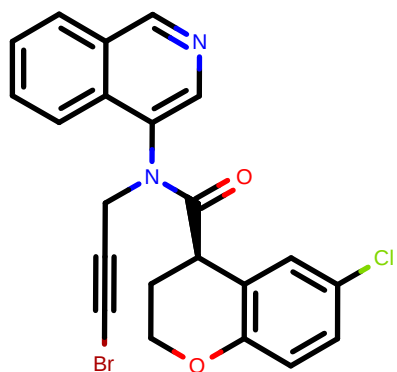


DAR-DIA-5ff57136-17_1



CID:

DAR-DIA-5ff57136-17_1

SMILES:

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

RUN:

RUN69

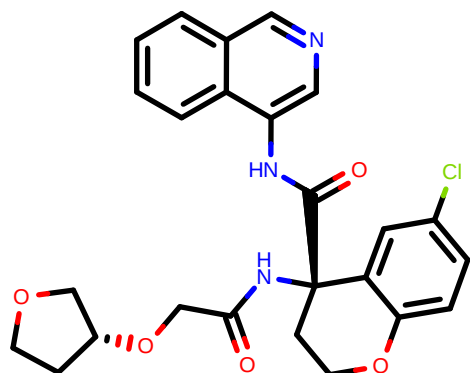
DDG (kcal/mol):

-4.13

dDDG (kcal/mol):

0.15

EN300-99391_1_1



CID:

EN300-99391_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@H]5CCOC5

RUN:

RUN1764

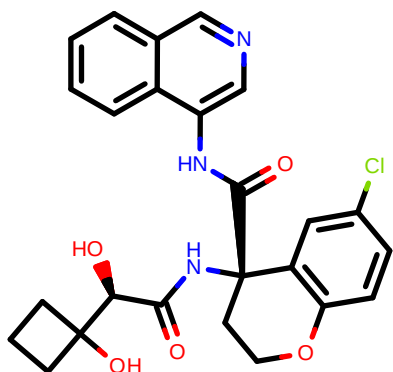
DDG (kcal/mol):

-4.03

dDDG (kcal/mol):

0.37

EN300-1073320_1_1



CID:

EN300-1073320_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5(CCC5)O)O

RUN:

RUN1756

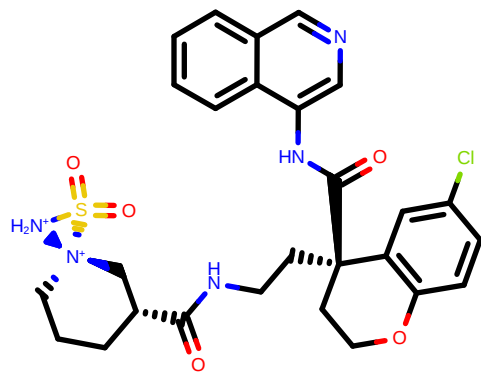
DDG (kcal/mol):

-3.92

dDDG (kcal/mol):

0.37

EN300-219496_3_1



CID:

EN300-219496_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C5(CCCN5)S(=O)(=O)N)N

RUN:

RUN1745

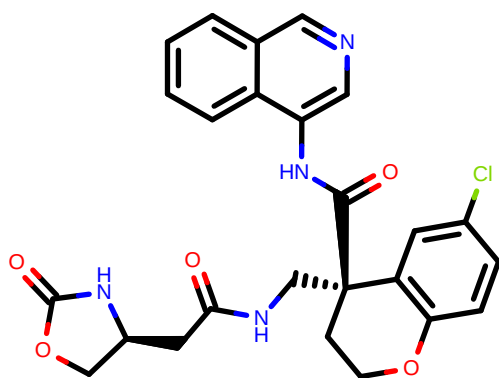
DDG (kcal/mol):

-3.76

dDDG (kcal/mol):

0.56

EN300-1703852_2_1



CID:

EN300-1703852_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@H]5OC(=O)N5

RUN:

RUN509

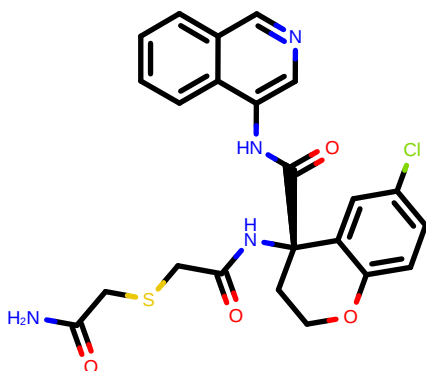
DDG (kcal/mol):

-3.70

dDDG (kcal/mol):

0.32

EN300-33513_1_1



CID:

EN300-33513_1_1

SMILES:

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

RUN:

RUN322

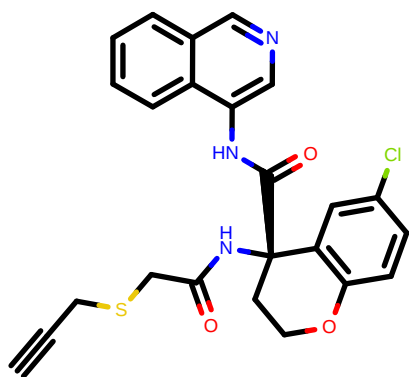
DDG (kcal/mol):

-3.66

dDDG (kcal/mol):

0.26

EN300-86878_1_1



CID:

EN300-86878_1_1

SMILES:

C#CCSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN585

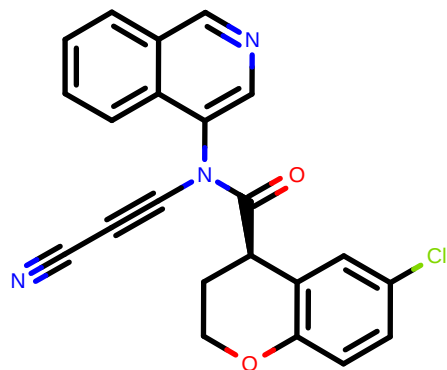
DDG (kcal/mol):

-3.57

dDDG (kcal/mol):

0.24

DAR-DIA-5ff57136-10_1



CID:

DAR-DIA-5ff57136-10_1

SMILES:

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

RUN:

RUN126

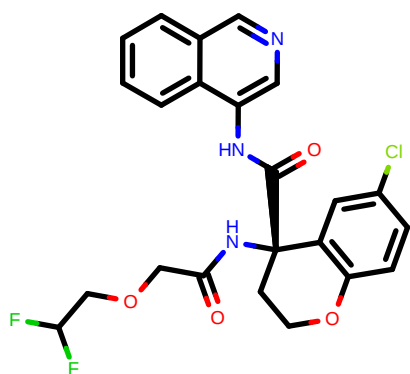
DDG (kcal/mol):

-3.55

dDDG (kcal/mol):

0.14

EN300-315792_1_1



CID: EN300-315792_1_1

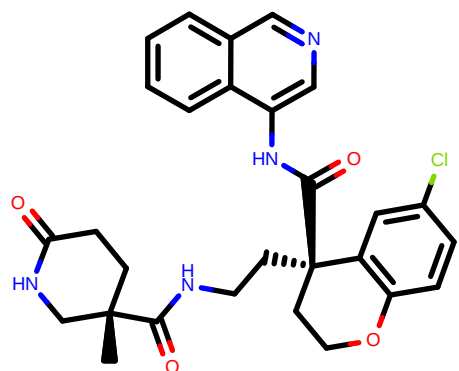
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F

RUN: RUN521

DDG (kcal/mol): -3.51

dDDG (kcal/mol): 0.26

EN300-195924_3_1



CID: EN300-195924_3_1

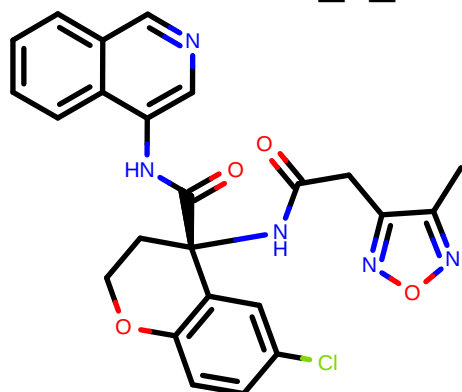
SMILES: C[C@@]1(CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN906

DDG (kcal/mol): -3.49

dDDG (kcal/mol): 0.40

EN300-254883_1_1



CID: EN300-254883_1_1

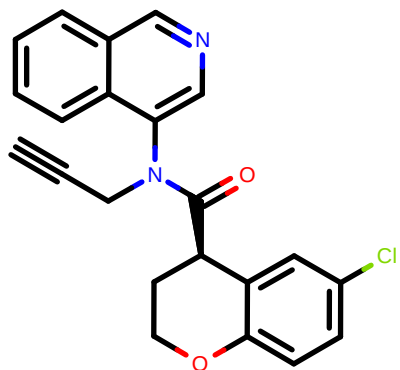
SMILES: Cc1c(non1)CC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1501

DDG (kcal/mol): -3.44

dDDG (kcal/mol): 0.23

DAR-DIA-5ff57136-13_1



CID: DAR-DIA-5ff57136-13_1

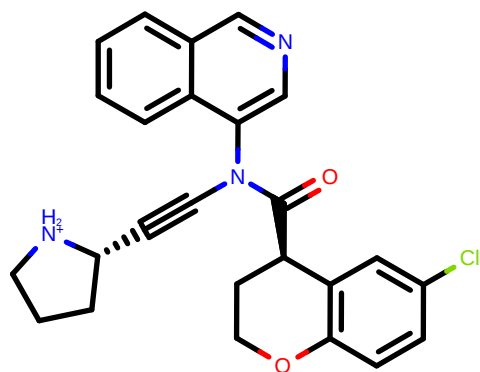
SMILES: C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN92

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.13

DAR-DIA-5ff57136-12_1



CID:

DAR-DIA-5ff57136-12_1

SMILES:

c1ccc2c(c1)cncc2N(C#C[C@H]3CCCC[NH2+](3)C(=O)[C@H]4CCOCc5c4cc(cc5)Cl

RUN:

RUN173

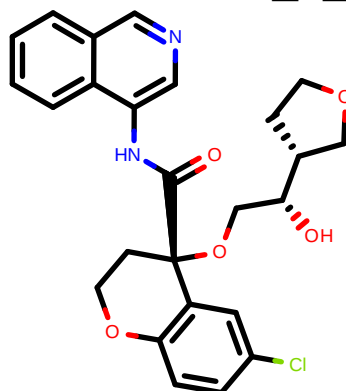
DDG (kcal/mol):

-3.41

dDDG (kcal/mol):

0.17

EN300-1911992_1_2



CID:

EN300-1911992_1_2

SMILES:

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

RUN:

RUN1751

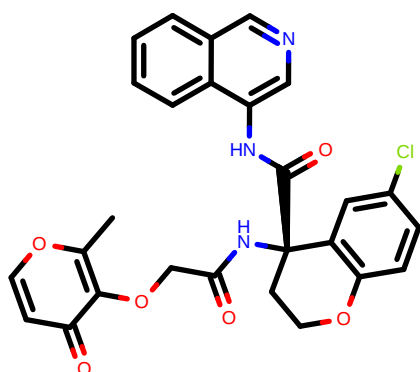
DDG (kcal/mol):

-3.40

dDDG (kcal/mol):

0.45

EN300-702714_1_1



CID:

EN300-702714_1_1

SMILES:

Cc1c(c(=O)ccoc1)OCC(=O)N[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN1341

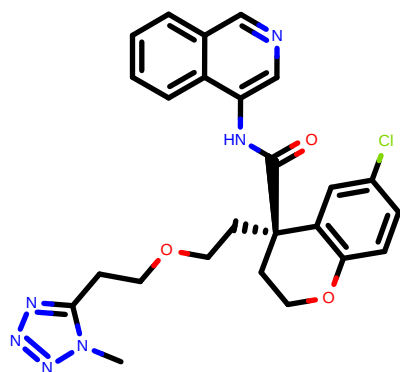
DDG (kcal/mol):

-3.39

dDDG (kcal/mol):

0.26

EN300-365398_3_1



CID:

EN300-365398_3_1

SMILES:

Cn1c(nnn1)CCOCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN624

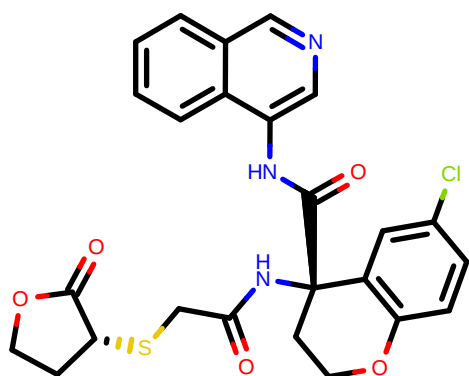
DDG (kcal/mol):

-3.35

dDDG (kcal/mol):

0.36

EN300-113218_1_1



CID: EN300-113218_1_1

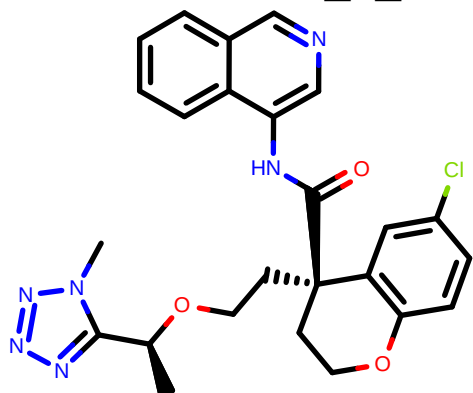
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@@H]5CCOC5=O

RUN: RUN1572

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.36

EN300-173006_3_1



CID: EN300-173006_3_1

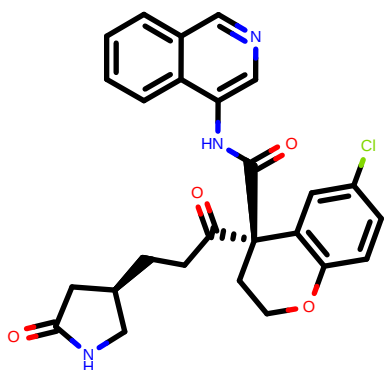
SMILES: C[C@@H](c1nnnn1C)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nnc5c4cccs5

RUN: RUN1124

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-21_1



CID: VLA-UCB-34f3ed0c-21_1

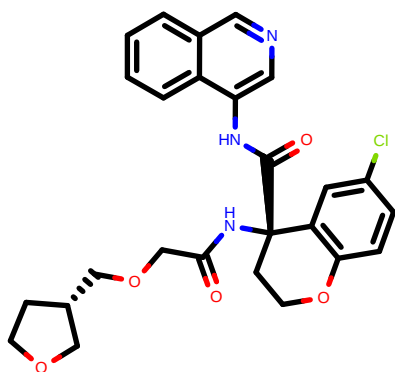
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NCS

RUN: RUN27

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.38

EN300-80522_1_2



CID: EN300-80522_1_2

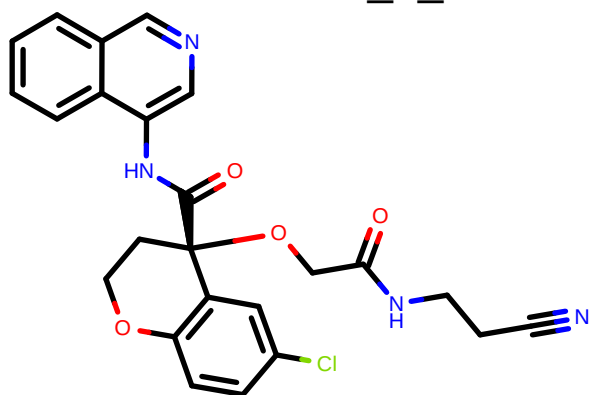
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCOC5

RUN: RUN1301

DDG (kcal/mol): -3.01

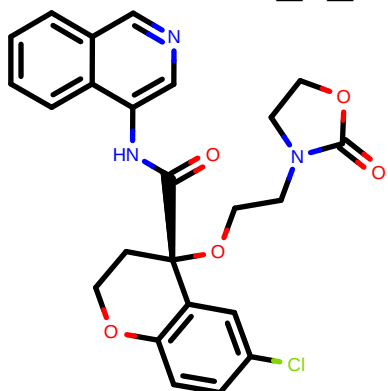
dDDG (kcal/mol): 0.28

EN300-10895_1_1



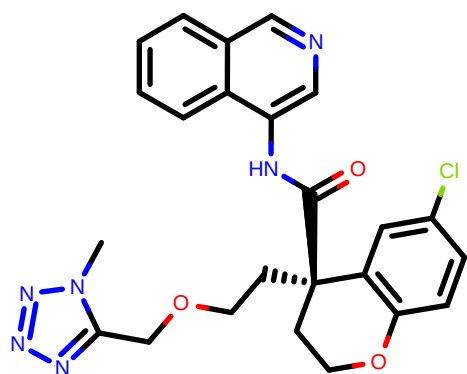
CID:	EN300-10895_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4Cl)OCC(=O)NCCC#N</chem>
RUN:	RUN357
DDG (kcal/mol):	-2.97
dDDG (kcal/mol):	0.24

EN300-370967_1_1



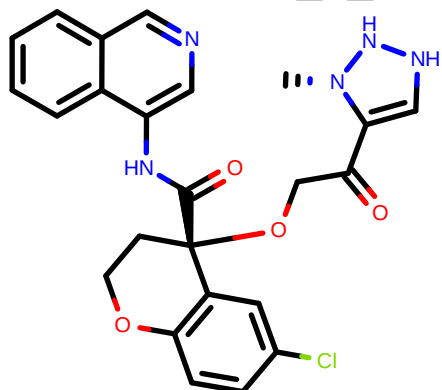
CID:	EN300-370967_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4Cl)OCCN5CCOC5=O</chem>
RUN:	RUN1647
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.25

EN300-62574_3_1



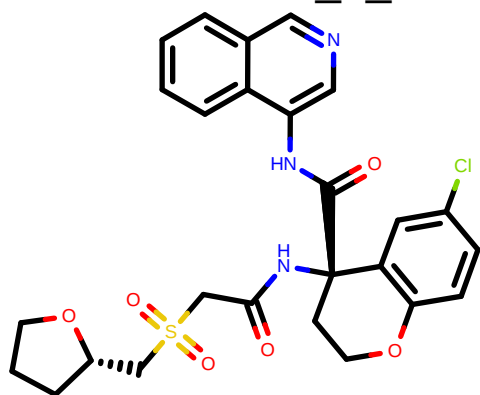
CID:	EN300-62574_3_1
SMILES:	<chem>Cn1c(nnn1)COC[C@@]2(CCOC3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1236
DDG (kcal/mol):	-2.93
dDDG (kcal/mol):	0.28

EN300-204936_1_1



CID:	EN300-204936_1_1
SMILES:	<chem>Cn1c(cnn1)C(=O)CO[C@@]2(CCOC3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN944
DDG (kcal/mol):	-2.92
dDDG (kcal/mol):	0.22

EN300-67023_1_1



CID:

EN300-67023_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C[C@@H]5CCCCO5

RUN:

RUN901

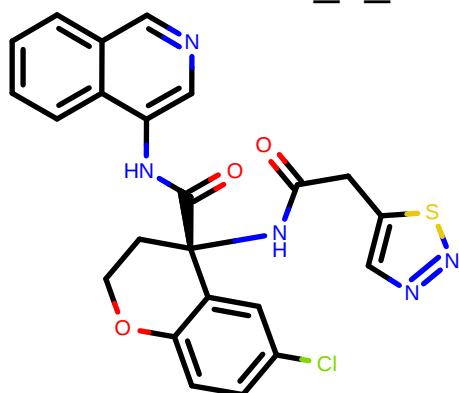
DDG (kcal/mol):

-2.89

dDDG (kcal/mol):

0.39

EN300-260152_1_1



CID:

EN300-260152_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnns5

RUN:

RUN1205

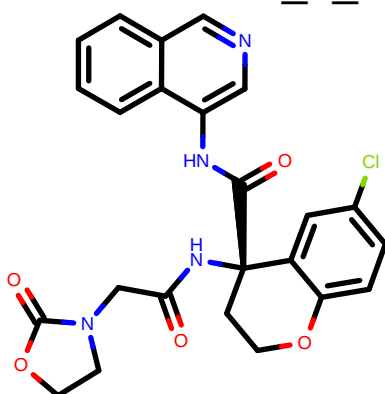
DDG (kcal/mol):

-2.87

dDDG (kcal/mol):

0.21

EN300-172179_1_1



CID:

EN300-172179_1_1

SMILES:

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

RUN:

RUN1149

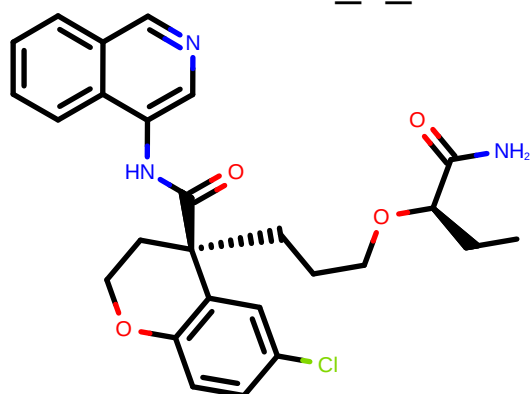
DDG (kcal/mol):

-2.86

dDDG (kcal/mol):

0.26

EN300-65839_4_2



CID:

EN300-65839_4_2

SMILES:

CC[C@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN:

RUN667

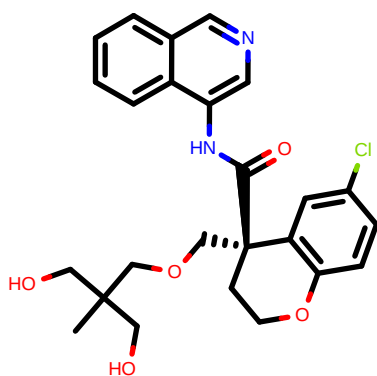
DDG (kcal/mol):

-2.85

dDDG (kcal/mol):

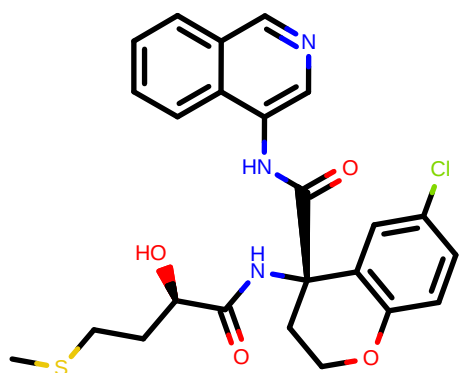
0.43

EN300-218116_2_1



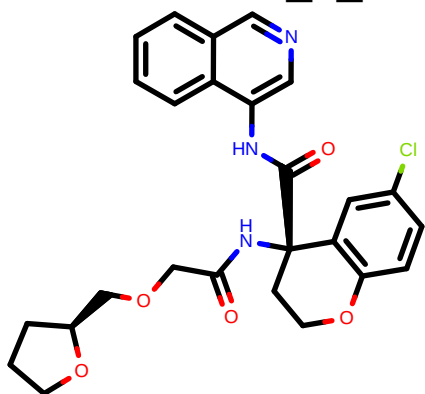
CID:	EN300-218116_2_1
SMILES:	<chem>CC(CO)(CO)COC[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1430
DDG (kcal/mol):	-2.85
dDDG (kcal/mol):	0.37

EN300-103144_1_2



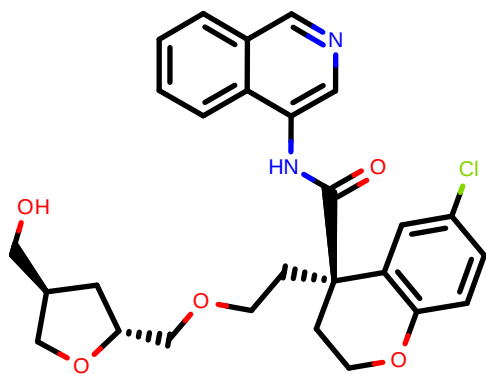
CID:	EN300-103144_1_2
SMILES:	<chem>CSCC[C@H](C(=O)N[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O</chem>
RUN:	RUN1453
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.33

EN300-60033_1_1



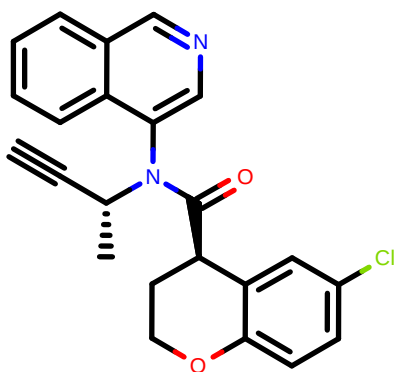
CID:	EN300-60033_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)NC(=O)COC[C@H]5CCCCO5</chem>
RUN:	RUN1541
DDG (kcal/mol):	-2.79
dDDG (kcal/mol):	0.27

EN300-6494158_3_2



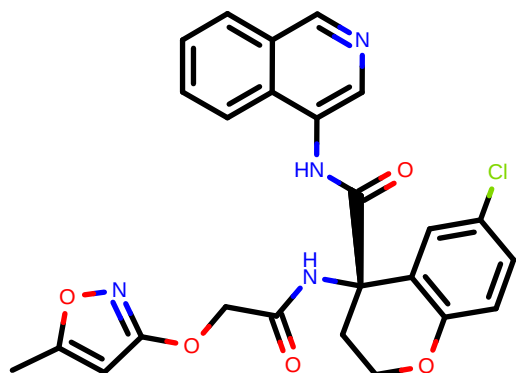
CID:	EN300-6494158_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCOC[C@H]5C[C@H](CO5)CO</chem>
RUN:	RUN1004
DDG (kcal/mol):	-2.77
dDDG (kcal/mol):	0.36

DAR-DIA-5ff57136-16_2



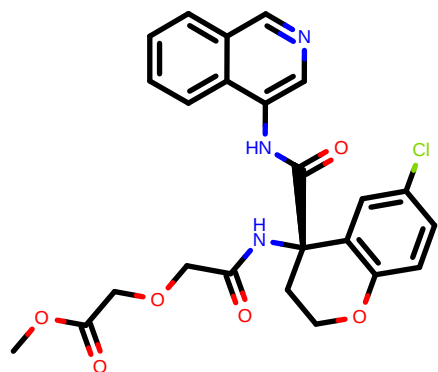
CID:	DAR-DIA-5ff57136-16_2
SMILES:	<chem>C[C@H](C#C)N(c1cncc2c1cccc2)C(=O)[C@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN192
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.15

EN300-12929_1_1



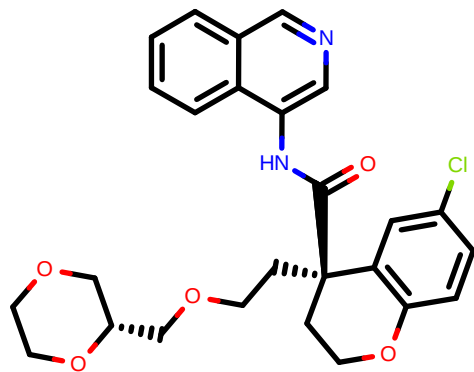
CID:	EN300-12929_1_1
SMILES:	<chem>Cc1cc(no1)OCC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1445
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.32

EN300-205635_1_1



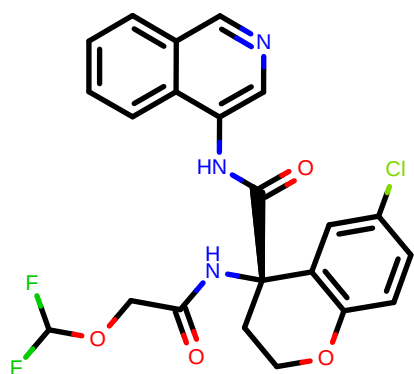
CID:	EN300-205635_1_1
SMILES:	<chem>COC(=O)COCC(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN402
DDG (kcal/mol):	-2.69
dDDG (kcal/mol):	0.24

EN300-139167_3_2



CID:	EN300-139167_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCOC5</chem>
RUN:	RUN664
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.37

EN300-179091_1_1



CID: EN300-179091_1_1

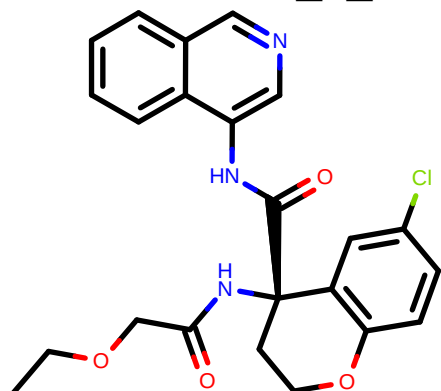
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)NC(=O)COC(F)F

RUN: RUN1732

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.33

EN300-21303_1_1



CID: EN300-21303_1_1

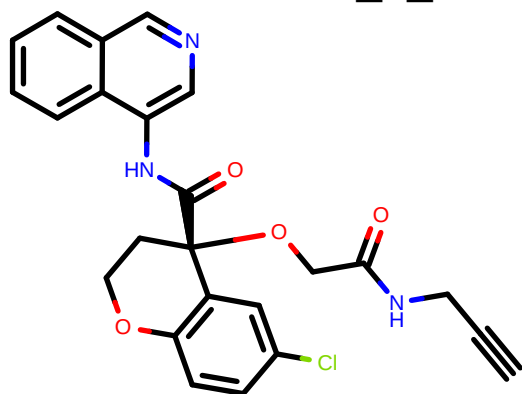
SMILES: CCOCC(=O)N[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN354

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.26

EN300-1659582_1_1



CID: EN300-1659582_1_1

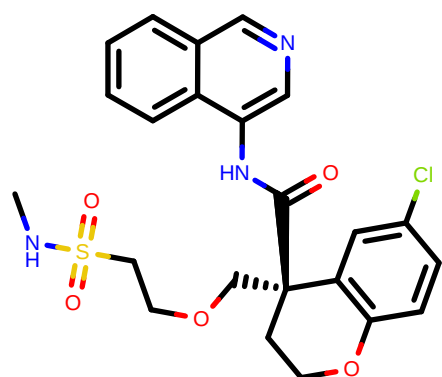
SMILES: C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN453

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.21

EN300-6482967_2_1



CID: EN300-6482967_2_1

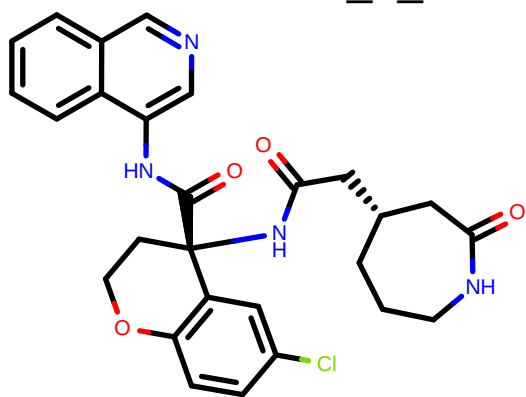
SMILES: CNS(=O)(=O)CCOC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN650

DDG (kcal/mol): -2.64

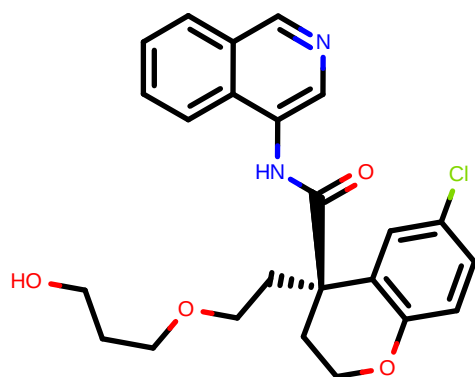
dDDG (kcal/mol): 0.37

EN300-195590_1_2



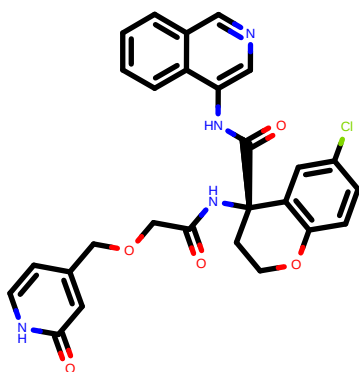
CID:	EN300-195590_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCNC(=O)C5</chem>
RUN:	RUN743
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.37

EN300-221518_3_1



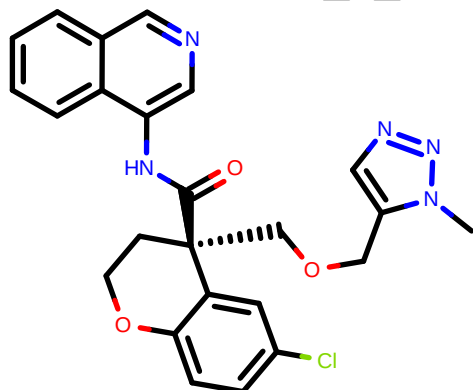
CID:	EN300-221518_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCCO</chem>
RUN:	RUN1404
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.22

EN300-316258_1_1



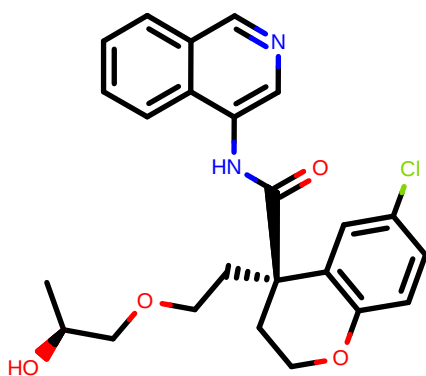
CID:	EN300-316258_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COCc5cc[nH]c(=O)c5</chem>
RUN:	RUN617
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.31

EN300-216673_2_1



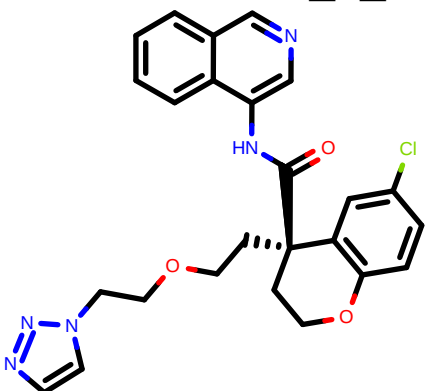
CID:	EN300-216673_2_1
SMILES:	<chem>Cn1c(cnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1350
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.28

EN300-185378_3_1



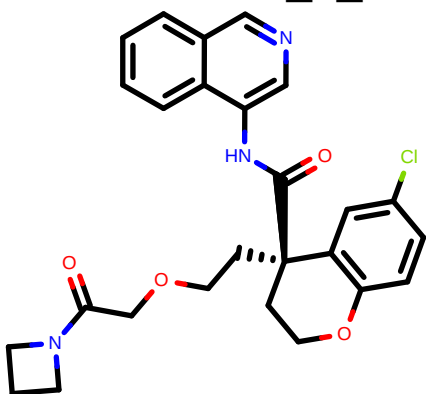
CID:	EN300-185378_3_1
SMILES:	<chem>C[C@@H](COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O</chem>
RUN:	RUN1428
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.29

EN300-1715993_3_1



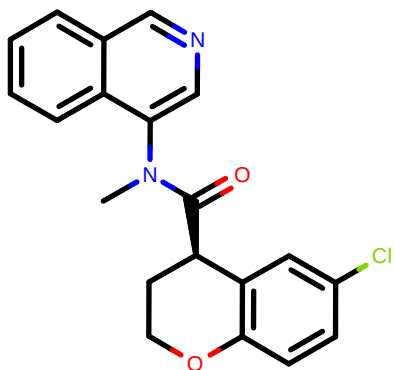
CID:	EN300-1715993_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCCn5ccnn5</chem>
RUN:	RUN1396
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.25

EN300-11195_3_1



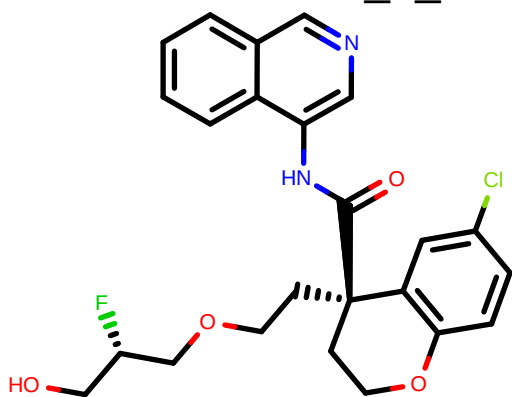
CID:	EN300-11195_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCCS</chem>
RUN:	RUN1356
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.29

MAK-UNK-3875bbc8-2_1



CID:	MAK-UNK-3875bbc8-2_1
SMILES:	<chem>CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN49
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.09

EN300-1600517_3_2



CID: EN300-1600517_3_2

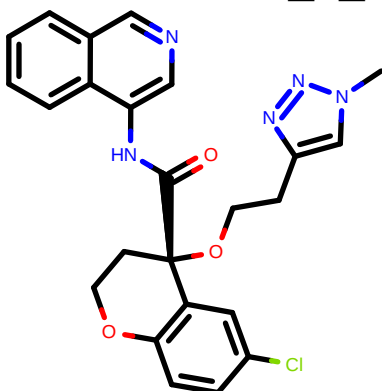
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)F

RUN: RUN1228

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.32

EN300-1600786_1_1



CID: EN300-1600786_1_1

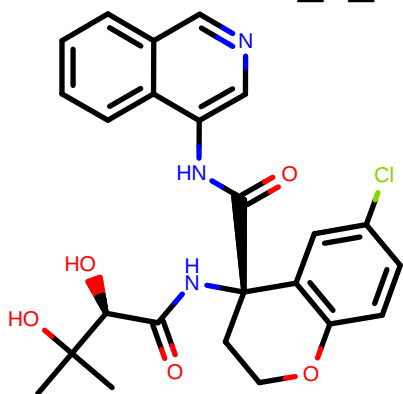
SMILES: Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1032

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.26

EN300-299532_1_2



CID: EN300-299532_1_2

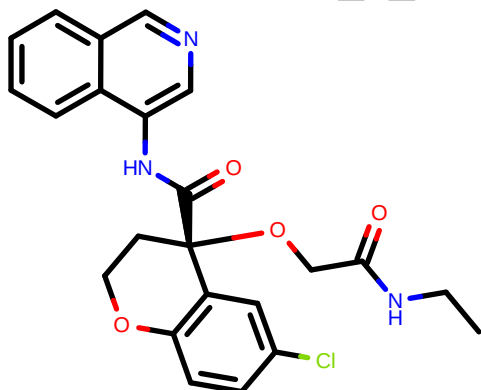
SMILES: CC(C)([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O

RUN: RUN1644

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.21

EN300-7003350_1_1



CID: EN300-7003350_1_1

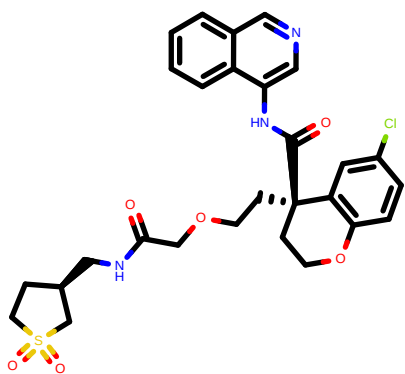
SMILES: CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN723

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.18

EN300-47606_3_1



CID:

EN300-47606_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C(=O)Oc3cc(ccc34)C)CCOC(=O)NC[C@@H](C)CCS(=O)(=O)CS

RUN:

