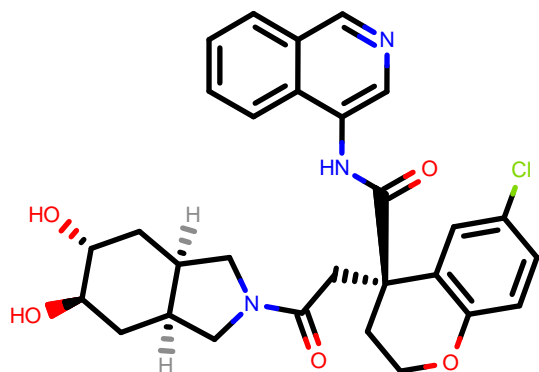
SMILES: c1ccc2c(c1)ncnc2N[C@@H](C(=O)N[C@@H]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c3cccc6)O

RUN: RUN6280

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.44

EN300-7355477_1_3_1



CID: EN300-7355477_1_3_1

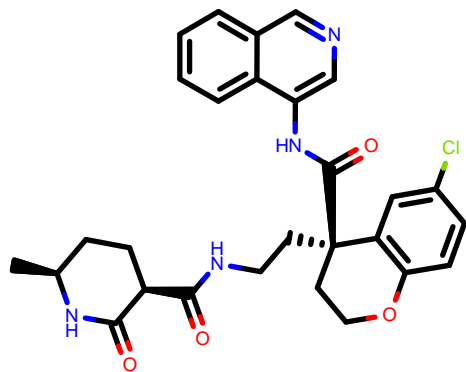
SMILES: c1ccc2c(c1)ncnc2N[C@@H](C(=O)N[C@@H]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncoc6c3cccc6)O

RUN: RUN6757

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.30

EN300-6505003_3_4_1



CID: EN300-6505003_3_4_1

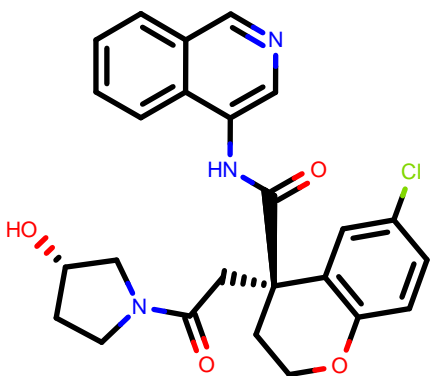
SMILES: C[C@@H]1CC[C@@H](C(=O)N1)C(=O)NCC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4cccc5

RUN: RUN4649

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.35

EN300-69312_1_1_1



CID: EN300-69312_1_1_1

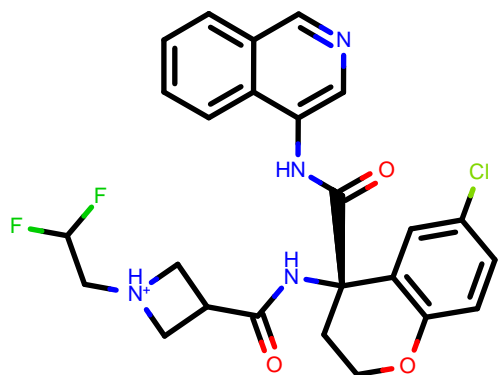
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)O

RUN: RUN7405

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.25

EDG-MED-90036822-64_1



CID: EDG-MED-90036822-64_1

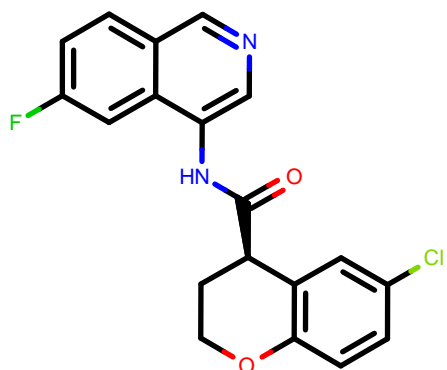
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CN(C5)C(F)F

RUN: RUN1649

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.26

ALP-POS-ce760d3f-7_1



CID: ALP-POS-ce760d3f-7_1

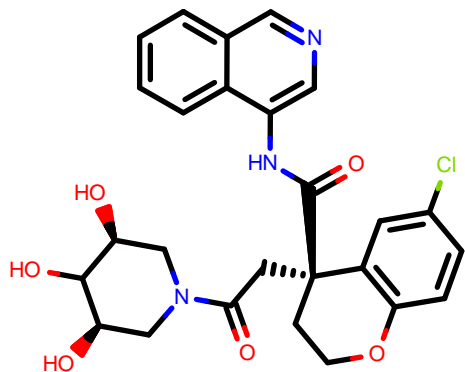
SMILES: c1cc2cnc(c2cc1F)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C1

RUN: RUN1300

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.04

EN300-299920_1_1_1



CID: EN300-299920_1_1_1

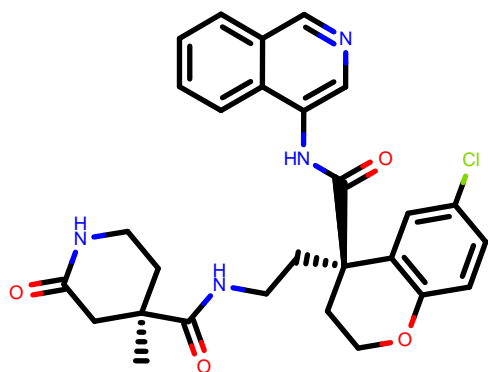
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C5)O

RUN: RUN5485

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.45

EN300-315854_3_2_1



CID: EN300-315854_3_2_1

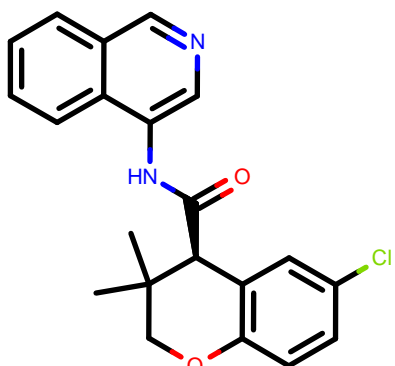
SMILES: C[C@@]1(CCN(C=O)C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN7089

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-3_1_1



CID: DAR-DIA-0d514e7d-3_1_1

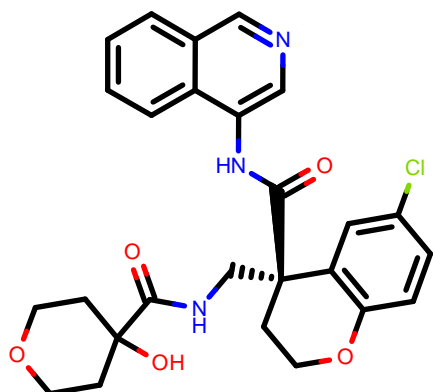
SMILES: CC1(COc2ccc(cc2[C@@]1C(=O)Nc3cnc4c3cccc4)Cl)C

RUN: RUN7167

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.22

EN300-69368_2_1_1



CID: EN300-69368_2_1_1

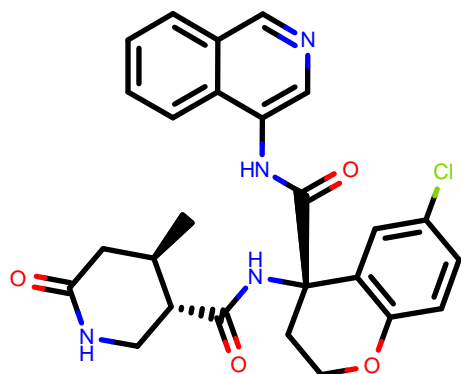
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COCCO5)O

RUN: RUN6903

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.32

EN300-95698_1_3_1



CID: EN300-95698_1_3_1

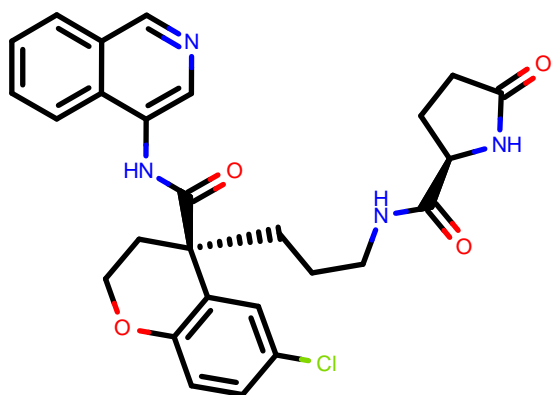
SMILES: C[C@@]1(CCN(C=O)N[C@@]1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN2853

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.22

EN300-54541_4_1_1



CID: EN300-54541_4_1_1

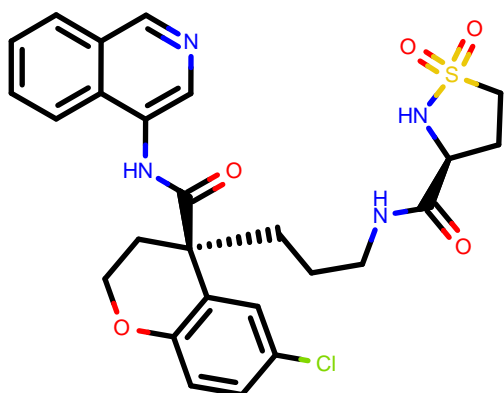
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN6638

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.34

EN300-45049_4_1_1



CID: EN300-45049_4_1_1

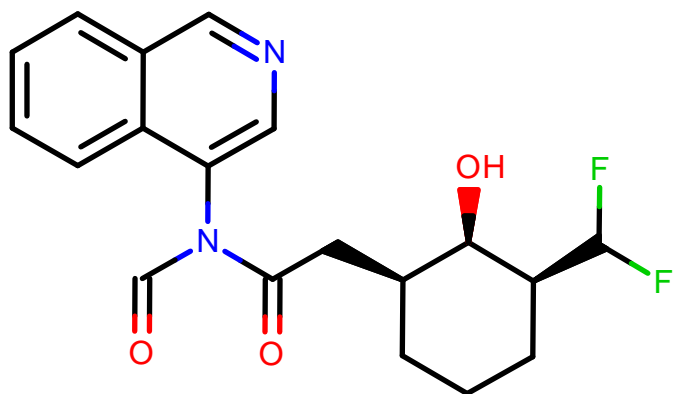
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5SCCS(=O)(=O)N5

RUN: RUN7572

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.34

MAK-UNK-c749d764-28_1



CID: MAK-UNK-c749d764-28_1

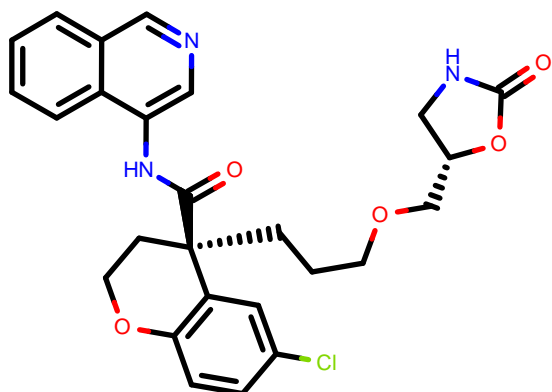
SMILES: c1ccc2c(c1)ncnc2N(C=O)C(=O)C[C@@H]3CCCC[C@@H]3[C@@H]3O[C@F]F

RUN: RUN1004

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.35

EN300-203293_4_1_1



CID: EN300-203293_4_1_1

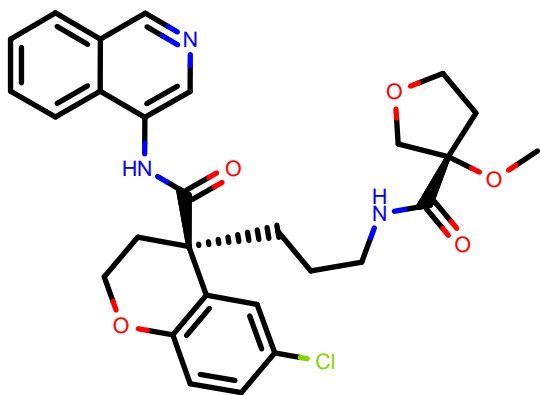
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CNCO5

RUN: RUN4677

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.36

EN300-174668_4_2_1



CID: EN300-174668_4_2_1

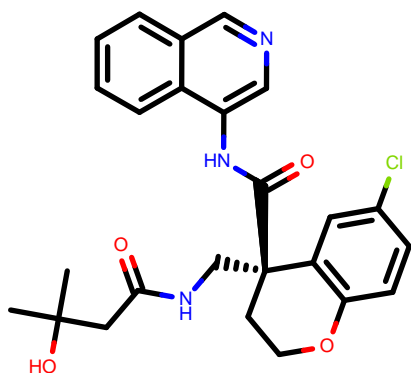
SMILES: CO[C@]1(COC1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5012

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.40

EN300-117931_2_1_1



CID: EN300-117931_2_1_1

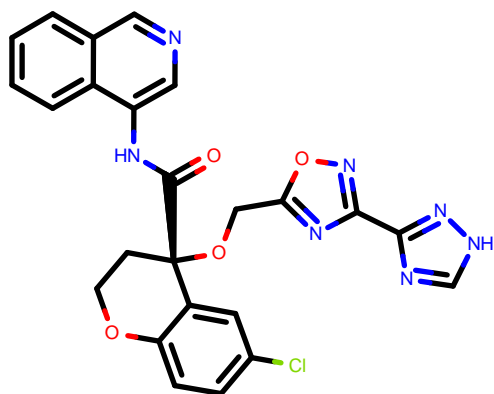
SMILES: CC(C)(CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN7187

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.26

EN300-92031_1_1_1



CID: EN300-92031_1_1_1

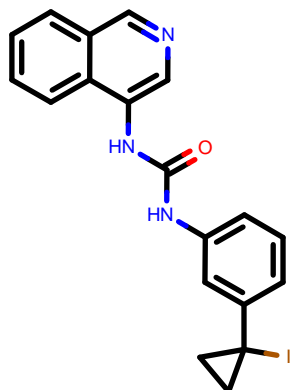
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(nc5)c6[nH]nnc6

RUN: RUN4704

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.26

DAR-DIA-0cde14eb-53_1



CID: DAR-DIA-0cde14eb-53_1

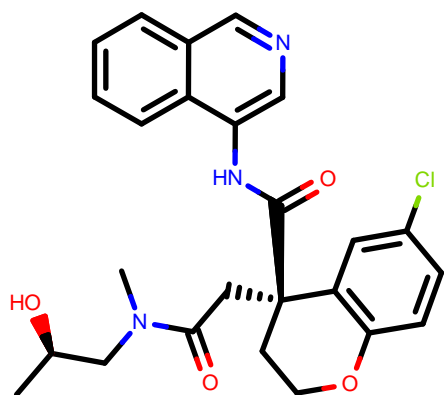
SMILES: c1ccc2c(c1)cncc2NC(=O)Nc3cccc(c3)C4(CC4)I

RUN: RUN5

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.34

EN300-209068_1_1_1



CID: EN300-209068_1_1_1

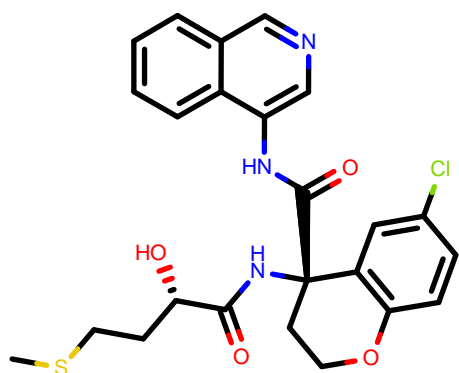
SMILES: C[C@@H](CN(C)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5663

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.30

EN300-103144_1_1_1



CID: EN300-103144_1_1_1

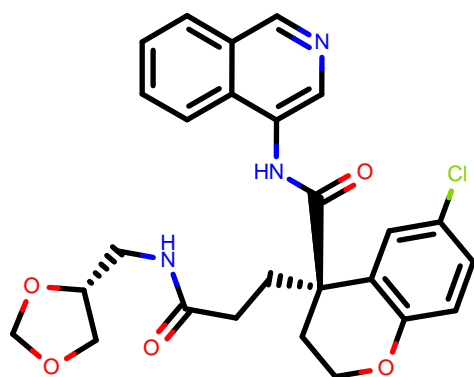
SMILES: CSCC[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN5969

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.29

EN300-253187_2_1_1



CID: EN300-253187_2_1_1

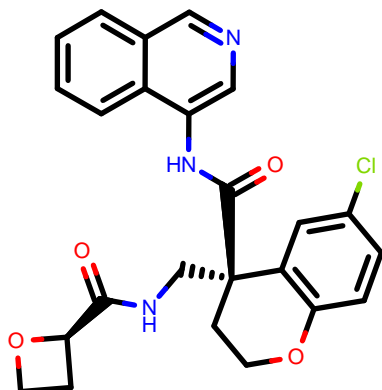
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H]5COC5O

RUN: RUN7445

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.28

EN300-85760_2_2_1



CID: EN300-85760_2_2_1

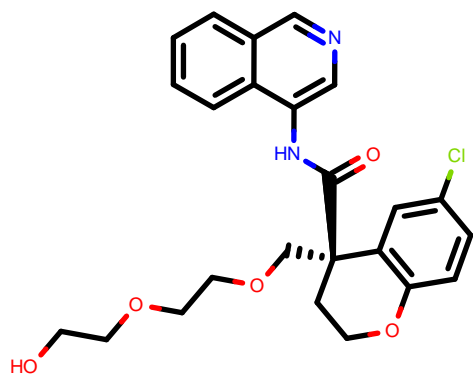
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COC5O

RUN: RUN5168

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.20

EN300-52467_2_1_1



CID: EN300-52467_2_1_1

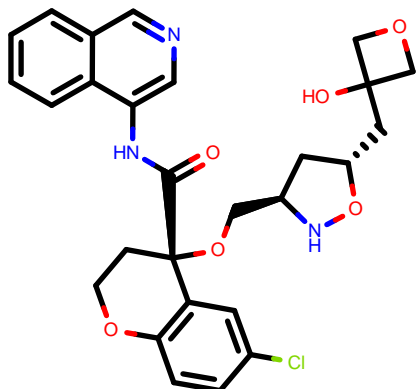
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCOCO

RUN: RUN4976

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.25

EN300-7457160_1_2_2



CID: EN300-7457160_1_2_2

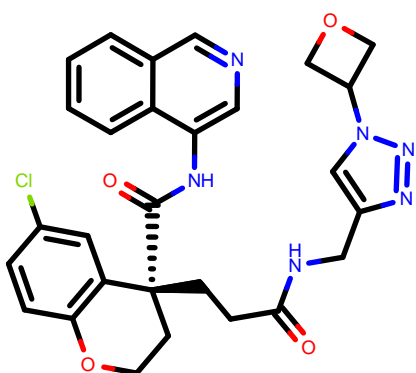
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[C@@H]6O5COC6O

RUN: RUN5669

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.36

EN300-1709745_2_1_1



CID: EN300-1709745_2_1_1

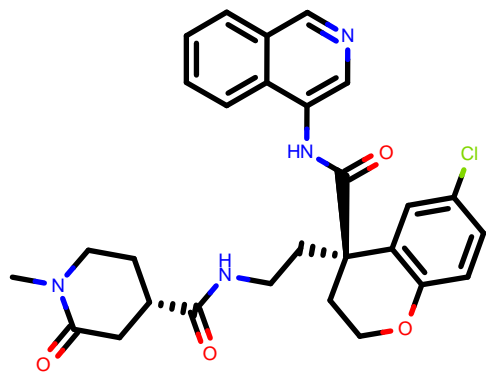
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cn(nn5)C6OC6

RUN: RUN5715

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.24

EN300-30458_3_1_1



CID: EN300-30458_3_1_1

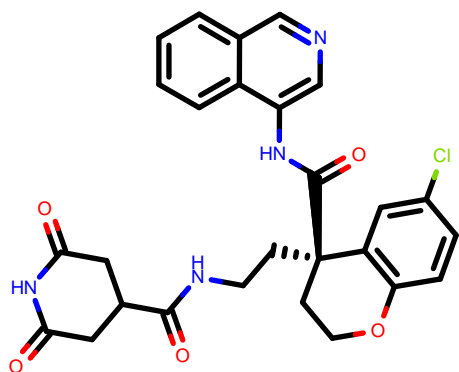
SMILES: CN1CC[C@@H](CC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c54cccc5

RUN: RUN7191

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.28

EN300-62192_3_1_1



CID: EN300-62192_3_1_1

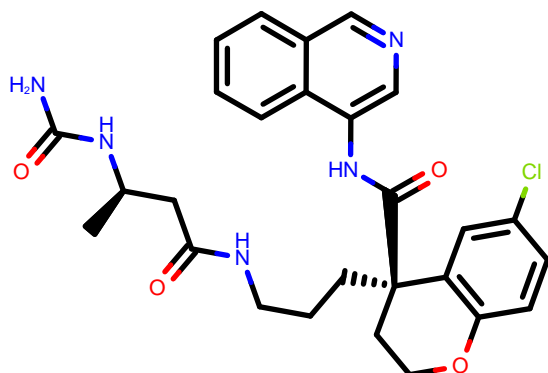
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCNC(=O)C5CC(=O)NC(=O)C5

RUN: RUN7805

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.33

EN300-268198_4_2_1



CID: EN300-268198_4_2_1

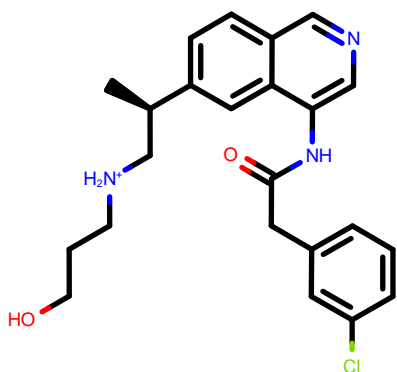
SMILES: C[C@H](CC(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4)NC(=O)N

RUN: RUN7778

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.35

MAK-UNK-ffc90da7-6_2



CID: MAK-UNK-ffc90da7-6_2

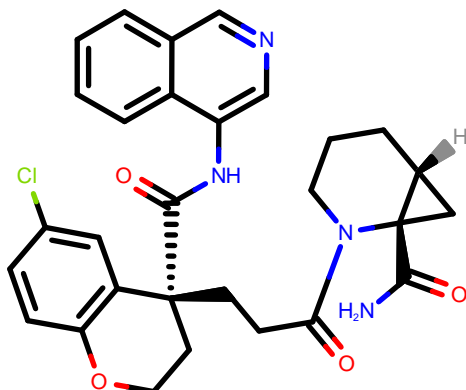
SMILES: C[C@H](C)[C](NH2+)[CCCO]c1ccc2nccc(c2c1)NC(=O)Cc3ccc(c3)Cl

RUN: RUN615

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.41

EN300-817777_2_1_1



CID: EN300-817777_2_1_1

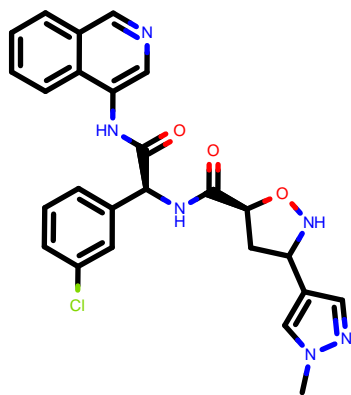
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)N5CC[C@H](C@)5(C)C1(=O)N

RUN: RUN6499

DDG (kcal/mol): -0.23

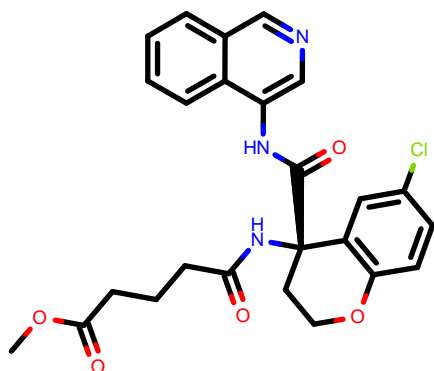
dDDG (kcal/mol): 0.31

EDJ-MED-ee07cf00-6_1



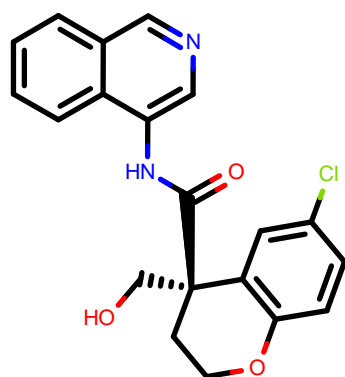
CID:	EDJ-MED-ee07cf00-6_1
SMILES:	<chem>Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@@H](c3ccccc3)C(=O)Nc4nccc5c4ccccc5</chem>
RUN:	RUN2670
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.48

EN300-24804_1_1_1



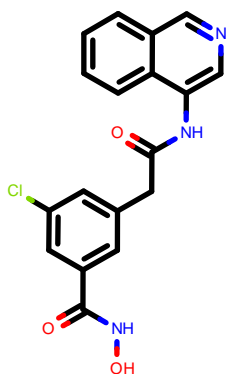
CID:	EN300-24804_1_1_1
SMILES:	<chem>COC(=O)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4</chem>
RUN:	RUN5700
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.21

EDG-MED-971238d3-2_1



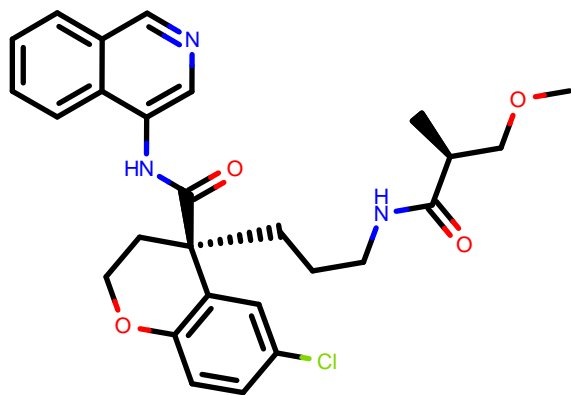
CID:	EDG-MED-971238d3-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO</chem>
RUN:	RUN1288
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.14

RAL-THA-1d44ff04-13_1



CID:	RAL-THA-1d44ff04-13_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(=O)NO</chem>
RUN:	RUN389
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.29

EN300-69162_4_1_1



CID: EN300-69162_4_1_1

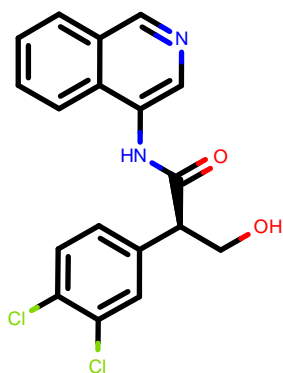
SMILES: C[C@@H](COC)C(=O)NCCC[C@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN6803

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.32

MAT-POS-fce787c2-11_1



CID: MAT-POS-fce787c2-11_1

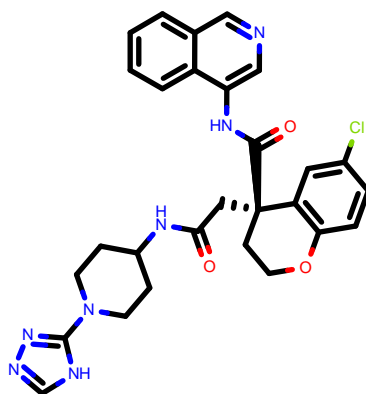
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](CO)c3ccc(c(c3)Cl)Cl

RUN: RUN1981

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EDJ-MED-d203f206-28_1



CID: EDJ-MED-d203f206-28_1

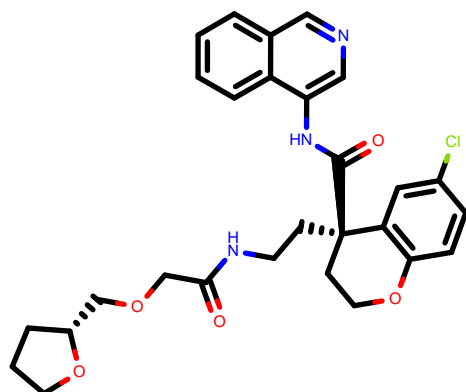
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CCN(CC5)c6[nH]nc6

RUN: RUN2446

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.29

EN300-60033_3_2_1



CID: EN300-60033_3_2_1

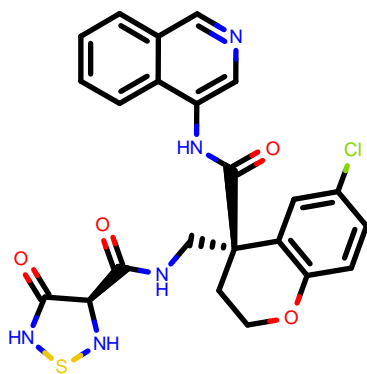
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@H]5CCCO5

RUN: RUN3813

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.31

EN300-261859_2_1_1



CID: EN300-261859_2_1_1

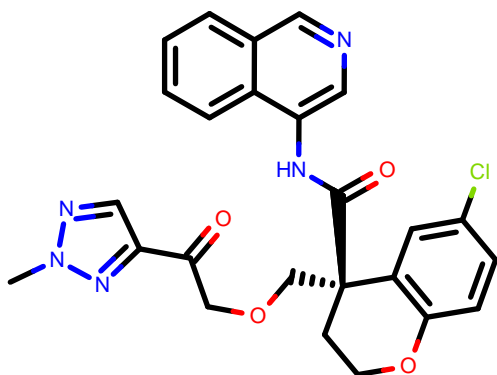
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C(=O)NSN5

RUN: RUN6360

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EN300-204935_2_1_1



CID: EN300-204935_2_1_1

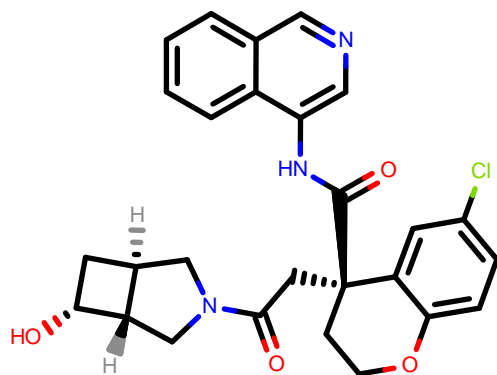
SMILES: Cn1ncc(n1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN7711

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-305294_1_7_1



CID: EN300-305294_1_7_1

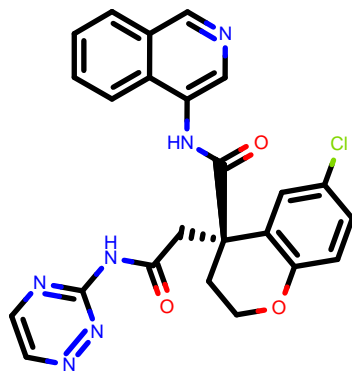
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H]7[C@@H]8C5O

RUN: RUN6394

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EDJ-MED-d203f206-18_1



CID: EDJ-MED-d203f206-18_1

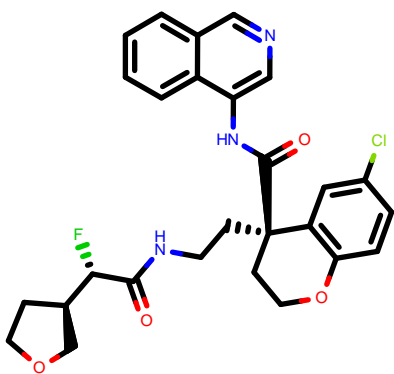
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nccn5

RUN: RUN2412

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EN300-783124_3_2_1



CID: EN300-783124_3_2_1

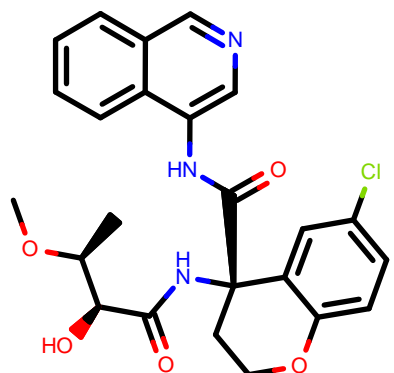
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C@H]([C@@H]5CCOC5)F

RUN: RUN6488

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-220194_1_1_1



CID: EN300-220194_1_1_1

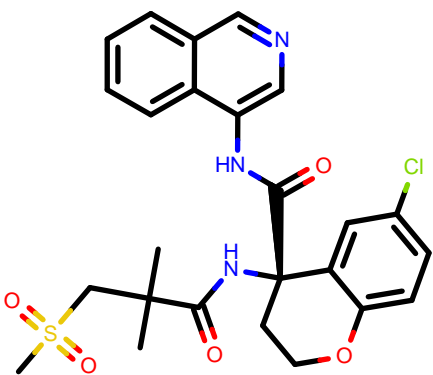
SMILES: C[C@@H]([C@@H]([C@@H](C=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)O)OC

RUN: RUN5324

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.29

EN300-188217_1_1_1



CID: EN300-188217_1_1_1

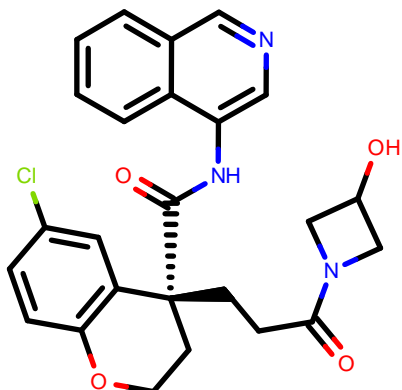
SMILES: CC(C)(CS(=O)(=O)C(=O)N[C@@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4

RUN: RUN6231

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-65115_2_1_1



CID: EN300-65115_2_1_1

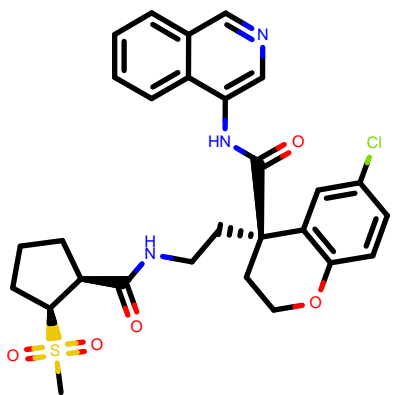
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC(C5)O

RUN: RUN7198

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

EN300-1387145_3_4_1



CID: EN300-1387145_3_4_1

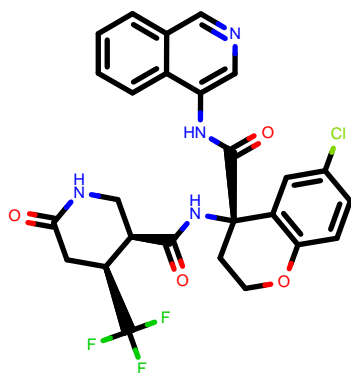
SMILES: CS(=O)(=O)C@H1CC[C@@H]1C(=O)NC[C@@]2(COC3C2cc(c3)C)C1=O)N4nc5c4ccc5

RUN: RUN5600

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.36

EN300-208959_1_1_1



CID: EN300-208959_1_1_1

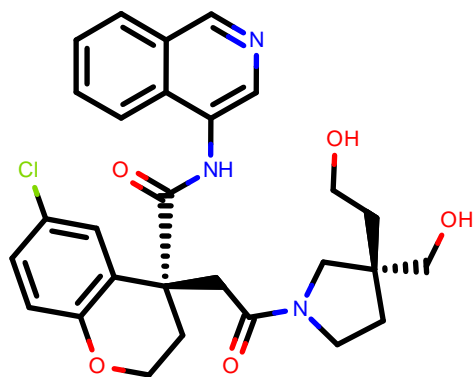
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3cc(c4)O)NC(=O)C[C@@]5H5C(F)(F)F

RUN: RUN6524

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.29

EN300-1707870_1_1_1



CID: EN300-1707870_1_1_1

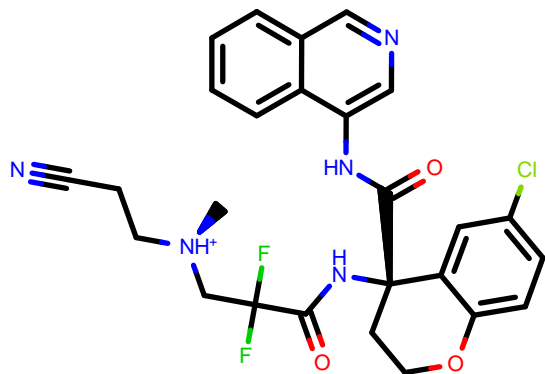
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COC4C3cc(c4)O)C(=O)N5CC[C@@]5(C)C(O)CO

RUN: RUN7635

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.43

EDG-MED-90036822-92_1



CID: EDG-MED-90036822-92_1

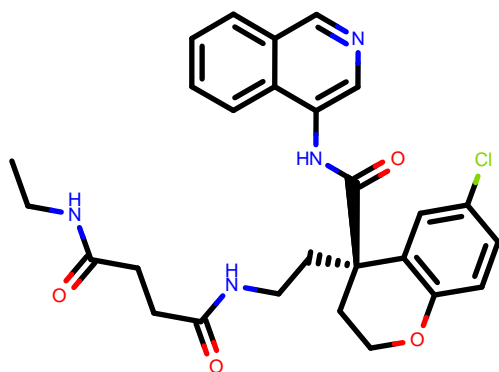
SMILES: C[N+]([C@@]1CCN)CC(C(=O)N[C@@]1(C)COC2c1cc(cc2)C)C(=O)Nc3nc4c3ccc4(F)F

RUN: RUN1737

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.33

EN300-68889_3_1_1



CID: EN300-68889_3_1_1

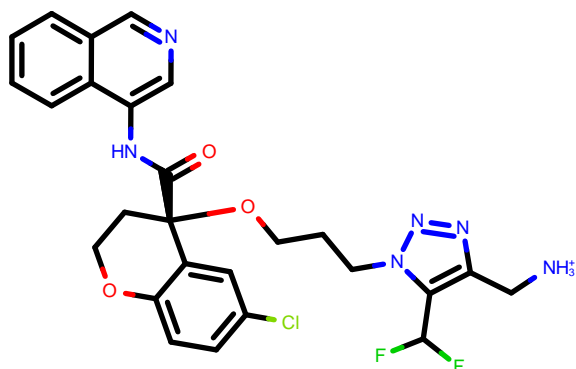
SMILES: CCNC(=O)CCC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN6164

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.30

ED_-GRI-5b13fbe2-54_1



CID: ED_-GRI-5b13fbe2-54_1

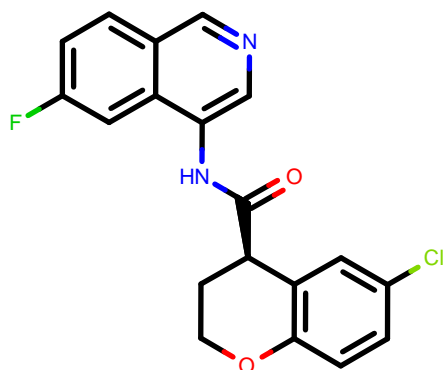
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCCc5c(c1n5)C[NH3+](F)F

RUN: RUN1523

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.39

ALP-POS-696356e4-1_1_1



CID: ALP-POS-696356e4-1_1_1

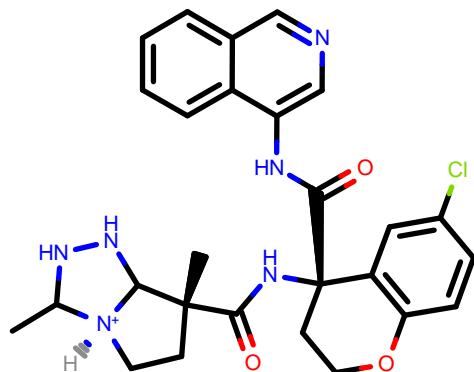
SMILES: c1cc2cnc(c2cc1F)NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)

RUN: RUN7511

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.04

EN300-7431629_1_1_1



CID: EN300-7431629_1_1_1

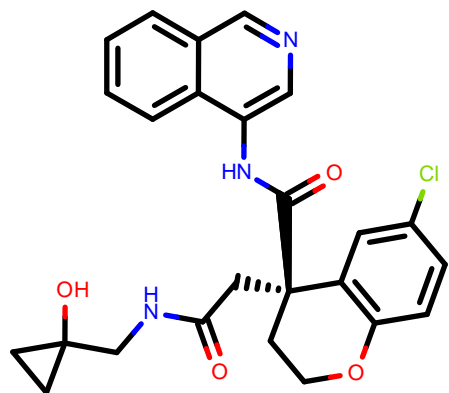
SMILES: Cc1nc2n1CC[C@@H]2(C)C(=O)N[C@@H]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5ccc6

RUN: RUN3742

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-1644703_1_1_1



CID: EN300-1644703_1_1_1

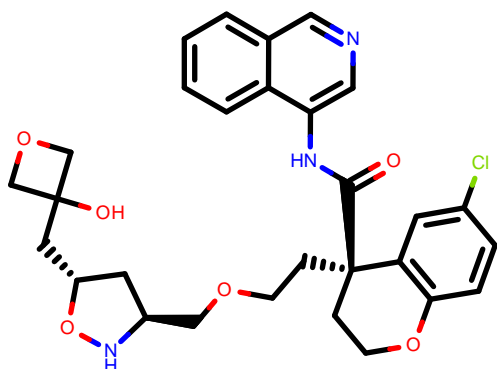
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)CC(=O)NCC5(C)CC5)O

RUN: RUN6555

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.24

EN300-7457160_3_1_1



CID: EN300-7457160_3_1_1

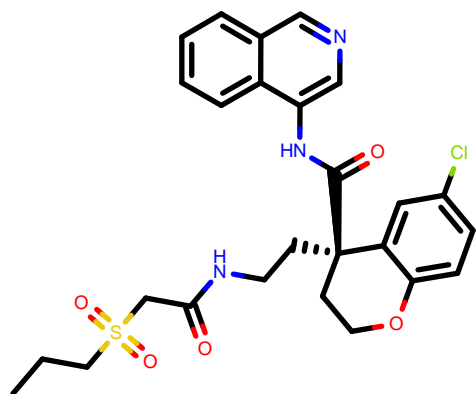
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)C1COC[C@@H]5C[C@@H](O)CC5)O

RUN: RUN3966

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.40

EN300-52325_3_1_1



CID: EN300-52325_3_1_1

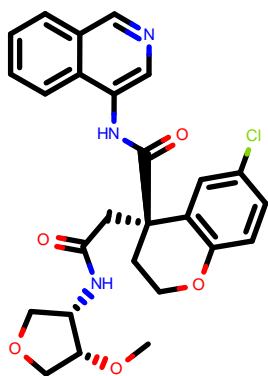
SMILES: CCCS(=O)(=O)CC(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4457