RUN1771

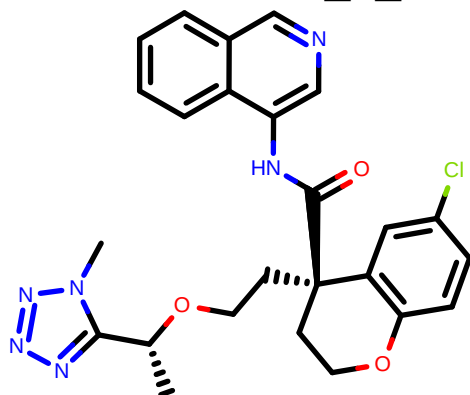
DDG (kcal/mol):

-2.50

dDDG (kcal/mol):

0.50

EN300-173006_3_2



CID:

EN300-173006_3_2

SMILES:

C[C@@H](c1nnnn1C)OCC[C@H]2(C(=O)Oc3cc(ccc34)C)C(=O)Nc4ncnc5c4cccc5

RUN:

RUN1715

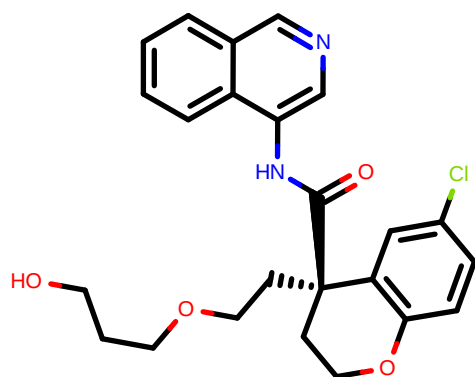
DDG (kcal/mol):

-2.49

dDDG (kcal/mol):

0.31

EN300-221518_3_1



CID:

EN300-221518_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C(=O)Oc3cc(ccc34)C)CCOCCCCO

RUN:

RUN1412

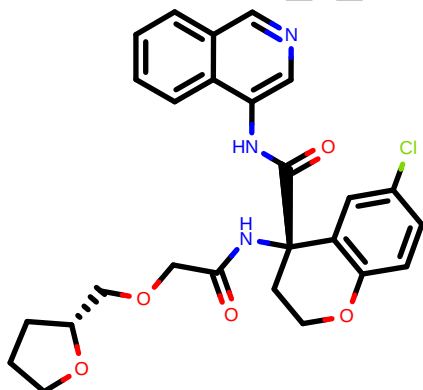
DDG (kcal/mol):

-2.48

dDDG (kcal/mol):

0.23

EN300-60033_1_2



CID:

EN300-60033_1_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H](C(=O)Oc3cc(ccc34)C)NC(=O)COC[C@H]5CCCCO5

RUN:

RUN1349

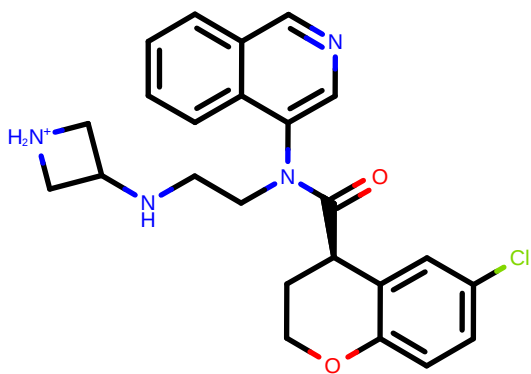
DDG (kcal/mol):

-2.47

dDDG (kcal/mol):

0.34

MAK-UNK-83e0a0b4-3_1



CID:

MAK-UNK-83e0a0b4-3_1

SMILES:

c1ccc2c(c1)cncc2N(CNCC3C[NH2+][C3])C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN:

RUN220

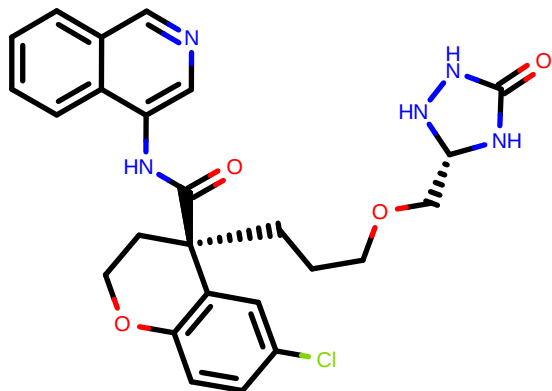
DDG (kcal/mol):

-2.47

dDDG (kcal/mol):

0.35

EN300-73772_4_1



CID:

EN300-73772_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]n5

RUN:

RUN308

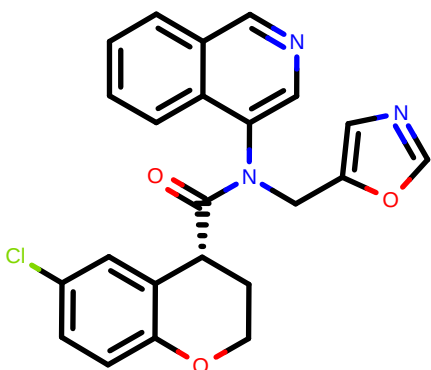
DDG (kcal/mol):

-2.46

dDDG (kcal/mol):

0.29

ALP-UNI-44c99a80-3_1



CID:

ALP-UNI-44c99a80-3_1

SMILES:

c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN:

RUN229

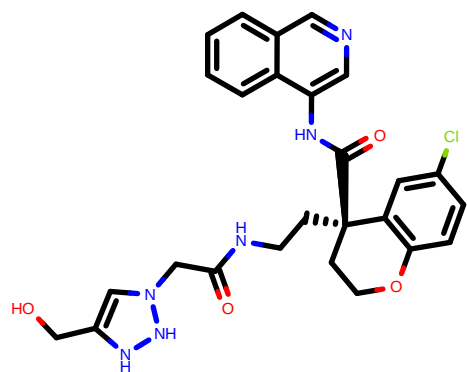
DDG (kcal/mol):

-2.45

dDDG (kcal/mol):

0.19

EN300-108236_3_1



CID:

EN300-108236_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc[nH]5CO

RUN:

RUN803

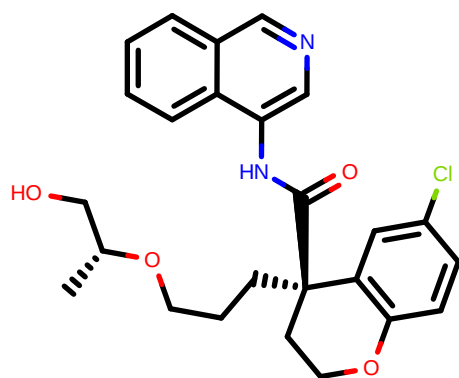
DDG (kcal/mol):

-2.43

dDDG (kcal/mol):

0.31

EN300-175186_4_2



CID: EN300-175186_4_2

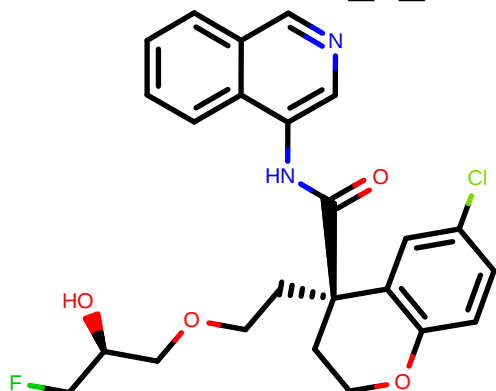
SMILES: C[C@H](CO)OCCC[C@]1(COC(=O)c2cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN460

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.30

EN300-1968342_3_1



CID: EN300-1968342_3_1

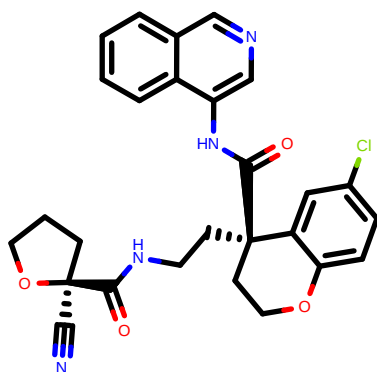
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(COC(=O)c4cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN916

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.36

EN300-3710141_3_1



CID: EN300-3710141_3_1

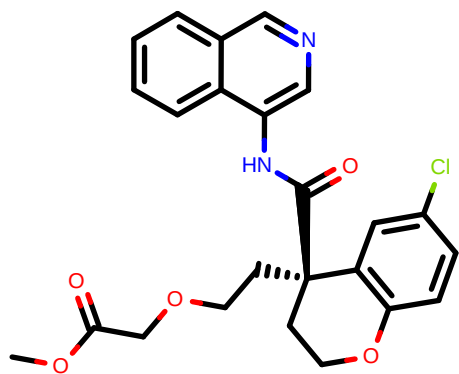
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(COC(=O)c4cc(cc4)Cl)CCNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN1002

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.30

EN300-19700_3_1



CID: EN300-19700_3_1

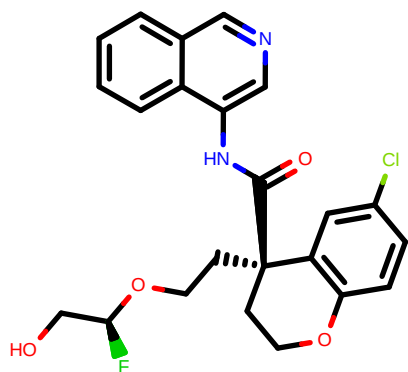
SMILES: COC(=O)COCC[C@]1(COC(=O)c2cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN1571

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.24

EN300-861925_3_2



CID: EN300-861925_3_2

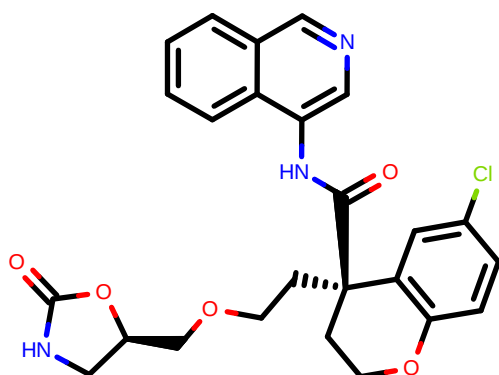
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H](CO)F

RUN: RUN1372

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.26

EN300-203293_3_2



CID: EN300-203293_3_2

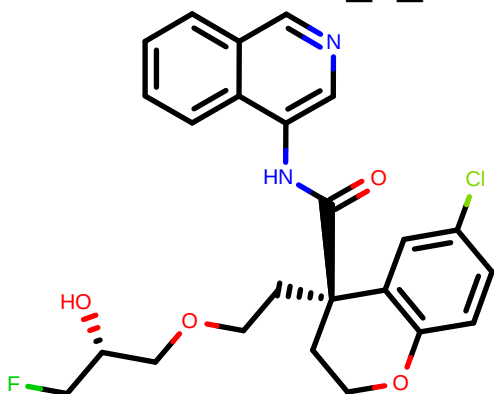
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5NC(=O)O5

RUN: RUN742

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.26

EN300-1968342_3_2



CID: EN300-1968342_3_2

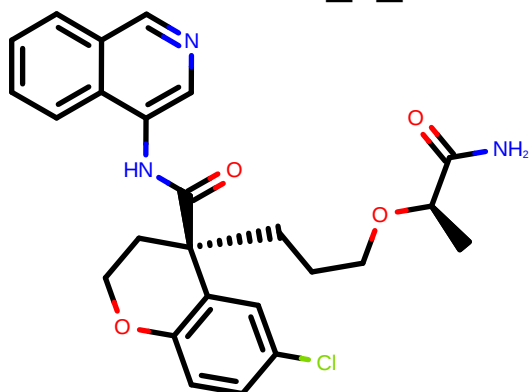
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN1548

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.36

EN300-17381_4_2



CID: EN300-17381_4_2

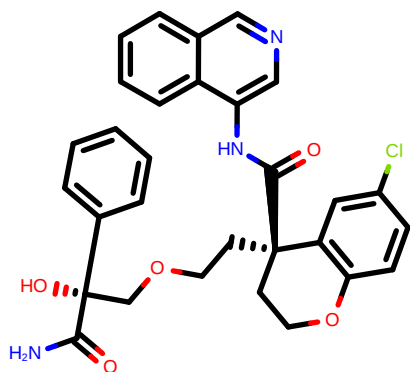
SMILES: C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN388

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.23

EN300-248526_3_1



CID: EN300-248526_3_1

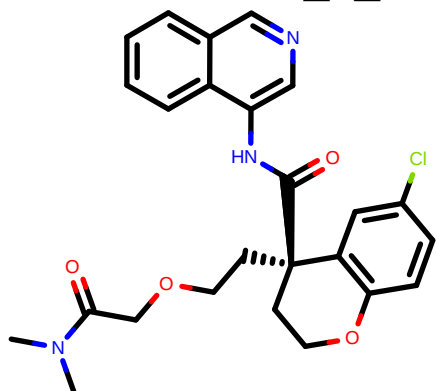
SMILES: c1ccc(cc1)[C@@]([C@@]1(COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(C(=O)N)O

RUN: RUN703

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.55

EN300-216063_3_1



CID: EN300-216063_3_1

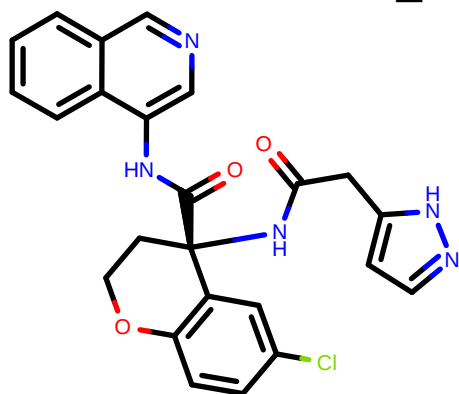
SMILES: CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1468

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-4_1



CID: VLA-UCB-34f3ed0c-4_1

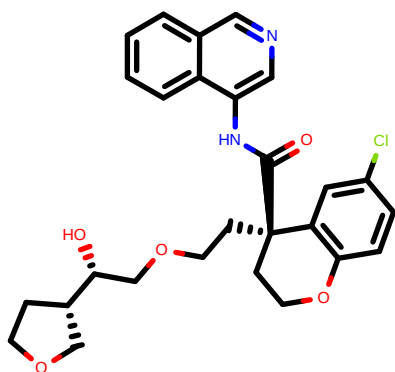
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]([C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cn[nH]5

RUN: RUN266

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.23

EN300-1911992_3_4



CID: EN300-1911992_3_4

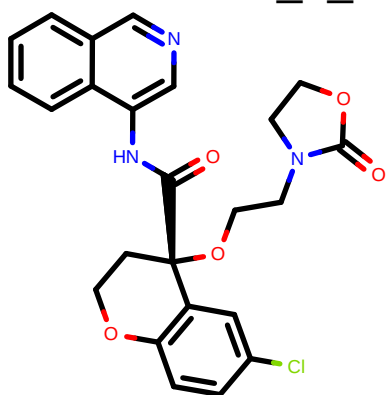
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]([C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]([C@H]5CCOC5)O

RUN: RUN449

DDG (kcal/mol): -2.31

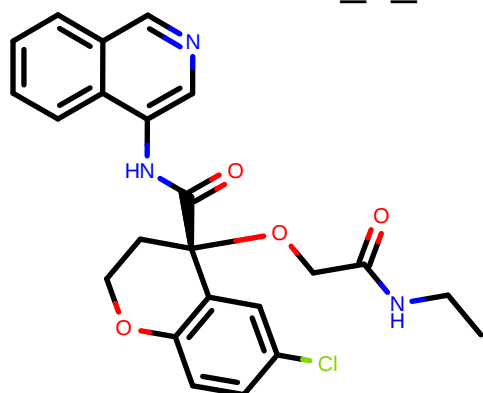
dDDG (kcal/mol): 0.36

EN300-370967_1_1



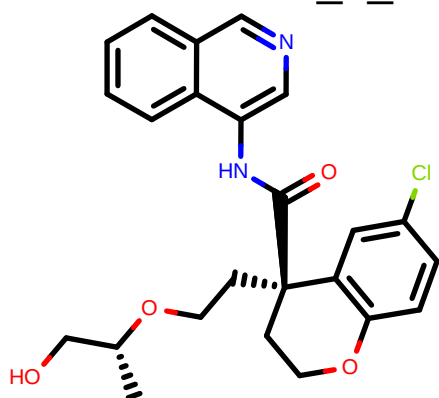
CID:	EN300-370967_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O</chem>
RUN:	RUN1655
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.27

EN300-7003350_1_1



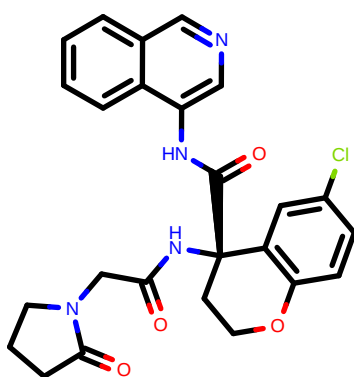
CID:	EN300-7003350_1_1
SMILES:	<chem>CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN738
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.20

EN300-175186_3_2



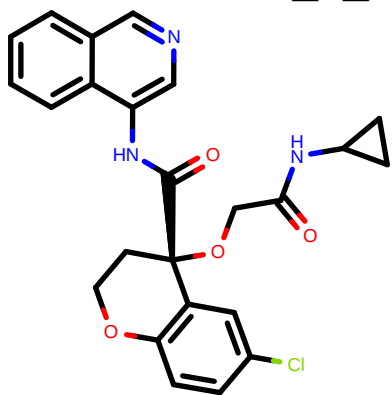
CID:	EN300-175186_3_2
SMILES:	<chem>C[C@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN1364
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.25

EN300-11934_1_1



CID:	EN300-11934_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O</chem>
RUN:	RUN1405
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.24

EN300-1253178_1_1



CID: EN300-1253178_1_1

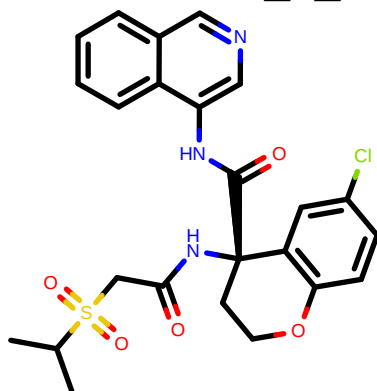
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN: RUN620

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.26

EN300-51028_1_1



CID: EN300-51028_1_1

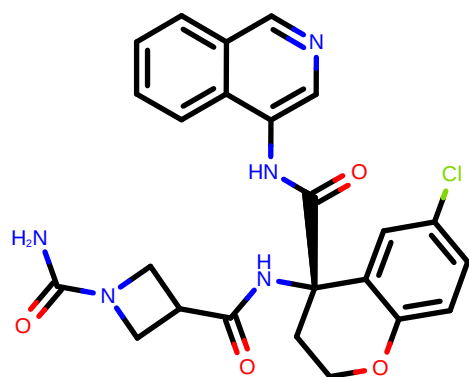
SMILES: CC(C)S(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN941

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.27

EN300-1248250_1_1



CID: EN300-1248250_1_1

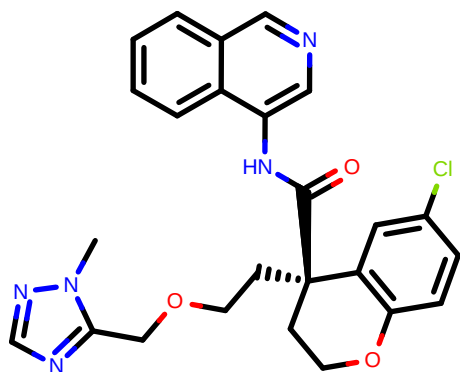
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CN(C5)C(=O)N

RUN: RUN1293

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.24

EN300-87334_3_1



CID: EN300-87334_3_1

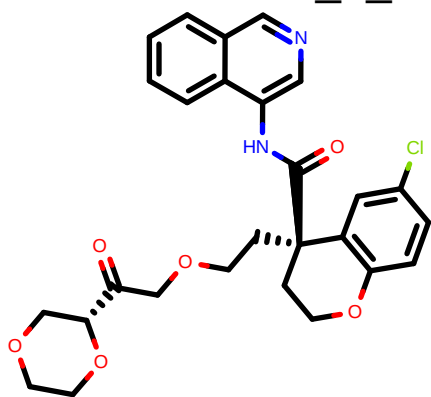
SMILES: Cn1c(ncn1)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1300

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.27

EN300-6238494_3_2



CID:

EN300-6238494_3_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)[C@H]5COCCO5

RUN:

RUN1076

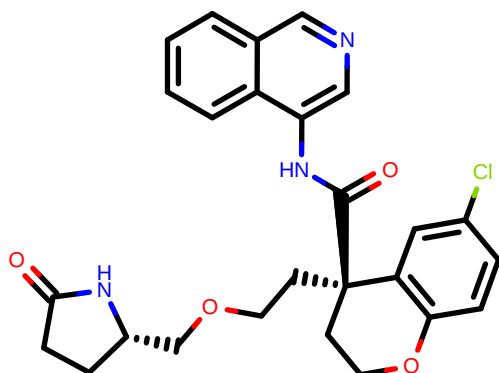
DDG (kcal/mol):

-2.23

dDDG (kcal/mol):

0.33

EN300-264301_3_1



CID:

EN300-264301_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCCC(=O)N5

RUN:

RUN860

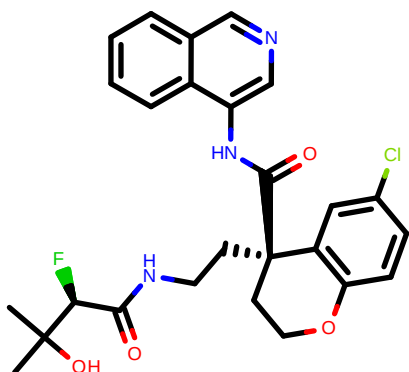
DDG (kcal/mol):

-2.22

dDDG (kcal/mol):

0.25

EN300-264744_3_2



CID:

EN300-264744_3_2

SMILES:

CC(C)[C@H](C)[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)F)O

RUN:

RUN1338

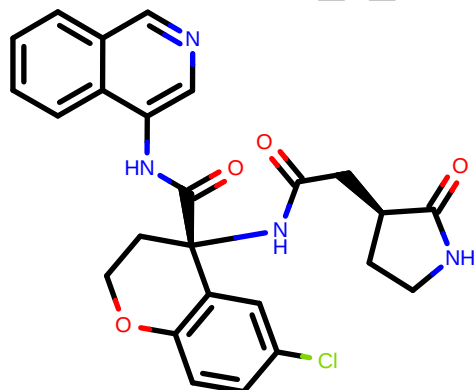
DDG (kcal/mol):

-2.21

dDDG (kcal/mol):

0.30

EN300-343474_1_1



CID:

EN300-343474_1_1

SMILES:

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

RUN:

RUN673

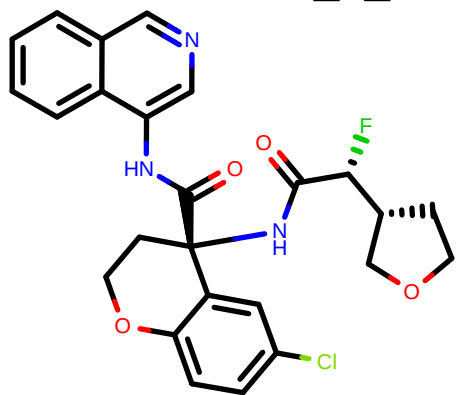
DDG (kcal/mol):

-2.21

dDDG (kcal/mol):

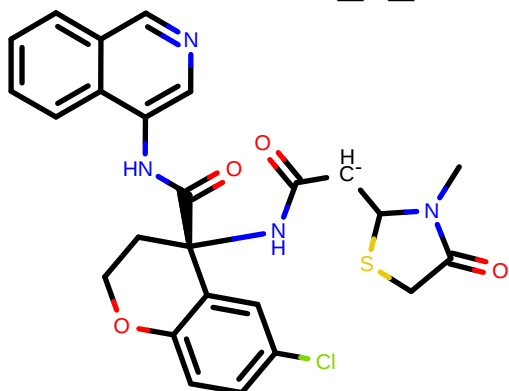
0.29

EN300-783124_1_1



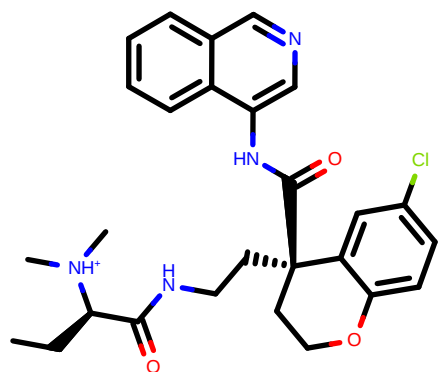
CID:	EN300-783124_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@@H]([C@@H]5CCOC5)F</chem>
RUN:	RUN1469
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.23

EN300-143564_1_2



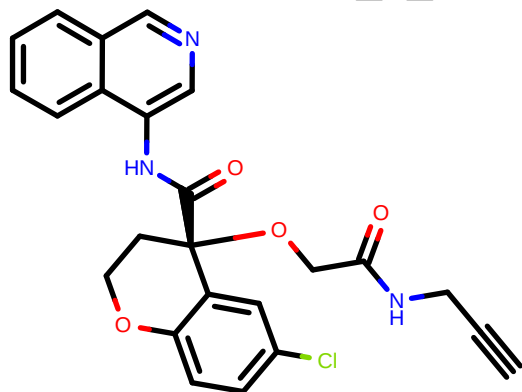
CID:	EN300-143564_1_2
SMILES:	<chem>CN1C(=O)CS/C1=C/C(=O)N[C@@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN529
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.22

EN300-110012_3_2



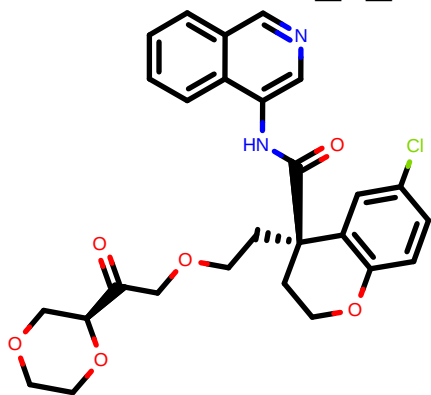
CID:	EN300-110012_3_2
SMILES:	<chem>CC[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cnc4c3cccc4)[NH+](C)C</chem>
RUN:	RUN654
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.42

EN300-1659582_1_1



CID:	EN300-1659582_1_1
SMILES:	<chem>C#CCNC(=O)CO[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN461
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.26

EN300-6238494_3_1



CID: EN300-6238494_3_1

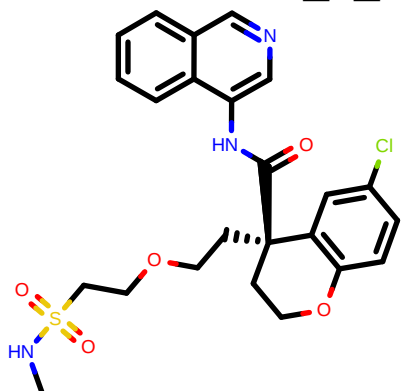
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)C@H]5COCCO5

RUN: RUN940

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.32

EN300-6482967_3_1



CID: EN300-6482967_3_1

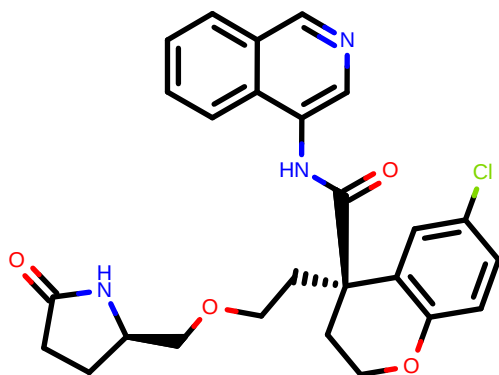
SMILES: CNS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN329

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.33

EN300-195756_3_2



CID: EN300-195756_3_2

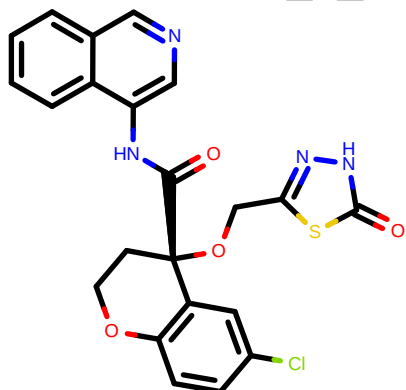
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC[C@H]5CCCC(=O)N5

RUN: RUN1084

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.24

EN300-171766_1_1



CID: EN300-171766_1_1

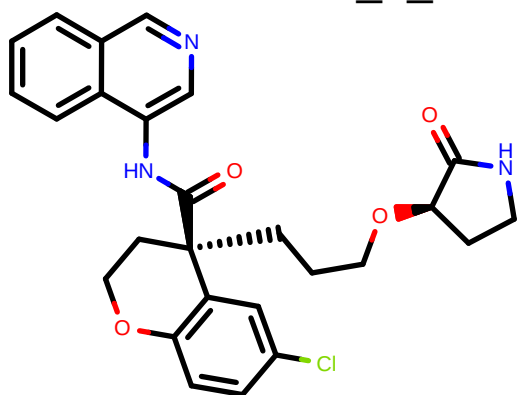
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5n[nH]c(=O)s5

RUN: RUN636

DDG (kcal/mol): -2.16

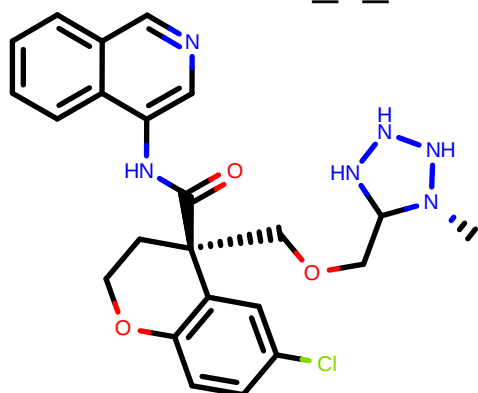
dDDG (kcal/mol): 0.22

EN300-6736413_4_1



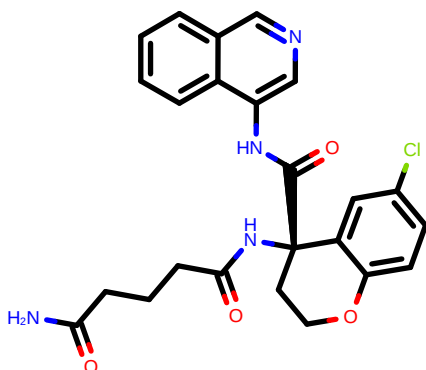
CID:	EN300-6736413_4_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O</chem>
RUN:	RUN983
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.34

EN300-62574_2_1



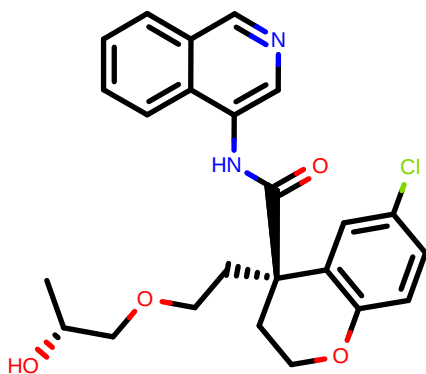
CID:	EN300-62574_2_1
SMILES:	<chem>Cn1c(nnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN1102
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.28

EN300-59478_1_1



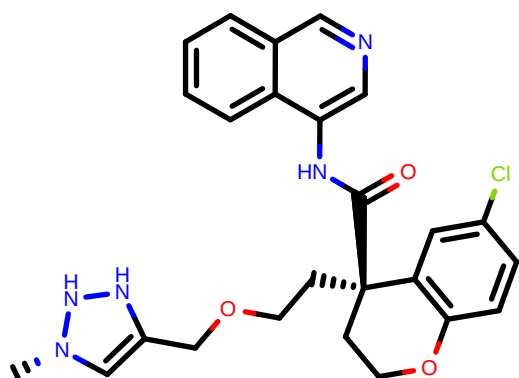
CID:	EN300-59478_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N</chem>
RUN:	RUN790
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.31

EN300-185378_3_2



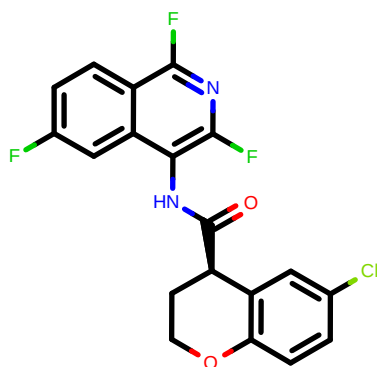
CID:	EN300-185378_3_2
SMILES:	<chem>C[C@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)O</chem>
RUN:	RUN1643
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.24

EN300-120282_3_1



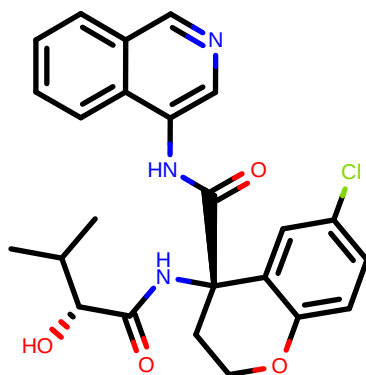
CID:	EN300-120282_3_1
SMILES:	<chem>Cn1cc(nn1)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1324
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.26

JOH-SUS-a69c159d-7_1



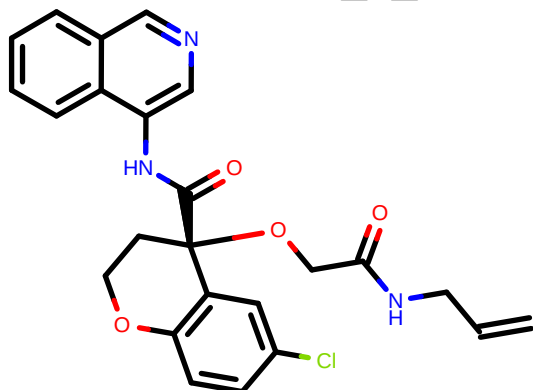
CID:	JOH-SUS-a69c159d-7_1
SMILES:	<chem>c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN71
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.06

EN300-115017_1_1



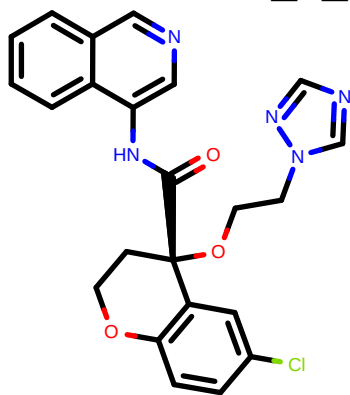
CID:	EN300-115017_1_1
SMILES:	<chem>CC(C)[C@H](C(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O</chem>
RUN:	RUN458
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.24

EN300-17184_1_1



CID:	EN300-17184_1_1
SMILES:	<chem>C=CCNC(=O)CO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN445
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.19

EN300-6255179_1_1



CID: EN300-6255179_1_1

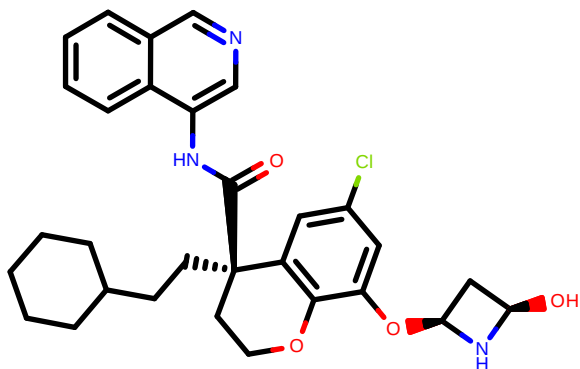
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnc5

RUN: RUN1088

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.19

VLA-UCB-50c39ae8-9_2



CID: VLA-UCB-50c39ae8-9_2

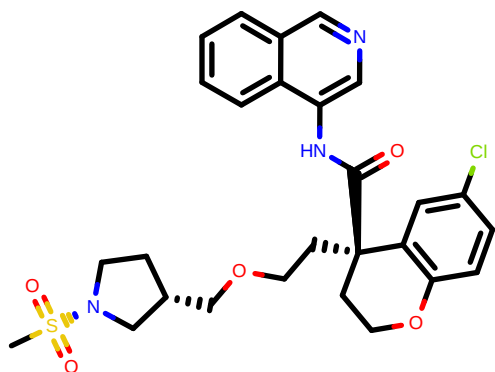
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)[C@H]5CC(=O)N5Cl)CCOC6CCCC6

RUN: RUN124

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.30

EN300-261986_3_1



CID: EN300-261986_3_1

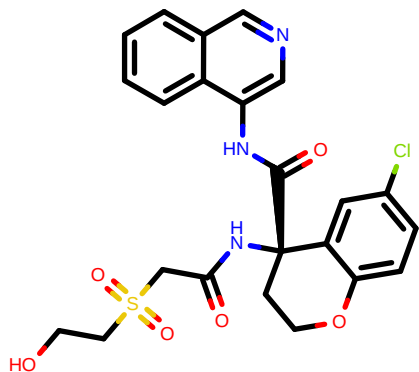
SMILES: CS(=O)(=O)N@1CC[C@@H]1[C@@]3(C1COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N6Acncc5c4ccccc5

RUN: RUN465

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.36

EN300-4293814_1_1



CID: EN300-4293814_1_1

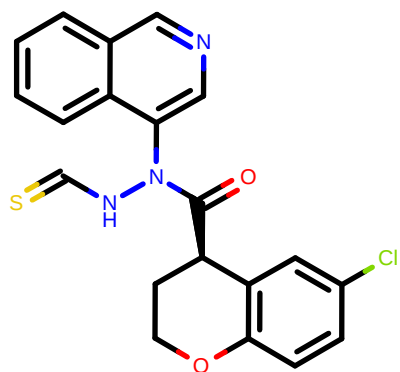
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)CCO

RUN: RUN466

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.48

DAR-DIA-5ff57136-18_1



CID: DAR-DIA-5ff57136-18_1

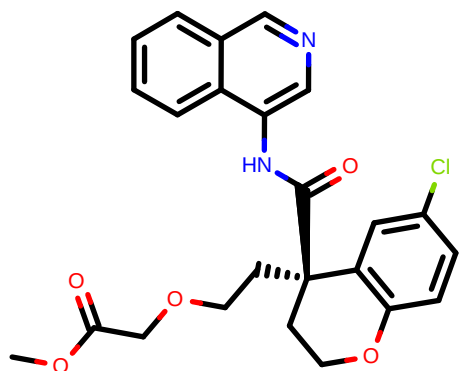
SMILES: c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)N=C=S

RUN: RUN101

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.13

EN300-19700_3_1



CID: EN300-19700_3_1

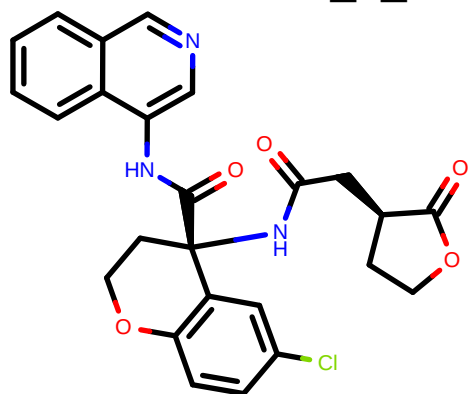
SMILES: COC(=O)COCC[C@]1(C(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1579