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.46

EN300-252683_1_1_1



CID: EN300-252683_1_1_1

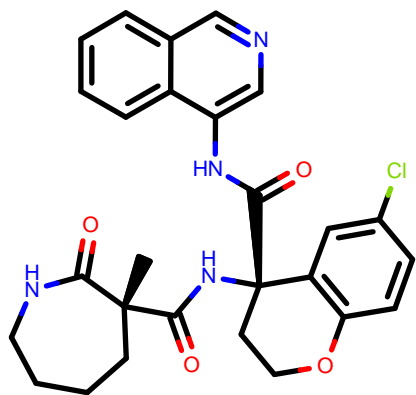
SMILES: CO[C@@H]1COC[C@@H]1NC(=O)[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN4566

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.26

EN300-6745081_1_2_1



CID: EN300-6745081_1_2_1

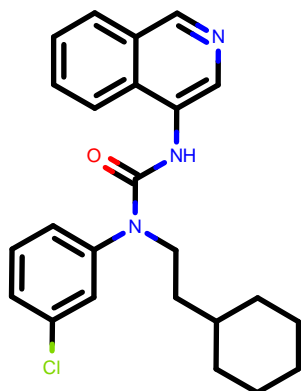
SMILES: C[C@]1(CCCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN5698

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.26

VLA-UCB-05e51b3f-14_1



CID: VLA-UCB-05e51b3f-14_1

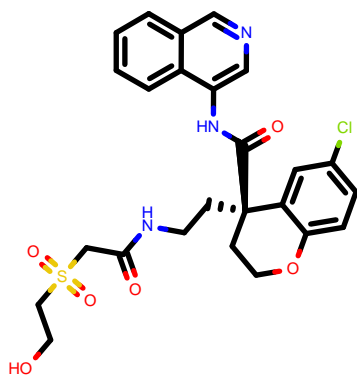
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cccc(c4)Cl

RUN: RUN295

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.34

EN300-4293814_3_1_1



CID: EN300-4293814_3_1_1

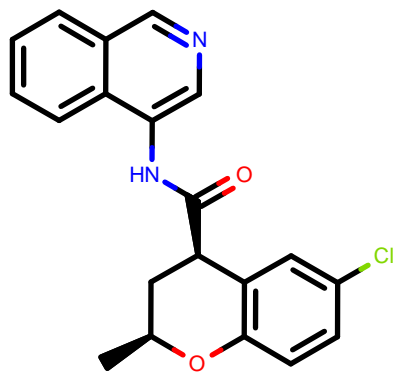
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)CCO

RUN: RUN3104

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.50

ALP-POS-d3acb8cc-1_1_1



CID: ALP-POS-d3acb8cc-1_1_1

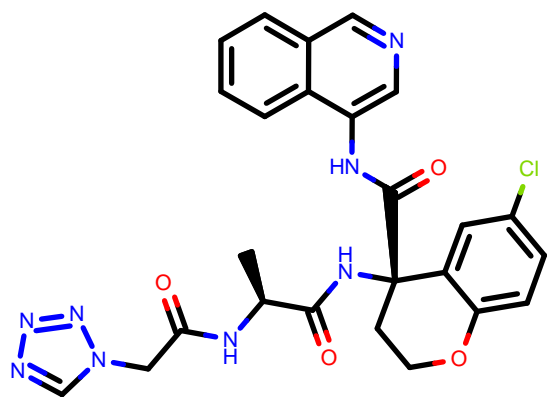
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN5524

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.09

EN300-651177_1_1_1



CID: EN300-651177_1_1_1

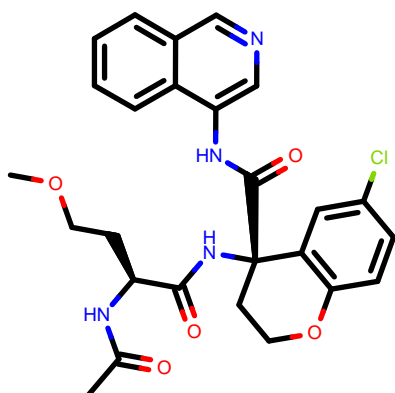
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)Cn5nnn5

RUN: RUN6842

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.37

EN300-62074_1_1_1



CID: EN300-62074_1_1_1

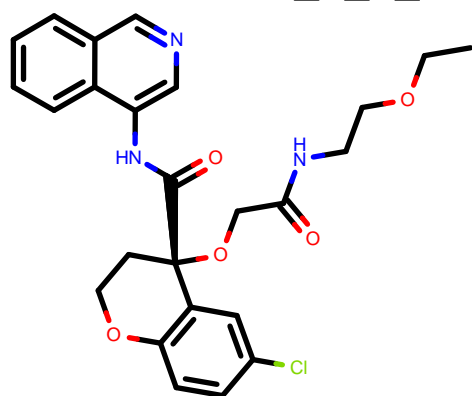
SMILES: CC(=O)N[C@@H](COC)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4278

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.28

EN300-103187_1_1_1



CID: EN300-103187_1_1_1

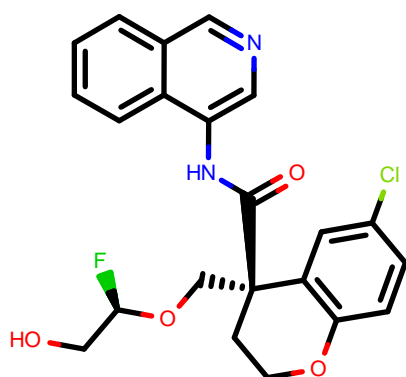
SMILES: CCOCCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5563

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.22

EN300-861925_2_1_1



CID: EN300-861925_2_1_1

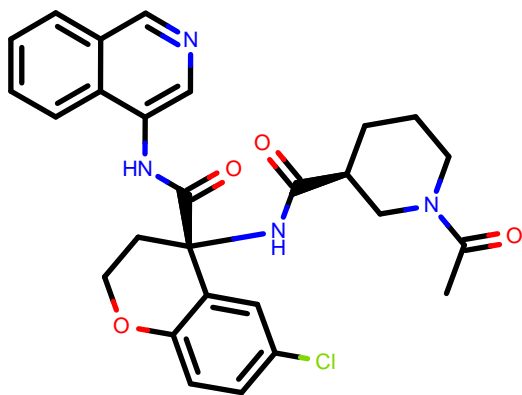
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H](CO)F

RUN: RUN7310

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.24

EN300-14752_1_1_1



CID: EN300-14752_1_1_1

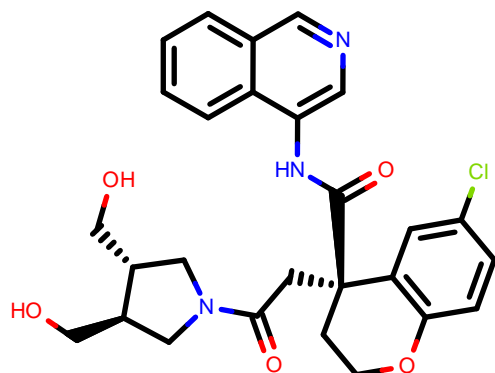
SMILES: CC(=O)N1CCC[C@@H](C1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN2739

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.16

EN300-314088_1_1_1



CID: EN300-314088_1_1_1

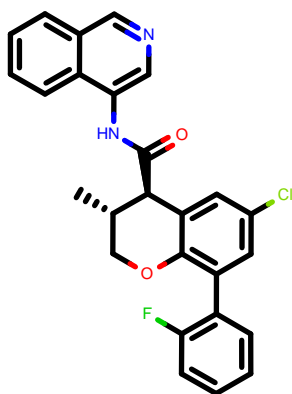
SMILES: c1ccc2c(e1)ncoc2NCl(O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@@H](C5)CO[CO]

RUN: RUN5707

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

DAR-DIA-0d514e7d-16_1



CID: DAR-DIA-0d514e7d-16_1

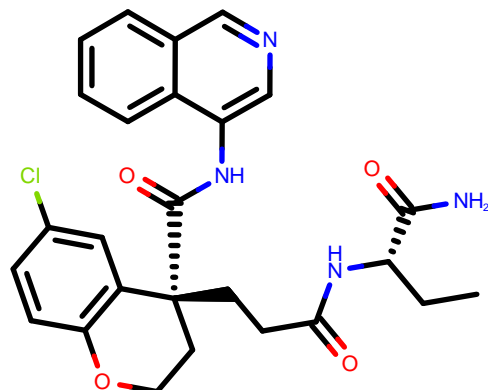
SMILES: C[C@@H]1COc2c(cc(cc2[C@@]3(CO)Nc3nccc4c3cccc4)Cl)c5ccccc5F

RUN: RUN796

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.21

EN300-7375395_2_1_1



CID: EN300-7375395_2_1_1

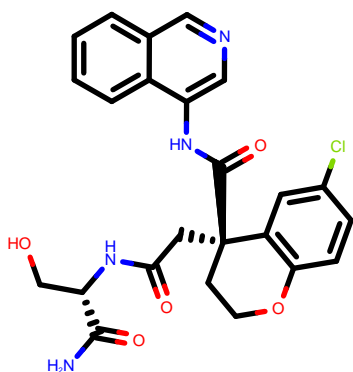
SMILES: CC[C@@H](C(=O)N)N[C(=O)CC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN7371

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-208204_1_1_1



CID: EN300-208204_1_1_1

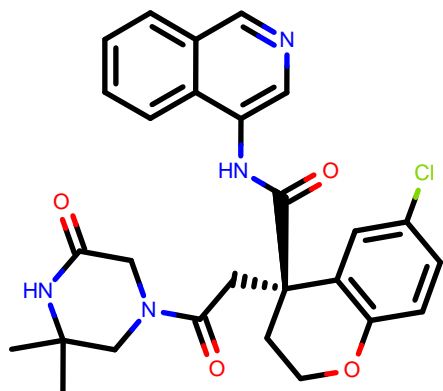
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)C(=O)N

RUN: RUN6233

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-7493939_1_1_1



CID: EN300-7493939_1_1_1

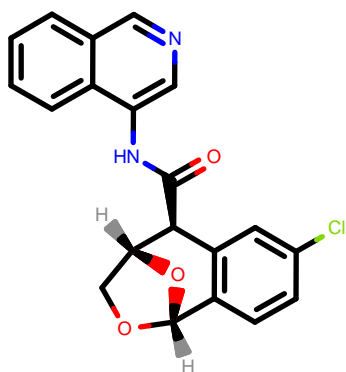
SMILES: CC1(CN(CC(=O)N1)C(=O)C)C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN4797

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

RAL-THA-c9f97604-2_1



CID: RAL-THA-c9f97604-2_1

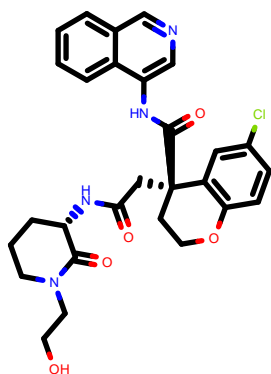
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4[C@@H]5OC[C@H]3O5)Cl

RUN: RUN457

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.21

EN300-141480_1_2_1



CID: EN300-141480_1_2_1

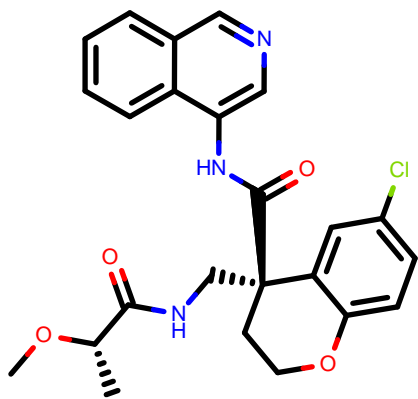
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCN(C5=O)CCO

RUN: RUN6338

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.33

EN300-51257_2_1_1



CID: EN300-51257_2_1_1

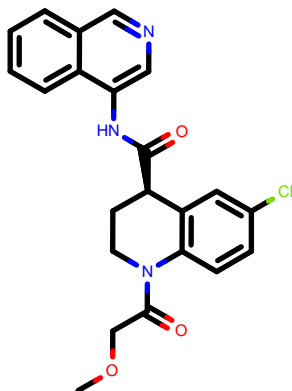
SMILES: C[C@@H](C(=O)NC[C@@H]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccc4)OC

RUN: RUN5473

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

RAL-THA-4aa06b95-5_2



CID: RAL-THA-4aa06b95-5_2

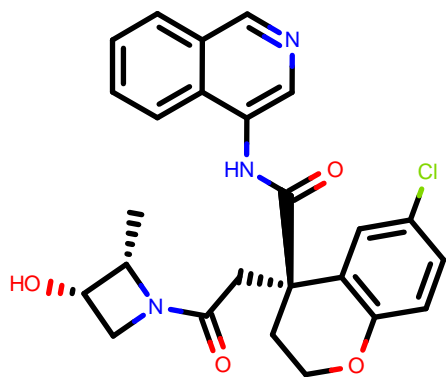
SMILES: COCC(=O)N1CC[C@H](c2c1ccc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN1169

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-7471076_1_4_1



CID: EN300-7471076_1_4_1

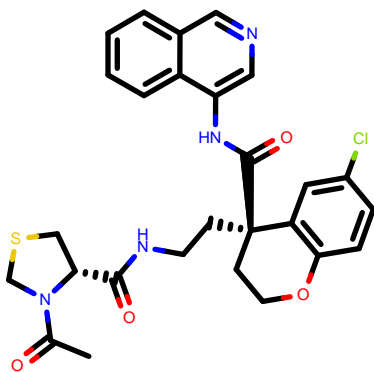
SMILES: C[C@H]1[C@H](CN1C(=O)C[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN5724

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

EN300-761220_3_1_1



CID: EN300-761220_3_1_1

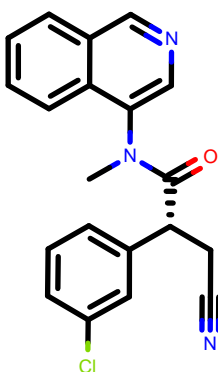
SMILES: CC(=O)N1CSC[C@@H]1C(=O)NCC[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccc5

RUN: RUN3659

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.31

JOH-UNI-3fc3434e-7_2



CID: JOH-UNI-3fc3434e-7_2

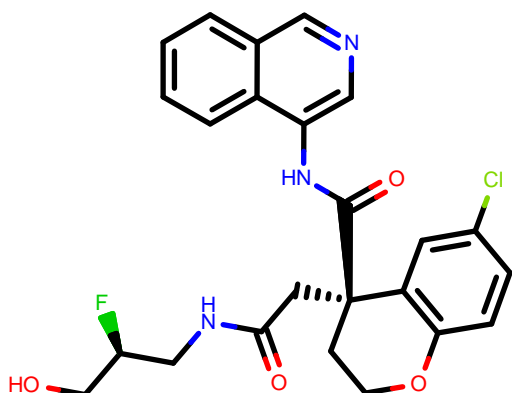
SMILES: CN(c1cncc2c1cccc2)C(=O)[C@H](CC#N)c3cccc(c3)Cl

RUN: RUN1778

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.23

EN300-7353973_1_1_1



CID: EN300-7353973_1_1_1

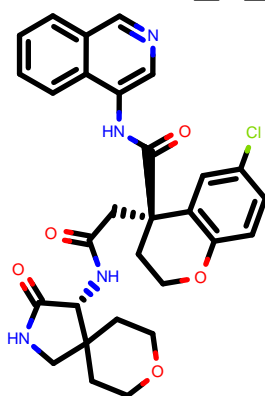
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC(C@H)(CO)F

RUN: RUN6458

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-310254_1_2_1



CID: EN300-310254_1_2_1

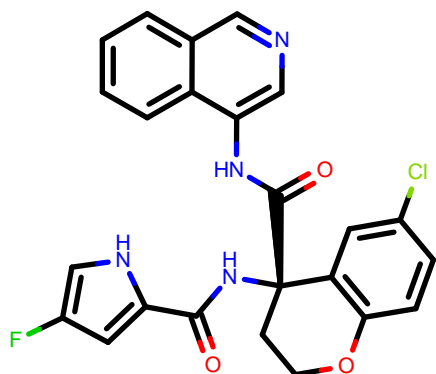
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC(C@H)5C(=O)NCC56CCCC6

RUN: RUN7716

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.45

EDG-MED-90036822-107_1



CID: EDG-MED-90036822-107_1

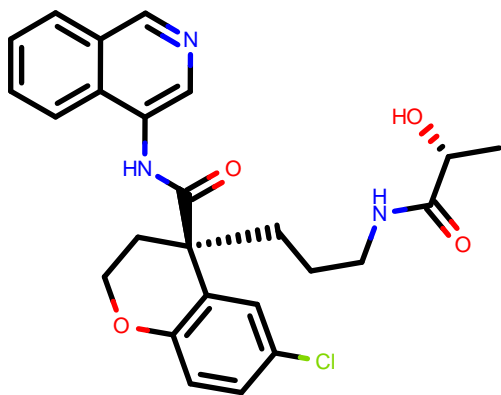
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(c(nH)5)F

RUN: RUN1694

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.21

EN300-19542_4_2_1



CID: EN300-19542_4_2_1

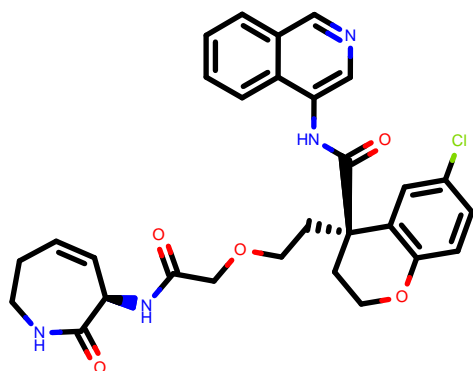
SMILES: C[C@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3ccc4)O

RUN: RUN3750

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.34

EN300-37195_3_1_1



CID: EN300-37195_3_1_1

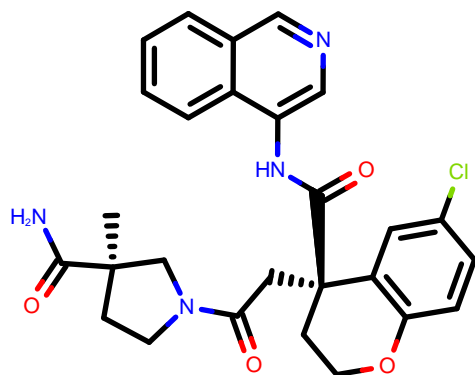
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)COC(=O)N[C@@]5C5CCCN5=O

RUN: RUN4744

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-194442_1_2_1



CID: EN300-194442_1_2_1

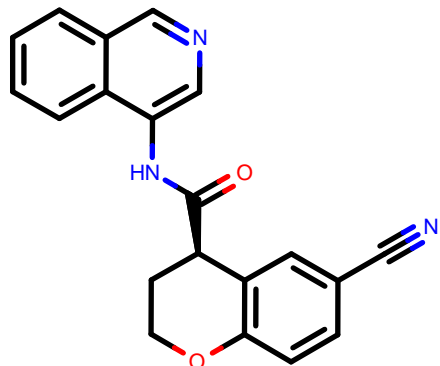
SMILES: C[C@]1(CCN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)O)C(=O)Nc4cncc5c4ccc5)C(=O)N

RUN: RUN4750

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.36

DAR-DIA-6a508060-3_1_1



CID: DAR-DIA-6a508060-3_1_1

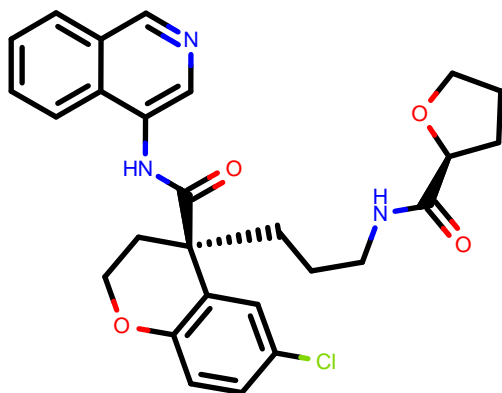
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C#N)C(=O)N

RUN: RUN6892

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.05

EN300-104395_4_1_1



CID: EN300-104395_4_1_1

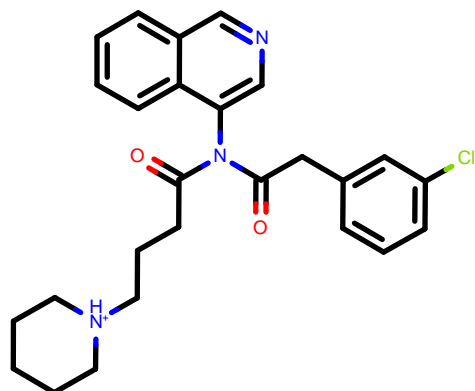
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@H]5CCCCO5

RUN: RUN6115

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

DAR-DIA-076fb6ea-12_1



CID: DAR-DIA-076fb6ea-12_1

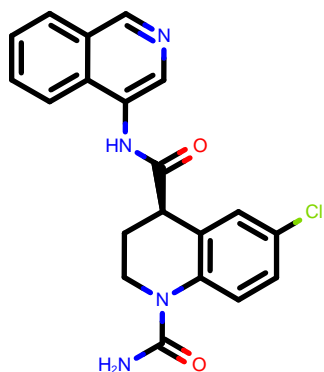
SMILES: c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)C=C/C[NH+]4CCCCC4