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.21

EN300-1072972_1_1



CID: EN300-1072972_1_1

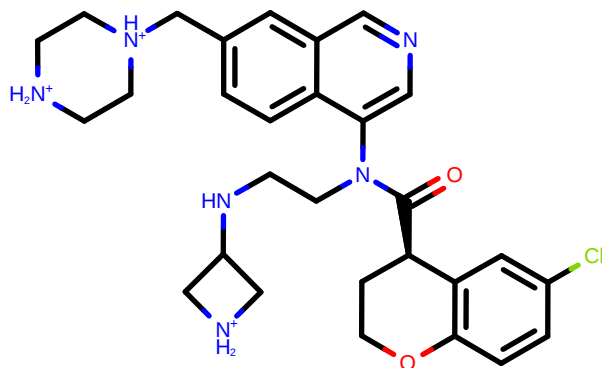
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COCc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCOC5=O

RUN: RUN1133

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.26

MAK-UNK-83e0a0b4-2_1



CID: MAK-UNK-83e0a0b4-2_1

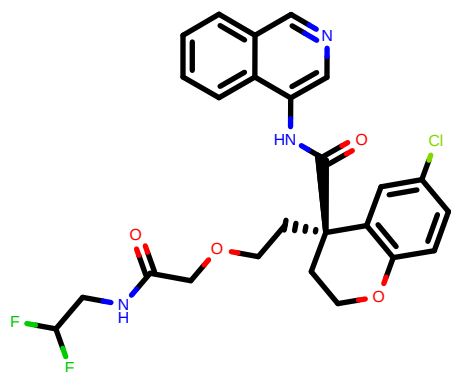
SMILES: c1cc2c(c1)cn3cc(NH2+)CC3cncc2N(CCNc4C[NH2+]C4)C(=O)[C@@H]5CCOCc6c5ccc6Cl

RUN: RUN34

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.50

EN300-120586_3_1



CID: EN300-120586_3_1

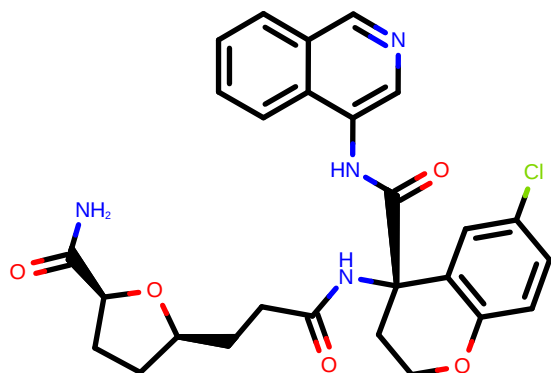
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCC(F)F

RUN: RUN369

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.30

EN300-364992_1_1



CID: EN300-364992_1_1

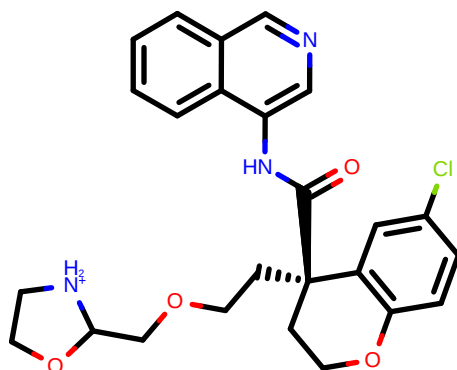
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H]5CC[C@H]5Cl=O

RUN: RUN696

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.38

EN300-317555_3_1



CID: EN300-317555_3_1

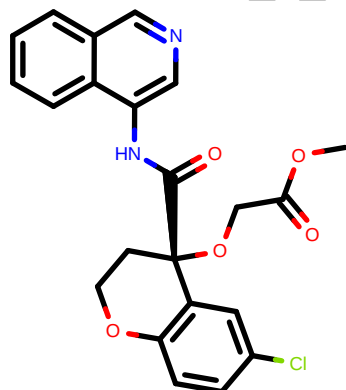
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5

RUN: RUN797

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.27

EN300-19700_1_1



CID: EN300-19700_1_1

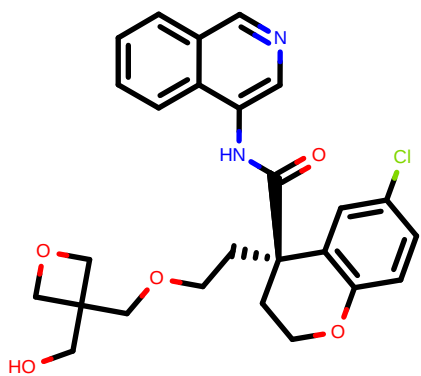
SMILES: COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN373

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.18

EN300-102347_3_1



CID:

EN300-102347_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)COC5CO

RUN:

RUN273

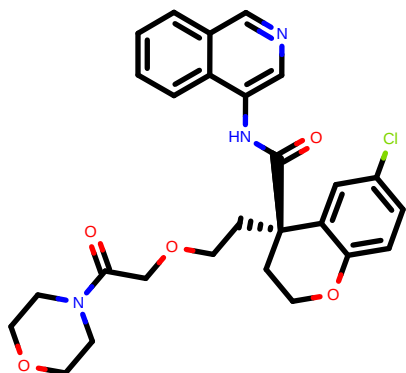
DDG (kcal/mol):

-1.94

dDDG (kcal/mol):

0.31

EN300-1241327_3_1



CID:

EN300-1241327_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5

RUN:

RUN829

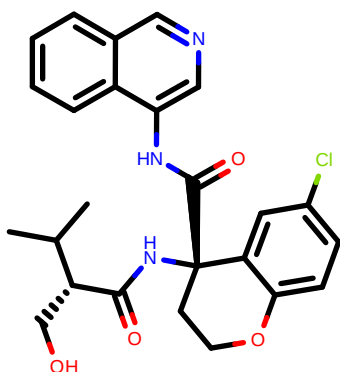
DDG (kcal/mol):

-1.94

dDDG (kcal/mol):

0.31

EN300-153257_1_1



CID:

EN300-153257_1_1

SMILES:

CC(C)[C@@H](CO)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN:

RUN1588

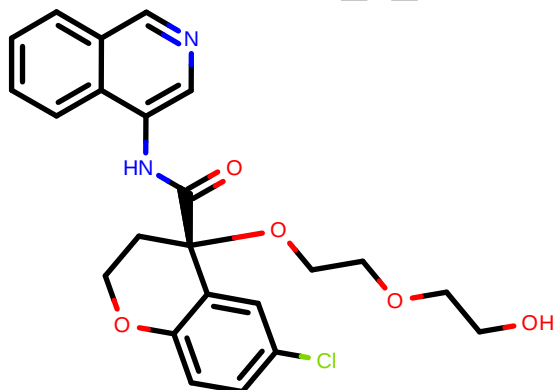
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

0.24

EN300-52467_1_1



CID:

EN300-52467_1_1

SMILES:

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

RUN:

RUN912

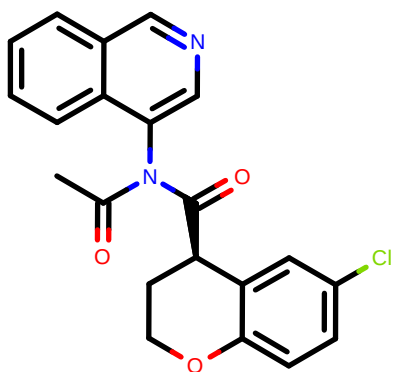
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

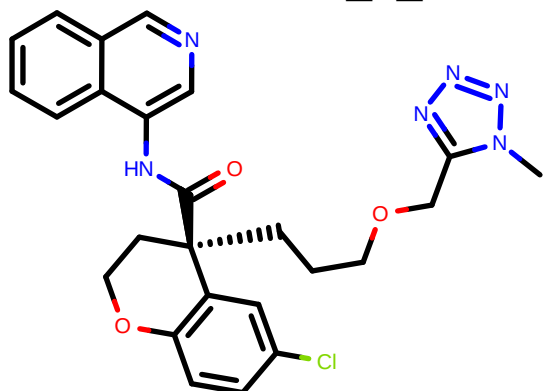
0.25

VLA-UCB-50c39ae8-1_1



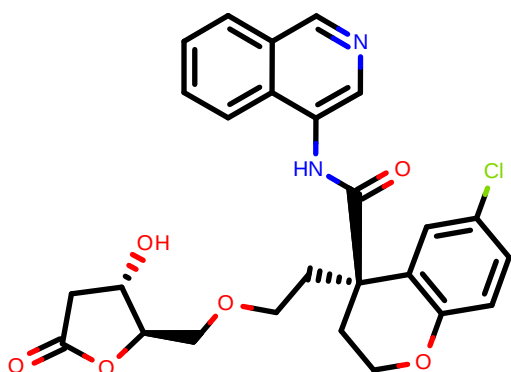
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	<chem>CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN94
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.13

EN300-62574_4_1



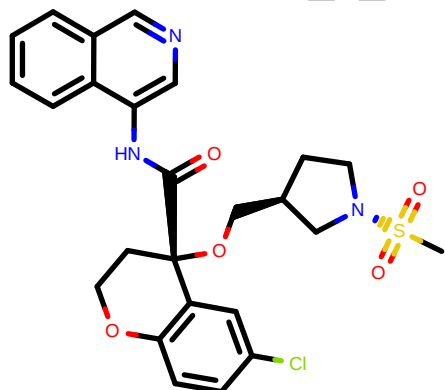
CID:	EN300-62574_4_1
SMILES:	<chem>Cn1c(nnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN332
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.39

EN300-6487407_3_1



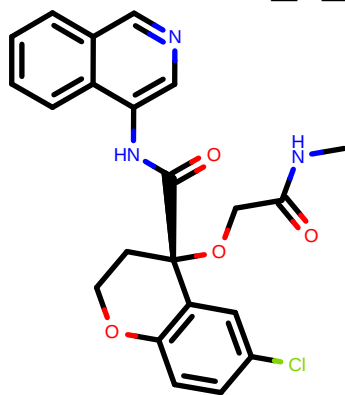
CID:	EN300-6487407_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5[C@H](CC(=O)O5)O</chem>
RUN:	RUN433
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.38

EN300-261986_1_1



CID:	EN300-261986_1_1
SMILES:	<chem>CS(=O)(=O)N[C@@]1CC[C@H](C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN524
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.29

EN300-2977549_1_1



CID: EN300-2977549_1_1

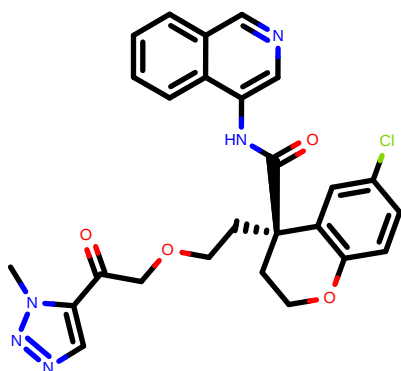
SMILES: CNC(=O)CO[C@]1(COC(=O)Cc2cc(Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1072

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.17

EN300-204936_3_1



CID: EN300-204936_3_1

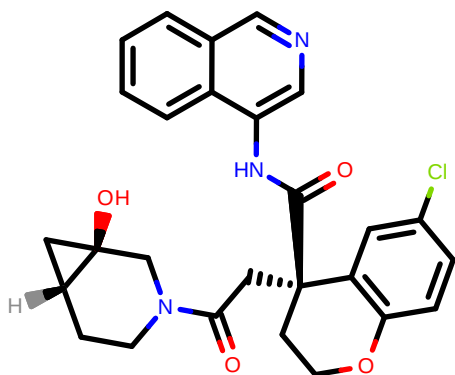
SMILES: Cn1c(cnn1)C(=O)COC[C@]2(COC(=O)Cc3cc(Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN345

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.29

EN300-1267093_1_1



CID: EN300-1267093_1_1

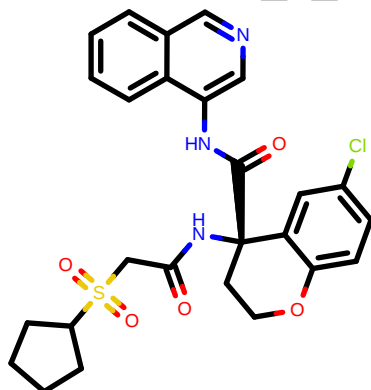
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(Cl)C(=O)Nc5cnc6C@@H(c6)C@5O

RUN: RUN1282

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.33

EN300-42154_1_1



CID: EN300-42154_1_1

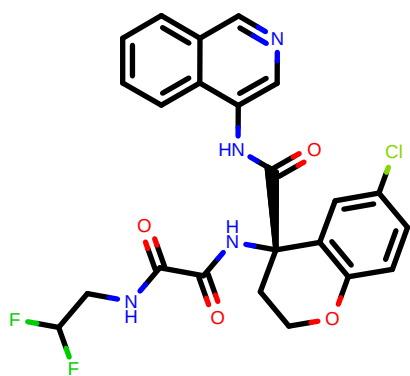
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(Cl)C(=O)Nc5cnc6C@@H(c6)C@5O

RUN: RUN877

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.32

EN300-128277_1_1



CID: EN300-128277_1_1

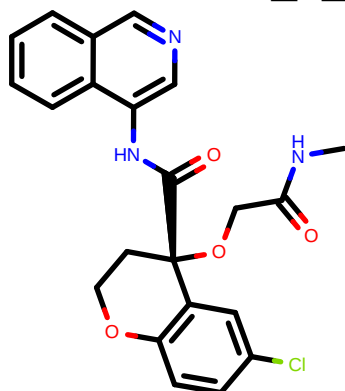
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NCC(F)(F)F

RUN: RUN1157

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.24

EN300-2977549_1_1



CID: EN300-2977549_1_1

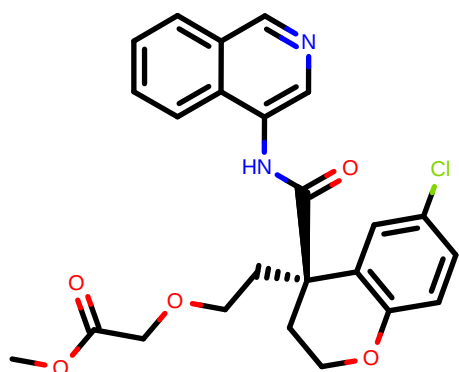
SMILES: CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1064

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.18

EN300-19700_3_1



CID: EN300-19700_3_1

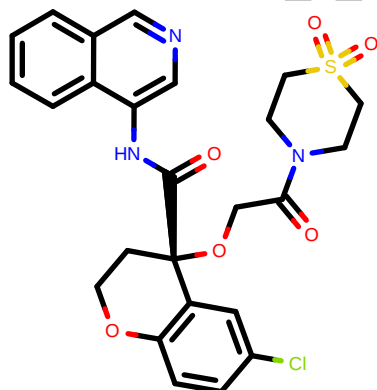
SMILES: COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1587

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.21

EN300-1265948_1_1



CID: EN300-1265948_1_1

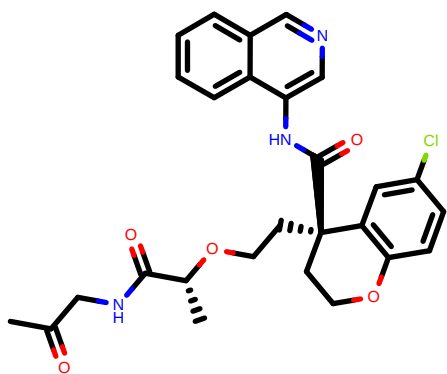
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN699

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.28

EN300-131093_3_2



CID:

EN300-131093_3_2

SMILES:

C[C@H](C(=O)NCC(=O)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN:

RUN1691

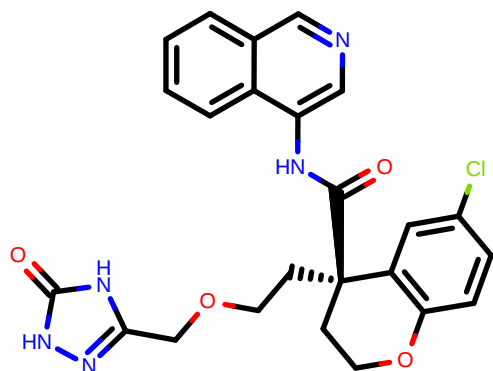
DDG (kcal/mol):

-1.85

dDDG (kcal/mol):

0.30

EN300-73772_3_1



CID:

EN300-73772_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]n5

RUN:

RUN1308

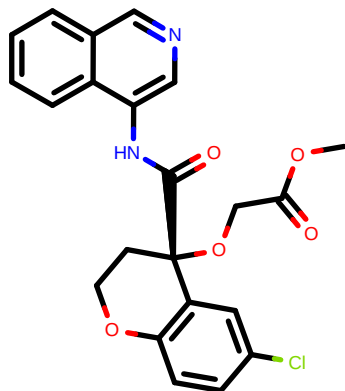
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.27

EN300-19700_1_1



CID:

EN300-19700_1_1

SMILES:

COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN:

RUN381

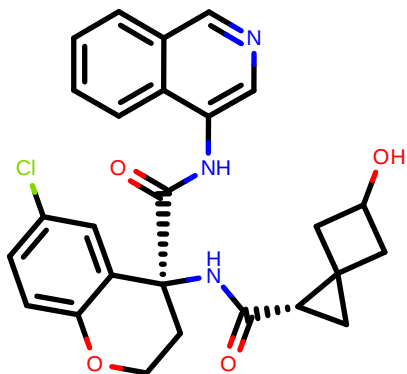
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.20

EN300-1717166_1_2



CID:

EN300-1717166_1_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC56CC(C6)O

RUN:

RUN861

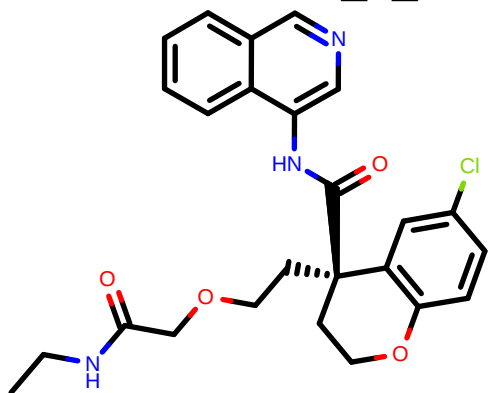
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.29

EN300-7003350_3_1



CID:

EN300-7003350_3_1

SMILES:

CCNC(=O)COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1484

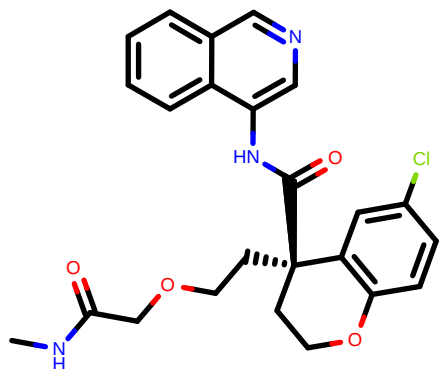
DDG (kcal/mol):

-1.83

dDDG (kcal/mol):

0.27

EN300-2977549_3_1



CID:

EN300-2977549_3_1

SMILES:

CNC(=O)COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1747

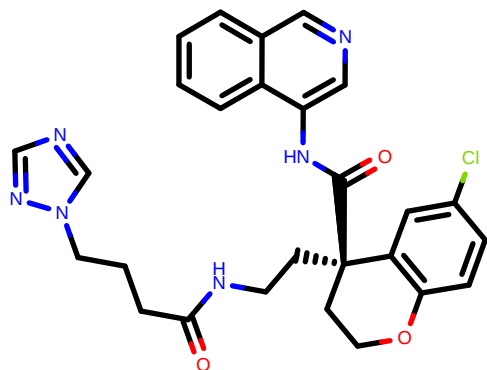
DDG (kcal/mol):

-1.82

dDDG (kcal/mol):

0.35

EN300-316216_3_1



CID:

EN300-316216_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCn5cnnc5

RUN:

RUN748

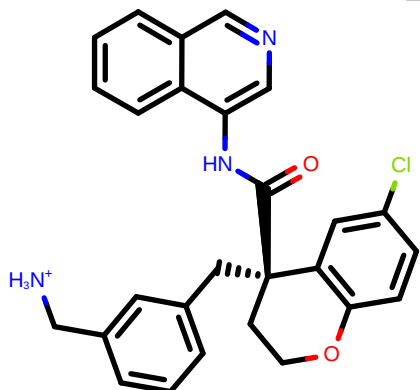
DDG (kcal/mol):

-1.81

dDDG (kcal/mol):

0.37

JAG-UCB-706446eb-8_1



CID:

JAG-UCB-706446eb-8_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)Cc5ccccc5[C+]([NH3+])

RUN:

RUN140

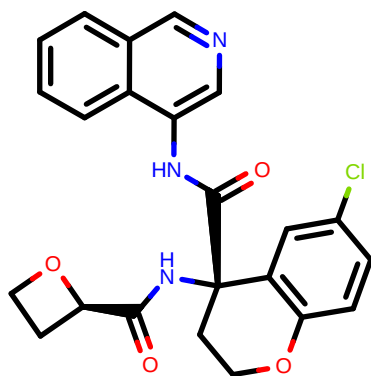
DDG (kcal/mol):

-1.81

dDDG (kcal/mol):

0.30

EN300-85760_1_2



CID:

EN300-85760_1_2

SMILES:

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

RUN:

RUN909

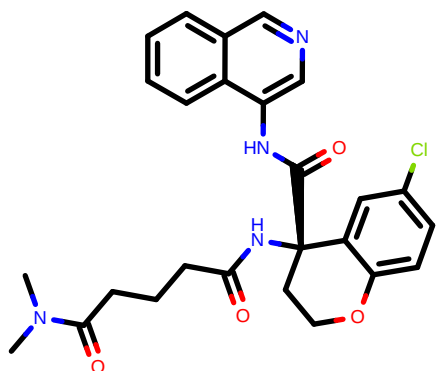
DDG (kcal/mol):

-1.81

dDDG (kcal/mol):

0.25

EN300-69215_1_1



CID:

EN300-69215_1_1

SMILES:

CN(C)C(=O)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncoc4c3ccoc4

RUN:

RUN274

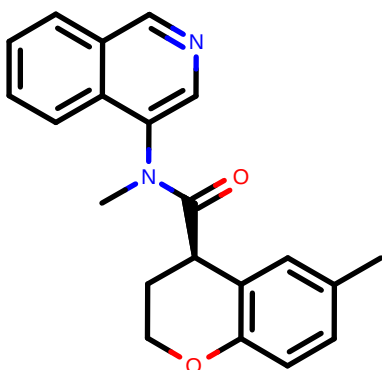
DDG (kcal/mol):

-1.80

dDDG (kcal/mol):

0.33

MAK-UNK-3875bbc8-1_1



CID:

MAK-UNK-3875bbc8-1_1

SMILES:

Cc1ccc2c(c1)[C@@@H](CCO2)C(=O)N(C)c3cncoc4c3ccccc4

RUN:

RUN32

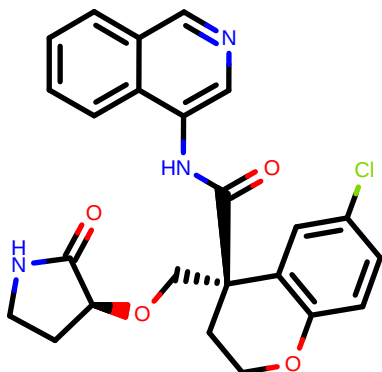
DDG (kcal/mol):

-1.80

dDDG (kcal/mol):

0.11

EN300-6736413_2_2



CID:

EN300-6736413_2_2

SMILES:

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

RUN:

RUN1182

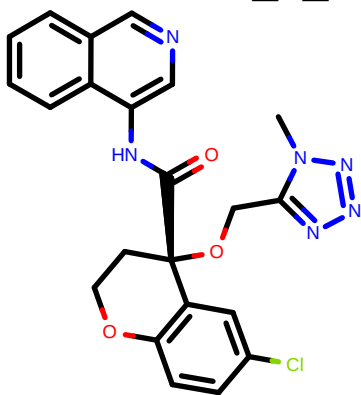
DDG (kcal/mol):

-1.79

dDDG (kcal/mol):

0.25

EN300-62574_1_1



CID:

EN300-62574_1_1

SMILES:

Cn1c(nnn1)CO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN1240

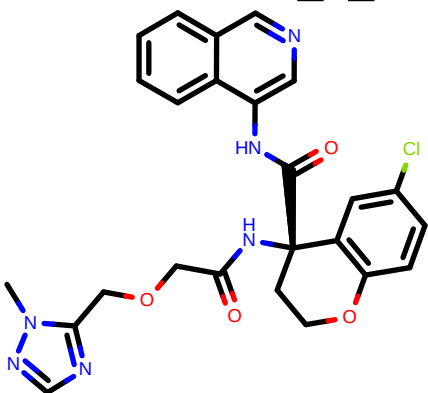
DDG (kcal/mol):

-1.77

dDDG (kcal/mol):

0.22

EN300-213358_1_1



CID:

EN300-213358_1_1

SMILES:

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

RUN:

RUN569

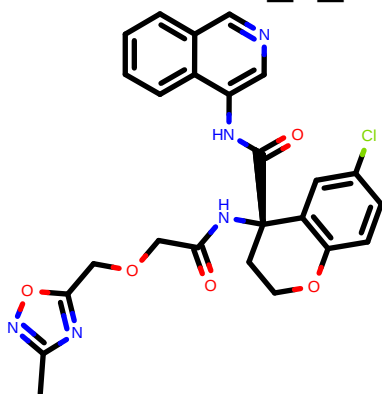
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

0.36

EN300-77006_1_1



CID:

EN300-77006_1_1

SMILES:

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

RUN:

RUN965

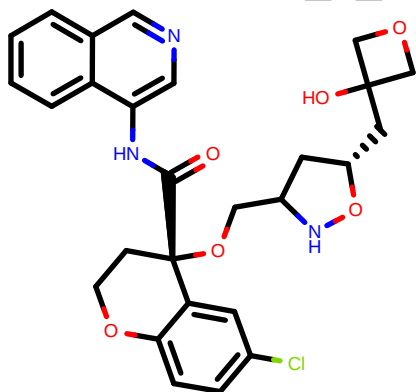
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

0.29

EN300-7457160_1_2



CID:

EN300-7457160_1_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOC4c3cc(cc4)Cl)OC5=NO[C@H](C5)C6(COC6)O

RUN:

RUN801

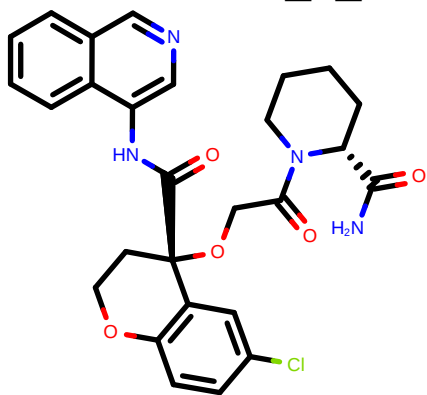
DDG (kcal/mol):

-1.75

dDDG (kcal/mol):

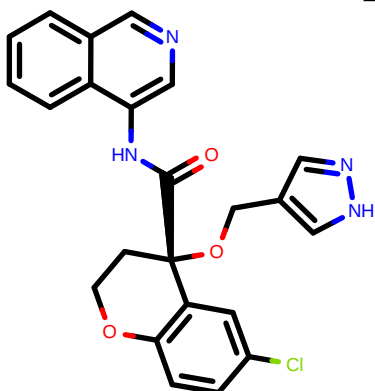
0.34

EN300-22879_1_1



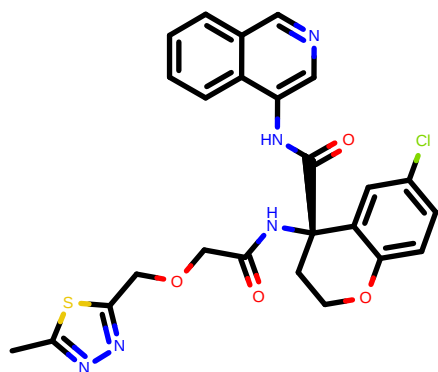
CID:	EN300-22879_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@@H]5C(=O)N</chem>
RUN:	RUN1687
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.29

EDJ-MED-28ec730d-4_1



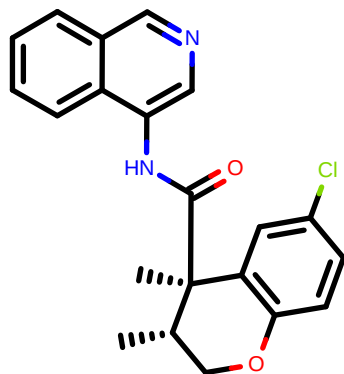
CID:	EDJ-MED-28ec730d-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5</chem>
RUN:	RUN65
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.20

EN300-206870_1_1



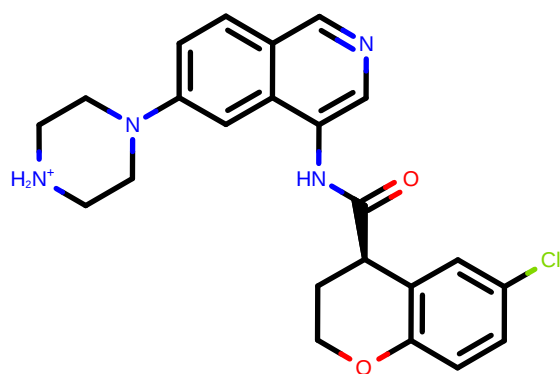
CID:	EN300-206870_1_1
SMILES:	<chem>Cc1nnc(s1)COC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN845
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.27

DAR-DIA-0d514e7d-28_1



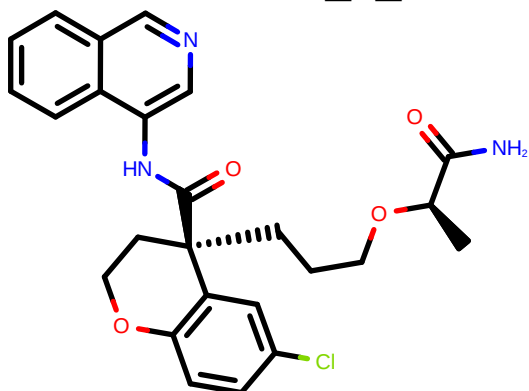
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@]1(C)C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN6
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.10

MAK-UNK-8be7dca9-4_1



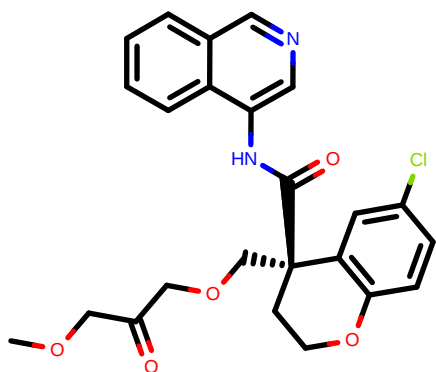
CID:	MAK-UNK-8be7dca9-4_1
SMILES:	<chem>c1cc2cncc(c2cc1N3CC[NH2+])CC3)NC(=O)[C@H]4CCOCc5c4cc(cc5)Cl</chem>
RUN:	RUN56
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.09

EN300-17381_4_2



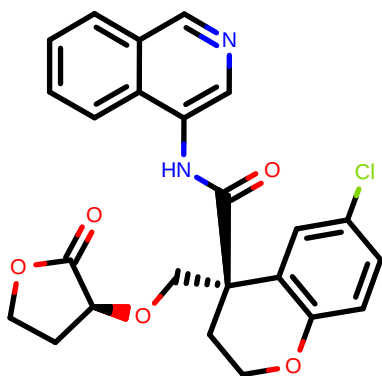
CID:	EN300-17381_4_2
SMILES:	<chem>C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN380
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.27

EN300-125140_2_1



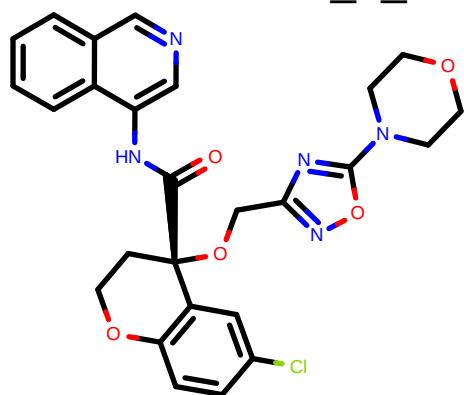
CID:	EN300-125140_2_1
SMILES:	<chem>COCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN918
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.35

EN300-20496_2_2



CID:	EN300-20496_2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCOC5=O</chem>
RUN:	RUN1166
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.22

EN300-1608590_1_1



CID: EN300-1608590_1_1

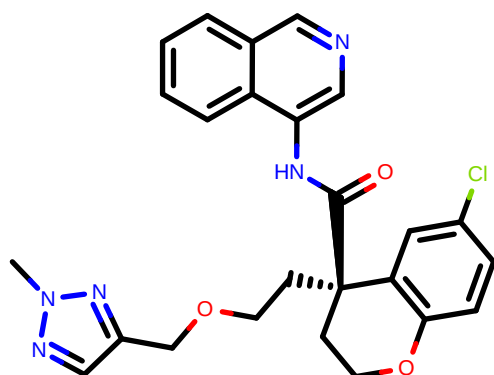
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(on5)N6CCOCC6

RUN: RUN1615

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.26

EN300-219020_3_1



CID: EN300-219020_3_1

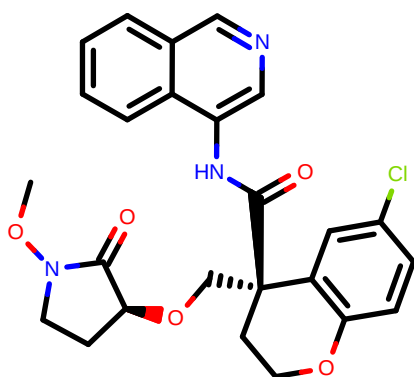
SMILES: Cn1ncc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1627

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.30

EN300-302058_2_1



CID: EN300-302058_2_1

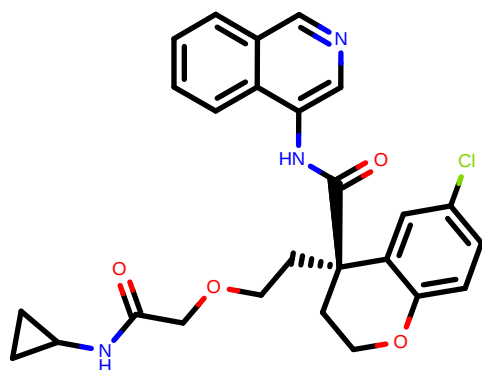
SMILES: CON1CC[C@@H](C1=O)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1629

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.29

EN300-1253178_3_1



CID: EN300-1253178_3_1

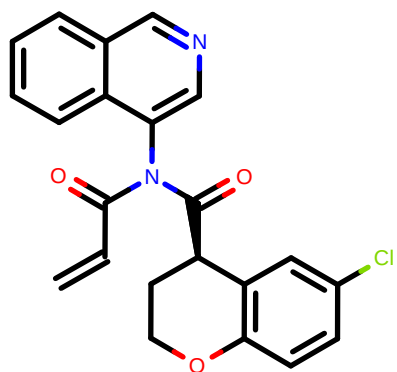
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC5CC5

RUN: RUN1675

DDG (kcal/mol): -1.65

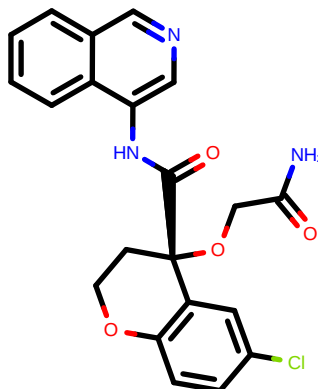
dDDG (kcal/mol): 0.25

VLA-UCB-50c39ae8-7_1



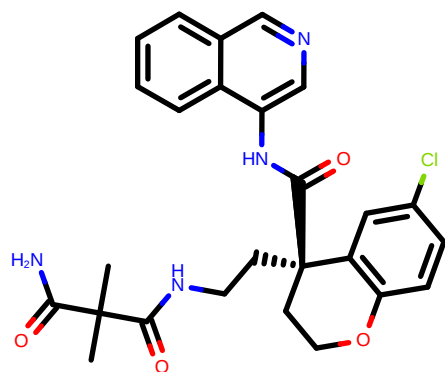
CID:	VLA-UCB-50c39ae8-7_1
SMILES:	<chem>C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN147
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.18

EN300-18249_1_1



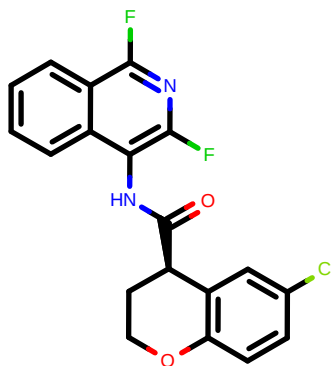
CID:	EN300-18249_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCC(=O)N</chem>
RUN:	RUN1128
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.16

EN300-182913_3_1



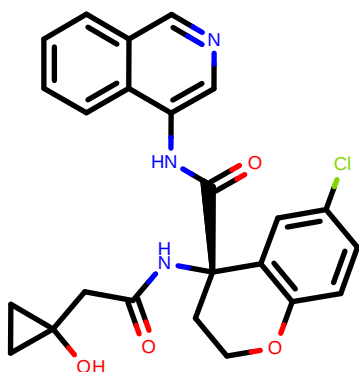
CID:	EN300-182913_3_1
SMILES:	<chem>CC(C)(C(=O)N)C(=O)NCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1649
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.31

JOH-SUS-a69c159d-6_1



CID:	JOH-SUS-a69c159d-6_1
SMILES:	<chem>c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN70
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.06

EN300-207873_1_1



CID: EN300-207873_1_1

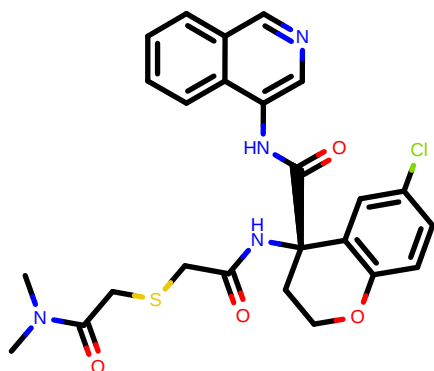
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)NC(=O)CC5(CC5)O

RUN: RUN338

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.22

EN300-12139_1_1



CID: EN300-12139_1_1

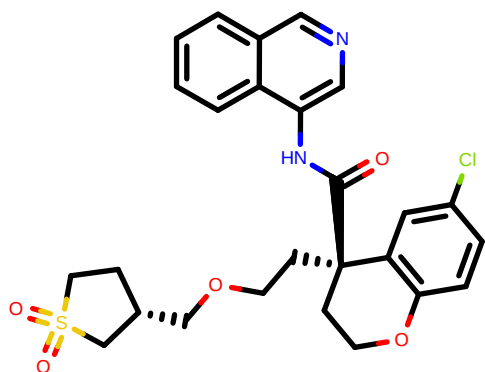
SMILES: CN(C)C(=O)CSCC(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccoc4