RUN: RUN1309

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.64

RAL-THA-4aa06b95-1_1



CID: RAL-THA-4aa06b95-1_1

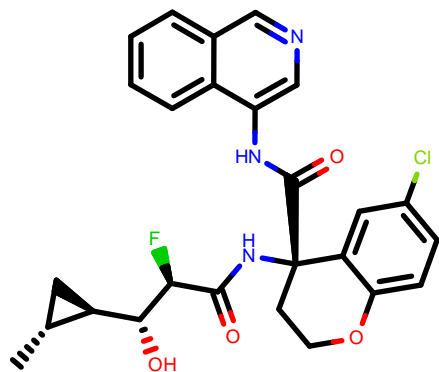
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)C(=O)N

RUN: RUN1120

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.25

EDG-MED-90036822-94_15



CID: EDG-MED-90036822-94_15

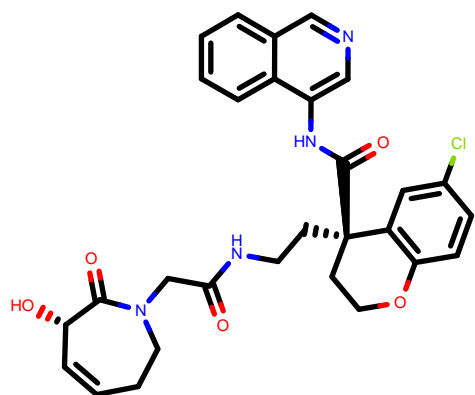
SMILES: C[C@@H]1[C@H]2[C@@H]3[C@H]4[C@@H]5C(=O)NC(=O)C3CCc2cc(cc2Cl)C1=O[N+]6CCCC5F6O

RUN: RUN1680

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-259849_3_1_1



CID: EN300-259849_3_1_1

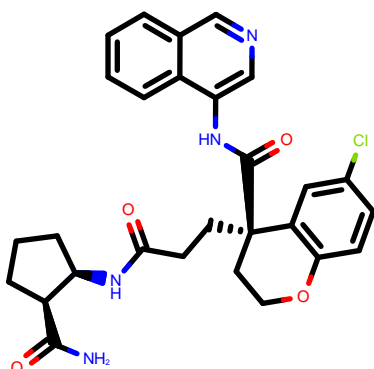
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc4)C)CNC(=O)CN5CCCC[C@@H]5C5=O

RUN: RUN4231

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.38

EN300-90531_2_1_1



CID: EN300-90531_2_1_1

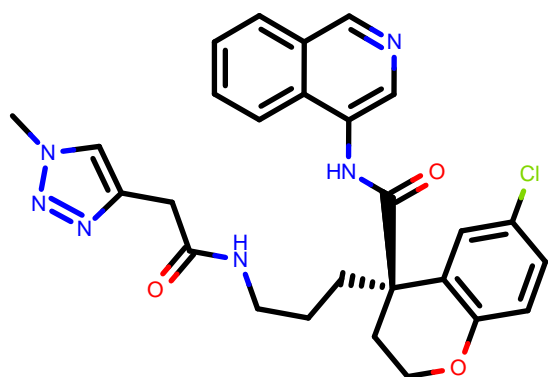
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc4)C)CNC(=O)N5CCCC[C@@H]5C5=O

RUN: RUN6434

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.38

EN300-1073264_4_1_1



CID: EN300-1073264_4_1_1

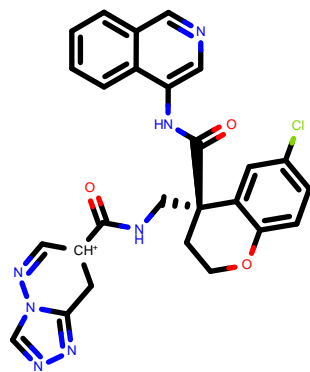
SMILES: Cn1cc(nn1)CC(=O)NCCC[C@@H]2(CCOc3cc2cc3)C)C(=O)Nc4ccc5cc4ccc5

RUN: RUN6854

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.36

ALP-UNI-0676e700-15_1



CID: ALP-UNI-0676e700-15_1

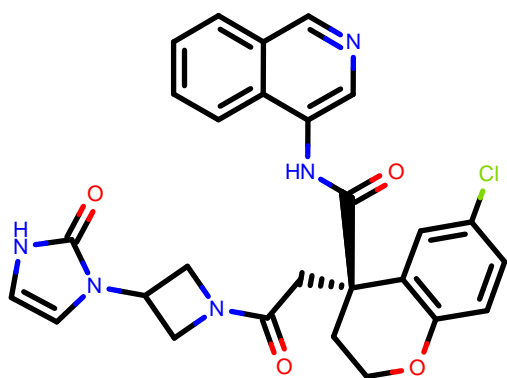
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4cc3cc4)C)CNC(=O)c5c6nnn6nc5

RUN: RUN2311

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.29

EN300-208993_1_1_1



CID: EN300-208993_1_1_1

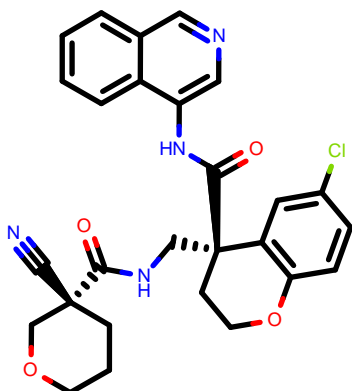
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)N6CCNC6=O

RUN: RUN5667

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.25

EN300-301925_2_1_1



CID: EN300-301925_2_1_1

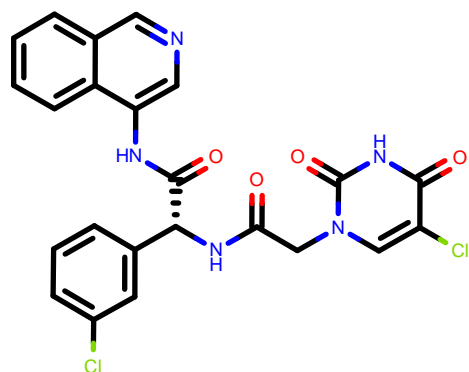
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN3535

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.25

EDJ-MED-ee07cf00-16_1



CID: EDJ-MED-ee07cf00-16_1

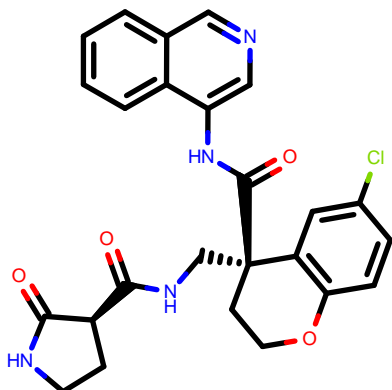
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)Cn4cc(c(=O)[nH]4)=OCl

RUN: RUN2673

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.47

EN300-94945_2_2_1



CID: EN300-94945_2_2_1

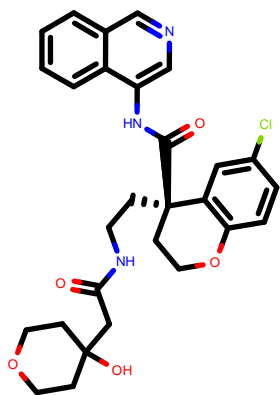
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5CNCNC5=O

RUN: RUN6239

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.24

EN300-151423_3_1_1



CID: EN300-151423_3_1_1

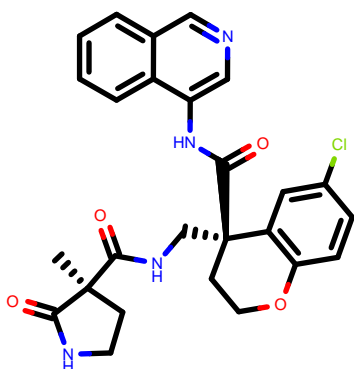
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOc4c3cc(cc4)C)CCNC(=O)CC5(CCCOCC5)O

RUN: RUN2869

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.35

EN300-207959_2_1_1



CID: EN300-207959_2_1_1

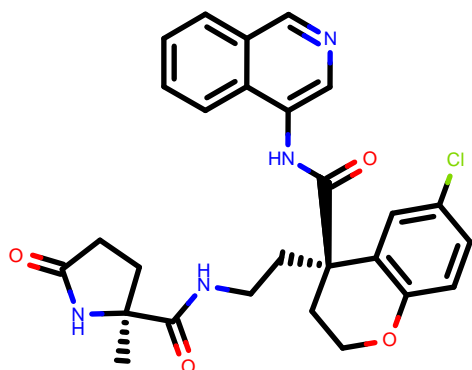
SMILES: C[C@@H]1(CCNC1=O)C(=O)N[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccoc5

RUN: RUN5014

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-370280_3_1_1



CID: EN300-370280_3_1_1

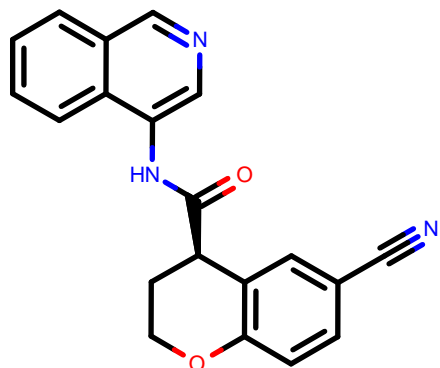
SMILES: C[C@@H]1(CCC(=O)N1)C(=O)N[C@@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccoc5

RUN: RUN4474

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

RAL-THA-05e671eb-7_1



CID: RAL-THA-05e671eb-7_1

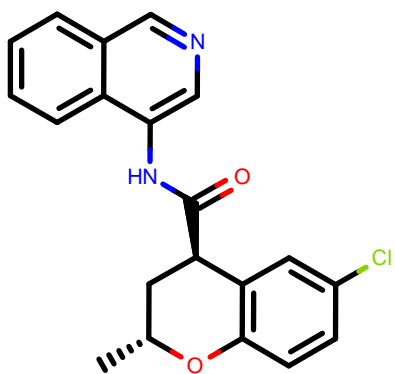
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C#N

RUN: RUN1871

DDG (kcal/mol): -0.16

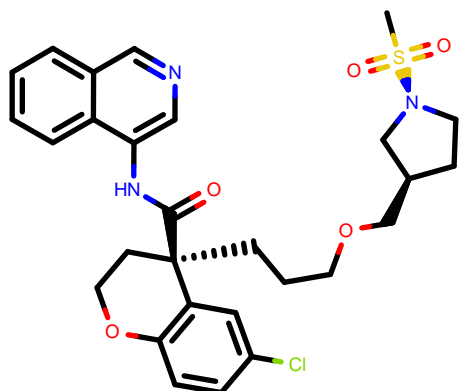
dDDG (kcal/mol): 0.09

ALP-POS-d3acb8cc-4_1



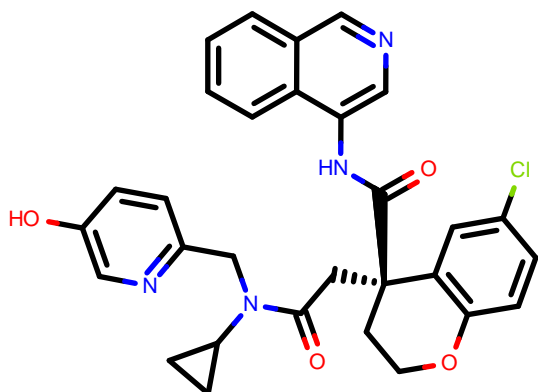
CID:	ALP-POS-d3acb8cc-4_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN980
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.04

EN300-261986_4_2_1



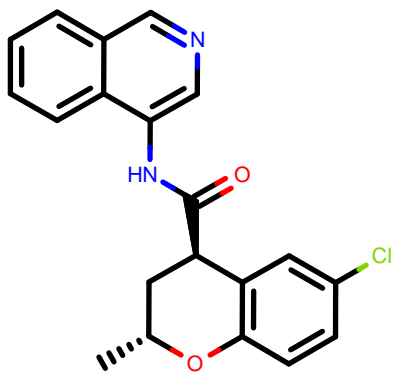
CID:	EN300-261986_4_2_1
SMILES:	<chem>CS(=O)(=O)[N@]1CC[C@H](C1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN7259
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.43

EDG-MED-ba1ac7b9-29_1



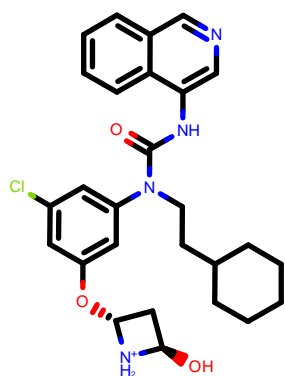
CID:	EDG-MED-ba1ac7b9-29_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ccc(cn5)O)C6CC6</chem>
RUN:	RUN2635
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.28

MAT-POS-8a69d52e-1_3_1



CID:	MAT-POS-8a69d52e-1_3_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN7557
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.04

MAT-POS-53907a1c-3_1



CID: MAT-POS-53907a1c-3_1

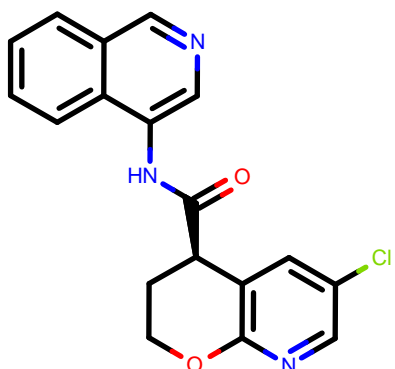
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cc(cc(c4)O)C@@H]5CC(=O)N5

RUN: RUN492

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.66

EDJ-MED-12f7f543-1_1



CID: EDJ-MED-12f7f543-1_1

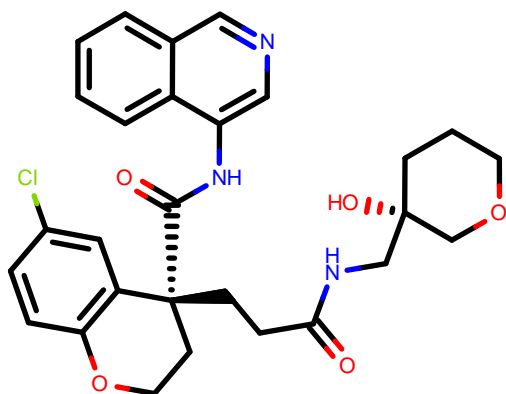
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cn4)Cl

RUN: RUN1227

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.22

EN300-193679_2_2_1



CID: EN300-193679_2_2_1

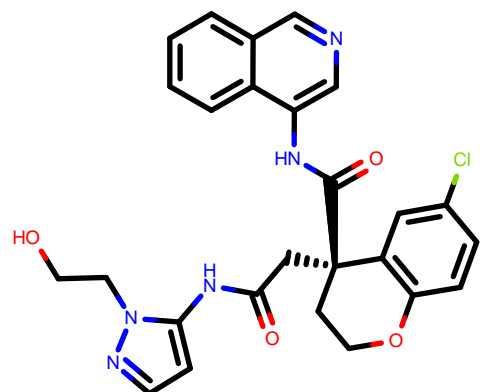
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)NC[C@@]5(CCCOC5)O

RUN: RUN4063

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-134536_1_1_1



CID: EN300-134536_1_1_1

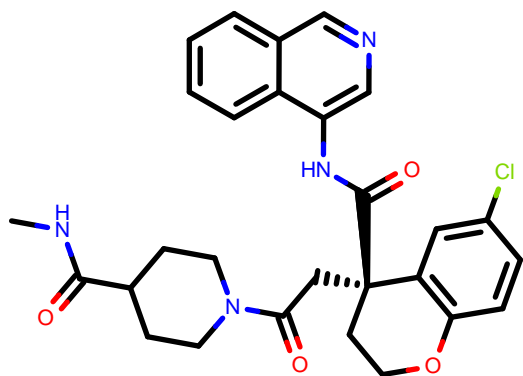
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ccn5CCO

RUN: RUN5938

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

EN300-24653_1_1_1



CID: EN300-24653_1_1_1

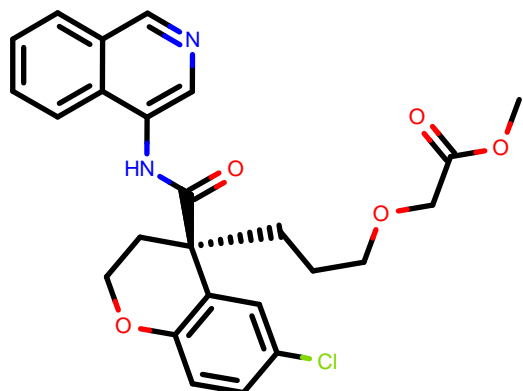
SMILES: CNC(=O)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN3250

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.34

EN300-19700_4_1_1



CID: EN300-19700_4_1_1

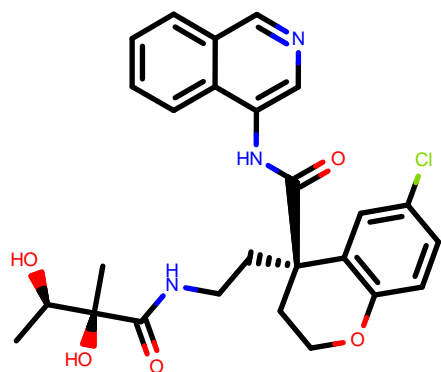
SMILES: COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN4733

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.31

EN300-202922_3_4_1



CID: EN300-202922_3_4_1

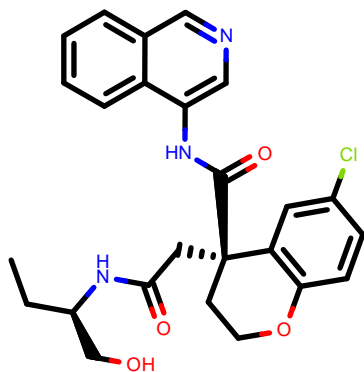
SMILES: C[C@H]([C@](C)(C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6918

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-19709_1_2_1



CID: EN300-19709_1_2_1

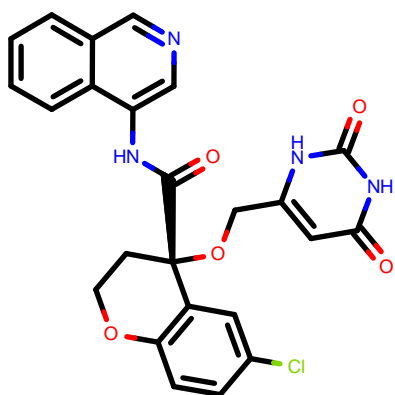
SMILES: CC[C@H](CO)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5221

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.39

EN300-11300_1_1_1



CID: EN300-11300_1_1_1

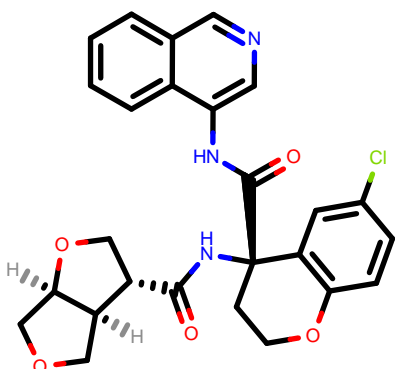
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN7652

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.28

EN300-6482296_1_4_1



CID: EN300-6482296_1_4_1

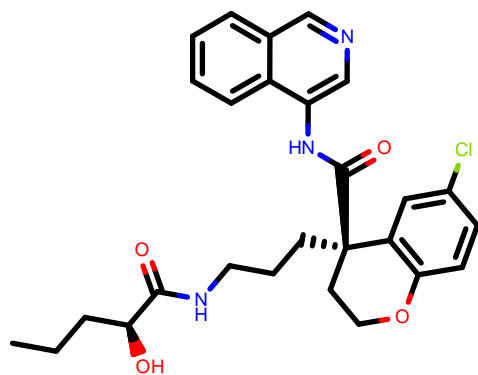
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5CO[C@@H]3[C@@H]5COO6

RUN: RUN3841

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.30

EN300-300217_4_2_1



CID: EN300-300217_4_2_1

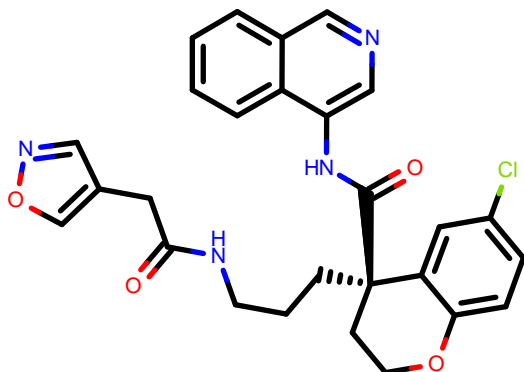
SMILES: C/C=C/[C@@H](C(=O)NCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN7653

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.38

EN300-315963_4_1_1



CID: EN300-315963_4_1_1

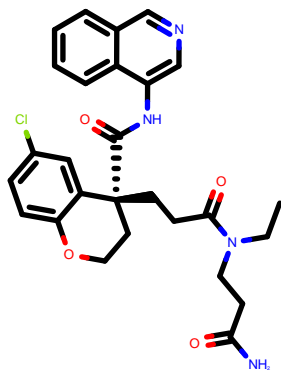
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5cncoc5

RUN: RUN4735

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.34

EN300-6766477_2_1_1



CID: EN300-6766477_2_1_1

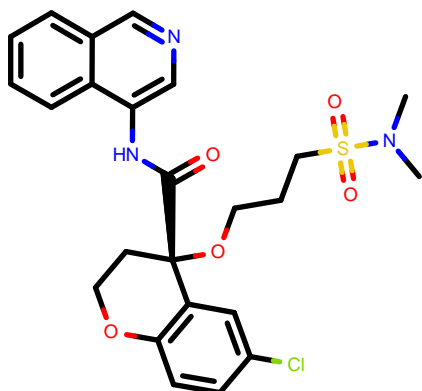
SMILES: CCN(CCC(=O)N)C(=O)CC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5985