RUN: RUN282

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.40

EN300-1448603_3_2



CID: EN300-1448603_3_2

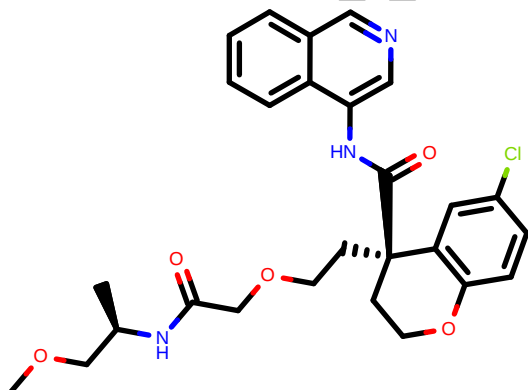
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4C3cc(cc4)Cl)CCOC[C@H]5SCCS(=O)(=O)C5

RUN: RUN1252

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.36

EN300-02067_3_2



CID: EN300-02067_3_2

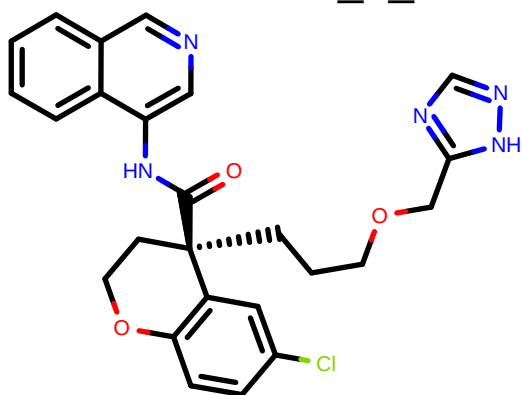
SMILES: C[C@H](COC)NC(=O)COC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccoc4

RUN: RUN711

DDG (kcal/mol): -1.62

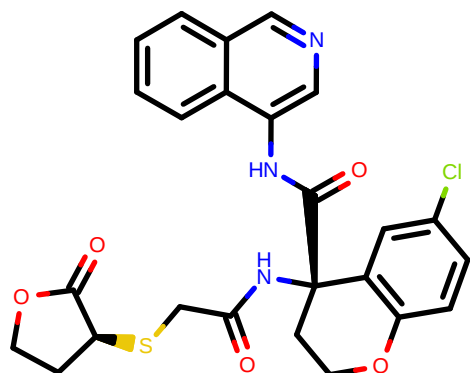
dDDG (kcal/mol): 0.34

EN300-306316_4_1



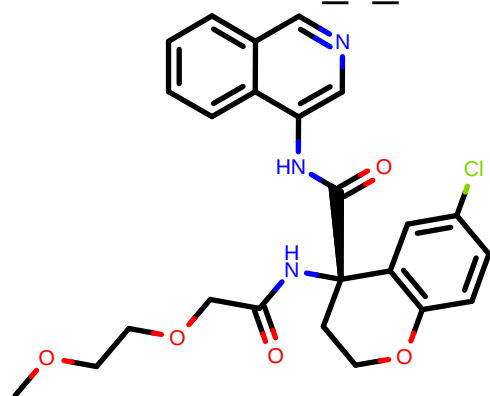
CID:	EN300-306316_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCc5[nH]jncn5</chem>
RUN:	RUN284
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.24

EN300-113218_1_2



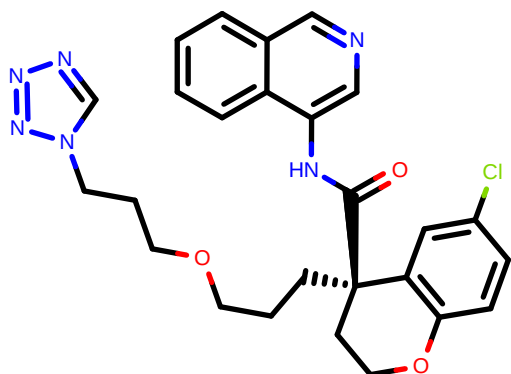
CID:	EN300-113218_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@H]5CCOCC5=O</chem>
RUN:	RUN513
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.26

EN300-20375_1_1



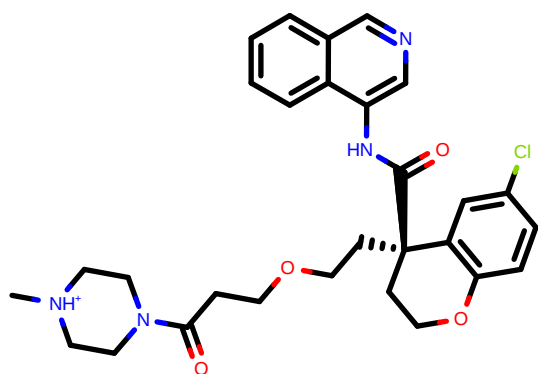
CID:	EN300-20375_1_1
SMILES:	<chem>COCOCOC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1117
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.26

EN300-1696962_4_1



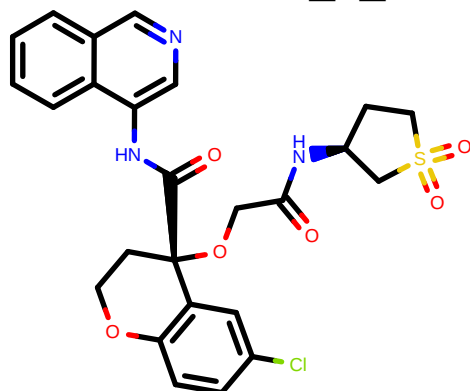
CID:	EN300-1696962_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCCN5cnnn5</chem>
RUN:	RUN1063
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.41

EN300-178293_3_1



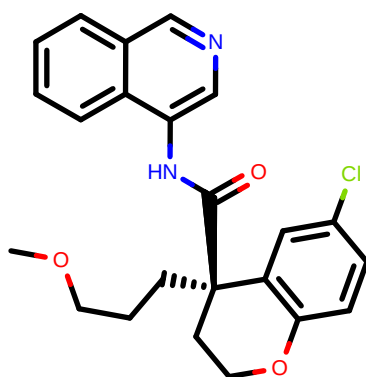
CID:	EN300-178293_3_1
SMILES:	<chem>C[NH+]1CCN(CC1)C(=O)COC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5</chem>
RUN:	RUN844
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.57

EN300-05512_1_2



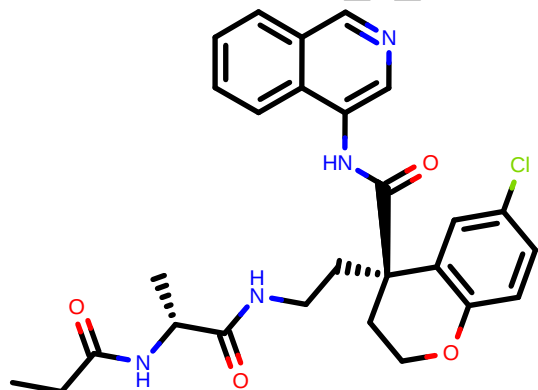
CID:	EN300-05512_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)OCC(=O)N[C@H]5CCS(=O)(=O)C5</chem>
RUN:	RUN349
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.33

EDJ-MED-28ec730d-1_1



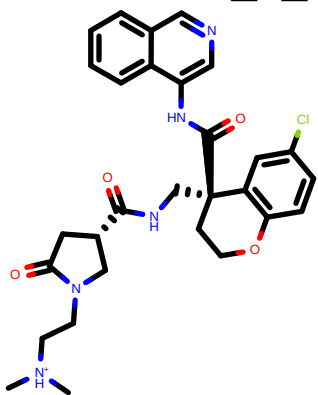
CID:	EDJ-MED-28ec730d-1_1
SMILES:	<chem>COCCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4</chem>
RUN:	RUN62
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.26

EN300-31148_3_2



CID:	EN300-31148_3_2
SMILES:	<chem>CCC(=O)N[C@H](C)C(=O)NCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4</chem>
RUN:	RUN1162
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.40

EN300-51735_2_2



CID: EN300-51735_2_2

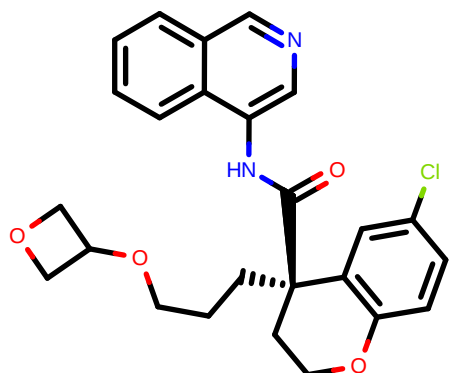
SMILES: C[NH+](C)CCN1C[C@H](CC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN645

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.34

EN300-317082_4_1



CID: EN300-317082_4_1

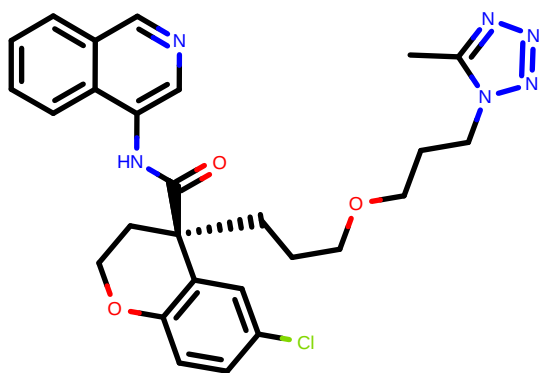
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCC5COC5

RUN: RUN1303

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.25

EN300-197715_4_1



CID: EN300-197715_4_1

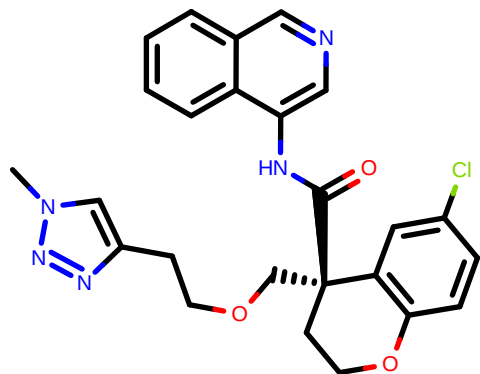
SMILES: Cc1nnnn1CCCOCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1543

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.33

EN300-1600786_2_1



CID: EN300-1600786_2_1

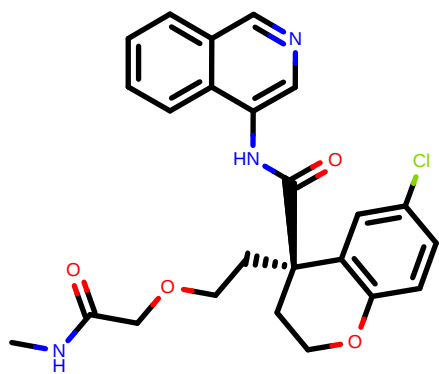
SMILES: Cn1cc(nn1)CCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1781

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.39

EN300-2977549_3_1



CID: EN300-2977549_3_1

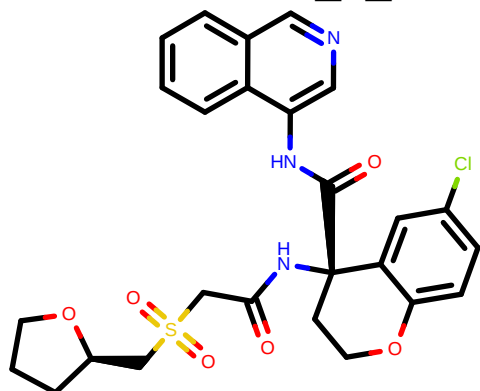
SMILES: CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN1739

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-67023_1_2



CID: EN300-67023_1_2

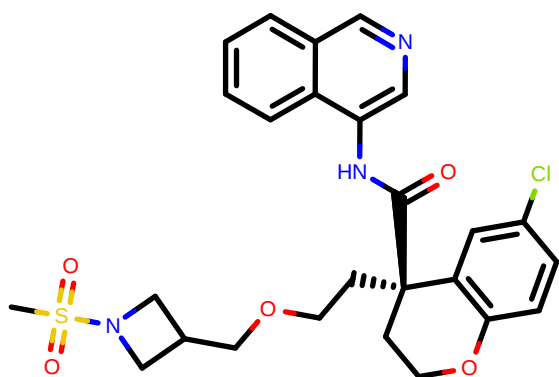
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C[C@H]5CCCCO5

RUN: RUN704

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.35

EN300-302290_3_1



CID: EN300-302290_3_1

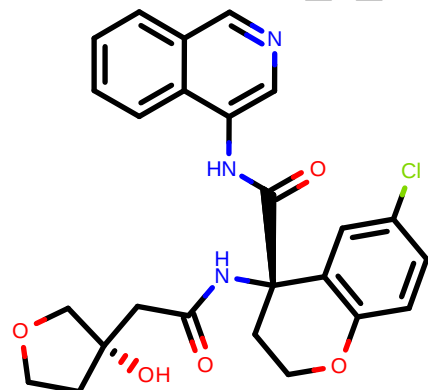
SMILES: CS(=O)(=O)N1CC(C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1220

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.36

EN300-360157_1_2



CID: EN300-360157_1_2

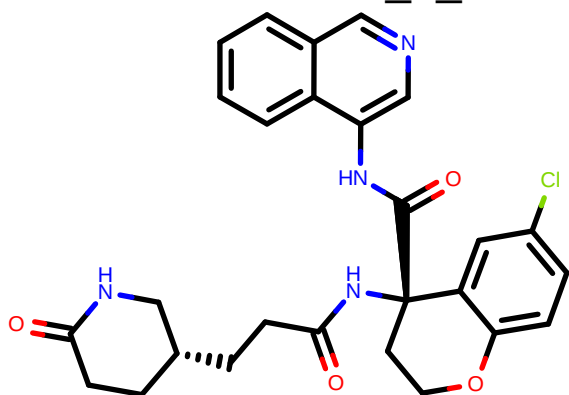
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@]5(CCOCS)O

RUN: RUN657

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.26

EN300-1215738_1_1



CID:

EN300-1215738_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC[C@@H]5CCCC(=O)NCS

RUN:

RUN973

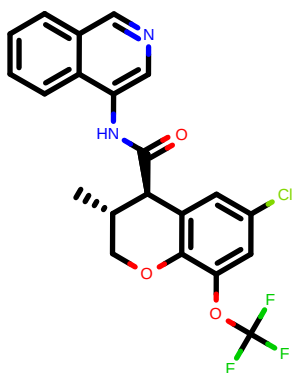
DDG (kcal/mol):

-1.55

dDDG (kcal/mol):

0.39

DAR-DIA-0d514e7d-18_1



CID:

DAR-DIA-0d514e7d-18_1

SMILES:

C[C@@H]1COc2c(cc(cc2OC(F)(F)F)Cl)[C@@H]1C(=O)Nc3cncc4c3ccccc4

RUN:

RUN123

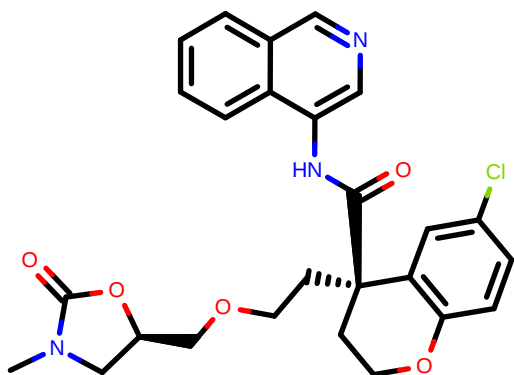
DDG (kcal/mol):

-1.55

dDDG (kcal/mol):

0.14

EN300-222969_3_1



CID:

EN300-222969_3_1

SMILES:

CN1C[C@@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN727

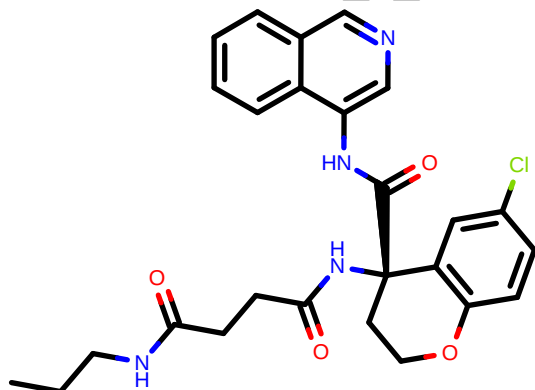
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.31

EN300-68740_1_1



CID:

EN300-68740_1_1

SMILES:

CCCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1229

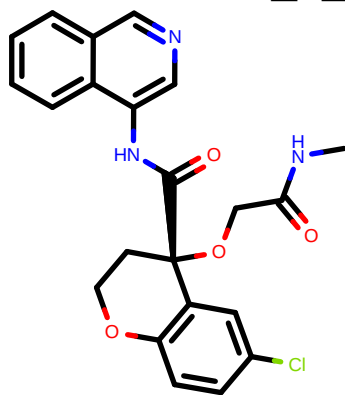
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.36

EN300-2977549_1_1



CID: EN300-2977549_1_1

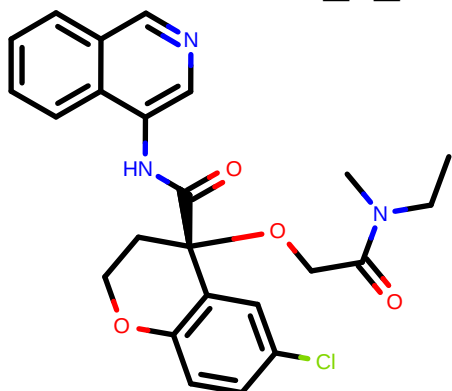
SMILES: CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1056

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.21

EN300-1253122_1_1



CID: EN300-1253122_1_1

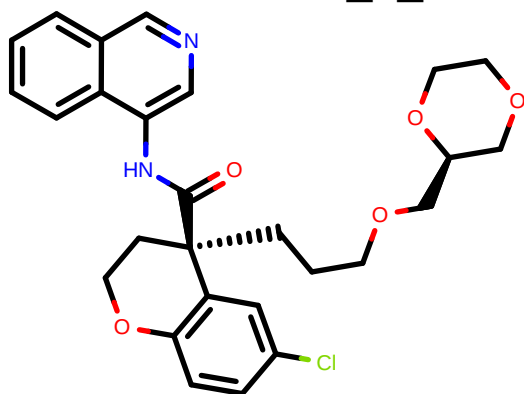
SMILES: CCN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN556

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-139167_4_1



CID: EN300-139167_4_1

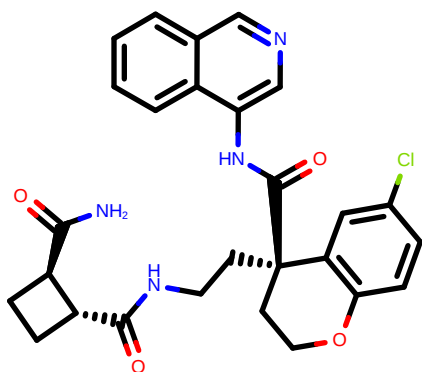
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCCCOC[C@H]5COCCO5

RUN: RUN515

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.31

EN300-217107_3_3



CID: EN300-217107_3_3

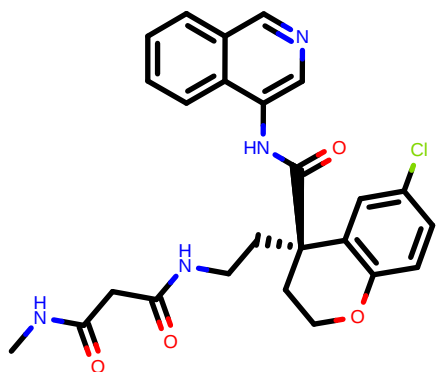
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC[C@H]5C1CC1=O

RUN: RUN503

DDG (kcal/mol): -1.53

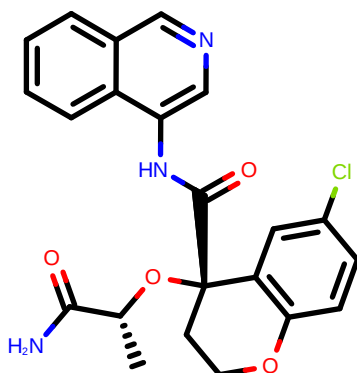
dDDG (kcal/mol): 0.32

EN300-128463_3_1



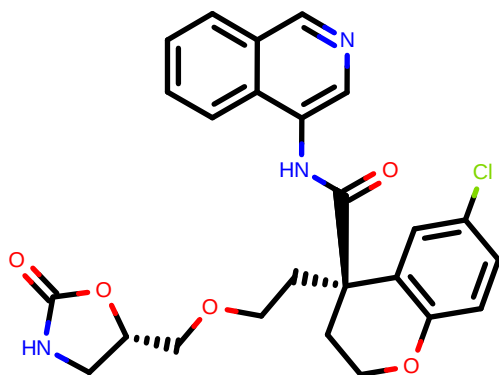
CID:	EN300-128463_3_1
SMILES:	<chem>CNC(=O)CC(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN1090
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.35

EN300-17381_1_2



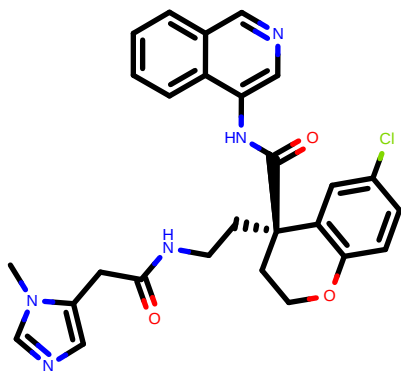
CID:	EN300-17381_1_2
SMILES:	<chem>C[C@H](C(=O)N)O[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN809
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.20

EN300-203293_3_1



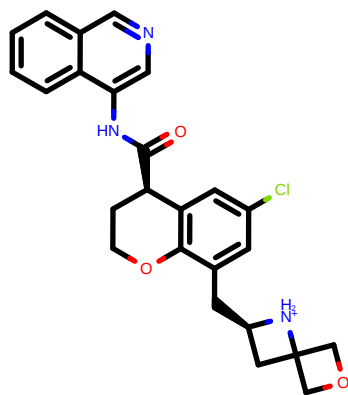
CID:	EN300-203293_3_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CNC(=O)O5</chem>
RUN:	RUN425
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.29

EN300-152418_3_1



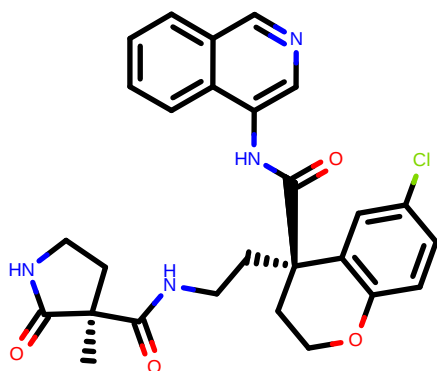
CID:	EN300-152418_3_1
SMILES:	<chem>Cn1cncc1CC(=O)NCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1170
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.33

DAR-DIA-23e5a6a0-8_1



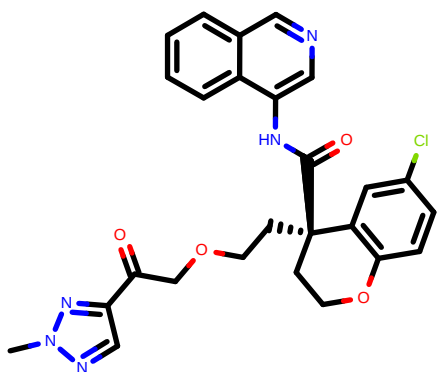
CID:	DAR-DIA-23e5a6a0-8_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6([NH2+][5])COC6)Cl</chem>
RUN:	RUN222
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.26

EN300-207959_3_2



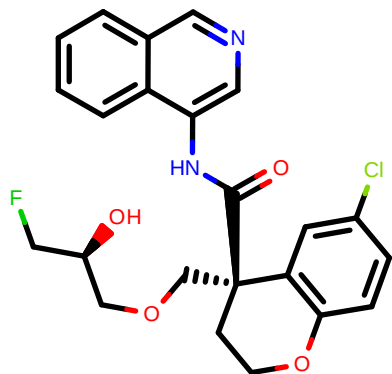
CID:	EN300-207959_3_2
SMILES:	<chem>C[C@@]1((CCNC1=O)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN1729
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.64

EN300-204935_3_1



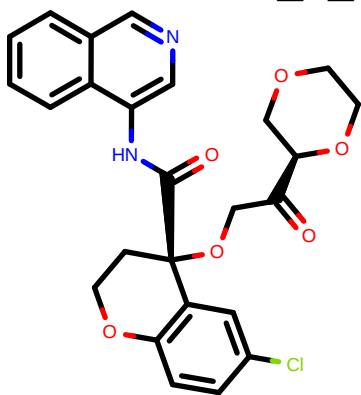
CID:	EN300-204935_3_1
SMILES:	<chem>Cn1ncc(n1)C(=O)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN688
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.34

EN300-1968342_2_1



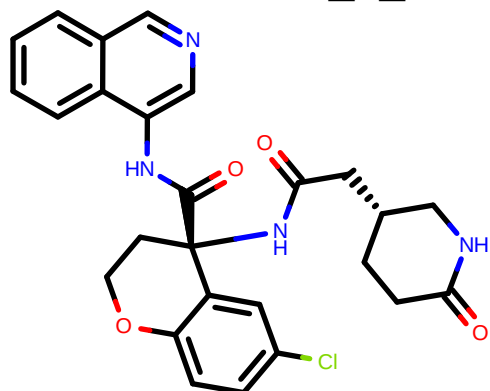
CID:	EN300-1968342_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O</chem>
RUN:	RUN483
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.32

EN300-6238494_1_2



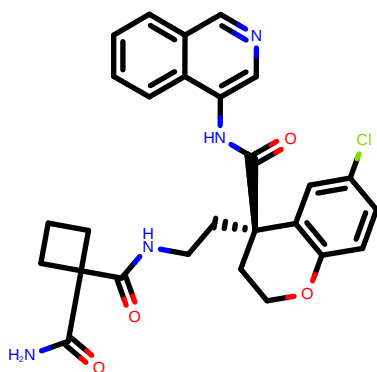
CID:	EN300-6238494_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5COCCO5</chem>
RUN:	RUN309
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.30

EN300-246992_1_2



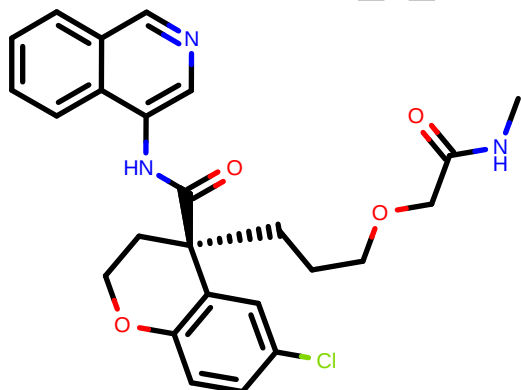
CID:	EN300-246992_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCNC(=O)NC5</chem>
RUN:	RUN474
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.24

EN300-68747_3_1



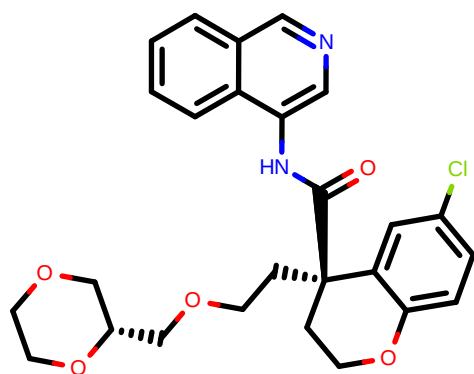
CID:	EN300-68747_3_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)C(=O)N</chem>
RUN:	RUN1330
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.34

EN300-2977549_4_1



CID:	EN300-2977549_4_1
SMILES:	<chem>CNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN611
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.30

EN300-139167_3_2



CID: EN300-139167_3_2

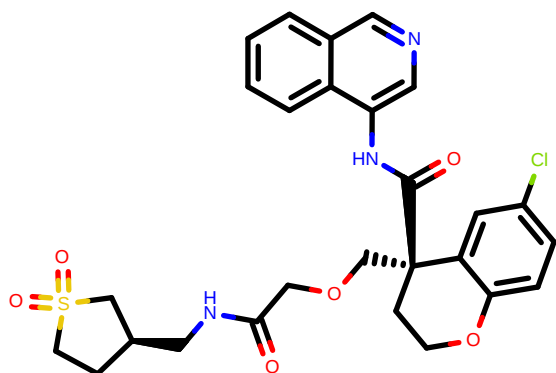
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)CCOC[C@H]5COC(CO5

RUN: RUN680

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.31

EN300-47606_2_2



CID: EN300-47606_2_2

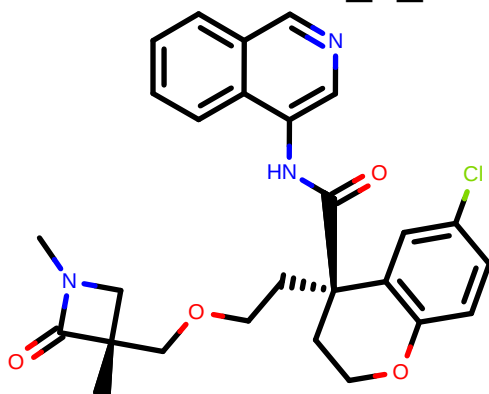
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)COC(=O)NC[C@H]5SCC(S(=O)(=O)C5

RUN: RUN1765

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.53

EN300-1273362_3_1



CID: EN300-1273362_3_1

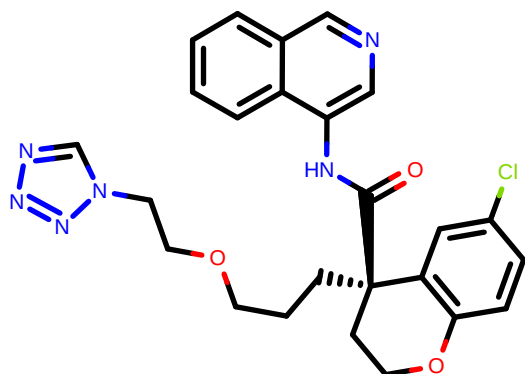
SMILES: C[C@@@]1(CN(C1=O)C)COC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN401

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.38

EN300-364679_4_1



CID: EN300-364679_4_1

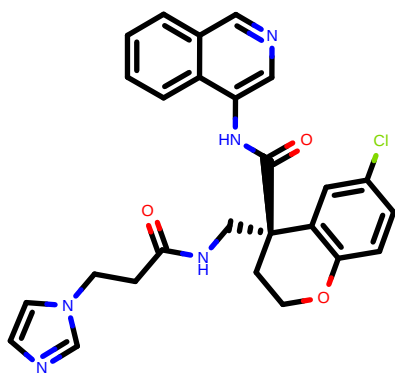
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)CCCCCn5cnnn5

RUN: RUN1750

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.40

EN300-75342_2_1



CID: EN300-75342_2_1

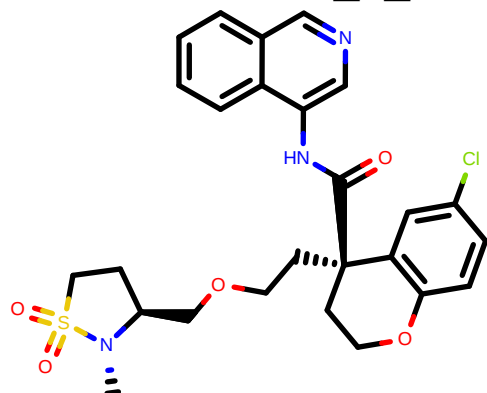
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cnc5

RUN: RUN724

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-393148_3_1



CID: EN300-393148_3_1

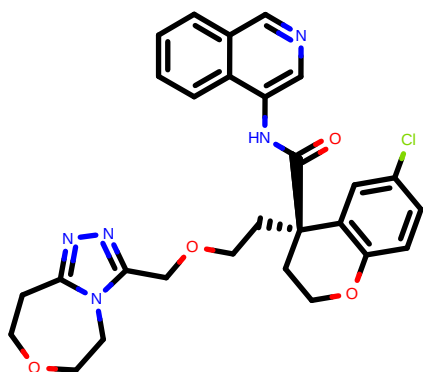
SMILES: C[N@]1[C@@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN385

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.29

EN300-310888_3_1



CID: EN300-310888_3_1

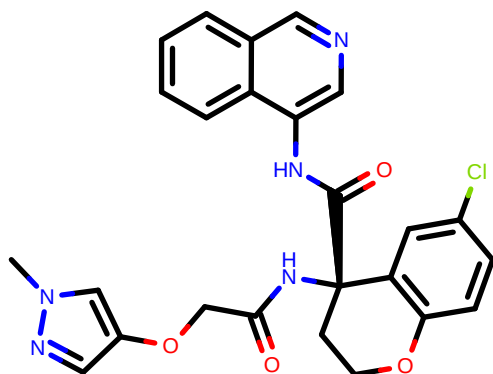
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nncc6n5CCOCC6

RUN: RUN1619

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.37

EN300-201553_1_1



CID: EN300-201553_1_1

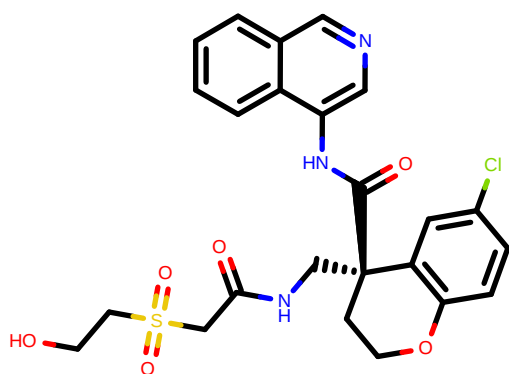
SMILES: Cn1cc(cn1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5

RUN: RUN814

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.25

EN300-4293814_2_1



CID: EN300-4293814_2_1

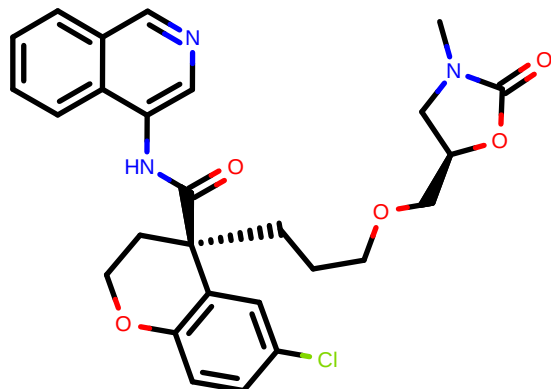
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS(=O)(=O)CCO

RUN: RUN398

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.64

EN300-222969_4_1



CID: EN300-222969_4_1

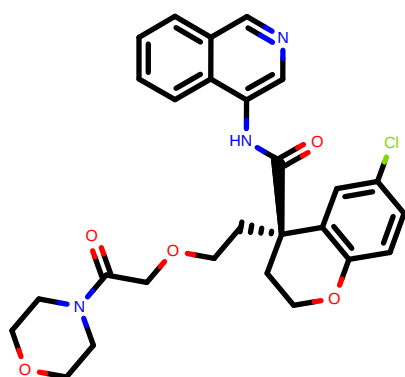
SMILES: CN1C[C@@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1375

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.53

EN300-1241327_3_1



CID: EN300-1241327_3_1

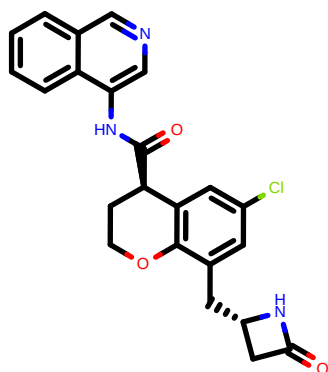
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCOCC5

RUN: RUN821

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.28

DAR-DIA-6a508060-5_3



CID: DAR-DIA-6a508060-5_3

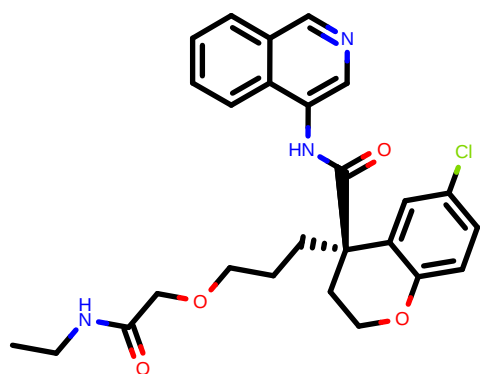
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CC(=O)N5Cl

RUN: RUN218

DDG (kcal/mol): -1.40

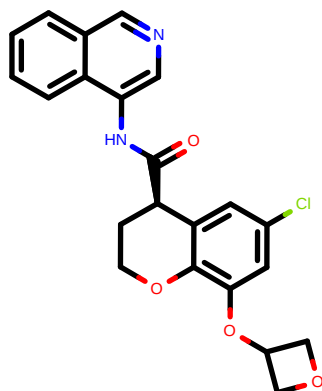
dDDG (kcal/mol): 0.16

EN300-7003350_4_1



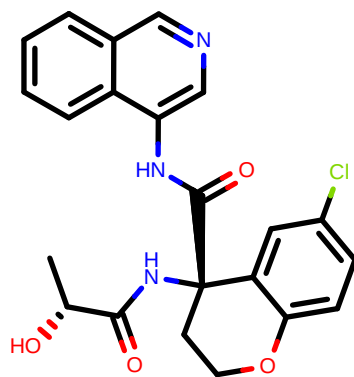
CID:	EN300-7003350_4_1
SMILES:	<chem>CCNC(=O)COCCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN1047
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.31

EDJ-MED-e4b030d8-4_1



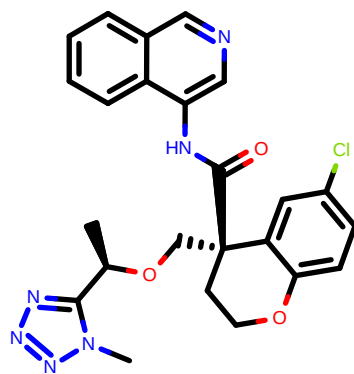
CID:	EDJ-MED-e4b030d8-4_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OC5COC5)Cl</chem>
RUN:	RUN150
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.21

EN300-77464_1_1



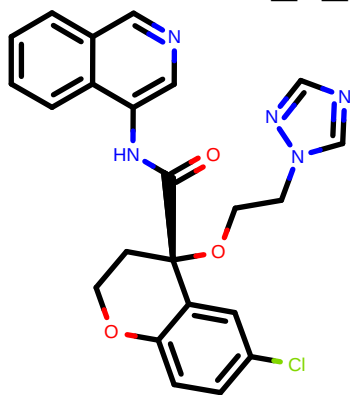
CID:	EN300-77464_1_1
SMILES:	<chem>C[C@H](C(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O</chem>
RUN:	RUN1397
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.24

EN300-173006_2_2



CID:	EN300-173006_2_2
SMILES:	<chem>C[C@H](c1nnnn1C)OC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1502
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.33

EN300-6255179_1_1



CID: EN300-6255179_1_1

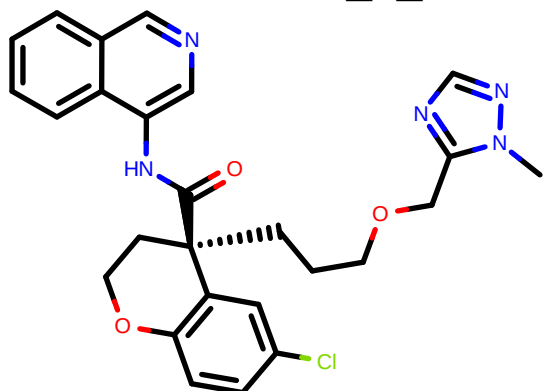
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnc5

RUN: RUN1096

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.25

EN300-87334_4_1



CID: EN300-87334_4_1

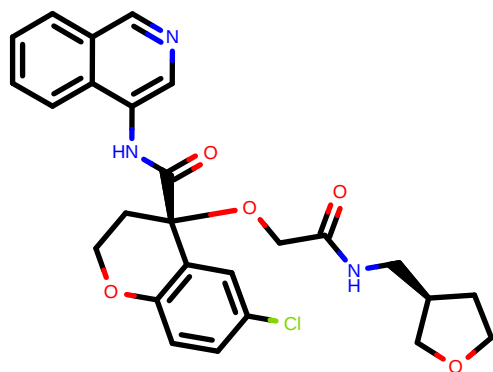
SMILES: Cn1c(ncn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN324

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.31

EN300-46832_1_2



CID: EN300-46832_1_2

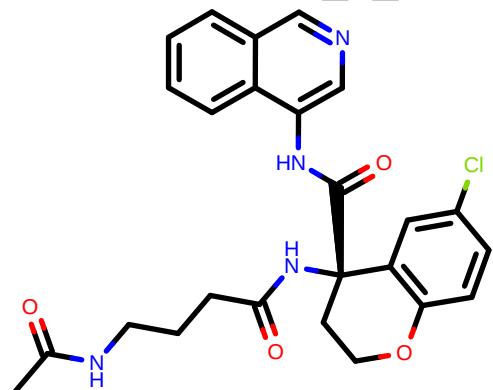
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5CCOC5

RUN: RUN1440

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.26

EN300-18564_1_1



CID: EN300-18564_1_1

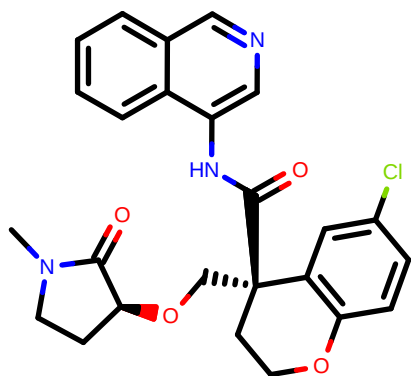
SMILES: CC(=O)NCCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN498

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.25

EN300-98648_2_1



CID:

EN300-98648_2_1

SMILES:

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

RUN:

RUN1685

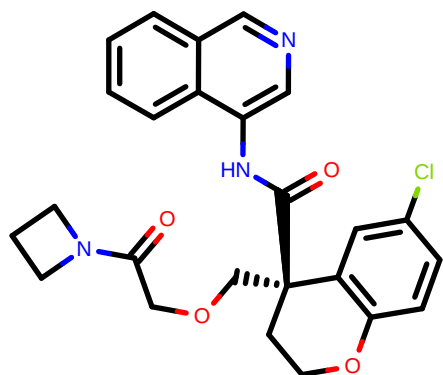
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.27

EN300-11195_2_1



CID:

EN300-11195_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC5

RUN:

RUN1142

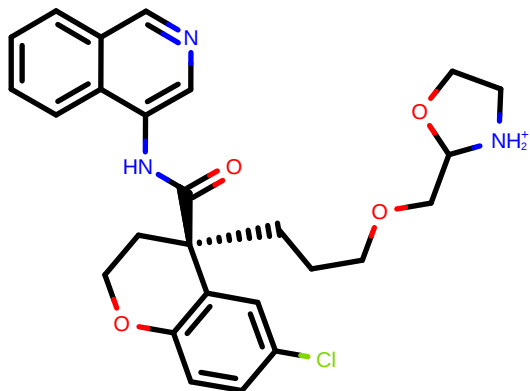
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.23

EN300-317555_4_1



CID:

EN300-317555_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5=NCCO5

RUN:

RUN500

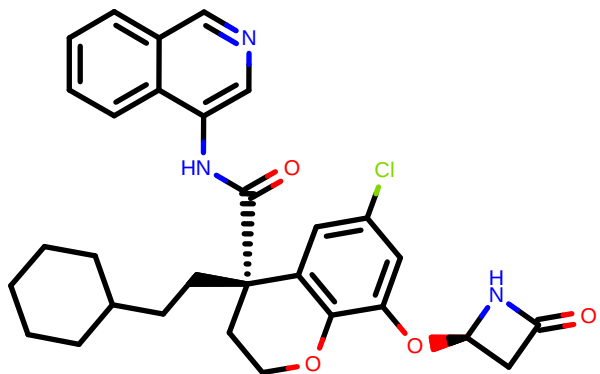
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.27

VLA-UCB-05e51b3f-12_1



CID:

VLA-UCB-05e51b3f-12_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CC(=O)N5C6CCCCC6

RUN:

RUN241

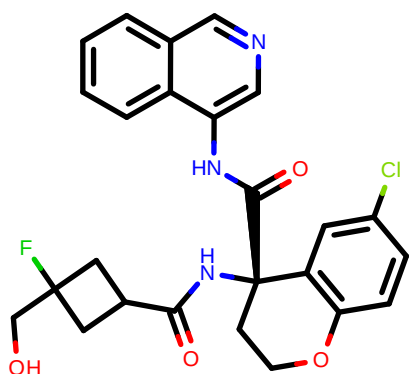
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.32

EN300-6746890_1_1



CID:

EN300-6746890_1_1

SMILES:

c1cc2c(c1)nc2NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@H]5C[C@@](C5)(F)CO)c1

RUN:

RUN1596

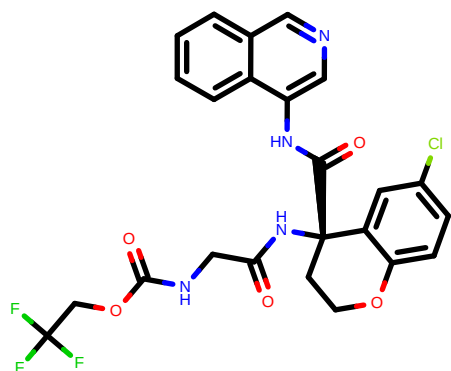
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.25

EN300-50488_1_1



CID:

EN300-50488_1_1

SMILES:

c1ccc2c(c1)nc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)OCC(F)(F)F

RUN:

RUN1005

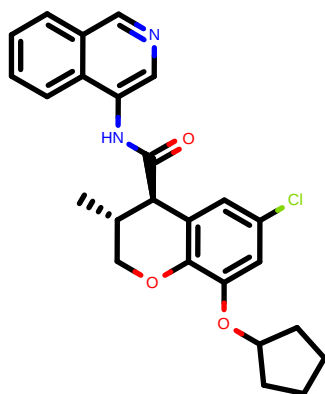
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.27

DAR-DIA-0d514e7d-4_1



CID:

DAR-DIA-0d514e7d-4_1

SMILES:

C[C@H]1COc2c(cc2OC3CCCC3)Cl)[C@H]1C(=O)Nc4cncc5c4cccc5

RUN:

RUN93

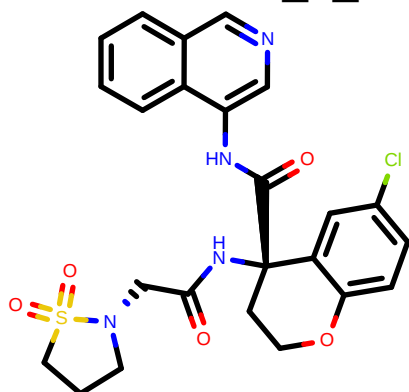
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.26

EN300-43206_1_1



CID:

EN300-43206_1_1

SMILES:

c1ccc2c(c1)nc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[N@]5CCCC5(=O)=O

RUN:

RUN1636

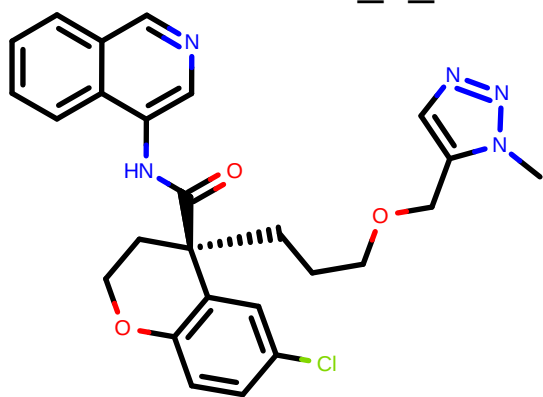
DDG (kcal/mol):

-1.34

dDDG (kcal/mol):

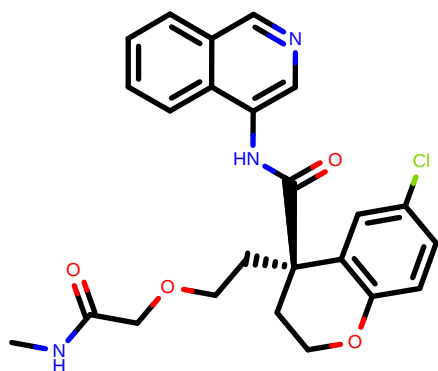
0.35

EN300-216673_4_1



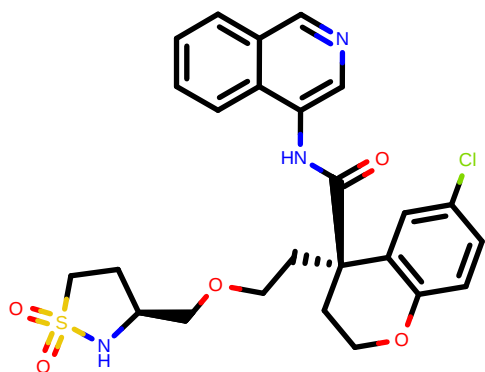
CID:	EN300-216673_4_1
SMILES:	<chem>Cn1c(cnn1)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN300
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.31

EN300-2977549_3_1



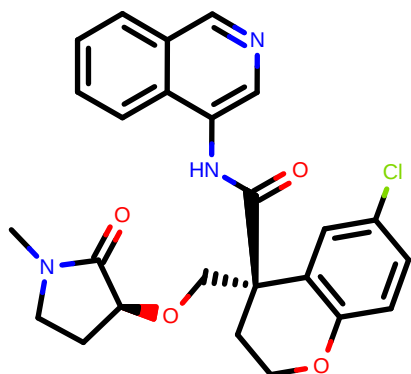
CID:	EN300-2977549_3_1
SMILES:	<chem>CNC(=O)COC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1755
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.27

EN300-1699871_3_1



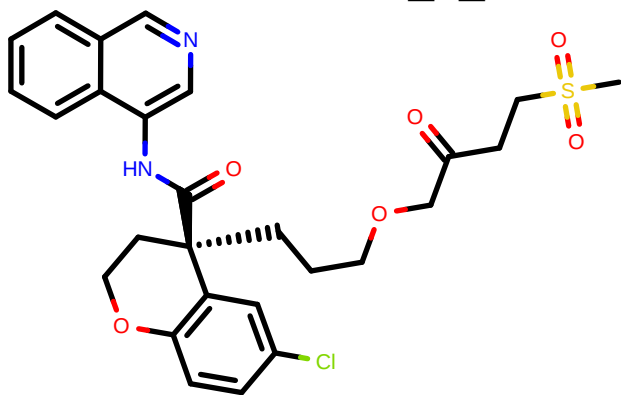
CID:	EN300-1699871_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC[C@@H]5CCCS(=O)(=O)N5</chem>
RUN:	RUN1140
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.34

EN300-98648_2_1



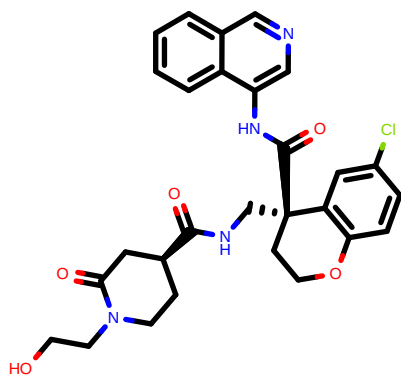
CID:	EN300-98648_2_1
SMILES:	<chem>CN1CC[C@@H](C1=O)OC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1693
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.26

EN300-1988306_4_1



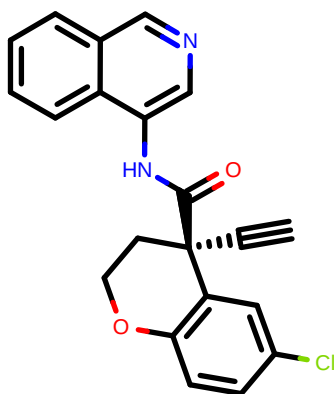
CID:	EN300-1988306_4_1
SMILES:	<chem>CS(=O)(=O)CCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1638
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.43

EN300-1723663_2_2



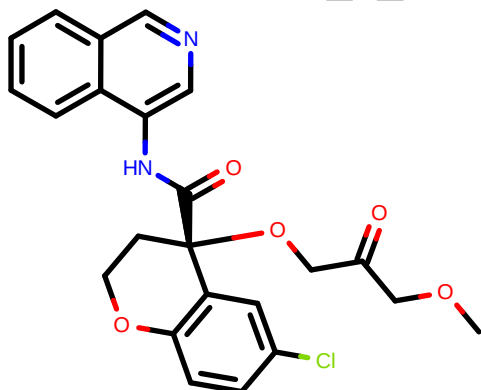
CID:	EN300-1723663_2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCN(C(=O)C5)CCO</chem>
RUN:	RUN358
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.34

PET-UNK-29afea89-1_1



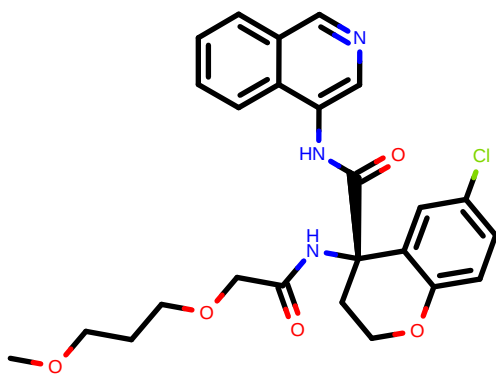
CID:	PET-UNK-29afea89-1_1
SMILES:	<chem>C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN40
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.10

EN300-125140_1_1



CID:	EN300-125140_1_1
SMILES:	<chem>COCC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN405
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.26

EN300-125769_1_1



CID: EN300-125769_1_1

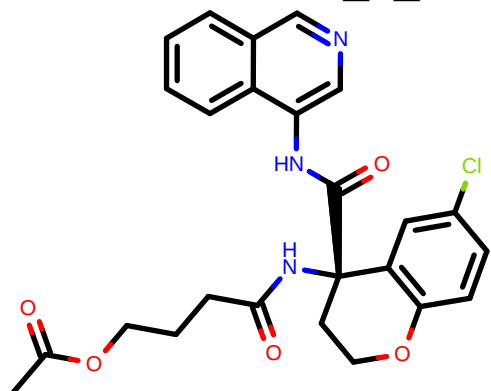
SMILES: COCCCOCC(=O)N[C@@]1(COC(=O)Cc2cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1365

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.31

EN300-1696058_1_1



CID: EN300-1696058_1_1

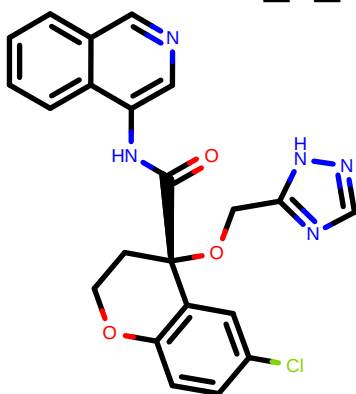
SMILES: CC(=O)OCCOC(=O)N[C@@]1(COC(=O)Cc2cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN394

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

EN300-306316_1_1



CID: EN300-306316_1_1

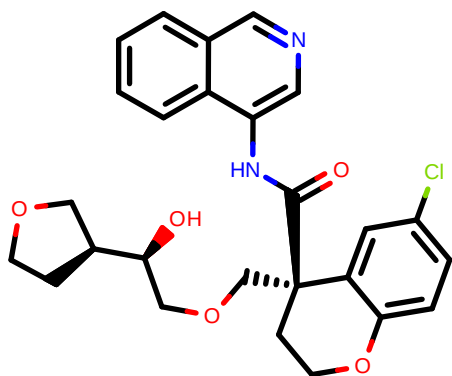
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC(=O)Cc4cc(cc4)Cl)OCc5[nH]nnc5

RUN: RUN668

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.23

EN300-1911992_2_3



CID: EN300-1911992_2_3

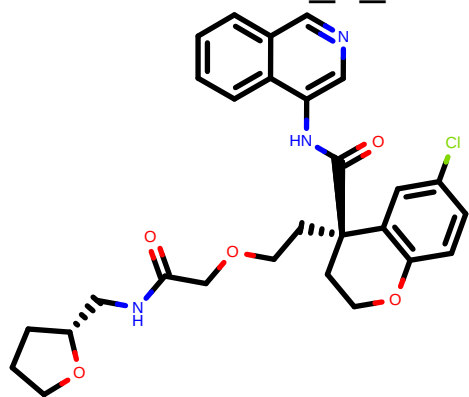
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC(=O)Cc4cc(cc4)Cl)COC[C@@H]5[C@@H](COC(=O)O)CO5

RUN: RUN1278

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.32

EN300-01527_3_2



CID:

EN300-01527_3_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@H]5CCCCO5

RUN:

RUN964

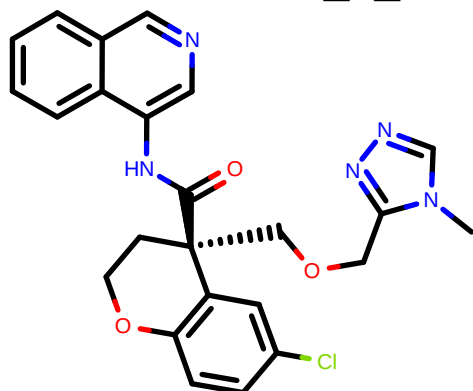
DDG (kcal/mol):

-1.28

dDDG (kcal/mol):

0.35

EN300-113112_2_1



CID:

EN300-113112_2_1

SMILES:

Cn1cnnc1COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN1438

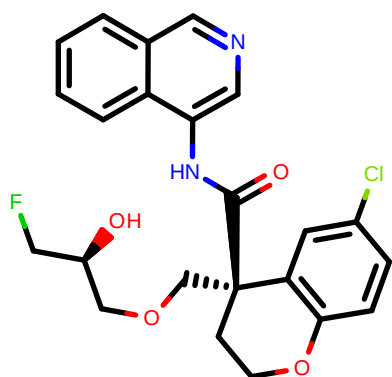
DDG (kcal/mol):

-1.27

dDDG (kcal/mol):

0.23

EN300-1968342_2_1



CID:

EN300-1968342_2_1

SMILES:

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

RUN:

RUN491

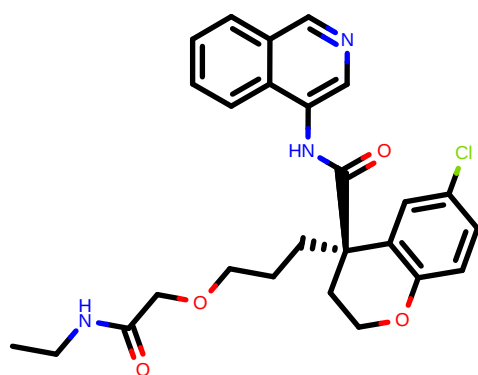
DDG (kcal/mol):

-1.27

dDDG (kcal/mol):

0.35

EN300-7003350_4_1



CID:

EN300-7003350_4_1

SMILES:

CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1031

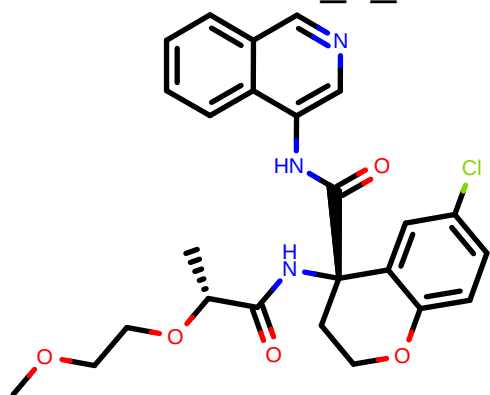
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.31

EN300-77359_1_2



CID: EN300-77359_1_2

SMILES:

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

RUN:

RUN1333

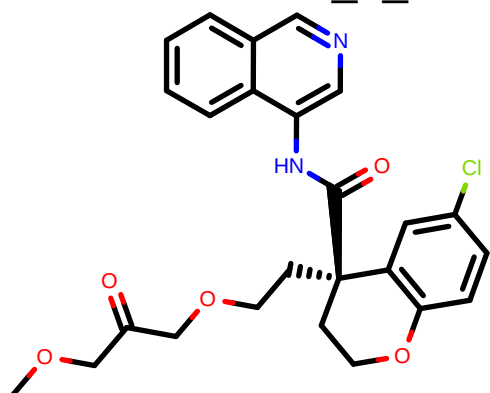
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.27

EN300-125140_3_1



CID: EN300-125140_3_1

SMILES:

COCC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN:

RUN735

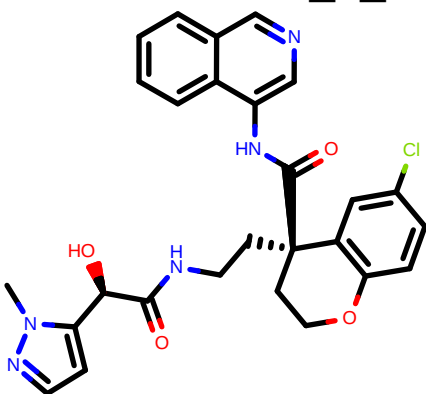
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.27

EN300-6473273_3_2



CID: EN300-6473273_3_2

SMILES:

Cn1c(cn1)[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN:

RUN1114

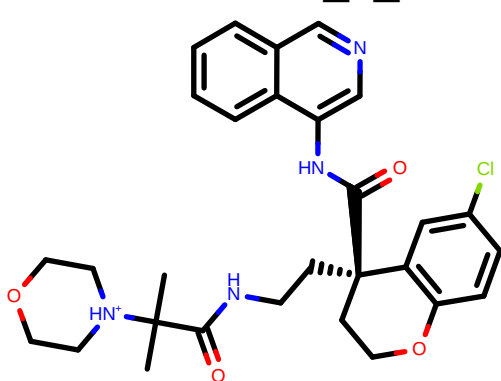
DDG (kcal/mol):

-1.26

dDDG (kcal/mol):

0.36

EN300-64247_3_1



CID: EN300-64247_3_1

SMILES:

CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)[NH+]5CCOCC5

RUN:

RUN630

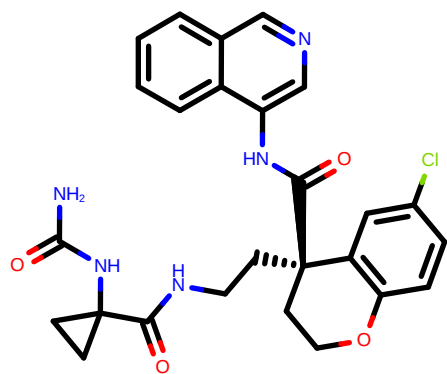
DDG (kcal/mol):

-1.25

dDDG (kcal/mol):

0.44

EN300-123614_3_1



CID:

EN300-123614_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCS)NC(=O)N

RUN:

RUN606

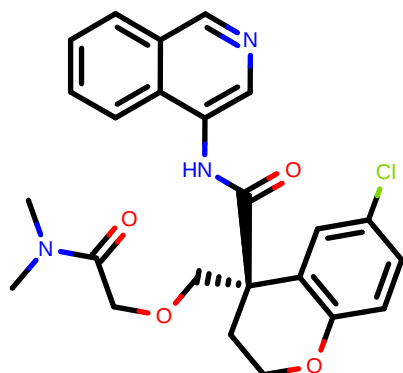
DDG (kcal/mol):

-1.25

dDDG (kcal/mol):

0.32

EN300-216063_2_1



CID:

EN300-216063_2_1

SMILES:

CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1206

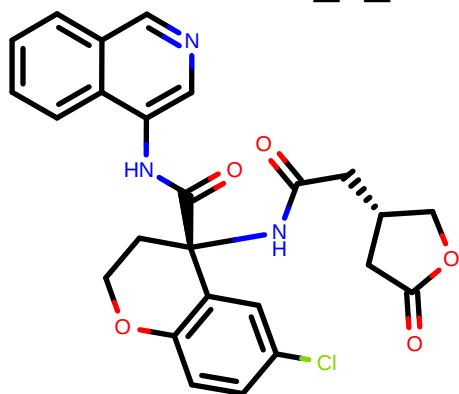
DDG (kcal/mol):

-1.25

dDDG (kcal/mol):

0.24

EN300-109535_1_2



CID:

EN300-109535_1_2

SMILES:

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

RUN:

RUN869

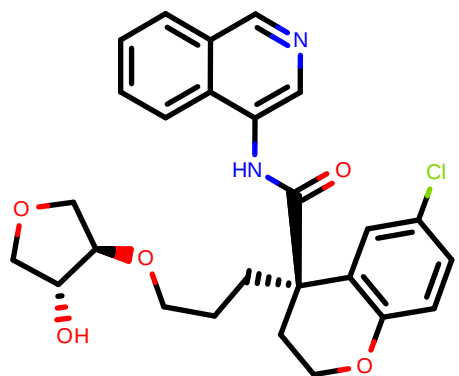
DDG (kcal/mol):

-1.25

dDDG (kcal/mol):

0.26

EN300-331828_4_1



CID:

EN300-331828_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5COC[C@H]5O

RUN:

RUN1447

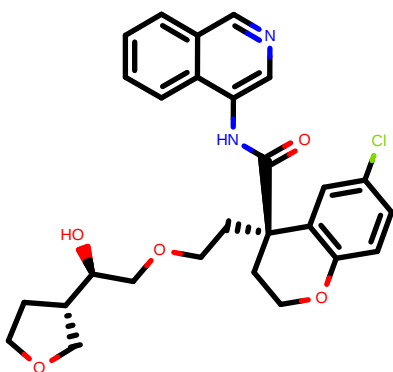
DDG (kcal/mol):

-1.24

dDDG (kcal/mol):

0.27

EN300-1911992_3_3



CID:

EN300-1911992_3_3

SMILES:

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

RUN:

RUN695

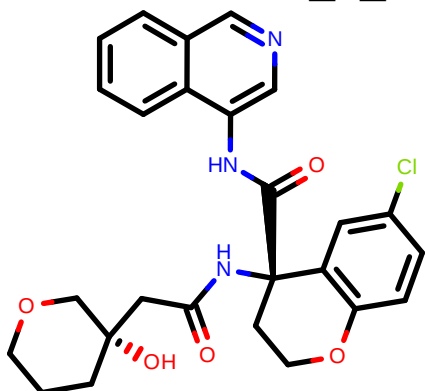
DDG (kcal/mol):

-1.23

dDDG (kcal/mol):

0.37

EN300-1071940_1_2



CID:

EN300-1071940_1_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H](C)5(CCCOC5)O

RUN:

RUN681

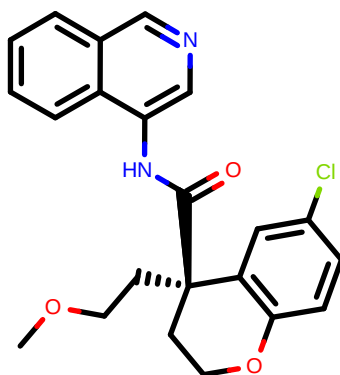
DDG (kcal/mol):

-1.23

dDDG (kcal/mol):

0.28

EDJ-MED-28ec730d-2_1



CID:

EDJ-MED-28ec730d-2_1

SMILES:

COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN77

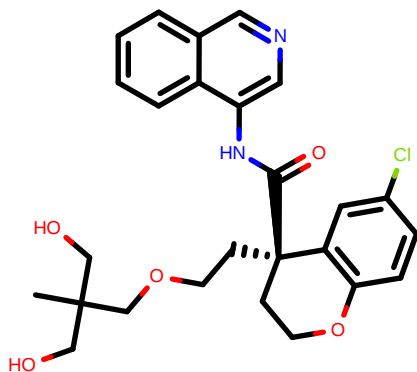
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.20

EN300-218116_3_1



CID:

EN300-218116_3_1

SMILES:

CC(CO)(CO)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN289

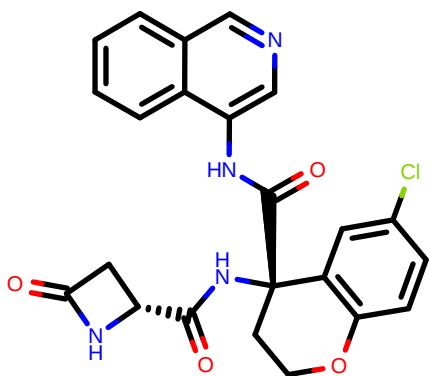
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.34

EN300-101505_1_2



CID:

EN300-101505_1_2

SMILES:

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

RUN:

RUN1277

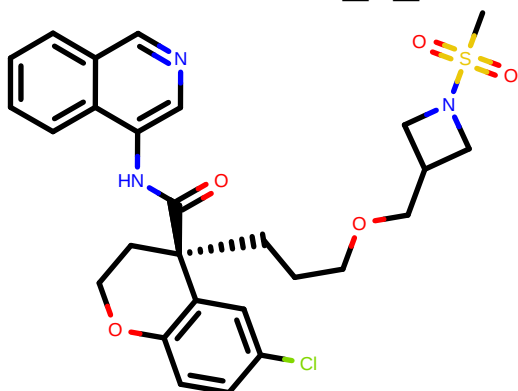
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.23

EN300-302290_4_1



CID:

EN300-302290_4_1

SMILES:

CS(=O)(=O)N1CC(C1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN:

RUN1199

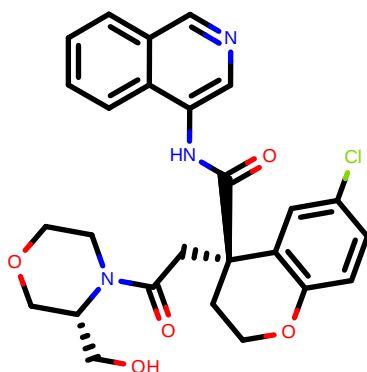
DDG (kcal/mol):

-1.21

dDDG (kcal/mol):

0.35

EN300-154201_1_2



CID:

EN300-154201_1_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO

RUN:

RUN1202

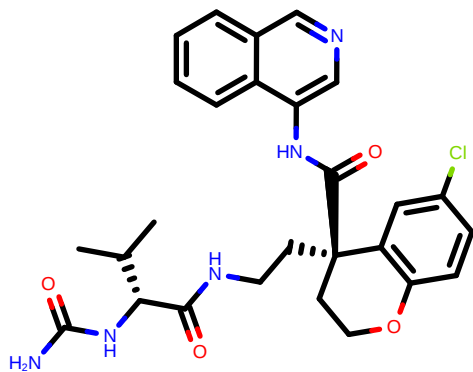
DDG (kcal/mol):

-1.21

dDDG (kcal/mol):

0.38

EN300-2972220_3_1



CID:

EN300-2972220_3_1

SMILES:

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

RUN:

RUN1362

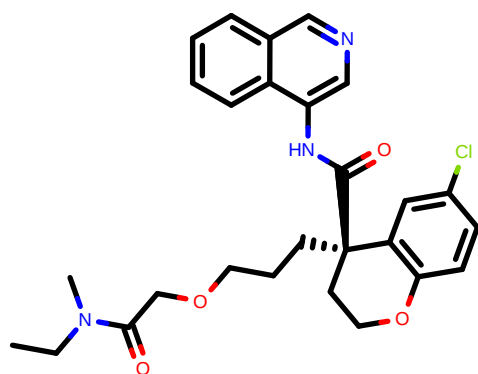
DDG (kcal/mol):

-1.21

dDDG (kcal/mol):

0.30

EN300-1253122_4_1



CID: EN300-1253122_4_1

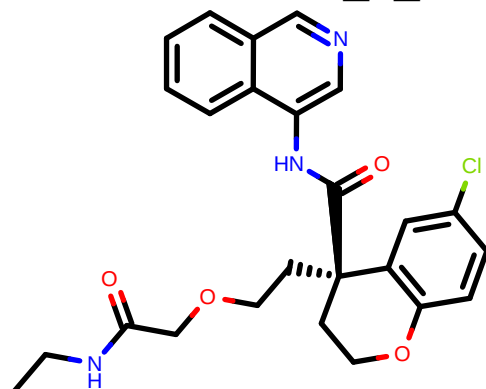
SMILES: CCN(C)C(=O)COCC[C@]1(C)C(=O)C2C1CC(C2)ClC(=O)Nc3cncc4c3cccc4

RUN: RUN698

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.34

EN300-7003350_3_1



CID: EN300-7003350_3_1

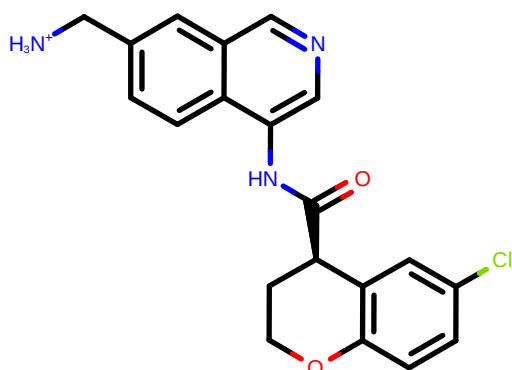
SMILES: CCNC(=O)COCC[C@]1(C)C(=O)C2C1CC(C2)ClC(=O)Nc3cncc4c3cccc4

RUN: RUN1500

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.27

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

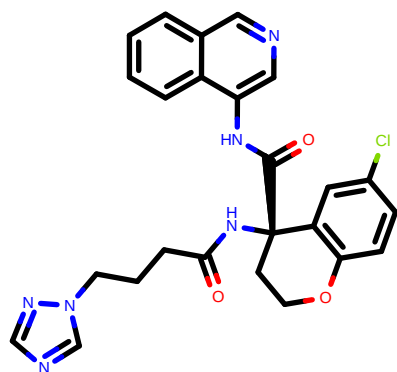
SMILES: c1cc2c(cc1C[NH3+])cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN19

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.14

EN300-316216_1_1



CID: EN300-316216_1_1

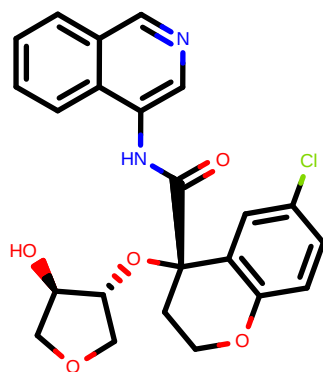
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4C3CC(C4)ClNC(=O)CCc5cncc5

RUN: RUN1740

DDG (kcal/mol): -1.21

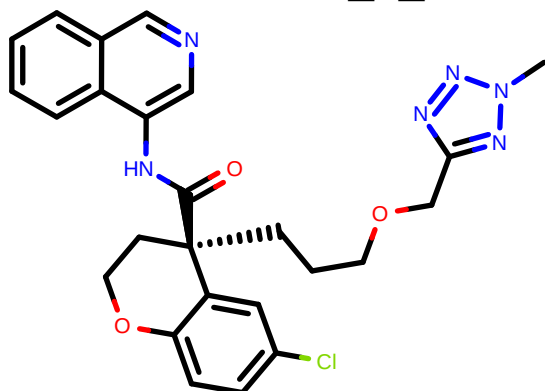
dDDG (kcal/mol): 0.43

EN300-331828_1_1



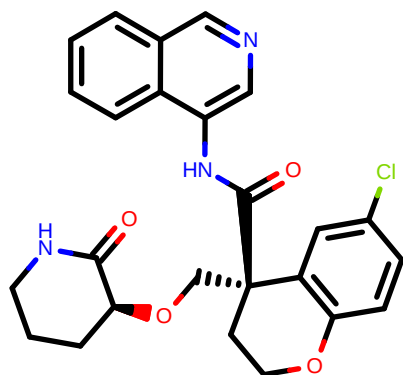
CID:	EN300-331828_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)O[C@@H]5COC[C@H]5O</chem>
RUN:	RUN1591
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.19

EN300-90225_4_1



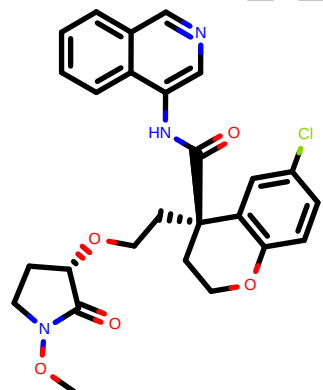
CID:	EN300-90225_4_1
SMILES:	<chem>Cn1nc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN587
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.32

EN300-107267_2_2



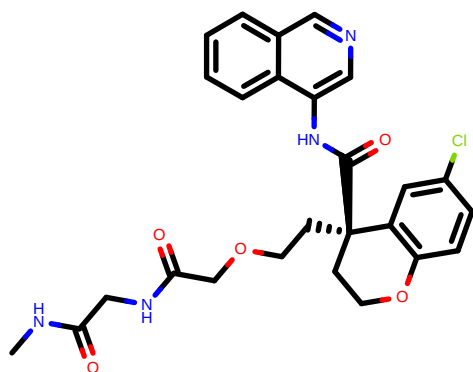
CID:	EN300-107267_2_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O</chem>
RUN:	RUN966
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.25

EN300-302058_3_1



CID:	EN300-302058_3_1
SMILES:	<chem>CON1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5</chem>
RUN:	RUN1707
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.27

EN300-23223_3_1



CID: EN300-23223_3_1

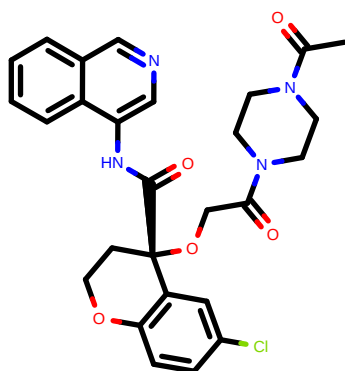
SMILES: CNC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1148

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.32

EN300-1724771_1_1



CID: EN300-1724771_1_1

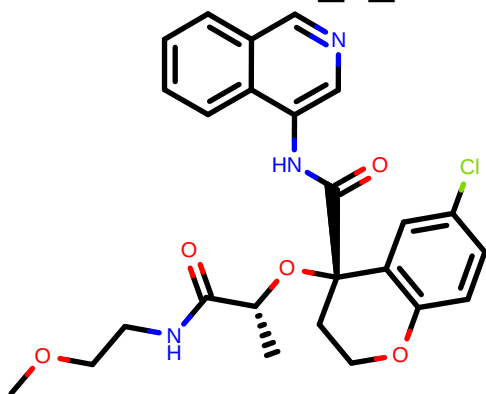
SMILES: CC(=O)N1CCN(CC1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN936