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.31

EN300-66432_1_1_1



CID: EN300-66432_1_1_1

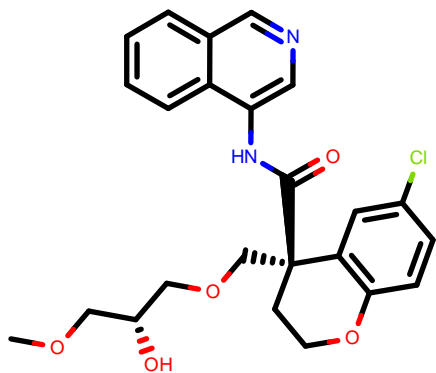
SMILES: CN(C)S(=O)(=O)CCCCO[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN5206

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.35

EN300-1915260_2_2_1



CID: EN300-1915260_2_2_1

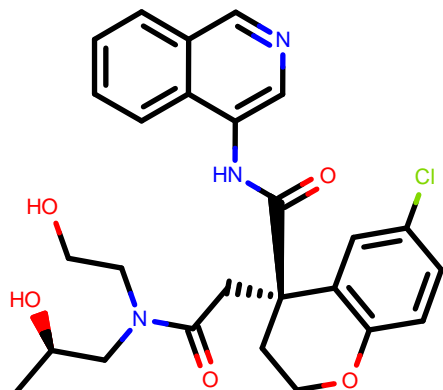
SMILES: COC[C@H](COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN7037

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.32

EN300-214038_1_2_1



CID: EN300-214038_1_2_1

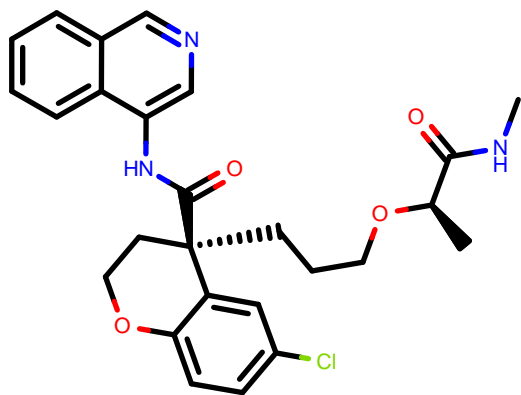
SMILES: C[C@H](CN(CCO)C(=O)C)C[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN4808

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.35

EN300-211482_4_2_1



CID: EN300-211482_4_2_1

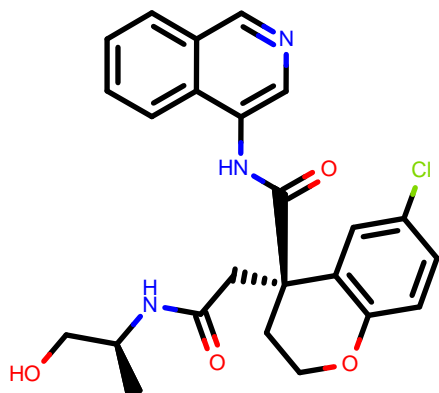
SMILES: C[C@H](C(=O)NC)OCCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6366

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.36

EN300-86282_1_1_1



CID: EN300-86282_1_1_1

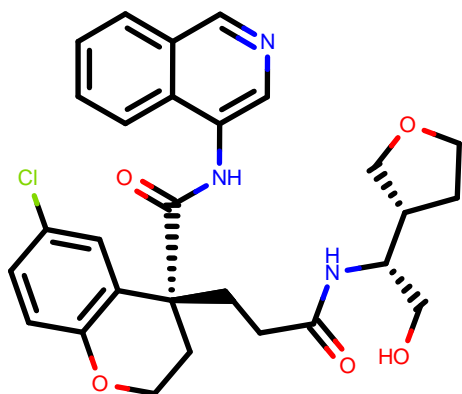
SMILES: C[C@@H](CO)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN6403

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.25

EN300-104493_2_3_1



CID: EN300-104493_2_3_1

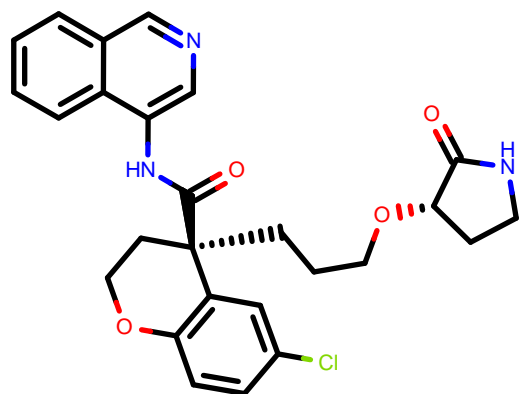
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(CO)N[C@@H](CO)C@H5CCOC5

RUN: RUN7126

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.41

EN300-6736413_4_2_1



CID: EN300-6736413_4_2_1

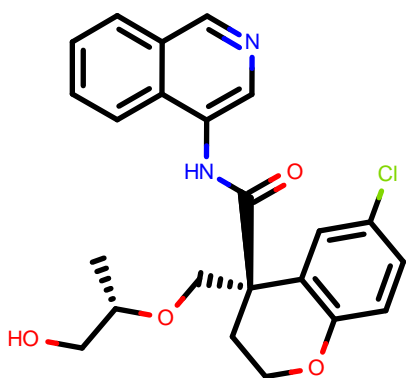
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(CO)N[C@@H]5CCNC5=O

RUN: RUN5815

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.31

EN300-175186_2_1_1



CID: EN300-175186_2_1_1

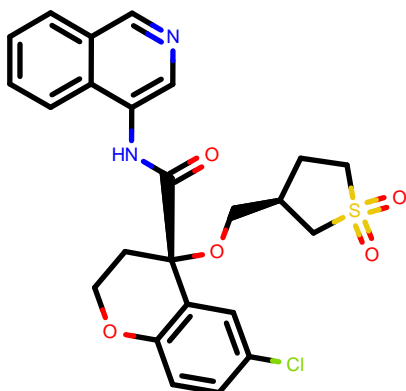
SMILES: C[C@@H](CO)OC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN6325

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.23

EN300-1448603_1_2_1



CID: EN300-1448603_1_2_1

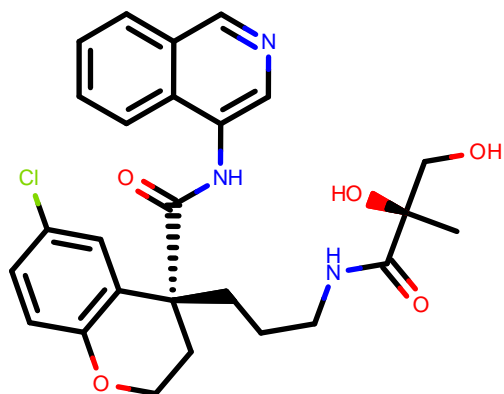
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN6215

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.32

EN300-89418_4_1_1



CID: EN300-89418_4_1_1

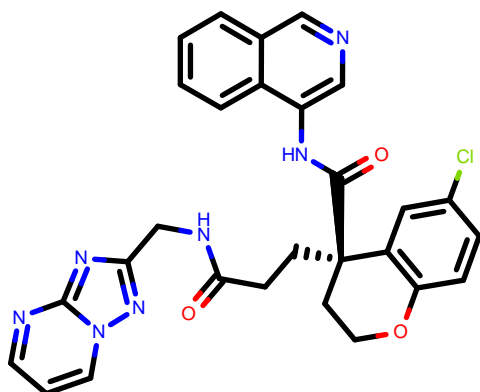
SMILES: C[C@@]1(CO)(C(=O)NCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN6921

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.67

EN300-250416_2_1_1



CID: EN300-250416_2_1_1

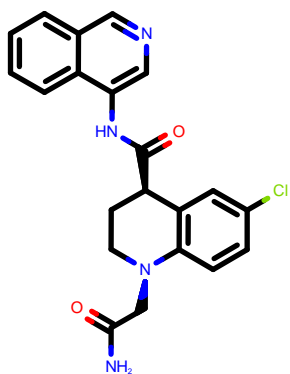
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCC(=O)NC5ncc6ncccc6n5

RUN: RUN6696

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.29

RAL-THA-8416115c-8_3



CID: RAL-THA-8416115c-8_3

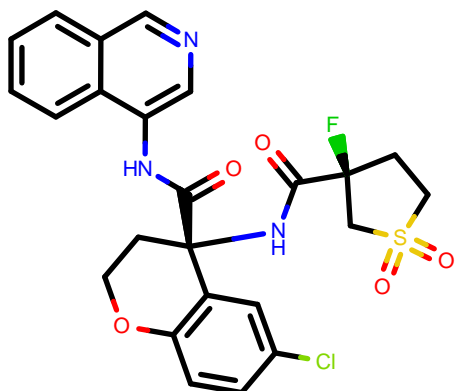
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@H]3CCN(c4c3cc(cc4)Cl)CC(=O)N

RUN: RUN1176

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.32

EN300-311920_1_1_1



CID: EN300-311920_1_1_1

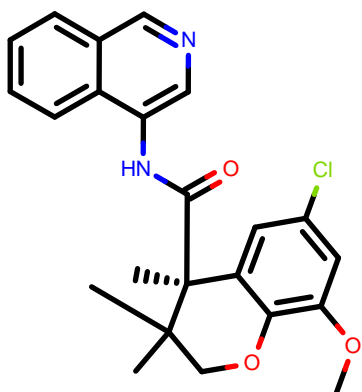
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCS(=O)(=O)C5)F

RUN: RUN6735

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.29

DAR-DIA-0d514e7d-27_1_1



CID: DAR-DIA-0d514e7d-27_1_1

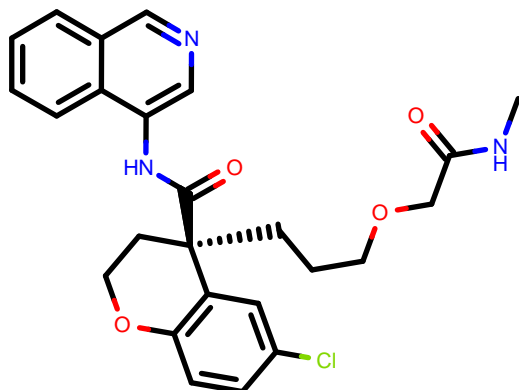
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)OC)Cl)C(=O)Nc3ncoc4c3cccc4

RUN: RUN7441

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.28

EN300-2977549_4_1_1



CID: EN300-2977549_4_1_1

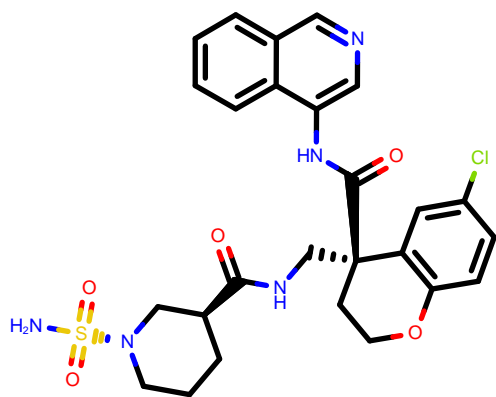
SMILES: CNC(=O)COCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4

RUN: RUN7272

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.31

EN300-219496_2_2_1



CID: EN300-219496_2_2_1

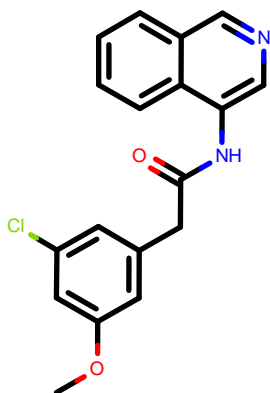
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3C(=O)C4=CC=CC=C4O[C@@H]3C(=O)N(C)C(S(=O)(=O)N)C5=CC=CC=C5

RUN: RUN6807

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.30

MAT-POS-3b92565d-2_1



CID: MAT-POS-3b92565d-2_1

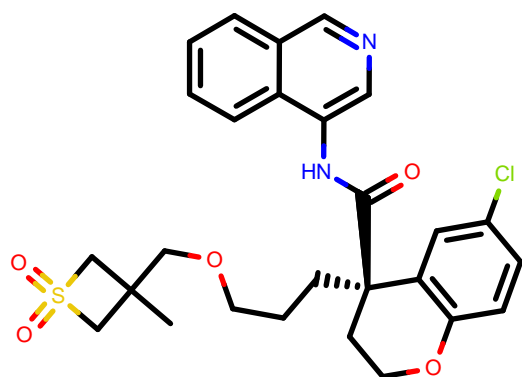
SMILES: COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2ccccc3

RUN: RUN29

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-1705754_4_1_1



CID: EN300-1705754_4_1_1

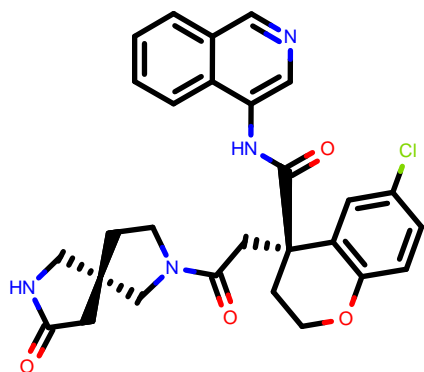
SMILES: CC1(CS(=O)(=O)C1)C(=O)C[C@@H]2(C(=O)OCC2)C(=O)Nc3cncc4c3ccccc4

RUN: RUN5624

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.48

EN300-187998_1_1_1



CID: EN300-187998_1_1_1

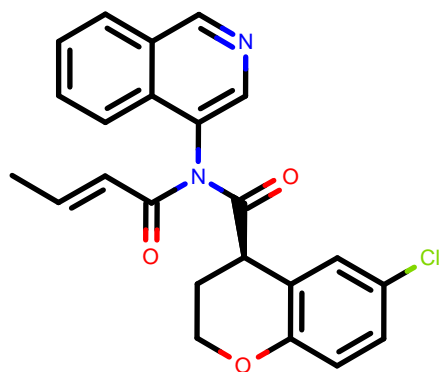
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3C(=O)C4=CC=CC=C4O[C@@H]3C(=O)N(C)C(S(=O)(=O)N)C5=CC=CC=C5

RUN: RUN7526

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.32

DAR-DIA-5ff57136-11_1_2



CID: DAR-DIA-5ff57136-11_1_2

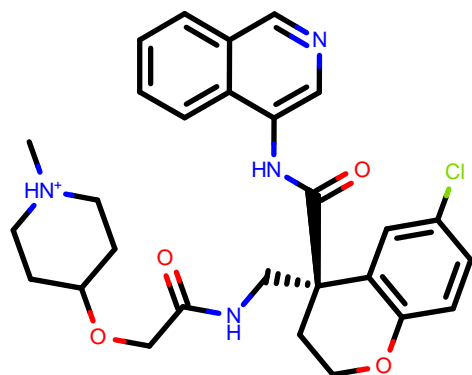
SMILES: C/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2764

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.24

EN300-237224_2_1_1



CID: EN300-237224_2_1_1

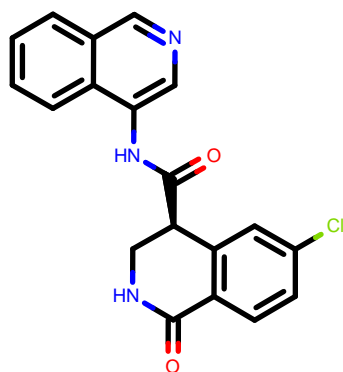
SMILES: C[NH+]1CCC(CC1)OCC(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN7019

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.32

MIC-UNK-91acba05-1_1



CID: MIC-UNK-91acba05-1_1

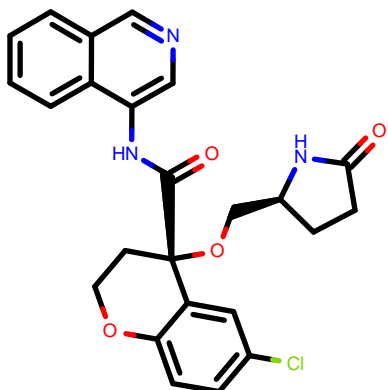
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CNC(=O)c4c3cc(cc4)Cl

RUN: RUN363

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.22

EN300-195756_1_1_1



CID: EN300-195756_1_1_1

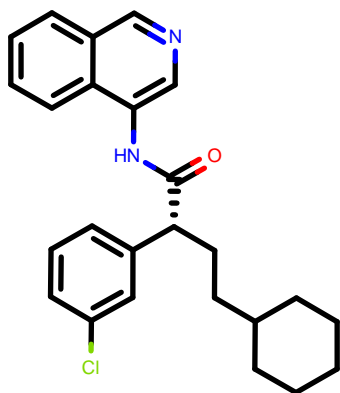
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCCC(=O)N5

RUN: RUN4938

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.21

ALP-POS-3b848b35-4_2



CID: ALP-POS-3b848b35-4_2

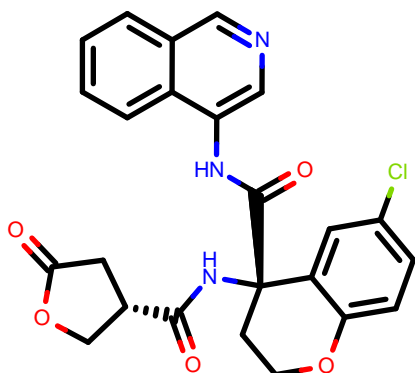
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl

RUN: RUN47

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.35

EN300-113234_1_2_1



CID: EN300-113234_1_2_1

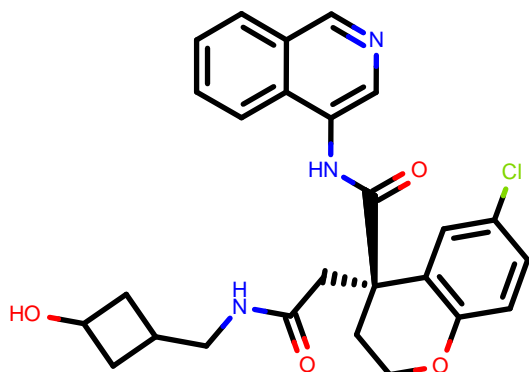
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)OC5

RUN: RUN5597

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.21

EN300-94856_1_1_1



CID: EN300-94856_1_1_1

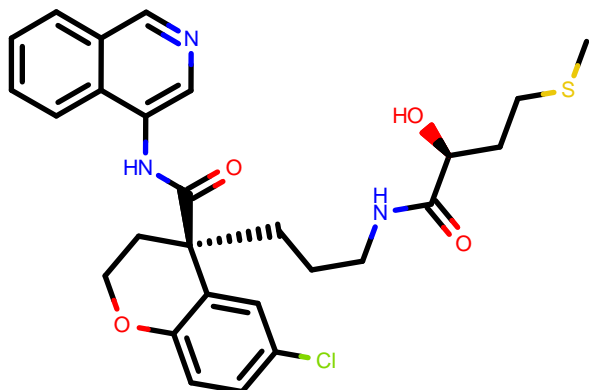
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5CC(O)O5

RUN: RUN6675

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.27

EN300-103144_4_1_1



CID: EN300-103144_4_1_1

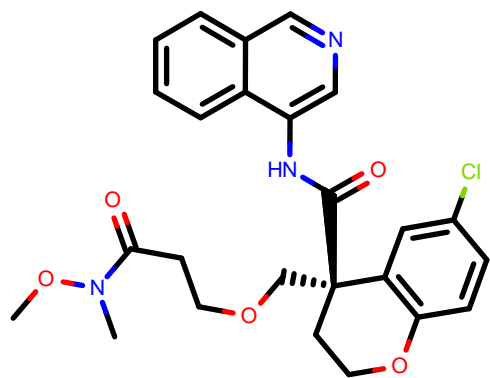
SMILES: CSCC[C@@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4)O

RUN: RUN2943

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.43

EN300-174603_2_1_1



CID: EN300-174603_2_1_1

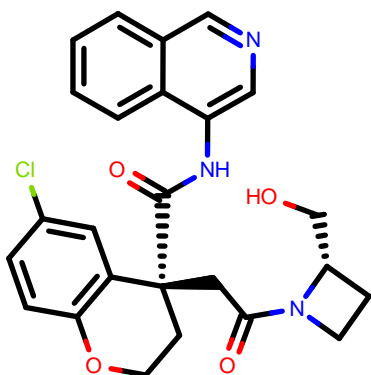
SMILES: CN(C(=O)CCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4)OC

RUN: RUN5582

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.26

EDG-MED-ba1ac7b9-2_3



CID: EDG-MED-ba1ac7b9-2_3

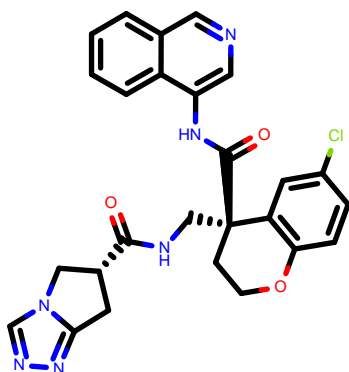
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO