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.28

EN300-23317_1_2



CID: EN300-23317_1_2

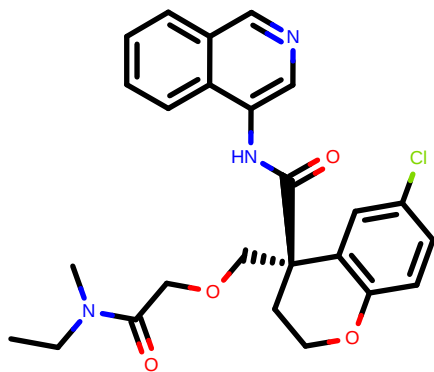
SMILES: C[C@H](C(=O)NCCOC)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1320

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.35

EN300-1253122_2_1



CID: EN300-1253122_2_1

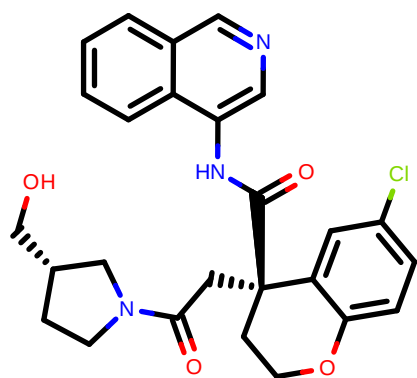
SMILES: CCN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1454

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.24

EN300-256053_1_1



CID: EN300-256053_1_1

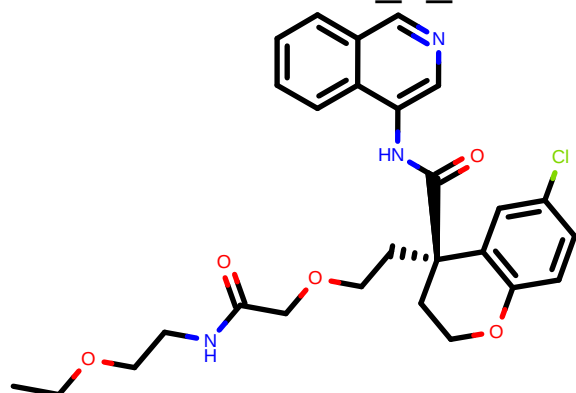
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO

RUN: RUN1458

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.25

EN300-103187_3_1



CID: EN300-103187_3_1

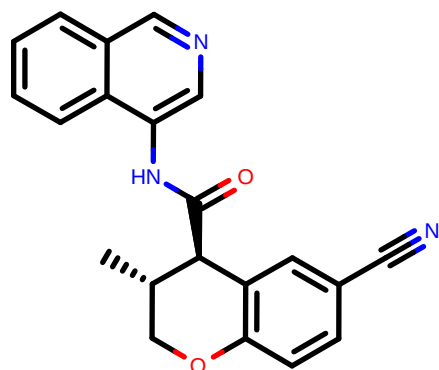
SMILES: CCOCCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN632

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.46

DAR-DIA-0d514e7d-8_1



CID: DAR-DIA-0d514e7d-8_1

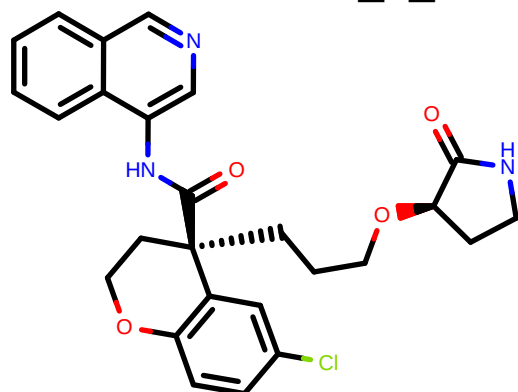
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cnc4c3ccccc4)C#N

RUN: RUN18

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.07

EN300-6736413_4_1



CID: EN300-6736413_4_1

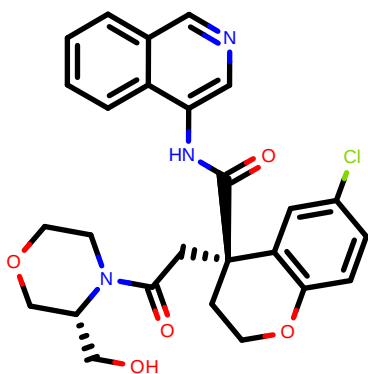
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@H]5CCNC5=O

RUN: RUN975

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.31

EN300-173903_1_1



CID: EN300-173903_1_1

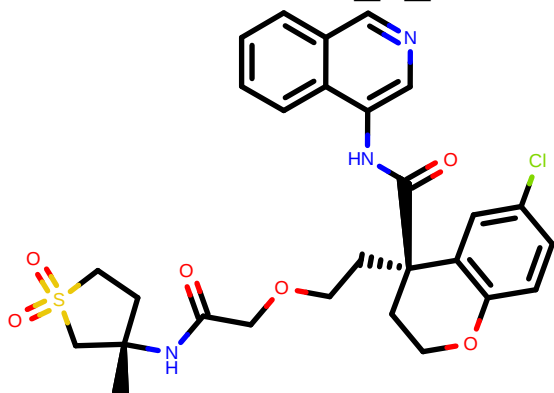
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO

RUN: RUN1210

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.32

EN300-10414_3_1



CID: EN300-10414_3_1

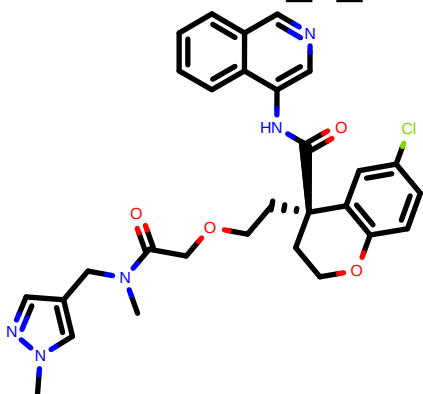
SMILES: C[C@@]1(CCS(=O)(=O)C1)NC(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN884

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.44

EN300-65978_3_1



CID: EN300-65978_3_1

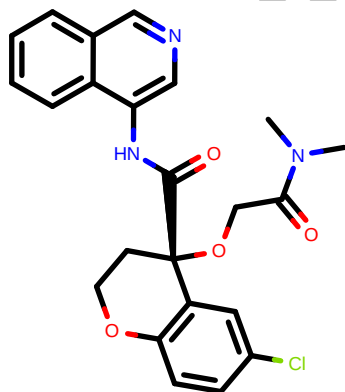
SMILES: Cn1cc(cn1)CN(C)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1731

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.55

EN300-216063_1_1



CID: EN300-216063_1_1

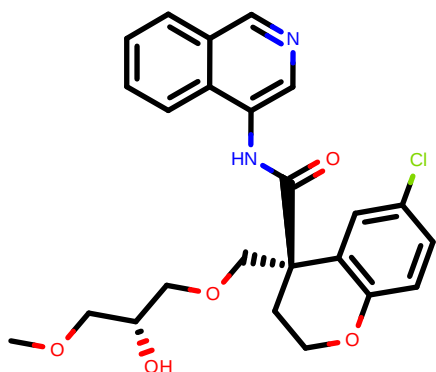
SMILES: CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN793

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.22

EN300-1915260_2_2



CID: EN300-1915260_2_2

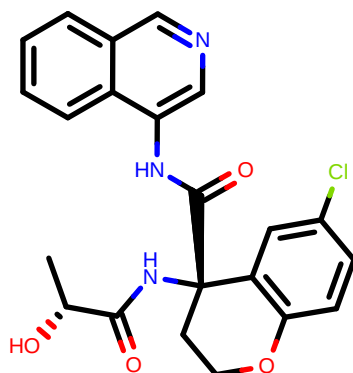
SMILES: COC[C@H](C(=O)N[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN1030

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.38

EN300-19542_1_2



CID: EN300-19542_1_2

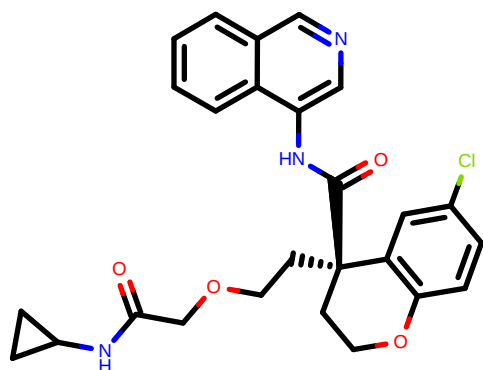
SMILES: C[C@H](C(=O)N[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN1389

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.20

EN300-1253178_3_1



CID: EN300-1253178_3_1

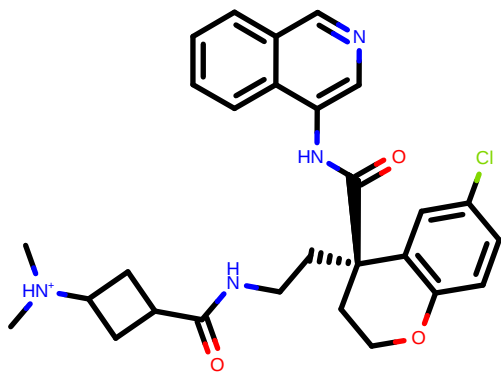
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(COC4c3cc(cc4)Cl)CCOCC(=O)NC5CC5

RUN: RUN1683

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-6739235_3_1



CID: EN300-6739235_3_1

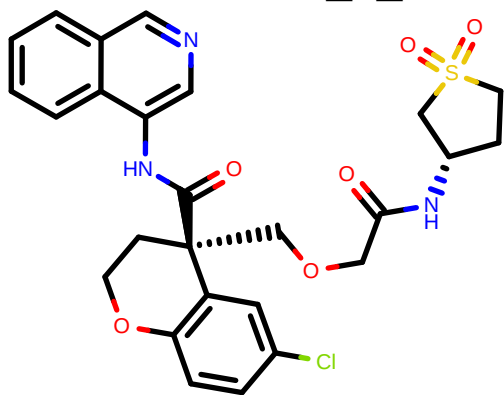
SMILES: C[NH+][C@H]1C[C@@H](C1)C(=O)NCC[C@]2(C3c4cc(c3)C9OCC2)C(=O)Nc4c5c(cnc4)cccc5C

RUN: RUN1274

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.34

EN300-05512_2_2



CID: EN300-05512_2_2

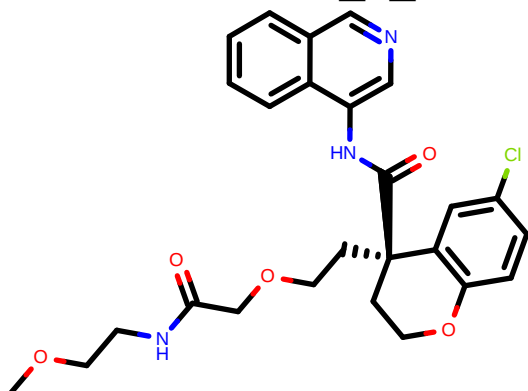
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@H]5CCS(=O)(=O)C5

RUN: RUN467

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.46

EN300-02015_3_1



CID: EN300-02015_3_1

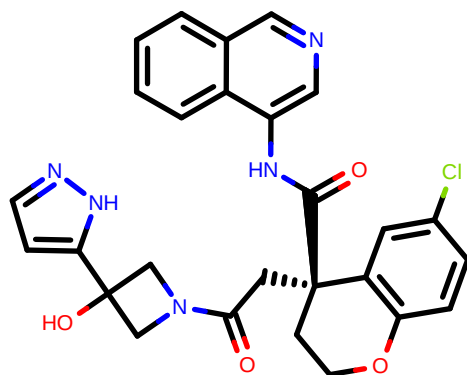
SMILES: COCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN393

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.34

EN300-1667046_1_1



CID: EN300-1667046_1_1

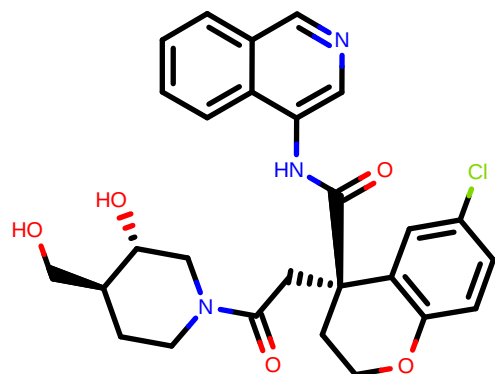
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cc[nH]6)O

RUN: RUN1673

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.29

EN300-95639_1_2



CID: EN300-95639_1_2

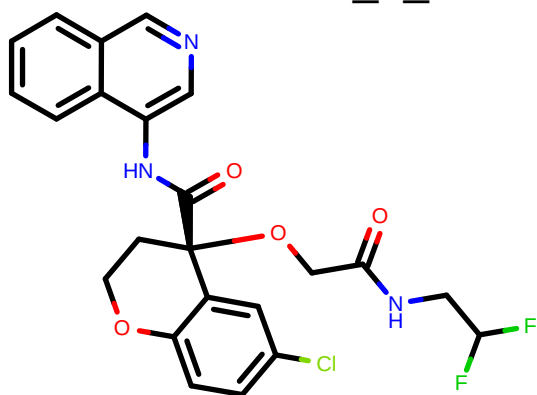
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cc[nH]6)O

RUN: RUN343

DDG (kcal/mol): -1.11

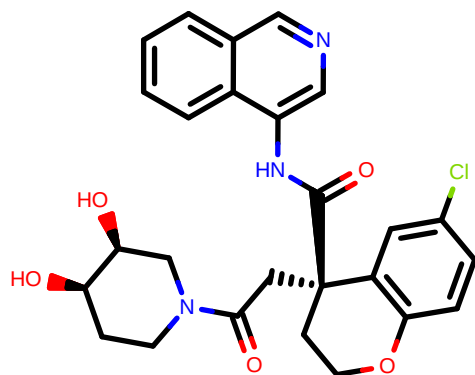
dDDG (kcal/mol): 0.39

EN300-120586_1_1



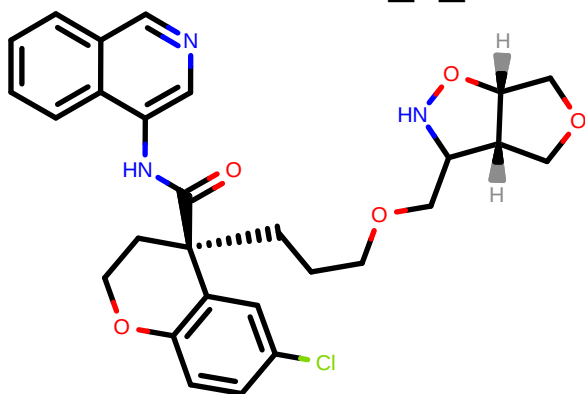
CID:	EN300-120586_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCC(F)F</chem>
RUN:	RUN429
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.26

EN300-349304_1_1



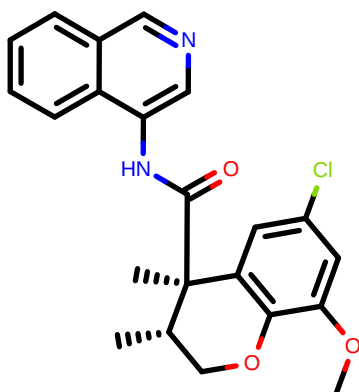
CID:	EN300-349304_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@H](C5)O)O</chem>
RUN:	RUN1082
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.28

EN300-7436306_4_1



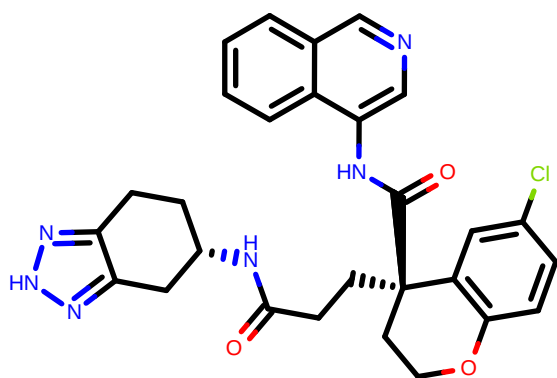
CID:	EN300-7436306_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NO[C@H]([C@H]5)COO6</chem>
RUN:	RUN839
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.34

DAR-DIA-0d514e7d-25_1



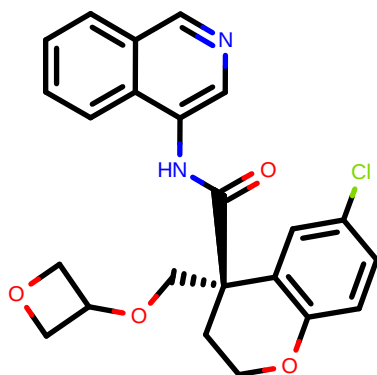
CID:	DAR-DIA-0d514e7d-25_1
SMILES:	<chem>C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN73
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.13

EN300-6491682_2_2



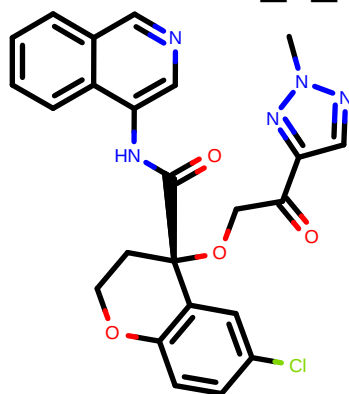
CID:	EN300-6491682_2_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCc6c(n1H)n6)C5</chem>
RUN:	RUN867
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.34

EN300-317082_2_1



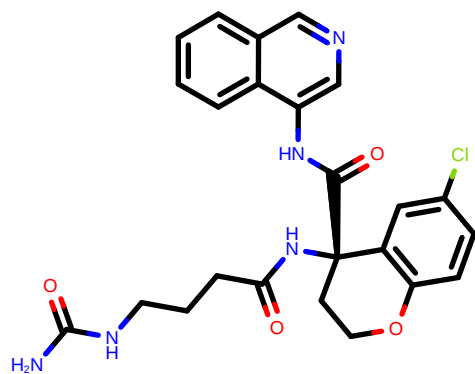
CID:	EN300-317082_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC5COC5</chem>
RUN:	RUN1462
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.22

EN300-204935_1_1



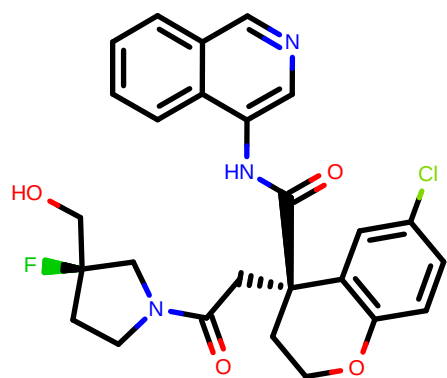
CID:	EN300-204935_1_1
SMILES:	<chem>Cn1ncc(n1)C(=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN1536
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.26

EN300-05620_1_1



CID:	EN300-05620_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCNC(=O)N</chem>
RUN:	RUN577
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.34

EN300-203118_1_1



CID:

EN300-203118_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@](C5)(CO)F

RUN:

RUN1737

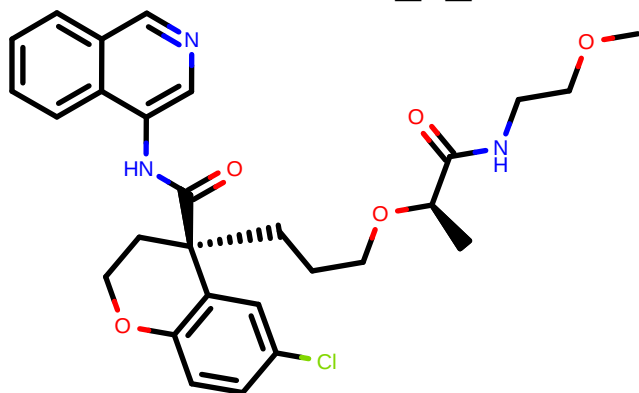
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.46

EN300-23317_4_2



CID:

EN300-23317_4_2

SMILES:

C[C@H](C(=O)NCCOC)OCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3ccoc4

RUN:

RUN1551

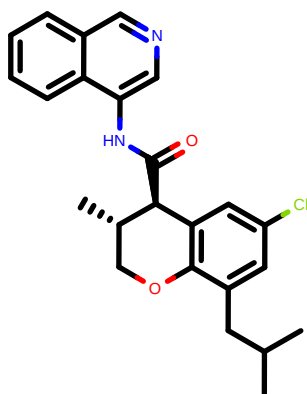
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.37

DAR-DIA-0d514e7d-24_1



CID:

DAR-DIA-0d514e7d-24_1

SMILES:

C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3ncc4c3ccoc4)C)CC(C)C

RUN:

RUN109

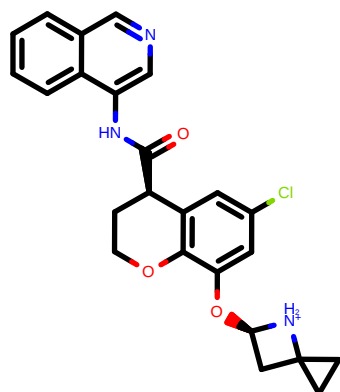
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.16

DAR-DIA-23e5a6a0-5_1



CID:

DAR-DIA-23e5a6a0-5_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC6([NH2+][5]CC6)Cl

RUN:

RUN84

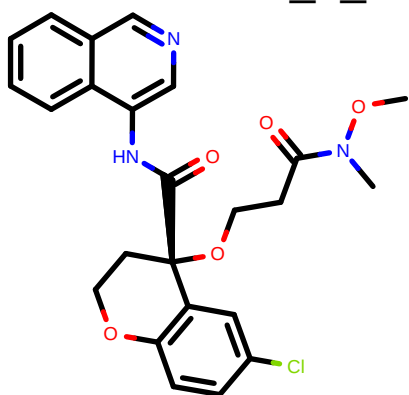
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

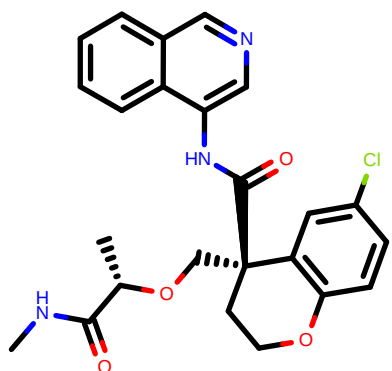
0.45

EN300-174603_1_1



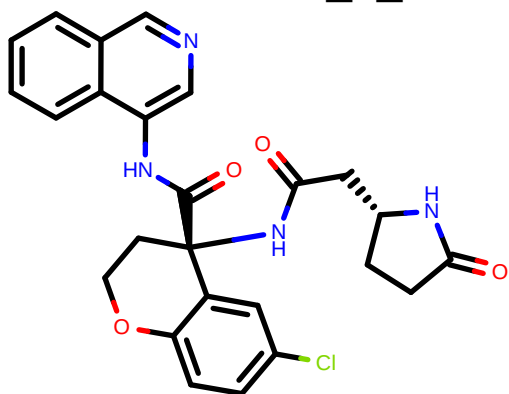
CID:	EN300-174603_1_1
SMILES:	<chem>CN(C(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC</chem>
RUN:	RUN1272
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.25

EN300-211482_2_1



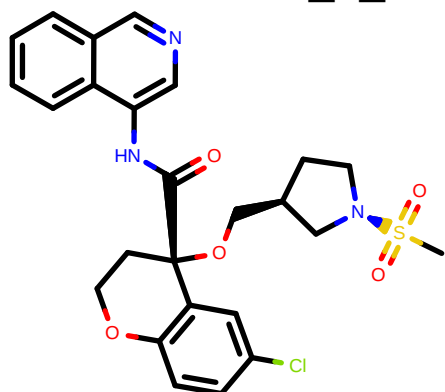
CID:	EN300-211482_2_1
SMILES:	<chem>C[C@@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1326
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.28

EN300-68203_1_2



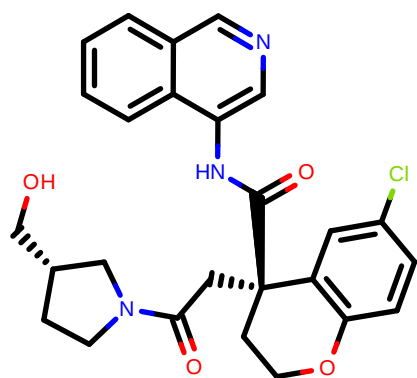
CID:	EN300-68203_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCC(=O)N5</chem>
RUN:	RUN1684
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.30

EN300-261986_1_1



CID:	EN300-261986_1_1
SMILES:	<chem>CS(=O)(=O)[N@@]1CC[C@H](C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN516
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.32

EN300-256053_1_1



CID:

EN300-256053_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)CO

RUN:

RUN1450

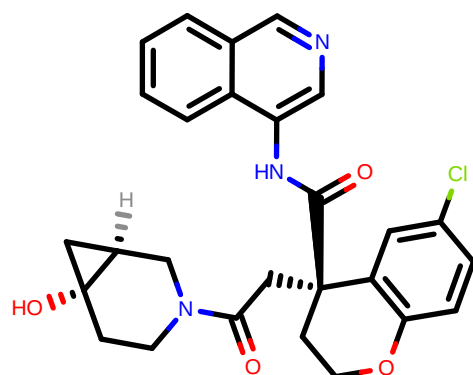
DDG (kcal/mol):

-1.01

dDDG (kcal/mol):

0.29

EN300-303908_1_1



CID:

EN300-303908_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)O

RUN:

RUN827

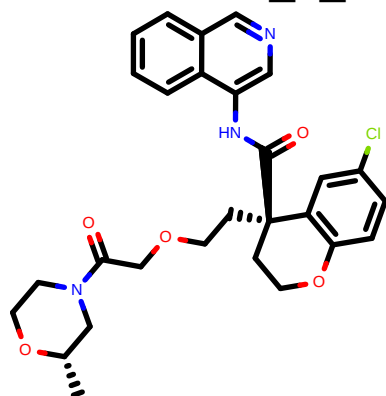
DDG (kcal/mol):

-1.00

dDDG (kcal/mol):

0.35

EN300-25572_3_2



CID:

EN300-25572_3_2

SMILES:

C[C@H]1CN(CCO1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4ccccc5

RUN:

RUN592

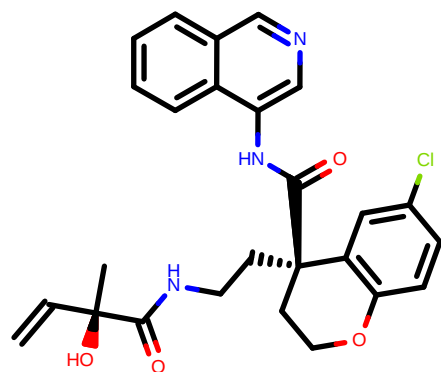
DDG (kcal/mol):

-0.99

dDDG (kcal/mol):

0.31

EN300-248888_3_1



CID:

EN300-248888_3_1

SMILES:

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

RUN:

RUN763

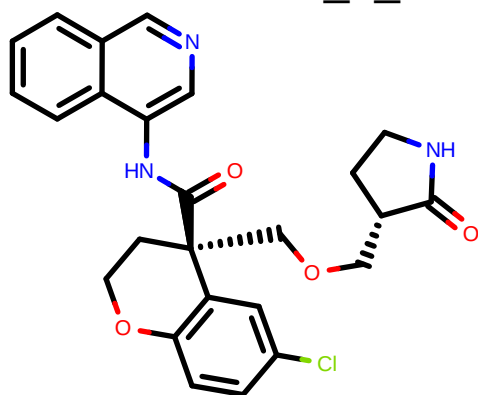
DDG (kcal/mol):

-0.99

dDDG (kcal/mol):

0.40

EN300-246248_2_1



CID: EN300-246248_2_1

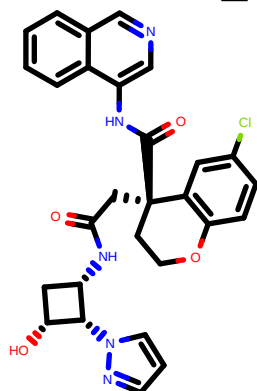
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O

RUN: RUN323

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-260696_1_8



CID: EN300-260696_1_8

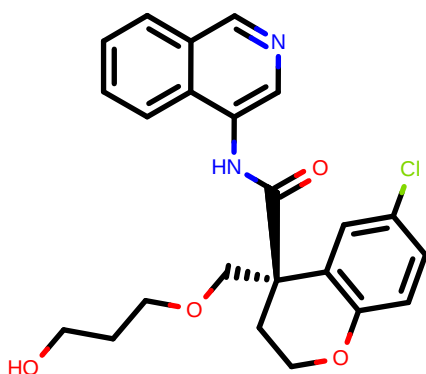
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]([C@@H]5m6ccc6)O

RUN: RUN1785

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.62

EN300-221518_2_1



CID: EN300-221518_2_1

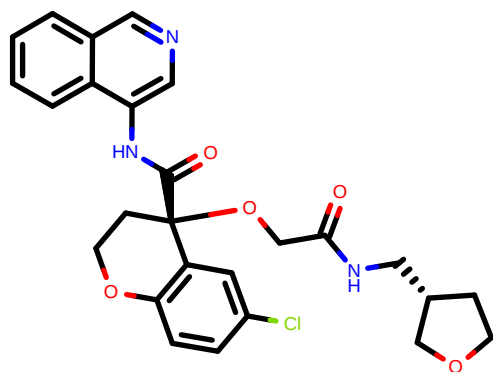
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(CO)CO

RUN: RUN823

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.23

EN300-46832_1_1



CID: EN300-46832_1_1

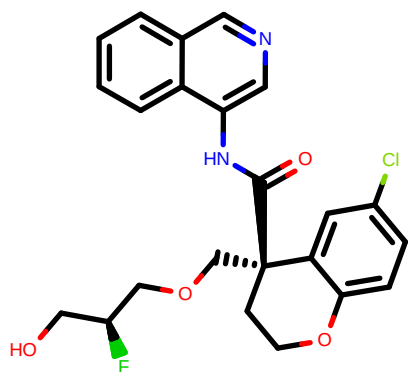
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCOC5

RUN: RUN1472

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-1600517_2_2



CID:

EN300-1600517_2_2

SMILES:

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

RUN:

RUN1134

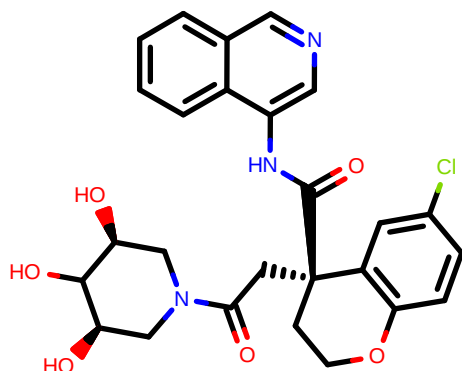
DDG (kcal/mol):

-0.98

dDDG (kcal/mol):

0.29

EN300-299920_1_1



CID:

EN300-299920_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C)[C@H](CO)O

RUN:

RUN1777

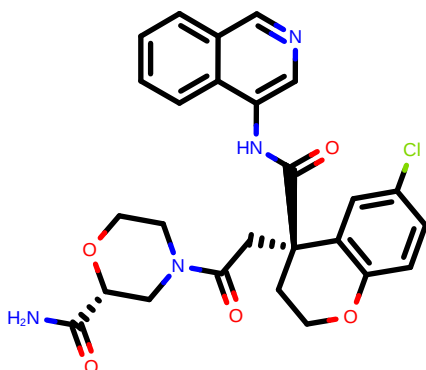
DDG (kcal/mol):

-0.98

dDDG (kcal/mol):

0.55

EN300-60862_1_2



CID:

EN300-60862_1_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)C(=O)N

RUN:

RUN866

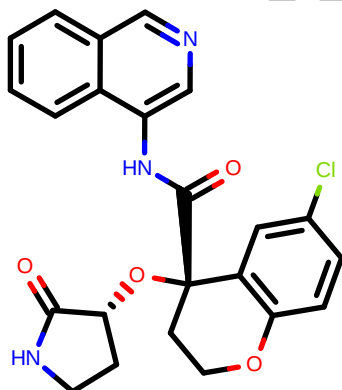
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.28

EN300-6736413_1_1



CID:

EN300-6736413_1_1

SMILES:

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

RUN:

RUN1679

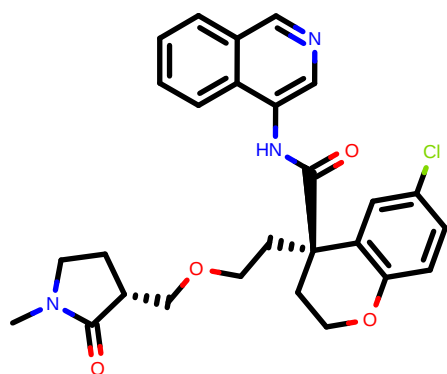
DDG (kcal/mol):

-0.96

dDDG (kcal/mol):

0.20

EN300-260816_3_1



CID: EN300-260816_3_1

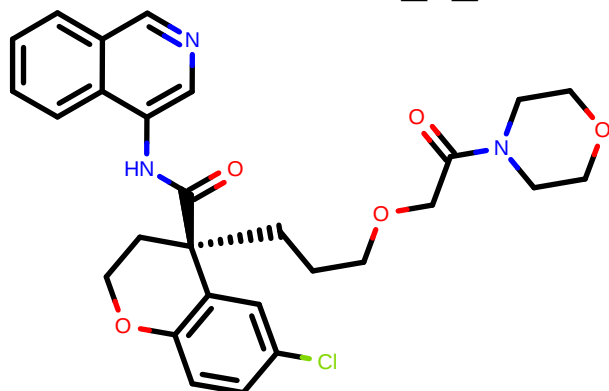
SMILES: CN1CC[C@@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN1763

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.52

EN300-1241327_4_1



CID: EN300-1241327_4_1

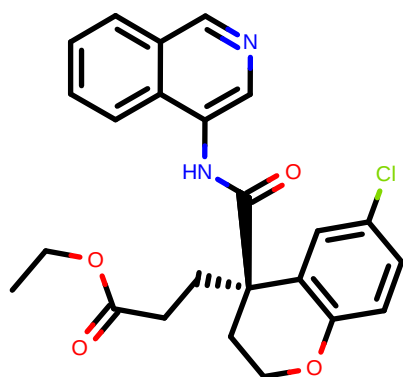
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5

RUN: RUN1183

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.33

JAG-UCB-706446eb-4_1



CID: JAG-UCB-706446eb-4_1

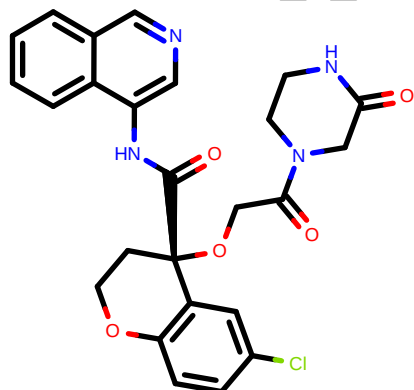
SMILES: CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.21

EN300-22884_1_1



CID: EN300-22884_1_1

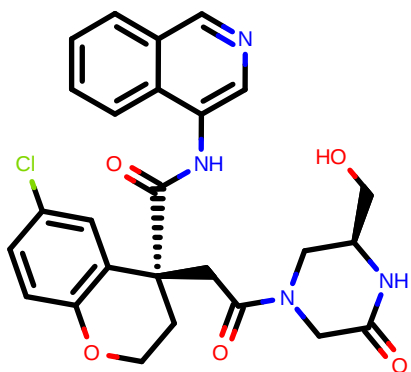
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCN(C(=O)O)C5

RUN: RUN707

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EN300-100700_1_1



CID: EN300-100700_1_1

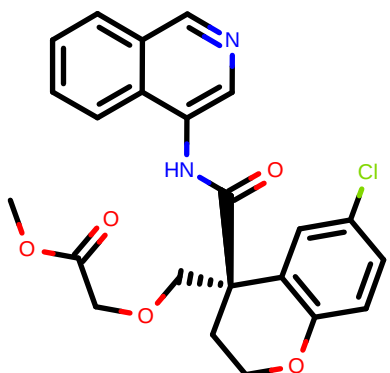
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](NC(=O)C5)CO

RUN: RUN1218

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.41

EN300-19700_2_1



CID: EN300-19700_2_1

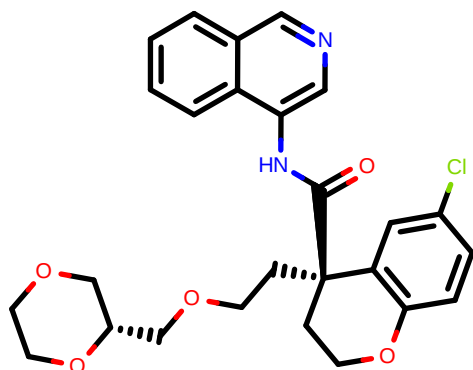
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1422

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.20

EN300-139167_3_2



CID: EN300-139167_3_2

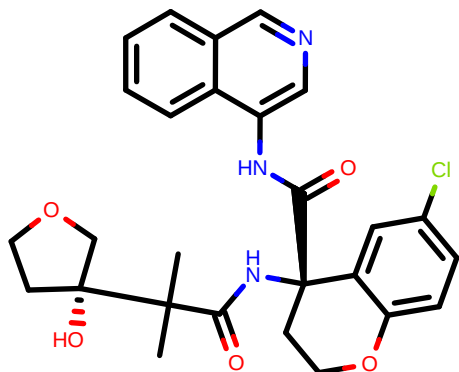
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCCO5

RUN: RUN672

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.32

EN300-1630093_1_2



CID: EN300-1630093_1_2

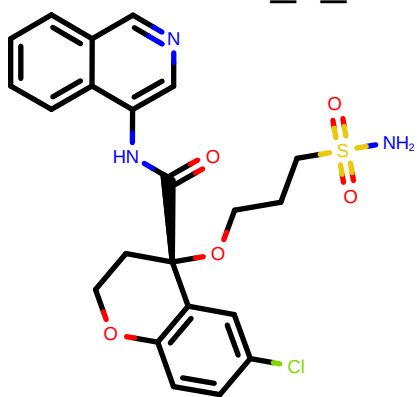
SMILES: CC(C)(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)[C@]5(CCOCC5)O

RUN: RUN1509

DDG (kcal/mol): -0.94

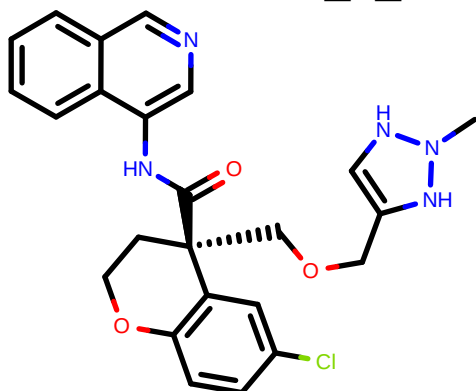
dDDG (kcal/mol): 0.24

EN300-79588_1_1



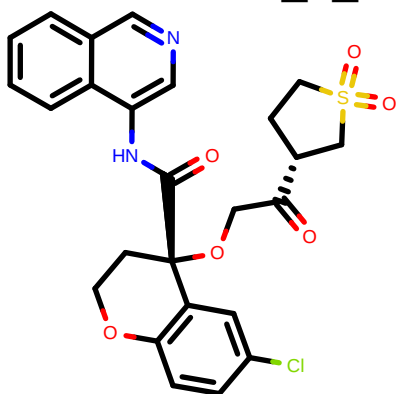
CID:	EN300-79588_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCS(=O)(=O)N</chem>
RUN:	RUN1120
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.29

EN300-219020_2_1



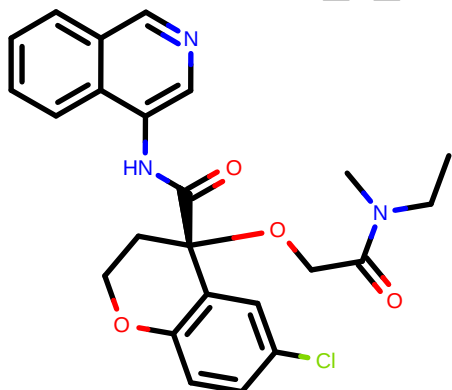
CID:	EN300-219020_2_1
SMILES:	<chem>Cn1ncc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1725
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.24

EN300-226314_1_1



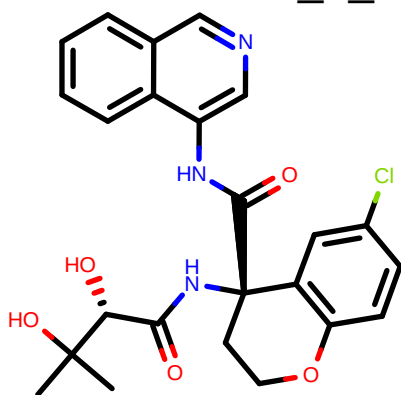
CID:	EN300-226314_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5SCCS(=O)(=O)C5</chem>
RUN:	RUN285
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.29

EN300-1253122_1_1



CID:	EN300-1253122_1_1
SMILES:	<chem>CCN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN548
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.25

EN300-299532_1_1



CID: EN300-299532_1_1

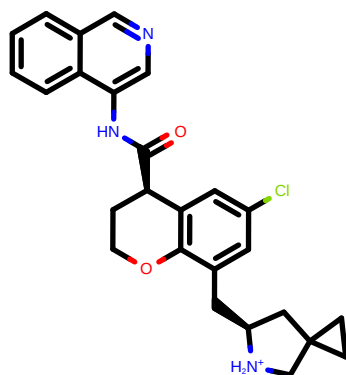
SMILES: CC(C)(C@H)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4O)O

RUN: RUN1141

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.27

DAR-DIA-23e5a6a0-9_2



CID: DAR-DIA-23e5a6a0-9_2

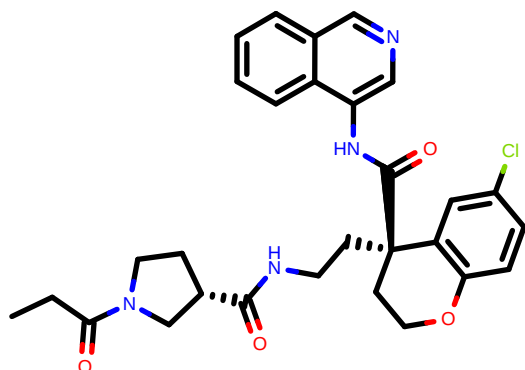
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C)COCc4c3cc(cc4C)[C@H]5CC6(CC6)C[NH2+][5]Cl

RUN: RUN157

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.29

EN300-114133_3_1



CID: EN300-114133_3_1

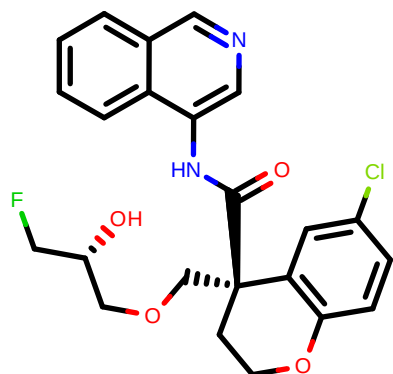
SMILES: CCC(=O)N1CC[C@H](C1)C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN1681

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.44

EN300-1968342_2_2



CID: EN300-1968342_2_2

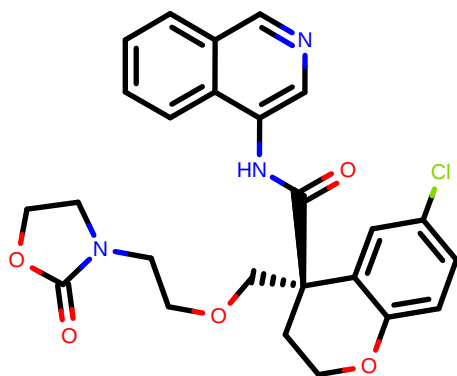
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN514

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.32

EN300-370967_2_1



CID: EN300-370967_2_1

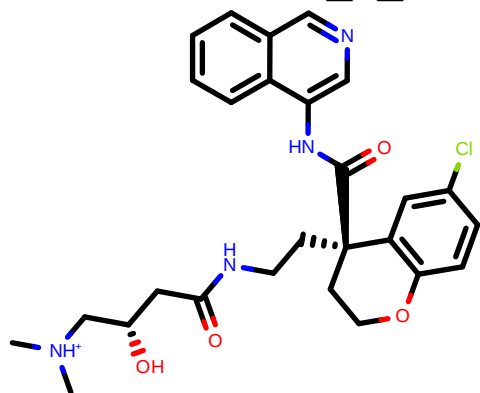
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCNC5CCOC5=O

RUN: RUN807

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-216916_3_2



CID: EN300-216916_3_2

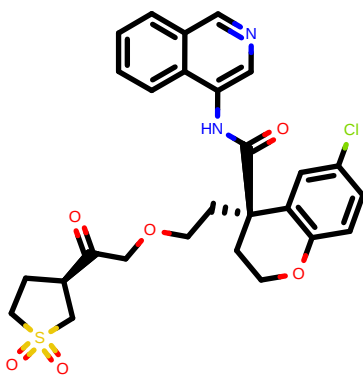
SMILES: C[NH+](C)C[C@H](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN1370

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.45

EN300-226314_3_1



CID: EN300-226314_3_1

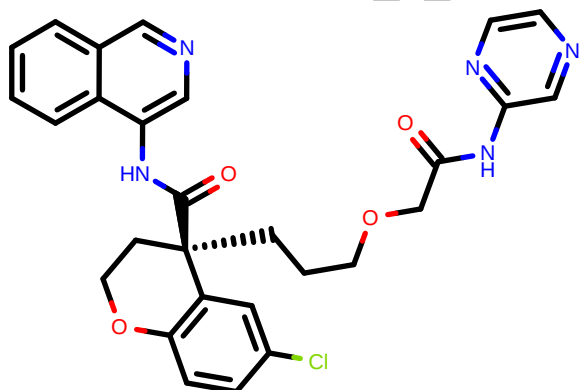
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@@H]5SCCS(=O)(=O)C5

RUN: RUN1156

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.37

EN300-105267_4_1



CID: EN300-105267_4_1

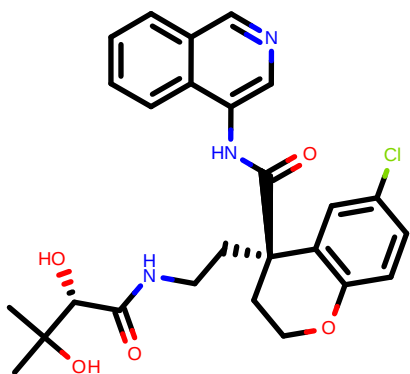
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5nccn5

RUN: RUN1135

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.31

EN300-299532_3_1



CID: EN300-299532_3_1

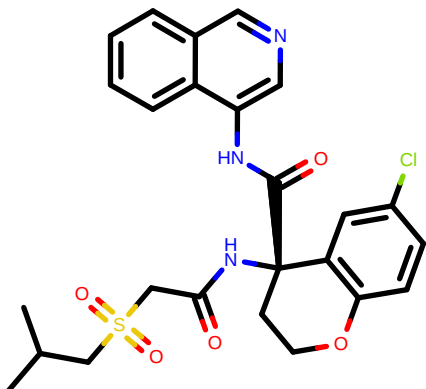
SMILES: CC(C)([C@@H](C(=O)NCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O

RUN: RUN1474

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.38

EN300-42243_1_1



CID: EN300-42243_1_1

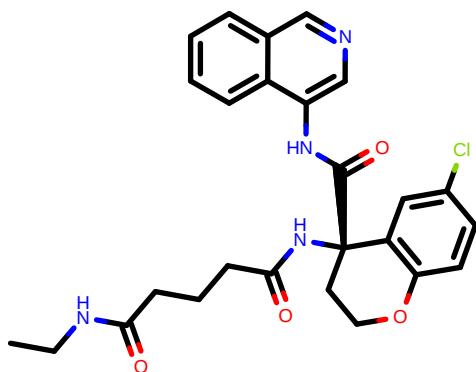
SMILES: CC(C)CS(=O)(=O)CC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN798

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-68635_1_1



CID: EN300-68635_1_1

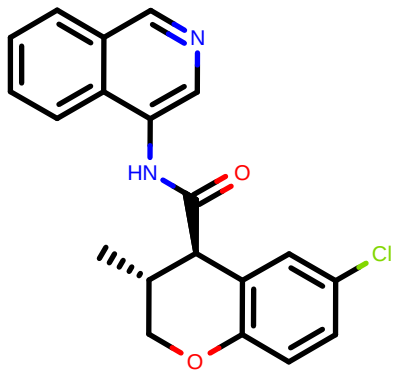
SMILES: CCNC(=O)CCCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN649

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.31

MAT-POS-8a69d52e-4_2



CID: MAT-POS-8a69d52e-4_2

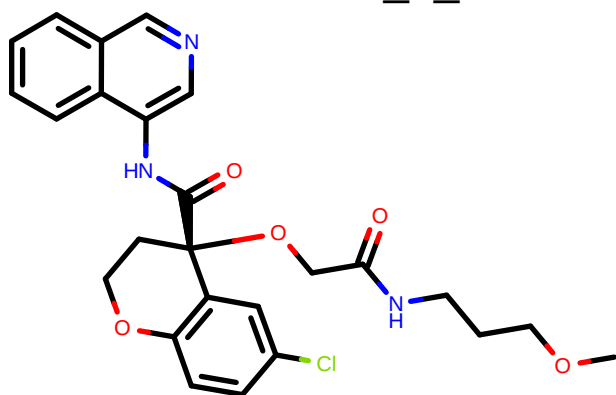
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN13

DDG (kcal/mol): -0.87

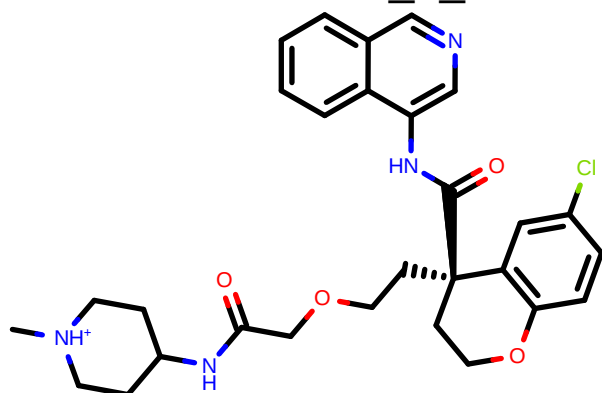
dDDG (kcal/mol): 0.06

EN300-04492_1_1



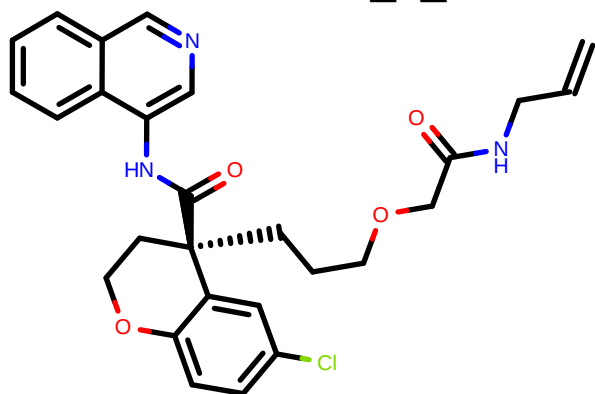
CID:	EN300-04492_1_1
SMILES:	<chem>COCCCCNC(=O)CO[C@]1(C)C(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1663
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.22

EN300-342462_3_1



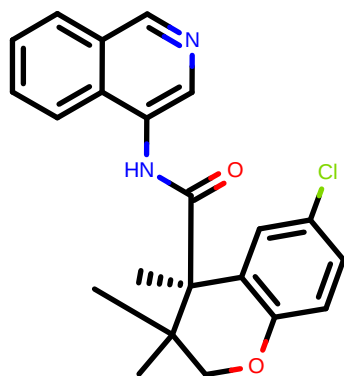
CID:	EN300-342462_3_1
SMILES:	<chem>C[NH+]1CCC(CC1)NC(=O)COC[C@]2(C)C(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1132
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.45

EN300-17184_4_1



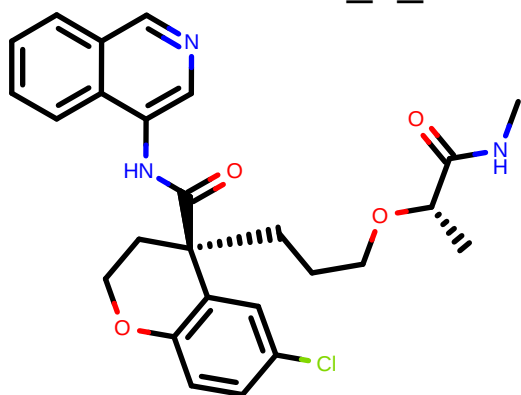
CID:	EN300-17184_4_1
SMILES:	<chem>C=CCNC(=O)COC[C@]1(C)C(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1567
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.38

DAR-DIA-0d514e7d-30_1



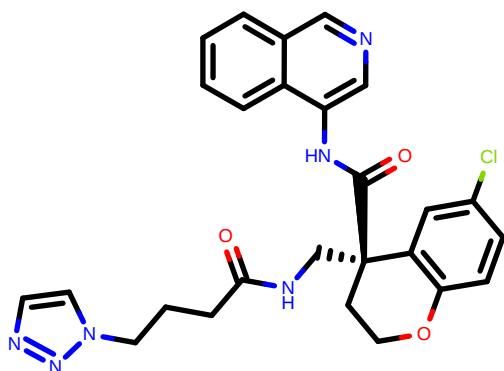
CID:	DAR-DIA-0d514e7d-30_1
SMILES:	<chem>C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN112
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.15

EN300-211482_4_1



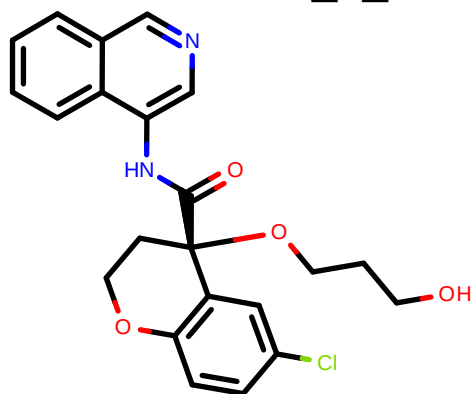
CID:	EN300-211482_4_1
SMILES:	<chem>C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4</chem>
RUN:	RUN1015
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.35

EN300-124301_2_1



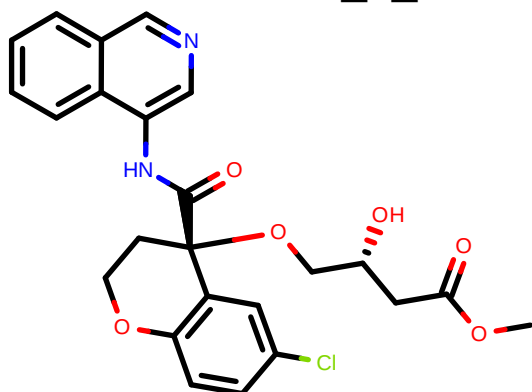
CID:	EN300-124301_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCc5cn5</chem>
RUN:	RUN754
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.32

EN300-221518_1_1



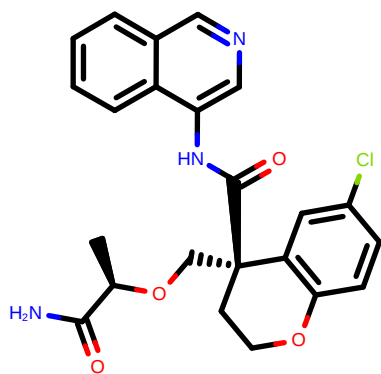
CID:	EN300-221518_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO</chem>
RUN:	RUN992
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.20

EN300-73662_1_1



CID:	EN300-73662_1_1
SMILES:	<chem>COC(=O)C[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)O</chem>
RUN:	RUN1288
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.32

EN300-17381_2_2



CID: EN300-17381_2_2

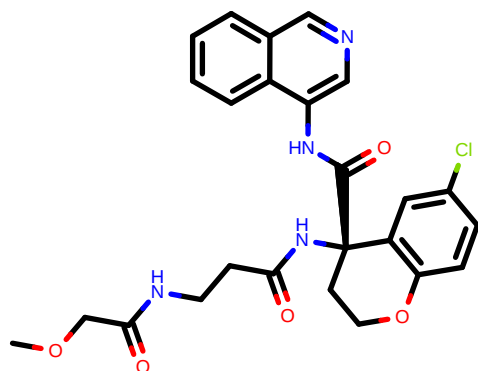
SMILES: C[C@H](C(=O)N)OC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1230

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.26

EN300-31242_1_1



CID: EN300-31242_1_1

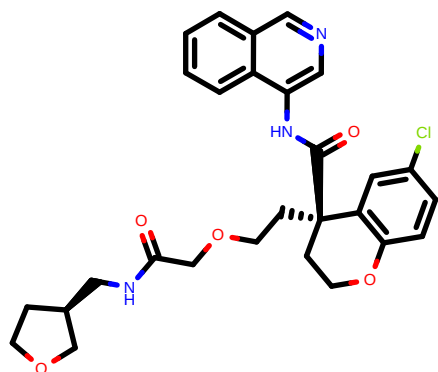
SMILES: COCC(=O)NCCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN553

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.28

EN300-46832_3_1



CID: EN300-46832_3_1

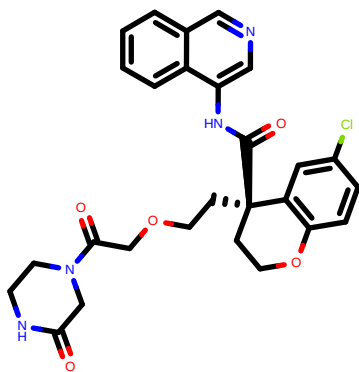
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@@H]5CCOC5

RUN: RUN1667

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.38

EN300-22884_3_1



CID: EN300-22884_3_1

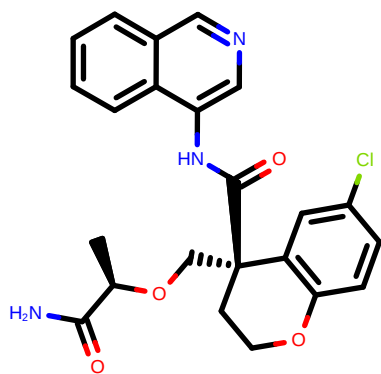
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCNC(=O)C5

RUN: RUN544

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.32

EN300-17381_2_2



CID:

EN300-17381_2_2

SMILES:

C[C@H](C(=O)N)OC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1246

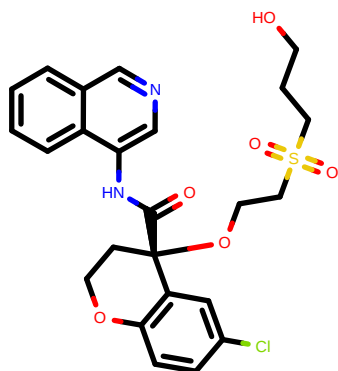
DDG (kcal/mol):

-0.83

dDDG (kcal/mol):

0.24

EN300-7456499_1_1



CID:

EN300-7456499_1_1

SMILES:

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

RUN:

RUN501

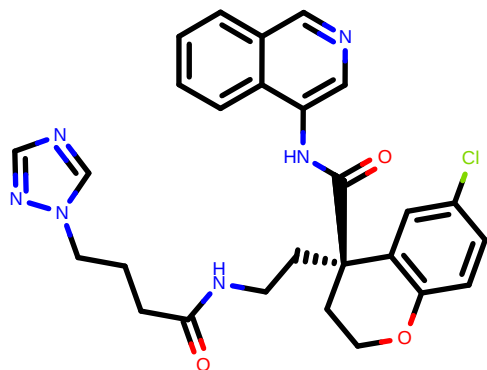
DDG (kcal/mol):

-0.82

dDDG (kcal/mol):

0.35

EN300-316216_3_1



CID:

EN300-316216_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCn5cnrn5

RUN:

RUN755

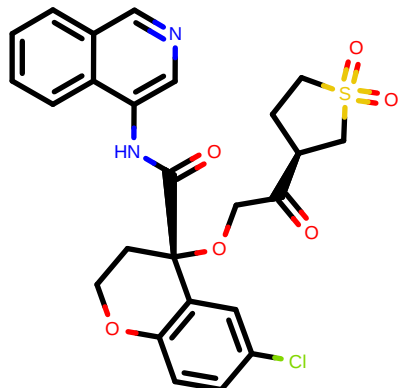
DDG (kcal/mol):

-0.82

dDDG (kcal/mol):

0.33

EN300-226314_1_2



CID:

EN300-226314_1_2

SMILES:

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

RUN:

RUN277

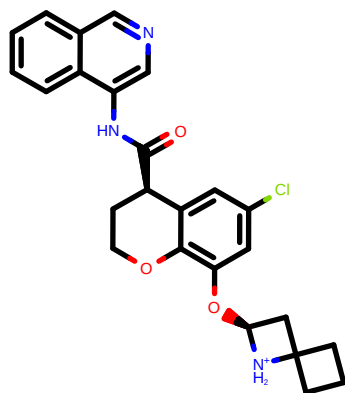
DDG (kcal/mol):

-0.81

dDDG (kcal/mol):

0.29

DAR-DIA-23e5a6a0-2_2



CID:

DAR-DIA-23e5a6a0-2_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOCc4ccc(cc4O)[C@H]5CC6([NH2+][5])CCC6)Cl

RUN:

RUN88

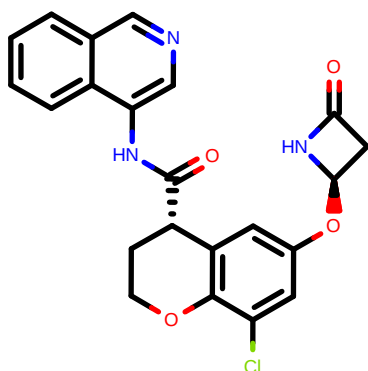
DDG (kcal/mol):

-0.81

dDDG (kcal/mol):

0.27

FRA-DIA-b66f7109-3_1



CID:

FRA-DIA-b66f7109-3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOCc4ccc(cc4Cl)O[C@H]5CC(=O)N5

RUN:

RUN187

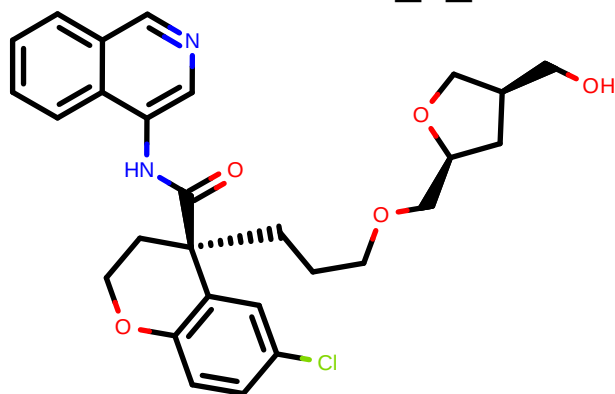
DDG (kcal/mol):

-0.80

dDDG (kcal/mol):

0.23

EN300-6494158_4_1



CID:

EN300-6494158_4_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4Cl)CCOC[C@H]5C[C@H]([C@H]5)CO

RUN:

RUN1007

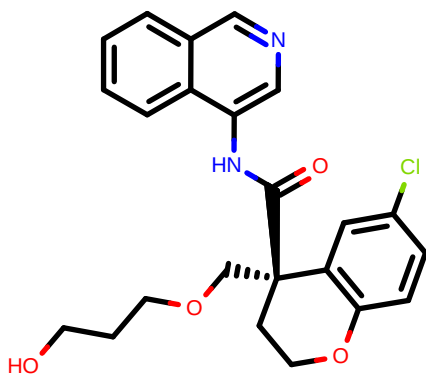
DDG (kcal/mol):

-0.80

dDDG (kcal/mol):

0.49

EN300-221518_2_1



CID:

EN300-221518_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4Cl)COCCCO

RUN:

RUN838

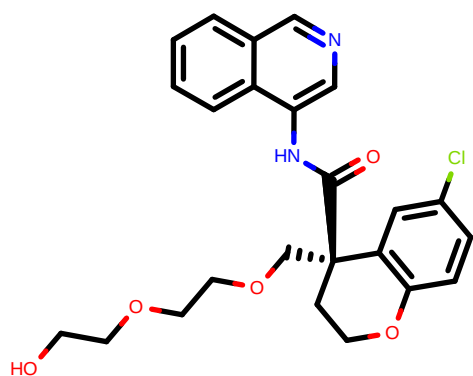
DDG (kcal/mol):

-0.80

dDDG (kcal/mol):

0.27

EN300-52467_2_1



CID:

EN300-52467_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCOCO

RUN:

RUN1581

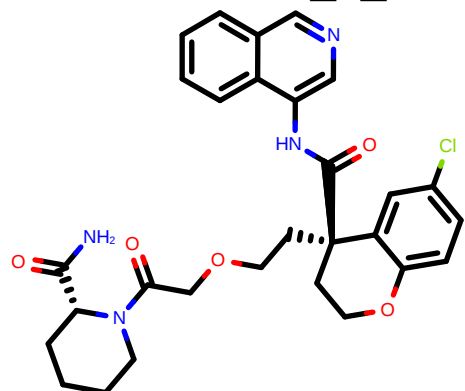
DDG (kcal/mol):

-0.80

dDDG (kcal/mol):

0.27

EN300-22879_3_1



CID:

EN300-22879_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC(=O)N5CCCC[C@@H]5C(=O)N

RUN:

RUN765

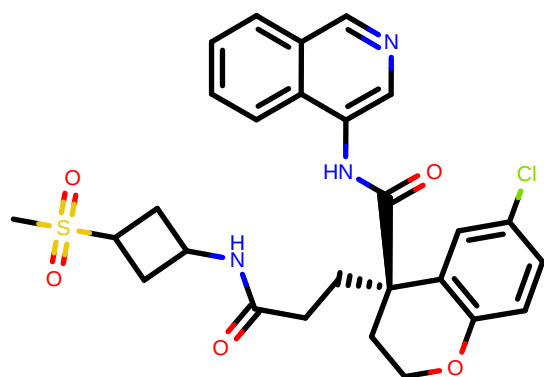
DDG (kcal/mol):

-0.80

dDDG (kcal/mol):

0.42

EN300-378760_2_1



CID:

EN300-378760_2_1

SMILES:

CS(=O)(=O)[C@@H]1C[C@@H]1C(=O)N[C@@]3(CCOc4c3cc(cc4)Cl)COCOC(=O)Nc4c5c(cnc4)ccccc5

RUN:

RUN1187

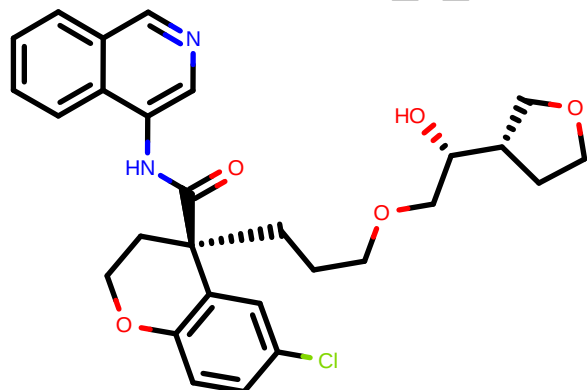
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.30

EN300-1911992_4_3



CID:

EN300-1911992_4_3

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H](C)[C@@H]5CCOC5O

RUN:

RUN675

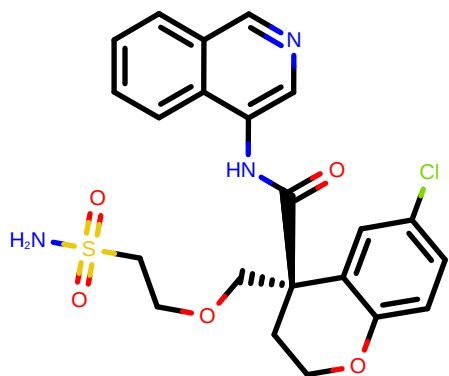
DDG (kcal/mol):

-0.79

dDDG (kcal/mol):

0.35

EN300-270710_2_1



CID: EN300-270710_2_1

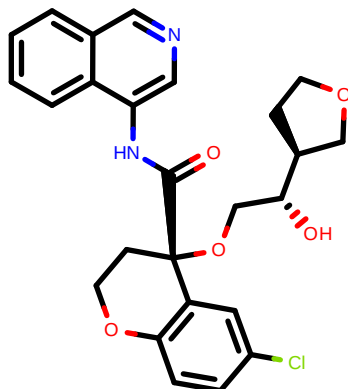
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(S(=O)(=O)N)CC

RUN: RUN1286

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.26

EN300-1911992_1_4



CID: EN300-1911992_1_4

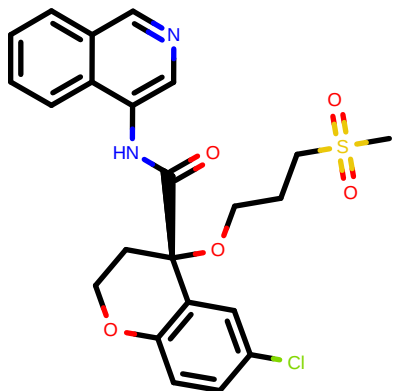
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]([C@H]5CCOC5O)

RUN: RUN1703

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.28

EN300-68794_1_1



CID: EN300-68794_1_1

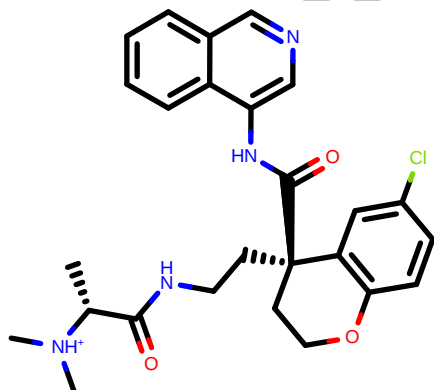
SMILES: CS(=O)(=O)CCCO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4

RUN: RUN652

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.28

EN300-312850_3_1



CID: EN300-312850_3_1

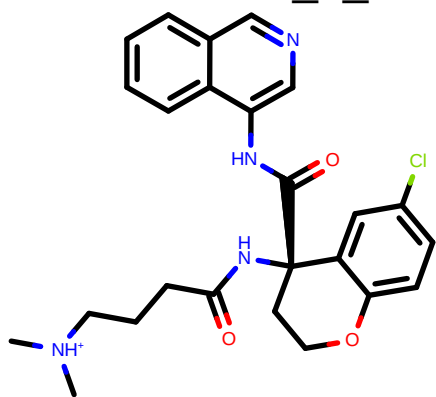
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4)[NH+](C)C

RUN: RUN407

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.41

EN300-42520_1_1



CID:

EN300-42520_1_1

SMILES:

C[NH+](C)CCCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN925

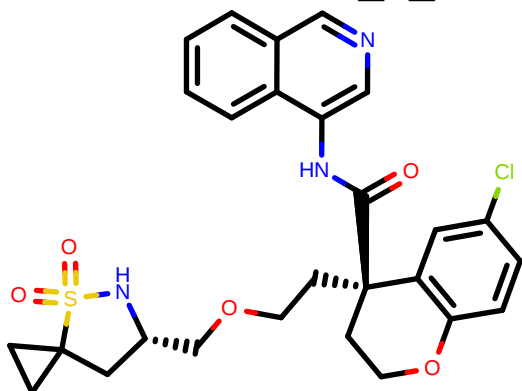
DDG (kcal/mol):

-0.77

dDDG (kcal/mol):

0.33

EN300-6504697_3_1



CID:

EN300-6504697_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COC6(CO6)S(=O)(=O)N5

RUN:

RUN892

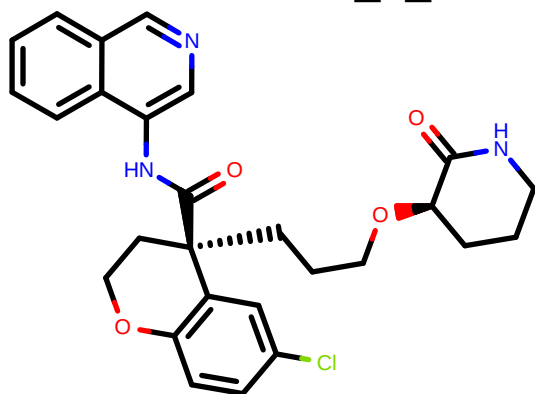
DDG (kcal/mol):

-0.77

dDDG (kcal/mol):

0.34

EN300-107267_4_1



CID:

EN300-107267_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNCC5=O

RUN:

RUN1670

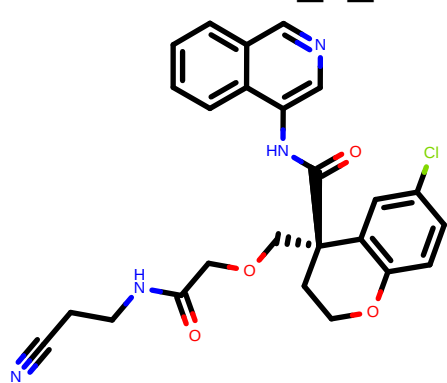
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.32

EN300-10895_2_1



CID:

EN300-10895_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCCC#N

RUN:

RUN690

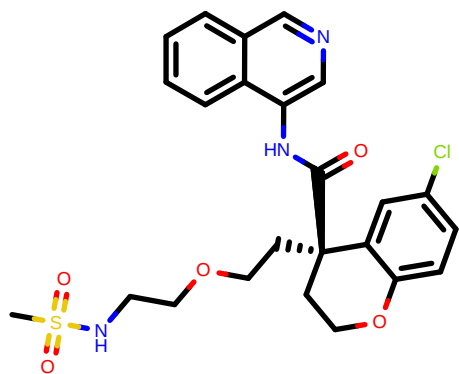
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.31

EN300-1238839_3_1



CID:

EN300-1238839_3_1

SMILES:

CS(=O)(=O)NCCOCC[C@]1(C)C(=O)C2C1CC(C2)C(C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1100

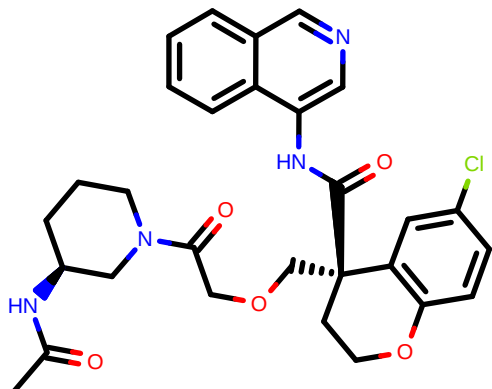
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.33

EN300-48886_2_2



CID:

EN300-48886_2_2

SMILES:

CC(=O)N[C@H]1CCCN(C1)C(=O)COC[C@]2(C)C(=O)C3C2CC(C3)C(C(=O)Nc4cncc5c4ccccc5

RUN:

RUN1741

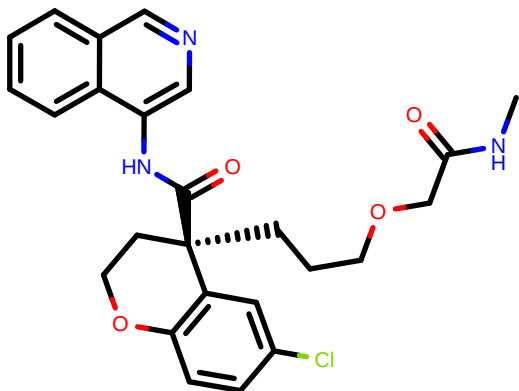
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.42

EN300-2977549_4_1



CID:

EN300-2977549_4_1

SMILES:

CNC(=O)COCC[C@]1(C)C(=O)C2C1CC(C2)C(C(=O)Nc3cncc4c3ccccc4

RUN:

RUN603

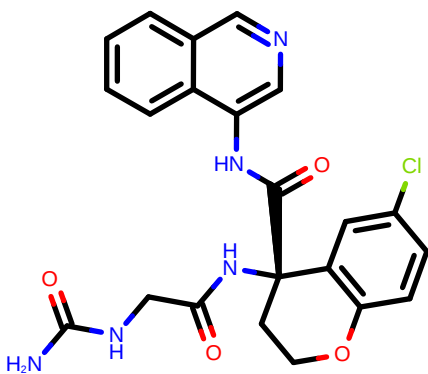
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.27

EN300-10397_1_1



CID:

EN300-10397_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4C3CC(C4)C(C(=O)Nc5cncc6c5ccccc6

RUN:

RUN1525

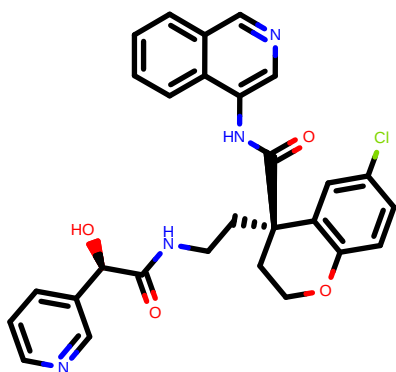
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.22

EN300-134855_3_1



CID: EN300-134855_3_1

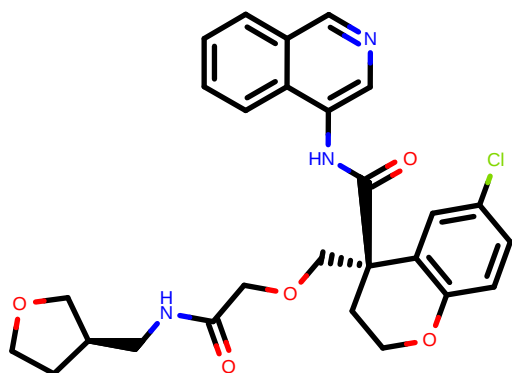
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](c5ccncc5)O