RUN: RUN2465

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.30

EN300-6745453_2_1_1



CID: EN300-6745453_2_1_1

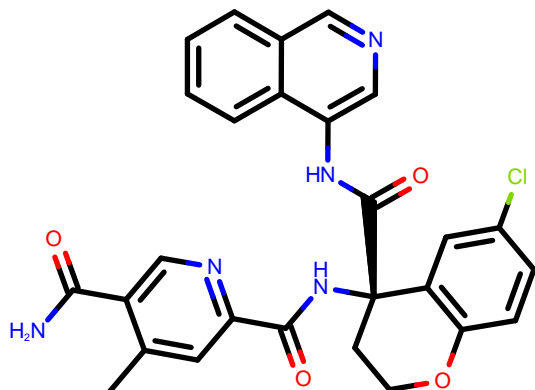
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5C[C@H]5CNn6c6

RUN: RUN6604

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.28

EN300-247617_1_1_1



CID: EN300-247617_1_1_1

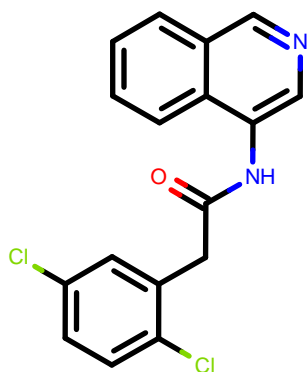
SMILES: Cc1cc(ncc1C(=O)N)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccc5

RUN: RUN4939

DDG (kcal/mol): -0.10

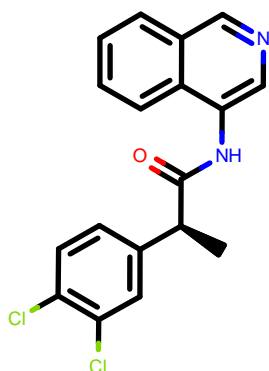
dDDG (kcal/mol): 0.23

PET-UNK-dd44aeb6-2_1



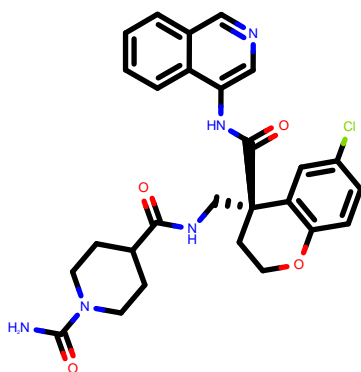
CID:	PET-UNK-dd44aeb6-2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)Cc3cc(ccc3Cl)Cl</chem>
RUN:	RUN336
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.26

MAT-POS-fce787c2-3_1



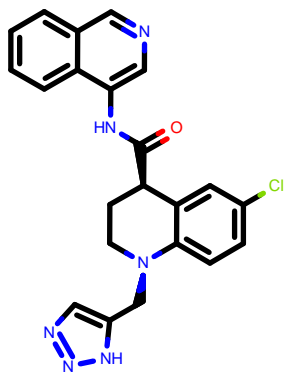
CID:	MAT-POS-fce787c2-3_1
SMILES:	<chem>C[C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3</chem>
RUN:	RUN1936
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.31

EN300-13489_2_1_1



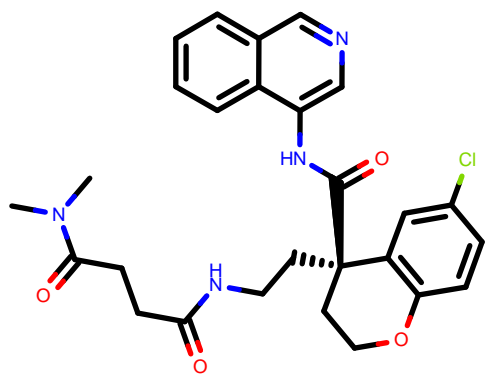
CID:	EN300-13489_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CCN(CC5)C(=O)N</chem>
RUN:	RUN7176
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.25

RAL-THA-8416115c-14_1



CID:	RAL-THA-8416115c-14_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)C5c[nH]n5</chem>
RUN:	RUN1205
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.35

EN300-176877_3_1_1



CID: EN300-176877_3_1_1

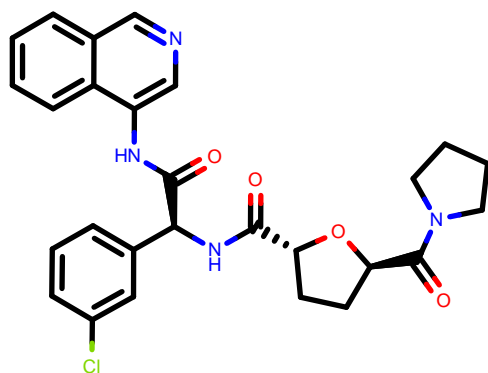
SMILES: CN(C)C(=O)CCC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN7135

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.27

EDJ-MED-ee07cf00-11_4



CID: EDJ-MED-ee07cf00-11_4

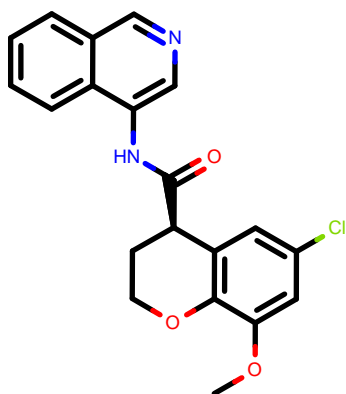
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](c3ccccc3)C(=O)Nc4cnc5c4c3cccc5

RUN: RUN2694

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.56

EDJ-MED-e4b030d8-7_1



CID: EDJ-MED-e4b030d8-7_1

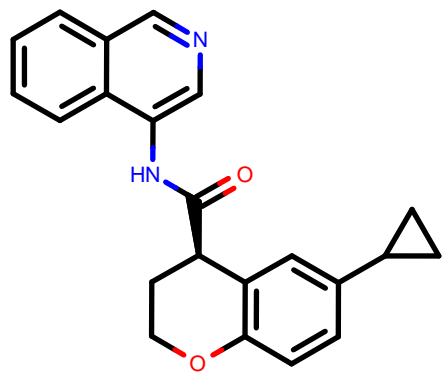
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN235

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.11

DAR-DIA-6a508060-8_1



CID: DAR-DIA-6a508060-8_1

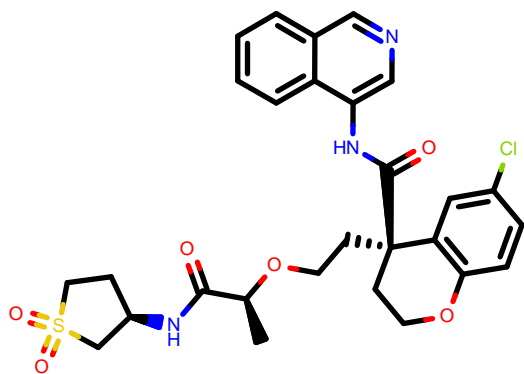
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C5CC5

RUN: RUN259

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.09

EN300-23318_3_1_1



CID: EN300-23318_3_1_1

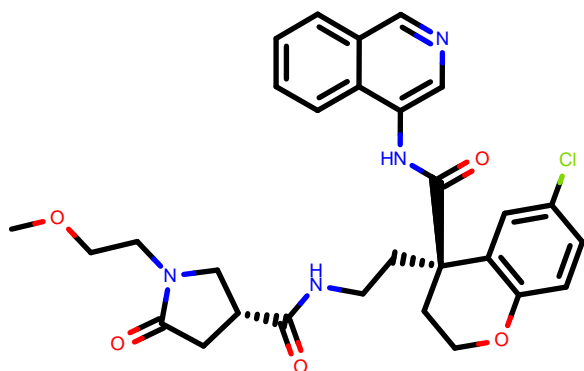
SMILES: C[C@@H](C(=O)N[C@@H](CCS(=O)(=O)C)OCC)[C@2](CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5588

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.40

EN300-31845_3_1_1



CID: EN300-31845_3_1_1

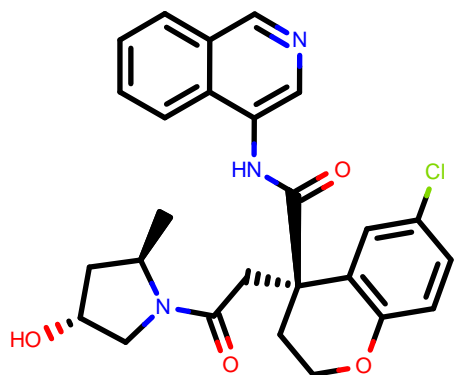
SMILES: COCCN1C[C@@H](CC1=O)C(=O)NCC[C@2](CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN5873

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.40

EN300-173562_1_3_1



CID: EN300-173562_1_3_1

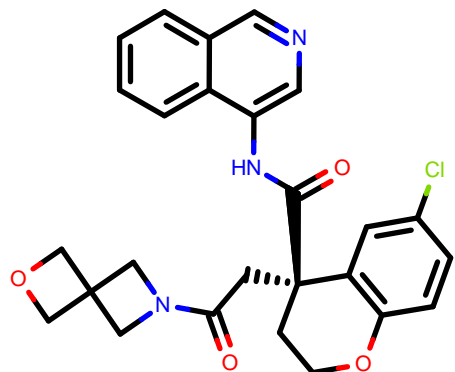
SMILES: C[C@@H]1C[C@H](CN1C(=O)C)[C@2](CCOc3c2cc(c3)Cl)C(=O)Nc4ccc5c4ccc5O

RUN: RUN3990

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.29

EN300-81038_1_1_1



CID: EN300-81038_1_1_1

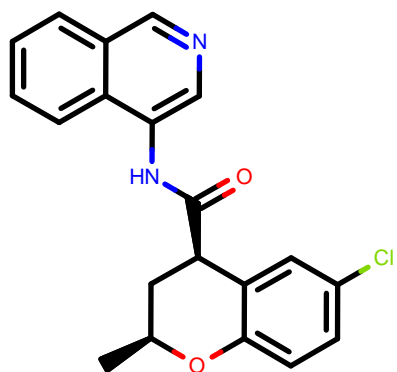
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(c4)Cl)CC(=O)N5CC6(C5)COC6

RUN: RUN6422

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.27

MAT-POS-8a69d52e-1_4_1



CID: MAT-POS-8a69d52e-1_4_1

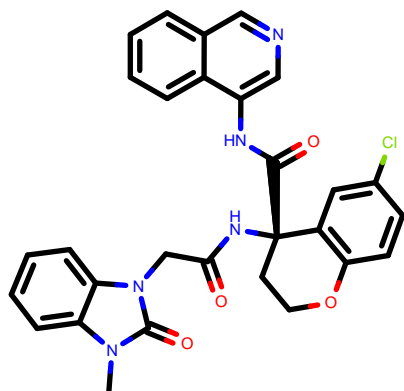
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5786

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.09

EN300-26603_1_1_1



CID: EN300-26603_1_1_1

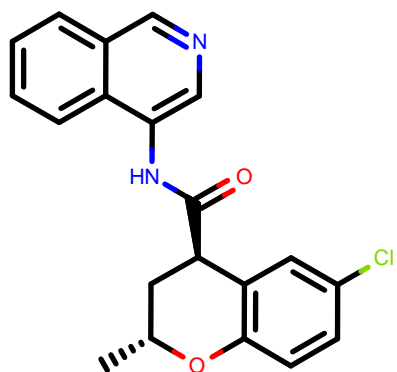
SMILES: Cn1c2cccc2n(c1=O)CC(=O)N[C@@]3(CCOc4c3cc(cc4O)C(=O)Nc5ncnc6c5cccc6

RUN: RUN4301

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.32

MAT-POS-8a69d52e-1_3



CID: MAT-POS-8a69d52e-1_3

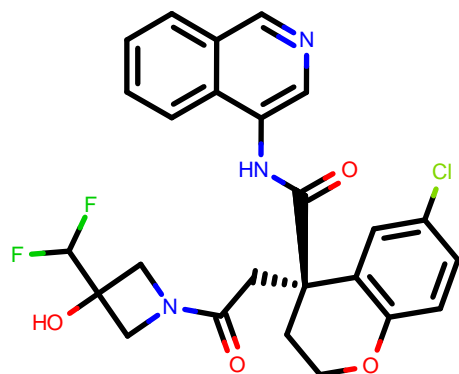
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN272

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.04

EN300-249245_1_1_1



CID: EN300-249245_1_1_1

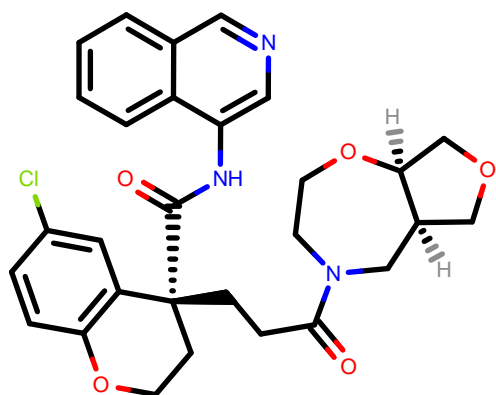
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)CC(=O)N5CC(C5)(C(F)F)O

RUN: RUN7640

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.24

EN300-395719_2_1_1



CID: EN300-395719_2_1_1

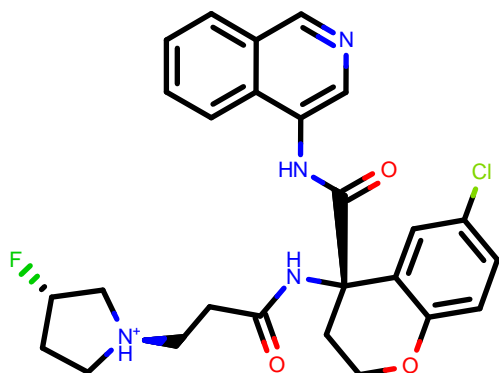
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCC(-O)N5CC[C@H]6COC[C@H]6C5

RUN: RUN5134

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.30

EDG-MED-90036822-109_2



CID: EDG-MED-90036822-109_2

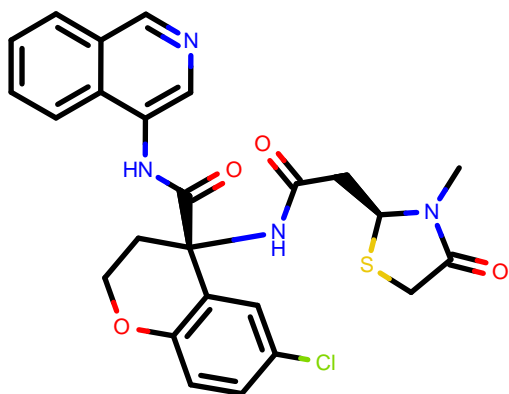
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC[N+](H)5CC[C@H]6C5F

RUN: RUN1748

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.31

EN300-143564_1_2_1



CID: EN300-143564_1_2_1

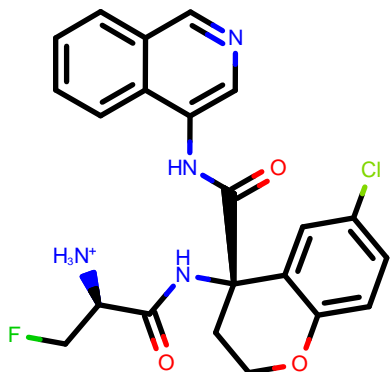
SMILES: CN1[C@@H]2(SCC1=O)CC(=O)N[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncnc5o4ccc5S

RUN: RUN2948

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.19

EDG-MED-90036822-5_1



CID: EDG-MED-90036822-5_1

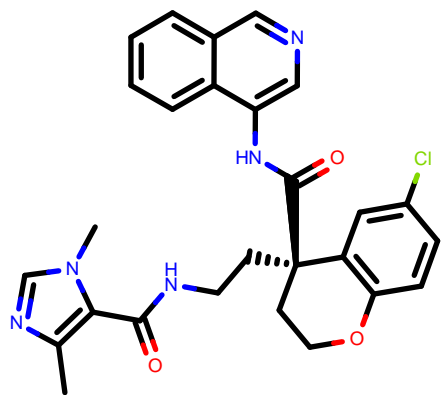
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](CF)[NH3+]

RUN: RUN1517

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.26

EN300-6498351_3_1_1



CID: EN300-6498351_3_1_1

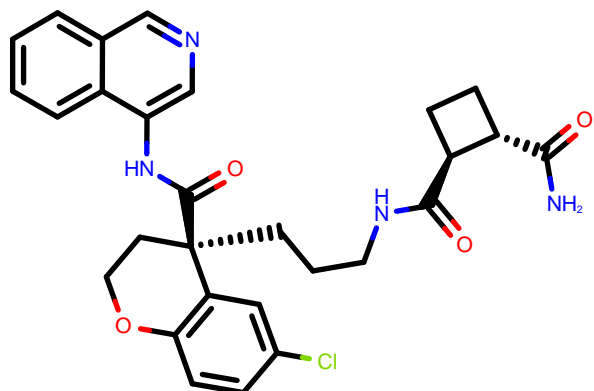
SMILES: Cc1c(n(c1)C)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN: RUN6753

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.35

EN300-217107_4_2_1



CID: EN300-217107_4_2_1

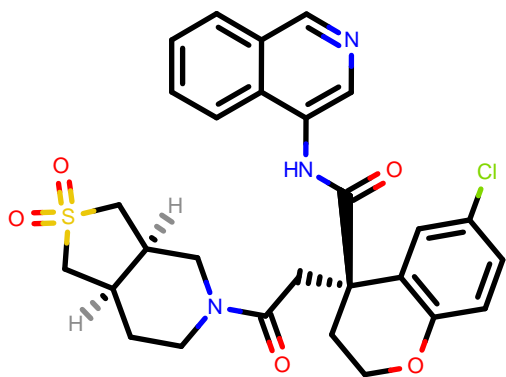
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(C1=O)[C@@H]5C[C@@]3(H)5Cl=O

RUN: RUN7631

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.37

KAD-UNI-80f122c8-3_7



CID: KAD-UNI-80f122c8-3_7

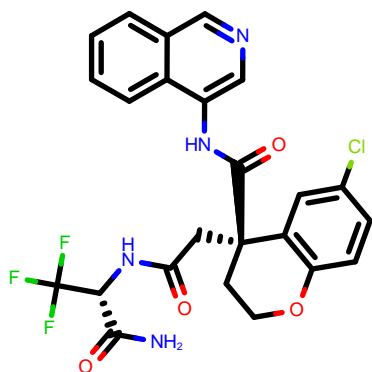
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(C1=O)N(C)C(F)F

RUN: RUN2190

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.30

EN300-6763470_1_2_1



CID: EN300-6763470_1_2_1

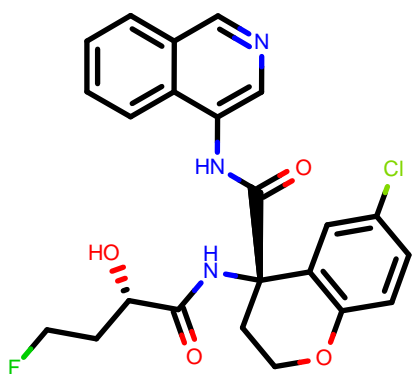
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(C)[C@@H]5C(F)(F)F

RUN: RUN7231

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.23

EDG-MED-90036822-51_2



CID: EDG-MED-90036822-51_2

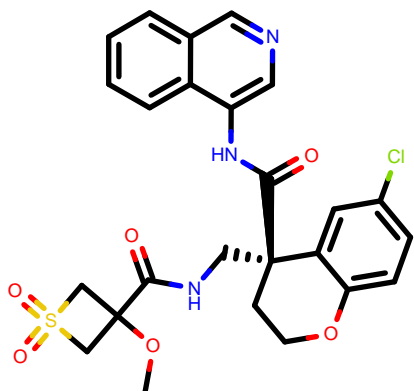
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](CCF)O

RUN: RUN1619

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.29

EN300-704025_2_1_1



CID: EN300-704025_2_1_1

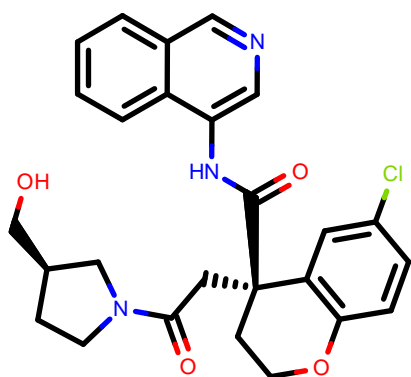
SMILES: COC1(CS(=O)(=O)C1)C(=O)NC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN4921

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.32

EN300-144970_1_1_1



CID: EN300-144970_1_1_1

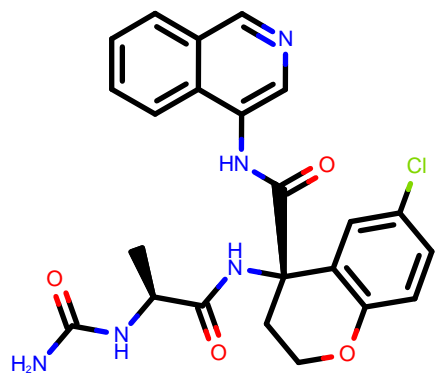
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO

RUN: RUN4554

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.27

EN300-152705_1_1_1



CID: EN300-152705_1_1_1

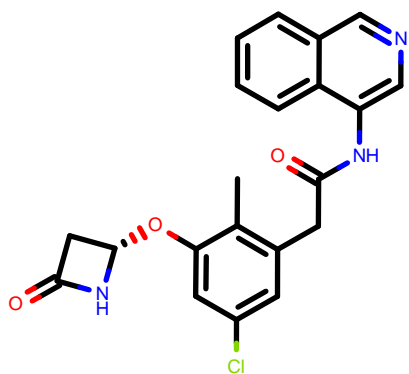
SMILES: C[C@@]H(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)NC(=O)N

RUN: RUN5652

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.22

EDJ-MED-50011917-2_2



CID: EDJ-MED-50011917-2_2

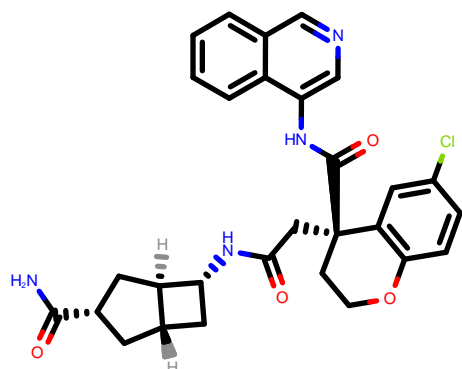
SMILES: Cc1c(cc(cc1O)[C@H]2CC(=O)N2)Cl)CC(=O)Nc3cncc4c3cccc4

RUN: RUN340

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.37

EN300-1268016_1_15_1



CID: EN300-1268016_1_15_1

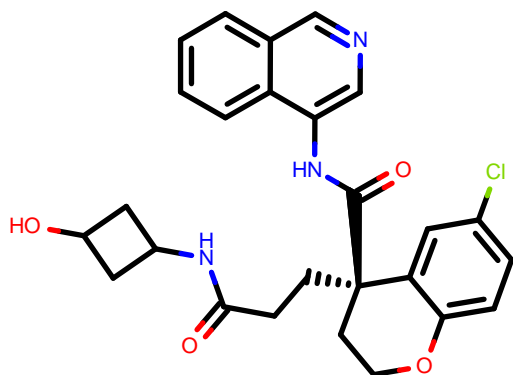
SMILES: c1ccc2c(e1)cncc2N(C(=O)C@@3[C@@O]c4ccc(cc4)C)C1=O)N[C@@H]5[C@@H]6[C@@H]7C[C@@H]8[C@H]9C[C@@H]9(C)C[C@@]8O

RUN: RUN6337

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.32

EN300-307592_2_1_1



CID: EN300-307592_2_1_1

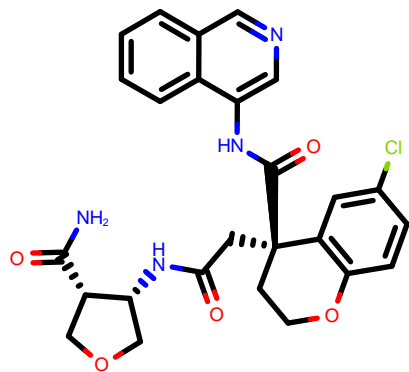
SMILES: c1ccc2c(e1)cncc2N(C(=O)C@@3[C@@O]c4ccc(cc4)C)C1=O)N[C@@H]5[C@@H]6[C@@H]7C[C@@H]9(C)C[C@@]8O

RUN: RUN7619

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.23

EN300-7435892_1_1_1



CID: EN300-7435892_1_1_1

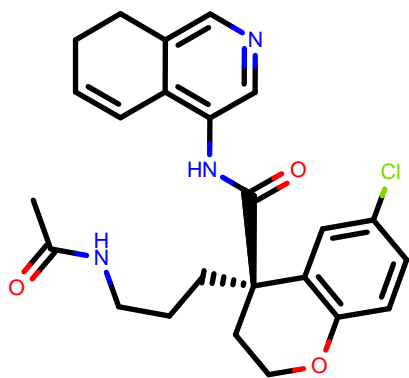
SMILES: c1ccc2c(e1)cncc2N(C(=O)C@@3[C@@O]c4ccc(cc4)C)C1=O)N[C@@H]5[C@@H]6[C@@H]7C[C@@H]9(C)C[C@@]8O

RUN: RUN7554

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.31

EN300-18074_4_1_1



CID: EN300-18074_4_1_1

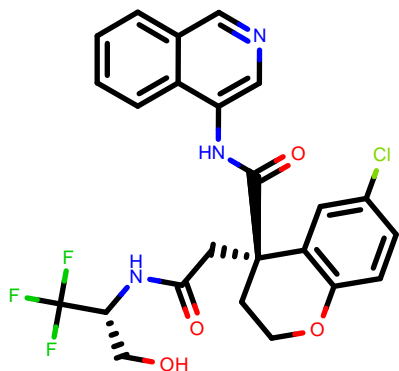
SMILES: CC(=O)NCCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN4302

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.28

EN300-296237_1_2_1



CID: EN300-296237_1_2_1

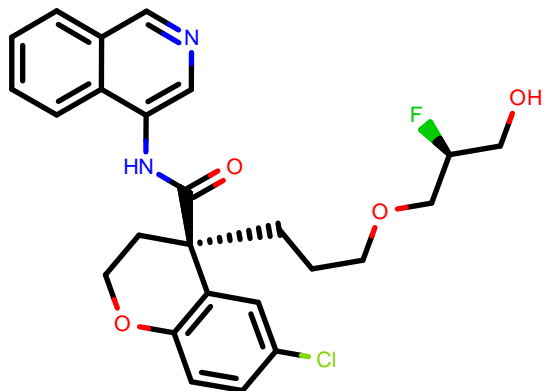
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)C(F)(F)F

RUN: RUN7464

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.43

EN300-1600517_4_2_1



CID: EN300-1600517_4_2_1

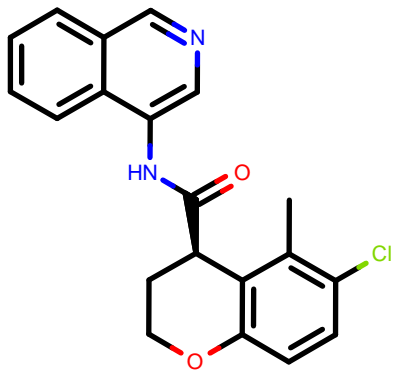
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)CCOC[C@H](CO)C(F)F

RUN: RUN5591

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.37

EDJ-MED-e4b030d8-8_1



CID: EDJ-MED-e4b030d8-8_1

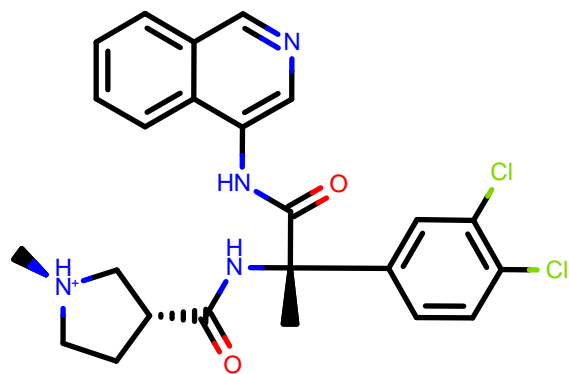
SMILES: Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN252

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.08

MAT-POS-e9e99895-13_6



CID: MAT-POS-e9e99895-13_6

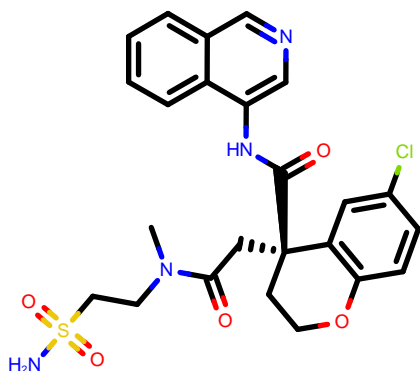
SMILES: C[C@](c1ccc(c1)Cl)C(=O)Nc2nc3c2ccc3NC(=O)C@@H4CCN@H+](C4)C

RUN: RUN2147

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.53

EN300-366974_1_1_1



CID: EN300-366974_1_1_1

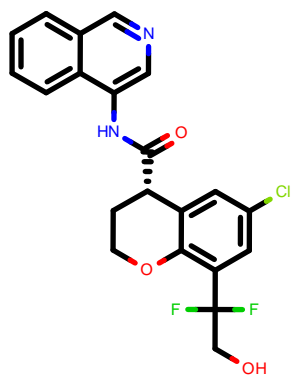
SMILES: CN(CCS(=O)=O)N(C=O)C[C@]1(C)COCc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4

RUN: RUN5530

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.27

MIC-UNK-08fa0751-1_2



CID: MIC-UNK-08fa0751-1_2

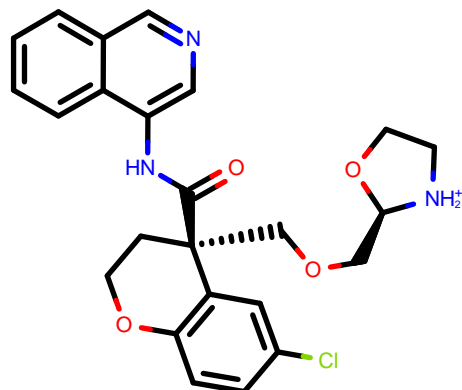
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@H]3CCOCc4c3cc(cc4C(CO)(F)F)Cl

RUN: RUN1369

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.38

EN300-317555_2_1_1



CID: EN300-317555_2_1_1

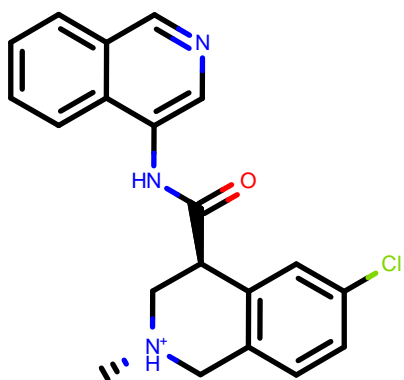
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(C)COCc4c3cc(cc4)Cl)COC(C)C[C@@H]5[NH2+][C]CO5

RUN: RUN4957

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.28

BEN-DND-f2e727cd-6_2



CID: BEN-DND-f2e727cd-6_2

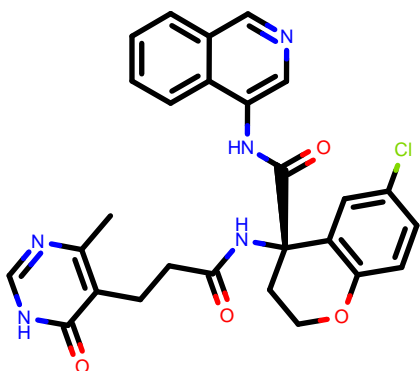
SMILES: C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN1041

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-33553_1_1_1



CID: EN300-33553_1_1_1

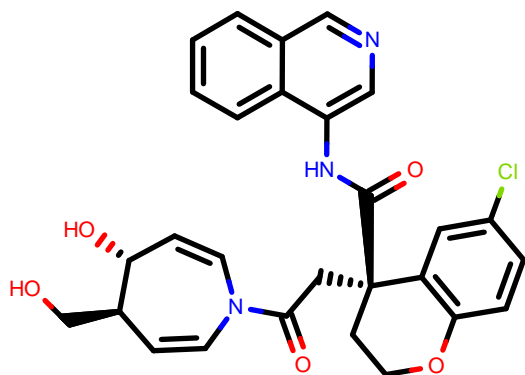
SMILES: Cc1c(c(=O)[nH]cn1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN6996

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-7353672_1_2_1



CID: EN300-7353672_1_2_1

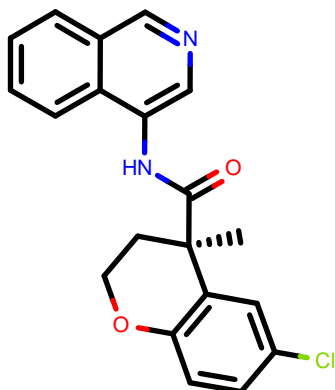
SMILES: c1ccc2c(c1)ncnc2N[C@@]3(C)[C@@]4(C)COC(C4)C(=O)N5CC[C@@H](C5)C(=O)CO

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

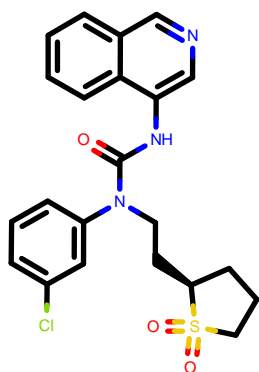
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN5557

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.11

MIC-UNK-cdc2493e-15_2



CID: MIC-UNK-cdc2493e-15_2

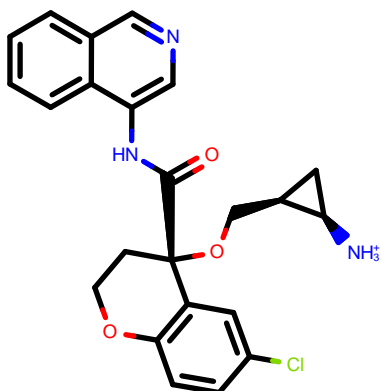
SMILES: c1ccc2c(c1)cncc2NC(=O)N(CC[C@H]3CCCS3(=O)=O)c4cccc(c4)Cl

RUN: RUN534

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.34

ED_-GRI-5b13fbe2-70_1



CID: ED_-GRI-5b13fbe2-70_1

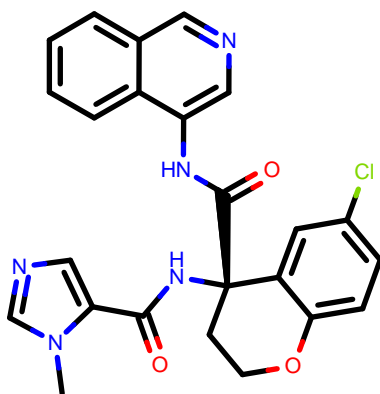
SMILES: c1ccc2c(c1)cncc2NC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@H]5[NH3+]

RUN: RUN1455

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-88417_1_1_1



CID: EN300-88417_1_1_1

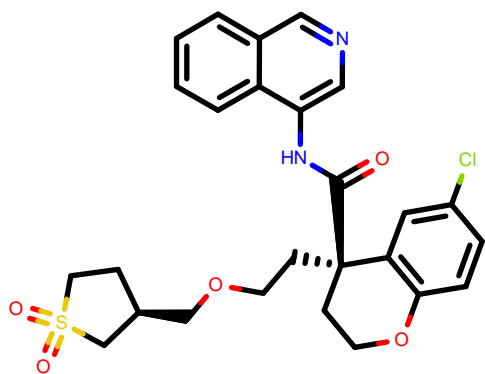
SMILES: Cn1cncc1C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN4680

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.23

EN300-1448603_3_1_1



CID: EN300-1448603_3_1_1

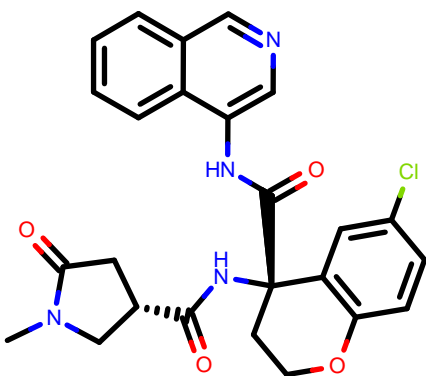
SMILES: c1ccc2c(c1)cncc2NC(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5SCCS(=O)(=O)C5

RUN: RUN5446

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.35

EN300-33601_1_2_1



CID: EN300-33601_1_2_1

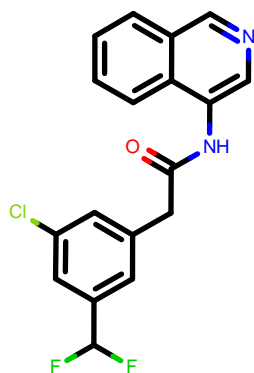
SMILES: CN1C[C@H](CC1=O)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5

RUN: RUN6155

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

MIC-UNK-16ccb665-3_1



CID: MIC-UNK-16ccb665-3_1

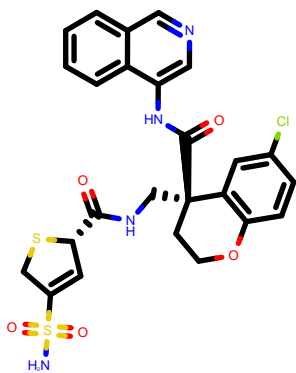
SMILES: c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(F)F

RUN: RUN2142

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.28

EN300-98099_2_1_1



CID: EN300-98099_2_1_1

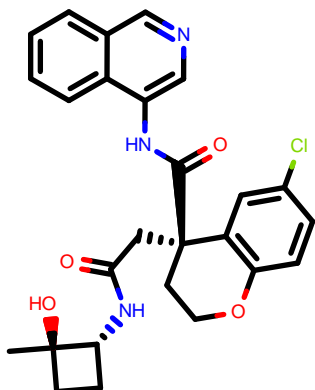
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(cs5)S(=O)(=O)N

RUN: RUN6518

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.40

EN300-262389_1_1_1



CID: EN300-262389_1_1_1

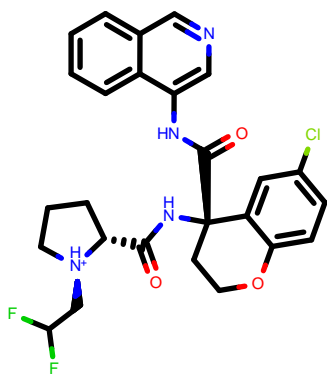
SMILES: C[C@@]1(CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5)O

RUN: RUN6192

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.32

EDG-MED-90036822-98_2



CID: EDG-MED-90036822-98_2

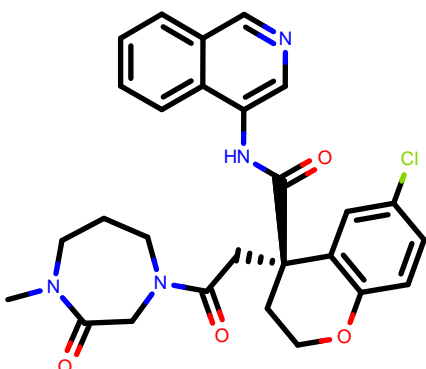
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H]5C(F)F

RUN: RUN1744

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

EN300-160143_1_1_1



CID: EN300-160143_1_1_1

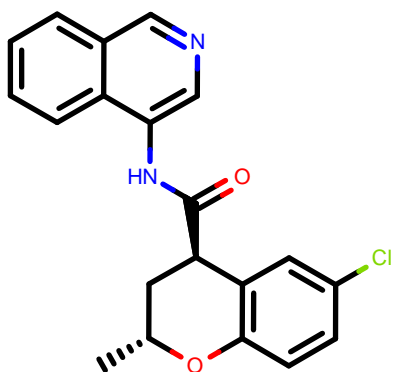
SMILES: CN1CCN(CC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN6130

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.26

ALP-POS-d3acb8cc-4_1_1



CID: ALP-POS-d3acb8cc-4_1_1

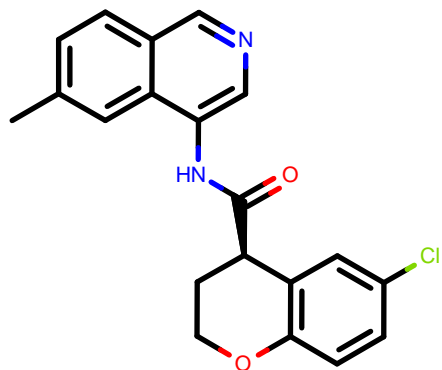
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN7815

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.04

ALF-EVA-5b152d2f-2_1



CID: ALF-EVA-5b152d2f-2_1

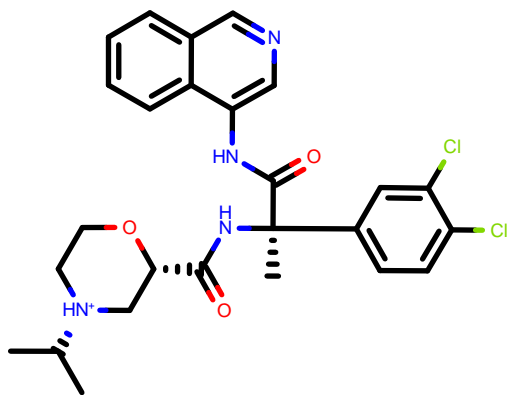
SMILES: Cc1ccc2ncc(c2c1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN2209

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.05

MAT-POS-e9e99895-2_5



CID: MAT-POS-e9e99895-2_5

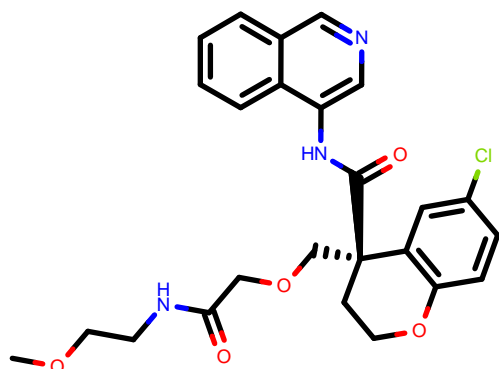
SMILES: CC(C)[N+]([O-])C(=O)C[C@@H](C1=O)N(C)[C@](C)(c2ccc(c1c2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN2143

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.64

EN300-02015_2_1_1



CID: EN300-02015_2_1_1

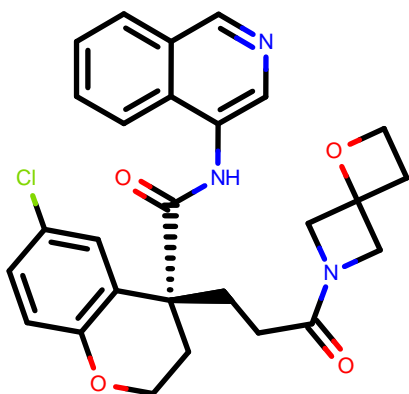
SMILES: COCCNC(=O)COC[C@]1(C)C(=O)C2=C1C(=O)Nc3ncc4c3cccc4

RUN: RUN6384

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.36

KAD-UNI-8a629cb0-26_1



CID: KAD-UNI-8a629cb0-26_1

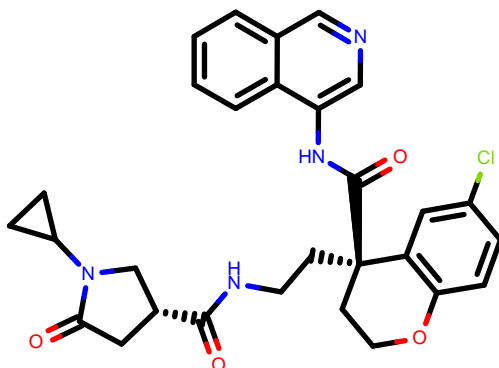
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(=O)C4=CC(=C(C4)C)CCC(=O)N5CC6(C5)CCO6

RUN: RUN1944

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.22

EN300-12440_3_1_1



CID: EN300-12440_3_1_1

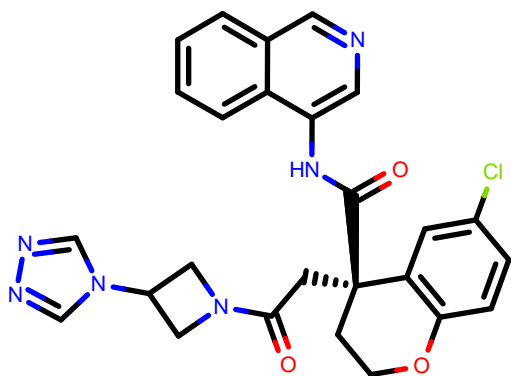
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(=O)C4=CC(=C(C4)C)CNC(=O)[C@@]5(C)CC6(C5)CCO6

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)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)n6mnc6

RUN:

RUN6795

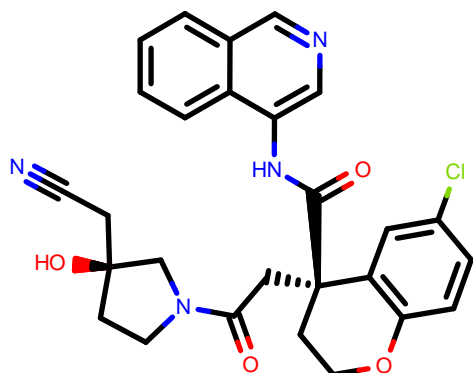
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.28

EN300-257405_1_1_1



CID: EN300-257405_1_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C@@)3(C#N)O

RUN:

RUN4131

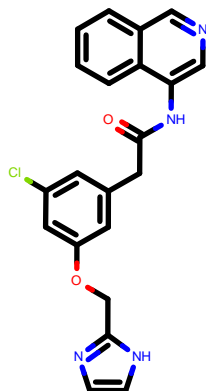
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.27

RAL-THA-1d44ff04-1_1



CID: RAL-THA-1d44ff04-1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCc4[nH]cnc4

RUN:

RUN402

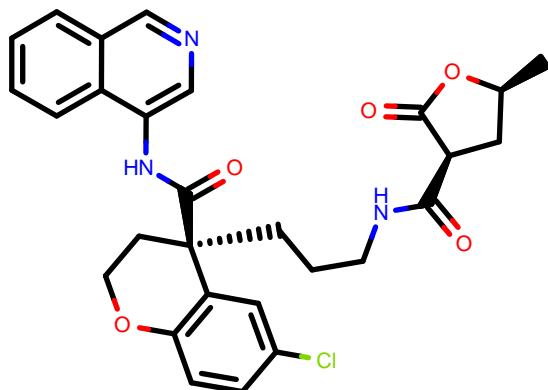
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.43

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)Nc4ncnc5c4ccc5

RUN:

RUN7322

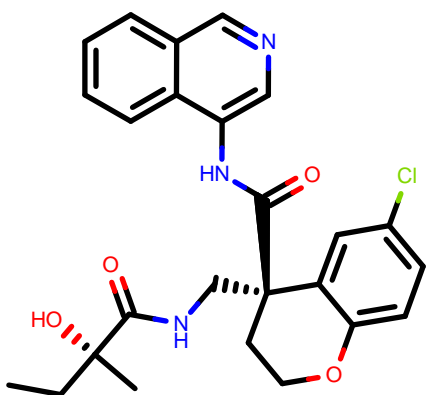
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.36

EN300-248888_2_1_1



CID: EN300-248888_2_1_1

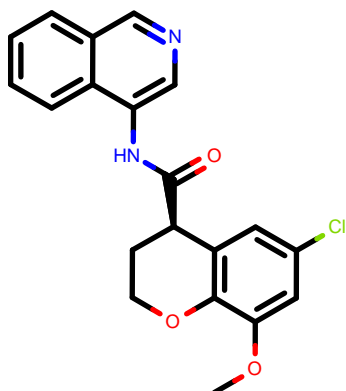
SMILES: C[C@@](C=C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3cccc4)O

RUN: RUN5105

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.32

DAR-DIA-6a508060-4_2



CID: DAR-DIA-6a508060-4_2

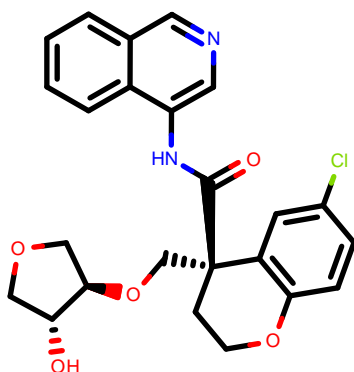
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3ncoc4c3cccc4)Cl

RUN: RUN289

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.11

EN300-331828_2_1_1



CID: EN300-331828_2_1_1

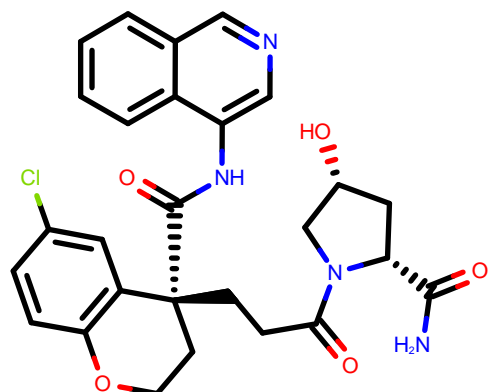
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5OCC[C@H]5O

RUN: RUN4217

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.25

EN300-07752_2_1_1



CID: EN300-07752_2_1_1

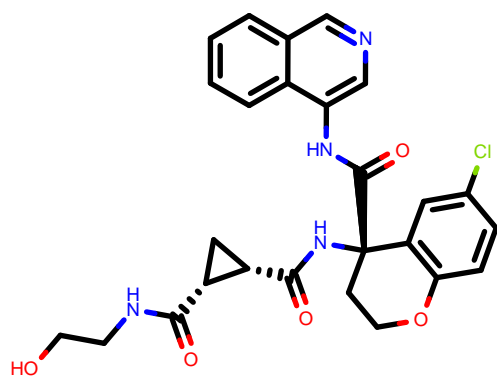
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN7744

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.46

EN300-6335413_1_1_1



CID: EN300-6335413_1_1_1

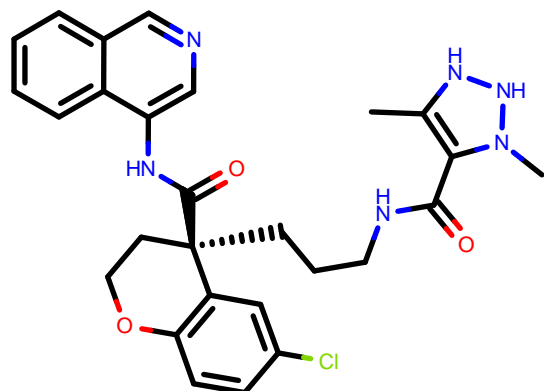
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C@H5C[C@H]5C(=O)NCCO

RUN: RUN4985

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.35

EN300-649738_4_1_1



CID: EN300-649738_4_1_1

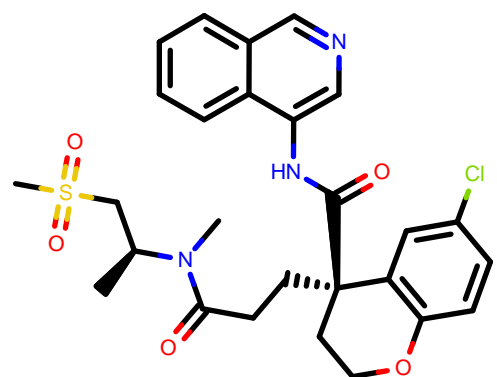
SMILES: Cc1c(n(n1)C)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccccc5

RUN: RUN7772

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.33

EN300-75209_2_1_1



CID: EN300-75209_2_1_1

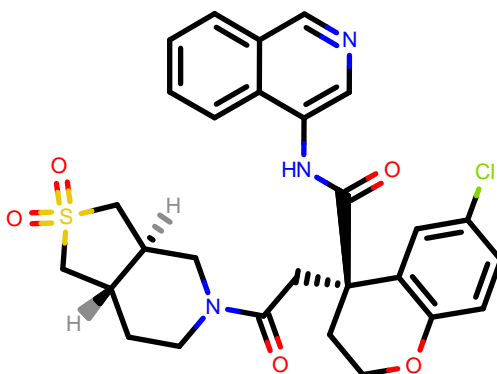
SMILES: C[C@@H](CS(=O)(=O)C)N(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccccc4

RUN: RUN6293

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.33

ALP-UNI-76695c4f-4_3



CID: ALP-UNI-76695c4f-4_3

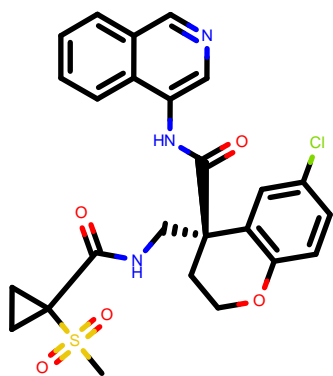
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H]6CS(=O)(=O)C6@H]6C5

RUN: RUN2046

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.37

EN300-191495_2_1_1



CID: EN300-191495_2_1_1

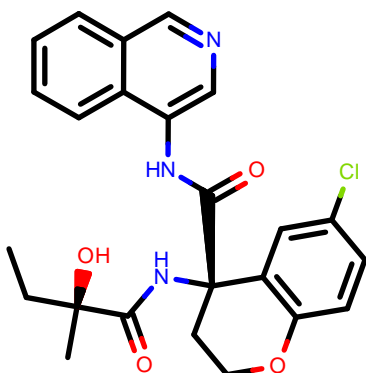
SMILES: CS(=O)(=O)C1(CC1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN3782

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.43

EN300-104746_1_1_1



CID: EN300-104746_1_1_1

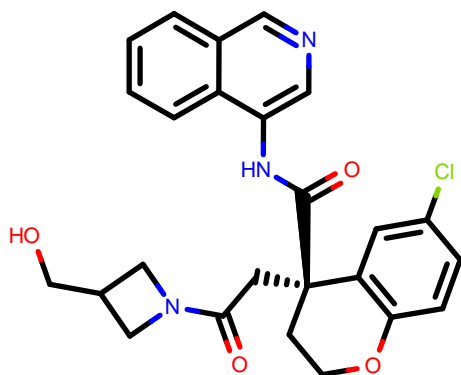
SMILES: CC[C@@H](C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN7586

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-7370063_1_1_1



CID: EN300-7370063_1_1_1

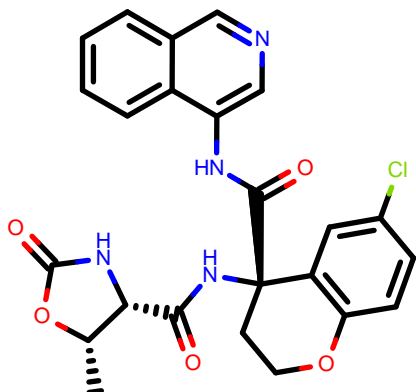
SMILES: c1ccc2c(c1)ncoc2N[C@@]1(C)[C@@]3(CCOc4c3cc(cc4)O)CC(=O)N5CC(C5)CO

RUN: RUN5881

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.23

EN300-172640_1_4_1



CID: EN300-172640_1_4_1

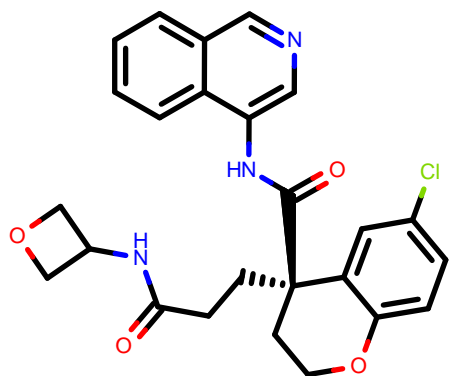
SMILES: C[C@H]1[C@H](NC(=O)O1)C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN6577

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.23

EN300-49064_2_1_1



CID: EN300-49064_2_1_1

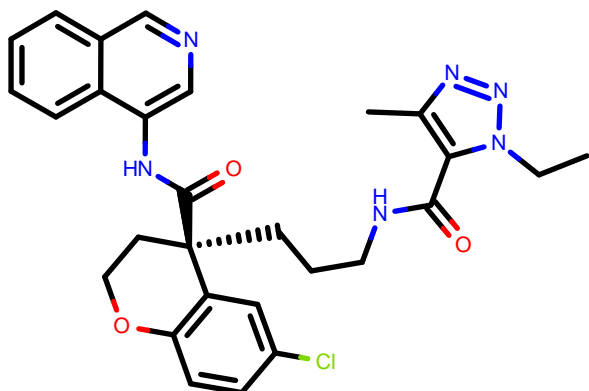
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5COC5

RUN: RUN6701

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.25

EN300-217526_4_1_1



CID: EN300-217526_4_1_1

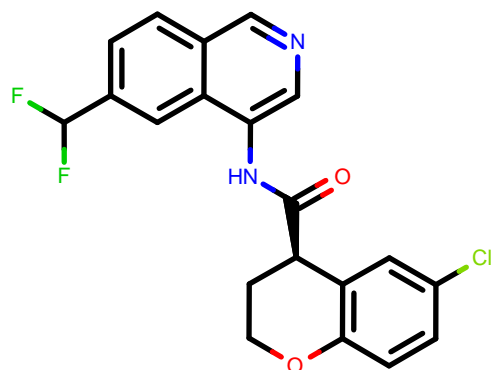
SMILES: CCn1c(c1nn1)C(=O)NCCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nnc5c4ccoc5

RUN: RUN7223

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.34

BEN-DND-c852c98b-7_1



CID: BEN-DND-c852c98b-7_1

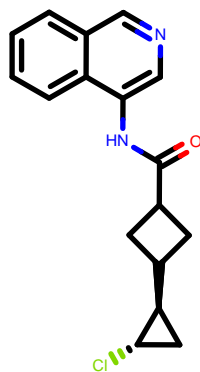
SMILES: c1cc2cncc(c2cc1C(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN1111

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.05

DAR-DIA-6a508060-11_2



CID: DAR-DIA-6a508060-11_2

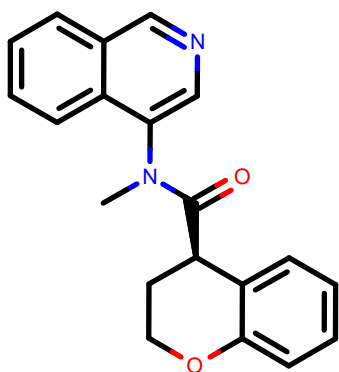
SMILES: c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@@H]4C[C@@H]4Cl

RUN: RUN275

DDG (kcal/mol): -0.02

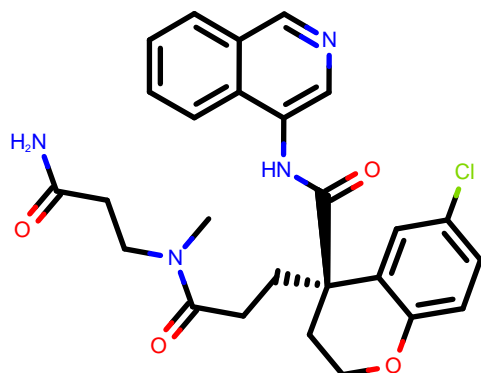
dDDG (kcal/mol): 0.25

MAK-UNK-3875bbc8-3_1



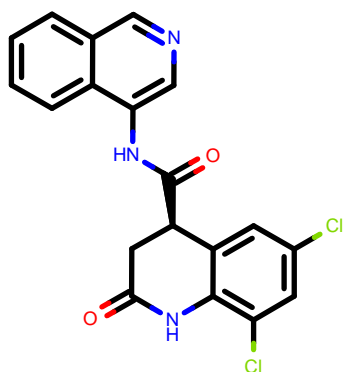
CID:	MAK-UNK-3875bbc8-3_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cccc4</chem>
RUN:	RUN706
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.10

EN300-209532_2_1_1



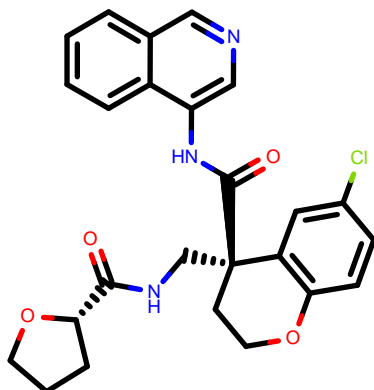
CID:	EN300-209532_2_1_1
SMILES:	<chem>CN(CCC(=O)N)C(=O)CC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN4021
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.29

MAT-POS-f39f51fd-1_1



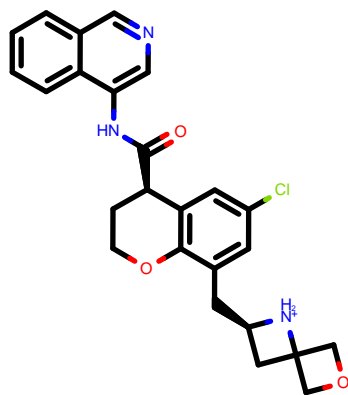
CID:	MAT-POS-f39f51fd-1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4Cl)Cl</chem>
RUN:	RUN2203
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.32

EN300-21009_2_1_1



CID:	EN300-21009_2_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCCO5</chem>
RUN:	RUN5200
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.28

DAR-DIA-23e5a6a0-8_1_1



CID: DAR-DIA-23e5a6a0-8_1_1

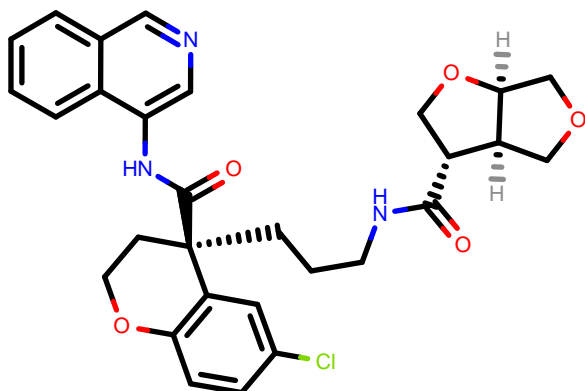
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4C)[C@@H]5CC6([NH2+][5]COC6)Cl

RUN: RUN7625

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.37

EN300-6482296_4_5_1



CID: EN300-6482296_4_5_1

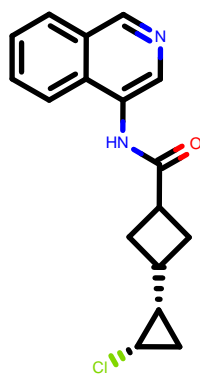
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCNC1=O)[C@@H]5CO[C@@H]6C[C@@H]5COC6

RUN: RUN6371

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.44

DAR-DIA-6a508060-11_1



CID: DAR-DIA-6a508060-11_1

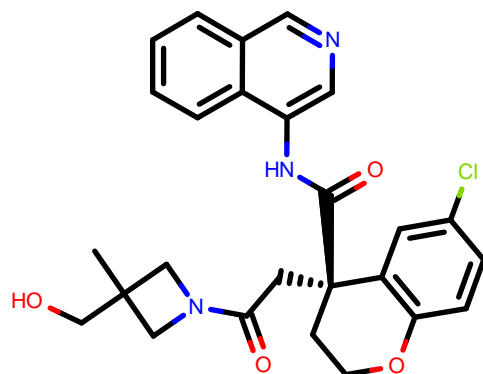
SMILES: c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@@H]4C[C@@H]4Cl

RUN: RUN270

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.21

EN300-244122_1_1_1



CID: EN300-244122_1_1_1

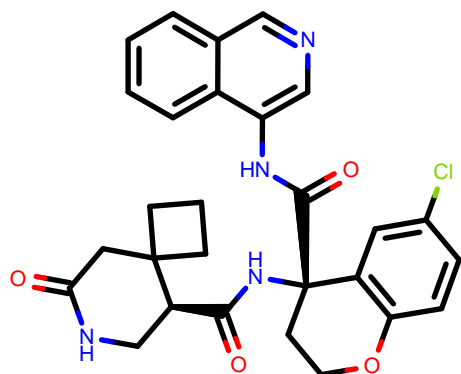
SMILES: CC1(CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4ccc5)CO

RUN: RUN4490

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.29

EN300-1704404_1_2_1



CID:	EN300-1704404_1_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)C@@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5CNC(=O)CC56CCC6</chem>
RUN:	RUN5327
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.27