RUN: RUN1258

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.47

EN300-46832_2_2



CID: EN300-46832_2_2

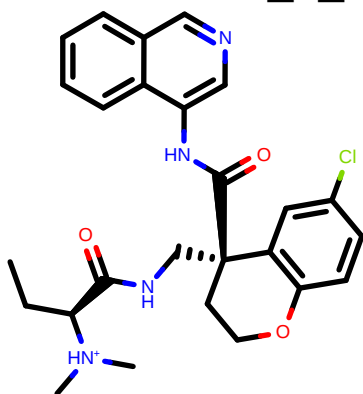
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@@H]5CCOC5

RUN: RUN618

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.33

EN300-110012_2_1



CID: EN300-110012_2_1

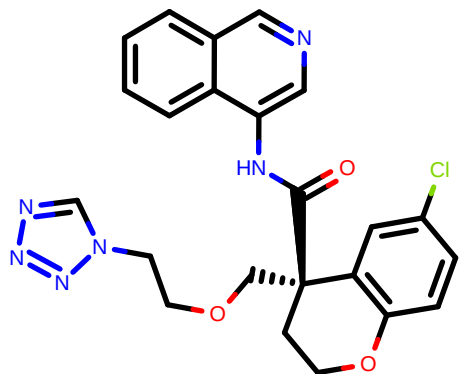
SMILES: CC[C@@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cc(c4)N)([NH+])(C)C

RUN: RUN1760

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.67

EN300-364679_2_1



CID: EN300-364679_2_1

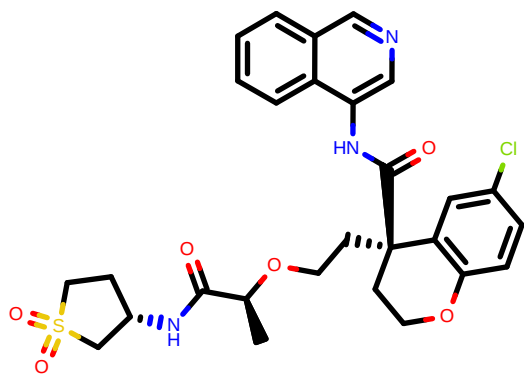
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nnn5

RUN: RUN1526

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.25

EN300-23318_3_3



CID: EN300-23318_3_3

SMILES:

C[C@H](C(=O)N[C@@H](CCS(=O)(=O)C1OCC1C2)C(=O)Nc3ccc4c3ccccc4

RUN:

RUN1348

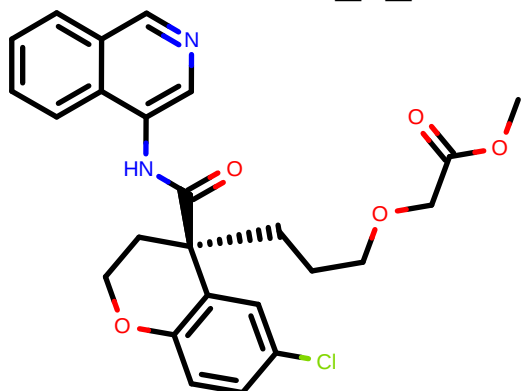
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.46

EN300-19700_4_1



CID: EN300-19700_4_1

SMILES:

COC(=O)COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4

RUN:

RUN436

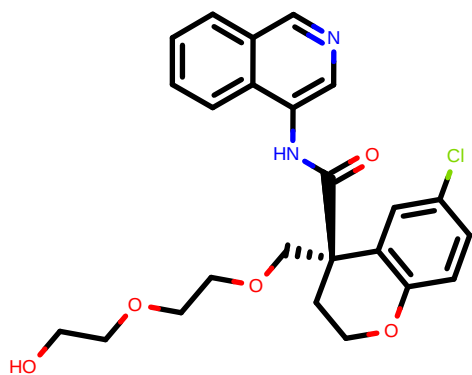
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.30

EN300-52467_2_1



CID: EN300-52467_2_1

SMILES:

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

RUN:

RUN1573

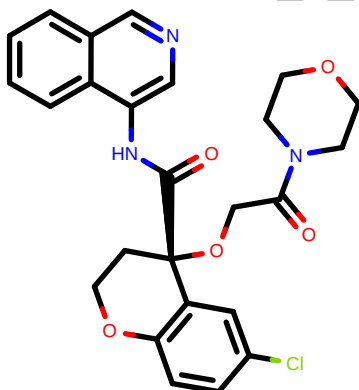
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.27

EN300-1241327_1_1



CID: EN300-1241327_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCOCC5

RUN:

RUN540

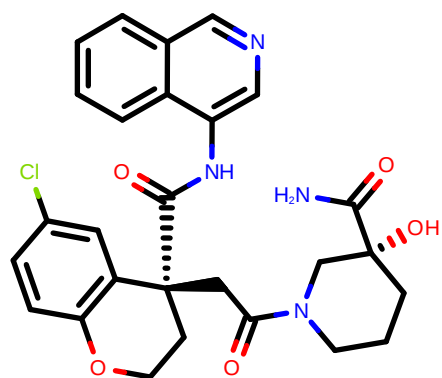
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.24

EN300-210553_1_1



CID: EN300-210553_1_1

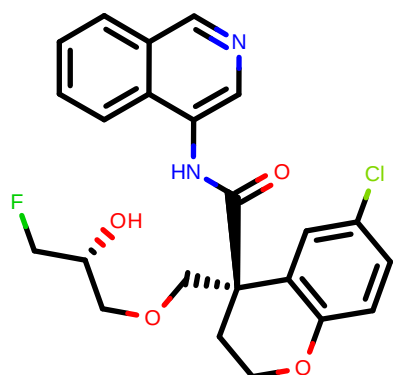
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@](C3)(C5)(C(=O)N)O

RUN: RUN1490

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.46

EN300-1968342_2_2



CID: EN300-1968342_2_2

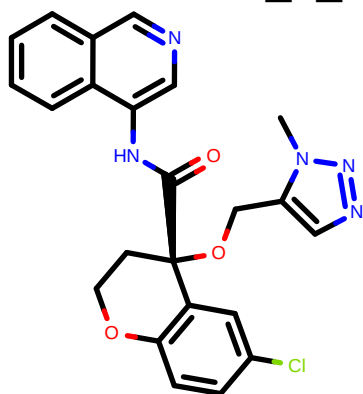
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN507

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.35

EN300-216673_1_1



CID: EN300-216673_1_1

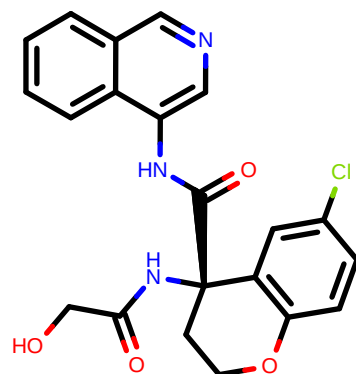
SMILES: Cn1c(cnn1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN564

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.25

EN300-19242_1_1



CID: EN300-19242_1_1

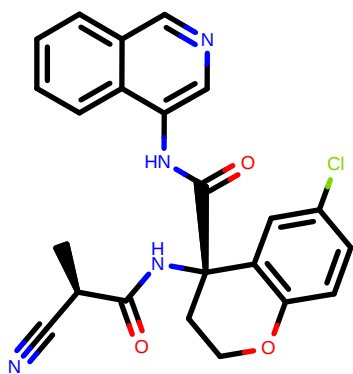
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO

RUN: RUN1780

DDG (kcal/mol): -0.71

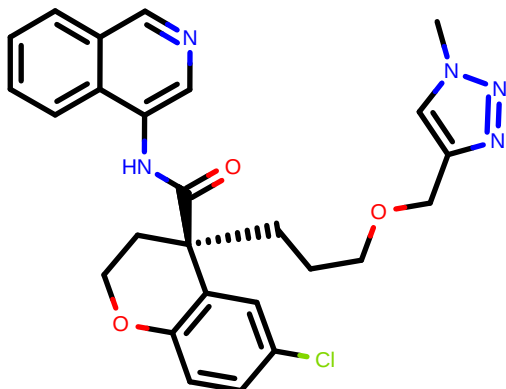
dDDG (kcal/mol): 0.26

EN300-72730_1_2



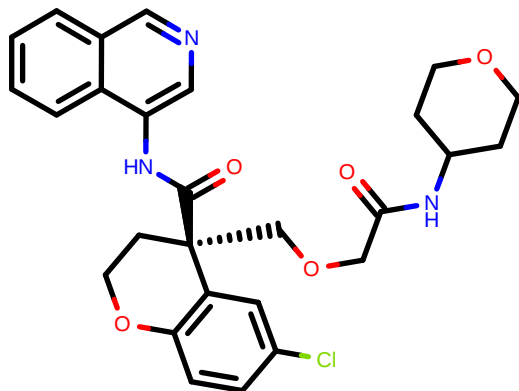
CID:	EN300-72730_1_2
SMILES:	<chem>C[C@H](C#N)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1261
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.22

EN300-120282_4_1



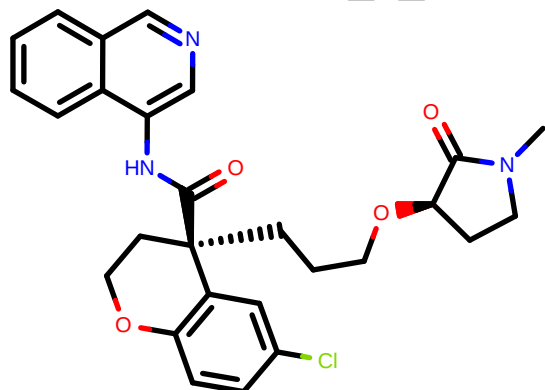
CID:	EN300-120282_4_1
SMILES:	<chem>Cn1cc(nn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN356
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.28

EN300-67573_2_1



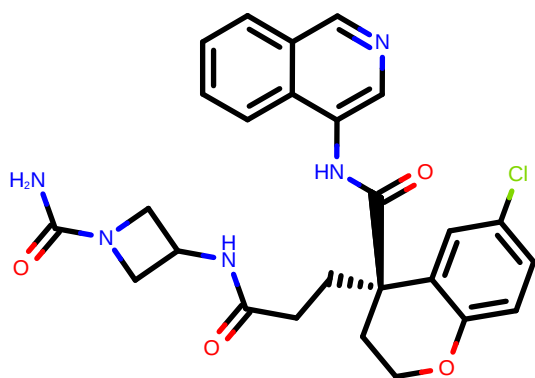
CID:	EN300-67573_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC5CCOCC5</chem>
RUN:	RUN626
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.28

EN300-98648_4_2



CID:	EN300-98648_4_2
SMILES:	<chem>CN1CC[C@H](C1=O)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1686
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.29

EN300-6472847_2_1



CID:

EN300-6472847_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)CCC(=O)NC5CN(C5)C(=O)N

RUN:

RUN663

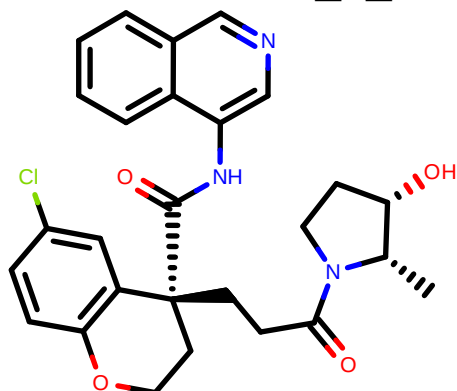
DDG (kcal/mol):

-0.69

dDDG (kcal/mol):

0.32

EN300-2008120_2_1



CID:

EN300-2008120_2_1

SMILES:

C[C@H]1[C@@H](CCN1C(=O)CC[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5O

RUN:

RUN1107

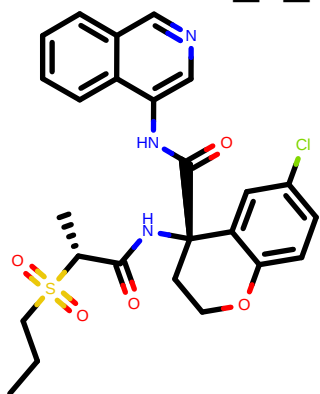
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.29

EN300-52768_1_2



CID:

EN300-52768_1_2

SMILES:

CCCS(=O)(=O)[C@@H](C)[C@H](C)C(=O)N[C@@]1(CCOc2cc1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1772

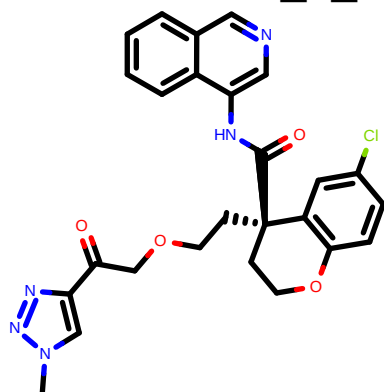
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.54

EN300-263153_3_1



CID:

EN300-263153_3_1

SMILES:

Cn1cc(nn1)C(=O)COC[C@@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN719

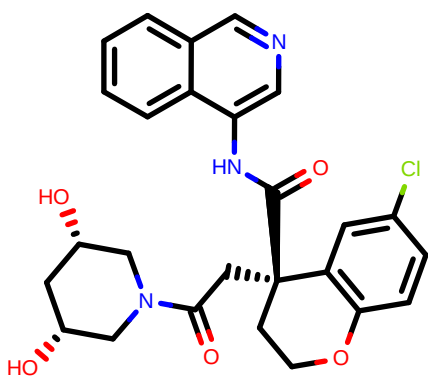
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.31

EN300-96886_1_1



CID:

EN300-96886_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@H](C(=O)N1CCCCC1N)C(=O)O1C2=CC=CC=C2O1

RUN:

RUN1410

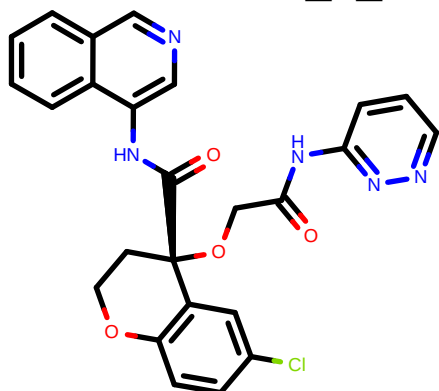
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.33

EN300-761618_1_1



CID:

EN300-761618_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@H](C(=O)N1CCCCC1N)C(=O)O1C2=CC=CC=C2O1

RUN:

RUN1607

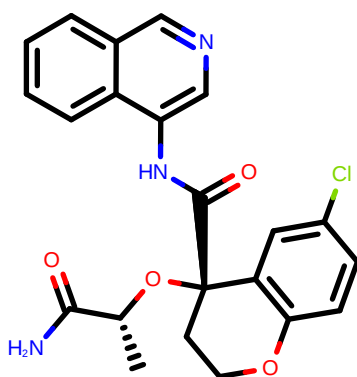
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.19

EN300-17381_1_2



CID:

EN300-17381_1_2

SMILES:

C[C@H](C(=O)N)O[C@H]1(C(=O)N1CCCCC1N)C(=O)O1C2=CC=CC=C2O1

RUN:

RUN817

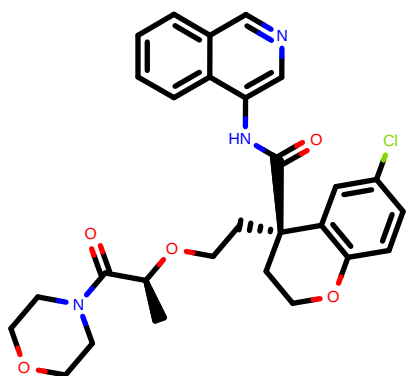
DDG (kcal/mol):

-0.67

dDDG (kcal/mol):

0.21

EN300-05754_3_1



CID:

EN300-05754_3_1

SMILES:

C[C@H](C(=O)N1CCCCC1N)O[C@H]1(C(=O)N1CCCCC1N)C(=O)O1C2=CC=CC=C2O1

RUN:

RUN956

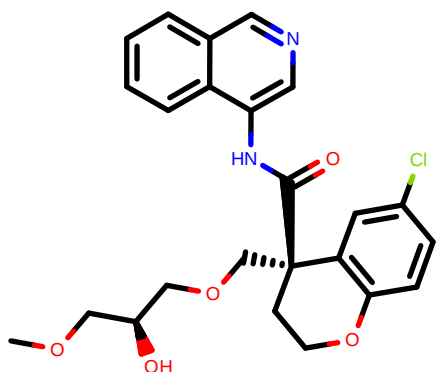
DDG (kcal/mol):

-0.66

dDDG (kcal/mol):

0.41

EN300-1915260_2_1



CID: EN300-1915260_2_1

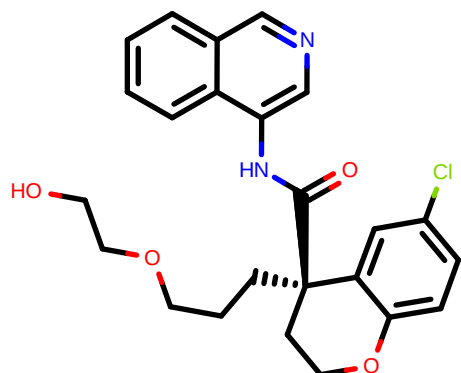
SMILES: COC[C@@H](COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)O

RUN: RUN934

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.40

EN300-21258_4_1



CID: EN300-21258_4_1

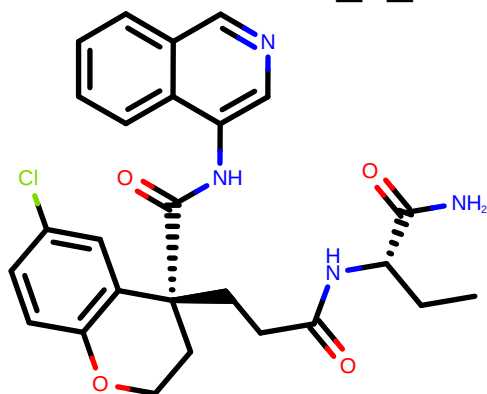
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN563

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.33

EN300-7375395_2_1



CID: EN300-7375395_2_1

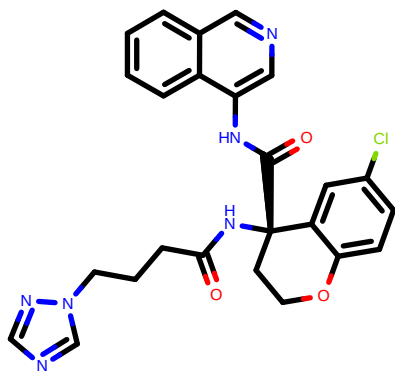
SMILES: CC[C@H](C(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1083

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.29

EN300-316216_1_1



CID: EN300-316216_1_1

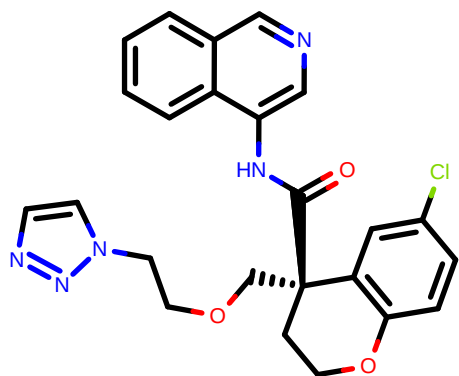
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5

RUN: RUN1748

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.38

EN300-1715993_2_1



CID: EN300-1715993_2_1

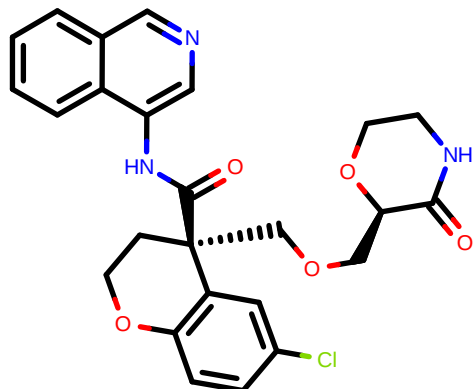
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cncn5

RUN: RUN1550

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.32

EN300-1706036_2_1



CID: EN300-1706036_2_1

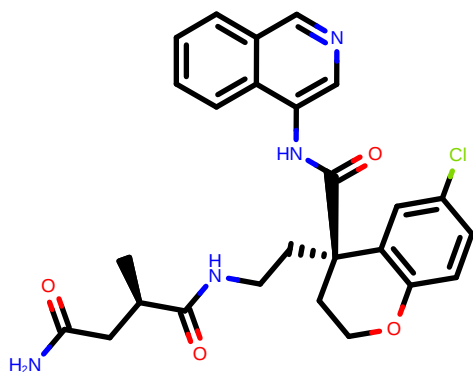
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C(=O)NCCO5

RUN: RUN1022

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.37

EN300-202757_3_2



CID: EN300-202757_3_2

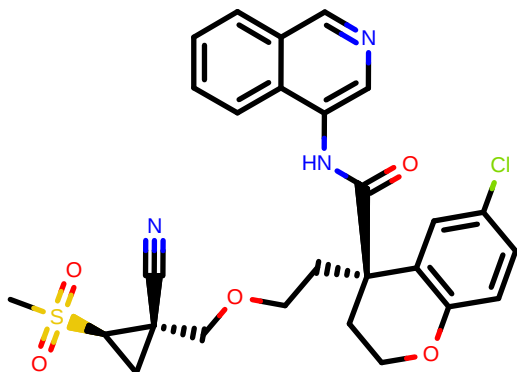
SMILES: C[C@H](CC(=O)N)C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN: RUN1761

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.49

EN300-633533_3_1



CID: EN300-633533_3_1

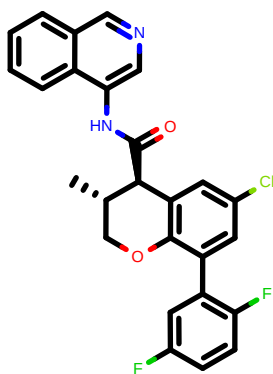
SMILES: CS(=O)(=O)[C@@H](C)[C@@H]1C[C@]1(COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5)C#N

RUN: RUN781

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.47

DAR-DIA-0d514e7d-15_1



CID:

DAR-DIA-0d514e7d-15_1

SMILES:

C[C@H]1COC2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3ccc4)Cl)c5cc(ccc5F)F

RUN:

RUN263

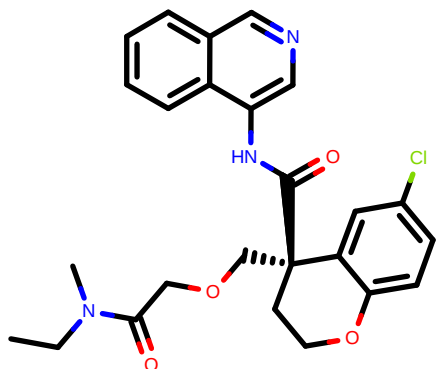
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.24

EN300-1253122_2_1



CID:

EN300-1253122_2_1

SMILES:

CCN(C)C(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4

RUN:

RUN1446

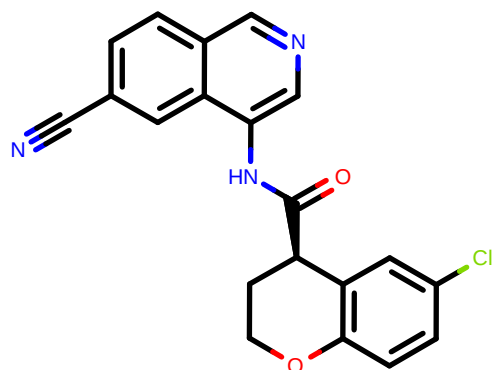
DDG (kcal/mol):

-0.63

dDDG (kcal/mol):

0.27

BEN-DND-c852c98b-1_1



CID:

BEN-DND-c852c98b-1_1

SMILES:

c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN:

RUN25

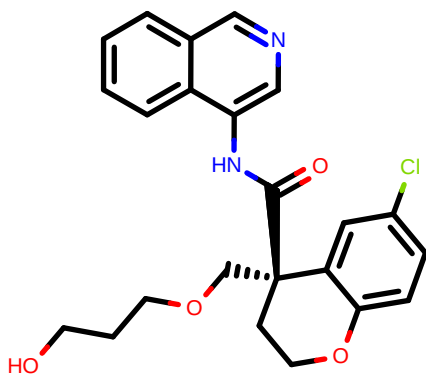
DDG (kcal/mol):

-0.61

dDDG (kcal/mol):

0.04

EN300-221518_2_1



CID:

EN300-221518_2_1

SMILES:

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

RUN:

RUN831

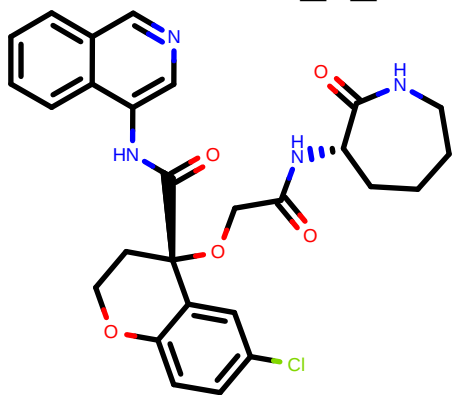
DDG (kcal/mol):

-0.61

dDDG (kcal/mol):

0.23

EN300-37195_1_2



CID: EN300-37195_1_2

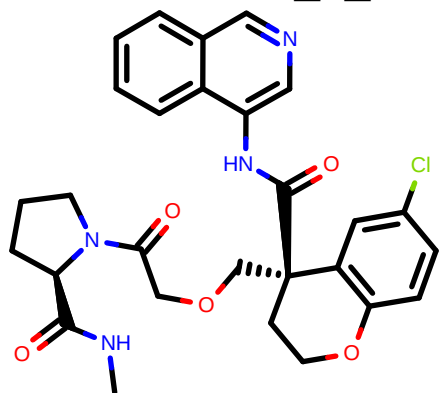
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN1232

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

EN300-48902_2_2



CID: EN300-48902_2_2

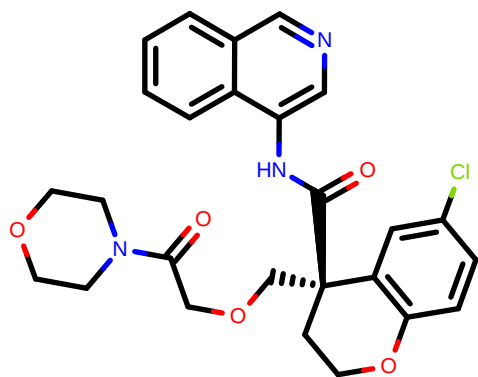
SMILES: CNC(=O)[C@@H]1CCCN1C(=O)COC[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncnc5c4cccc5

RUN: RUN729

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.43

EN300-1241327_2_1



CID: EN300-1241327_2_1

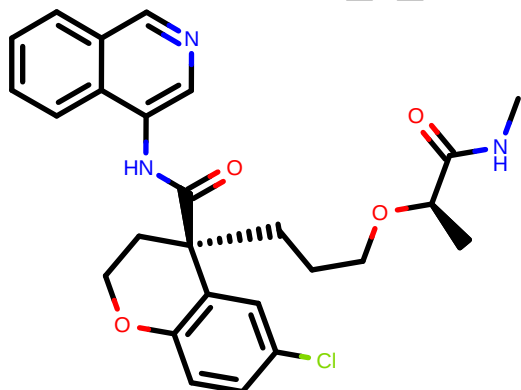
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COCC(=O)N5CCOCC5

RUN: RUN411

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.42

EN300-211482_4_2



CID: EN300-211482_4_2

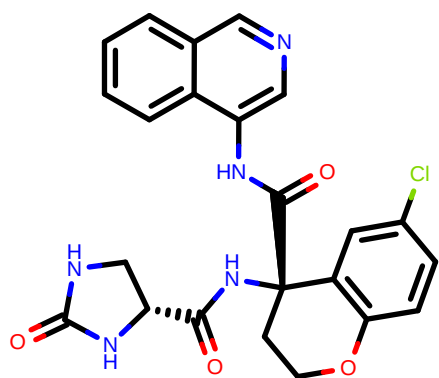
SMILES: C[C@@H](C(=O)NC)OCCC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN364

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.29

EN300-222145_1_1



CID: EN300-222145_1_1

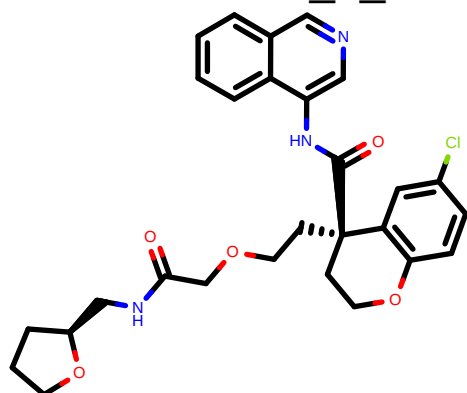
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)N5

RUN: RUN1557

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.22

EN300-01527_3_1



CID: EN300-01527_3_1

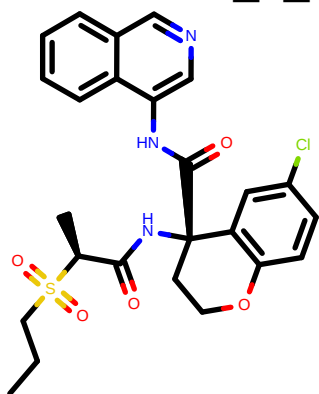
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@H]5CCCCO5

RUN: RUN1020

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.36

EN300-52768_1_1



CID: EN300-52768_1_1

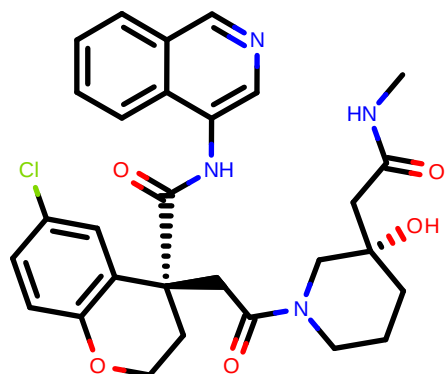
SMILES: CCCS(=O)(=O)[C@@]3(C)[C@H](C)C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN1612

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.46

EN300-259062_1_2



CID: EN300-259062_1_2

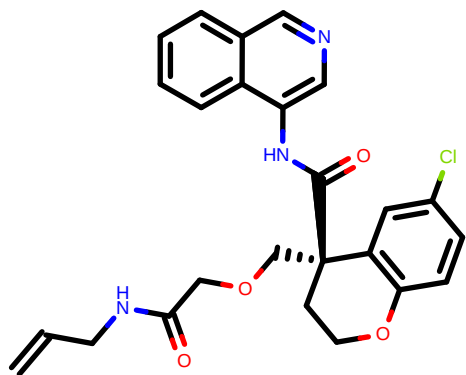
SMILES: CNC(=O)C[C@@]1(C)CCCNC1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5O

RUN: RUN1058

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.34

EN300-17184_2_1



CID: EN300-17184_2_1

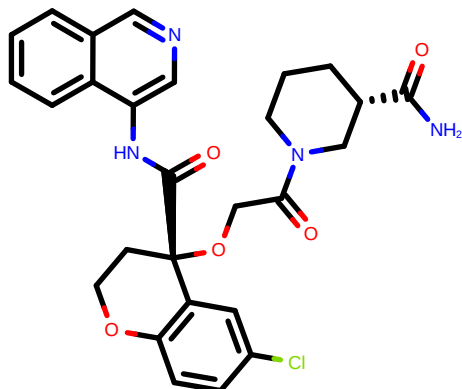
SMILES: C=CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN315

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.22

EN300-22880_1_1



CID: EN300-22880_1_1

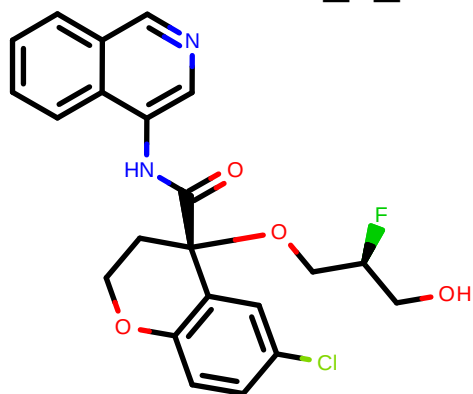
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@H](C5)C(=O)N

RUN: RUN1759

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.50

EN300-1600517_1_2



CID: EN300-1600517_1_2

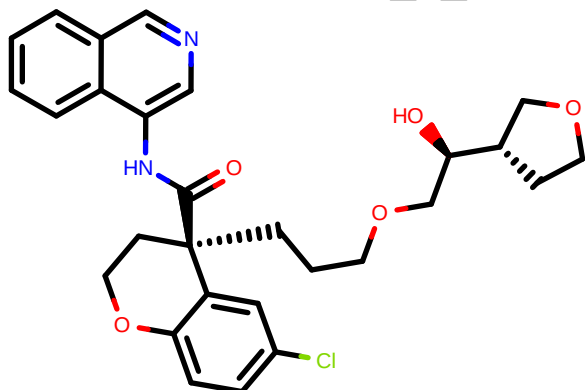
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CO)F

RUN: RUN1208

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.26

EN300-1911992_4_4



CID: EN300-1911992_4_4

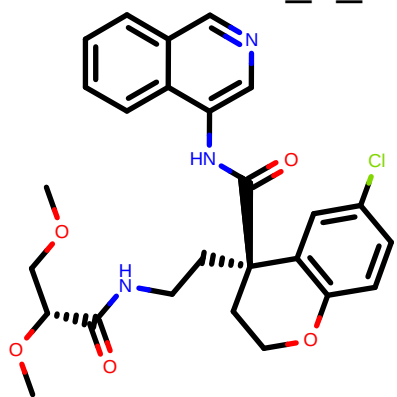
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H](C)[C@H]5CCOC5O

RUN: RUN903

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.39

EN300-305282_3_2



CID:

EN300-305282_3_2

SMILES:

COC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OC

RUN:

RUN1506

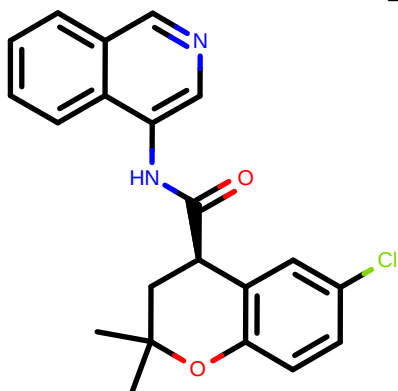
DDG (kcal/mol):

-0.53

dDDG (kcal/mol):

0.40

ADA-UCB-dc2b944c-16_1



CID:

ADA-UCB-dc2b944c-16_1

SMILES:

CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3cccc4)C

RUN:

RUN43

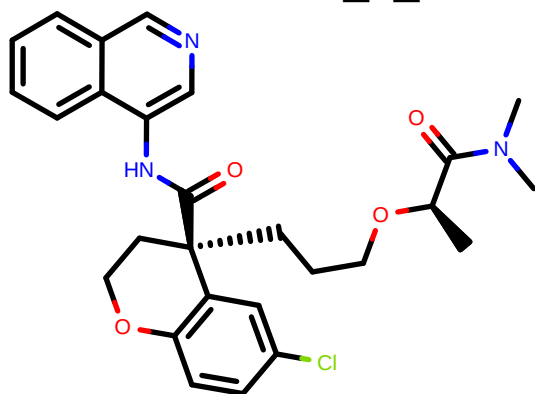
DDG (kcal/mol):

-0.53

dDDG (kcal/mol):

0.10

EN300-14458_4_2



CID:

EN300-14458_4_2

SMILES:

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

RUN:

RUN316

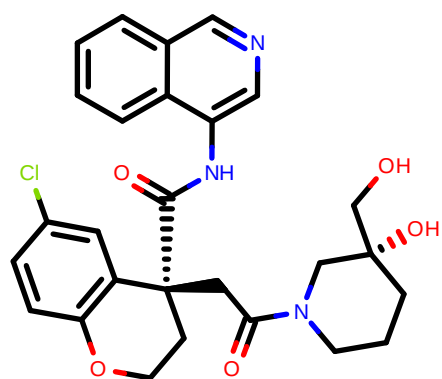
DDG (kcal/mol):

-0.52

dDDG (kcal/mol):

0.30

EN300-251396_1_1



CID:

EN300-251396_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@]6(C5)(CO)O

RUN:

RUN431

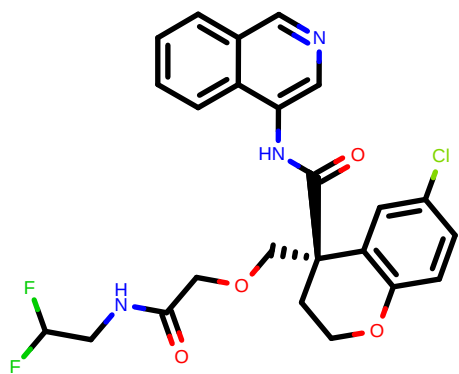
DDG (kcal/mol):

-0.52

dDDG (kcal/mol):

0.39

EN300-120586_2_1



CID: EN300-120586_2_1

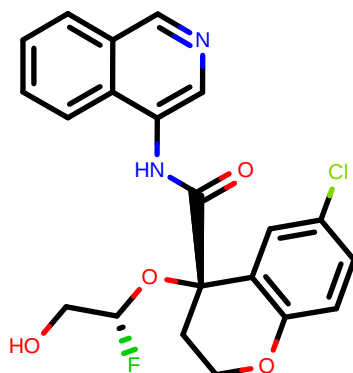
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NCC(F)F

RUN: RUN371

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.31

EN300-861925_1_1



CID: EN300-861925_1_1

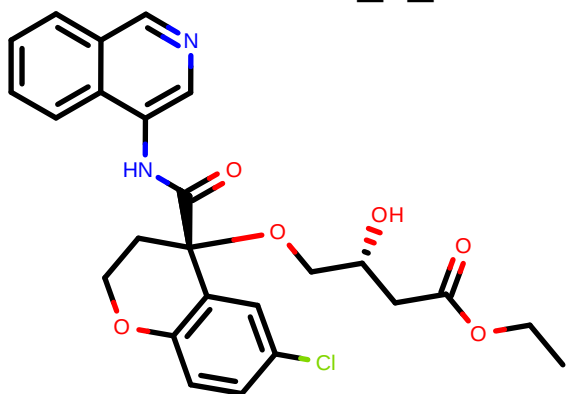
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H](CO)F

RUN: RUN1711

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.28

EN300-82539_1_2



CID: EN300-82539_1_2

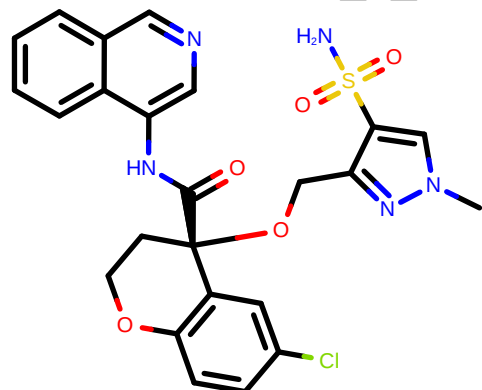
SMILES: CCOC(=O)C[C@@H](CO)[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4O

RUN: RUN960

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.27

EN300-7355737_1_1



CID: EN300-7355737_1_1

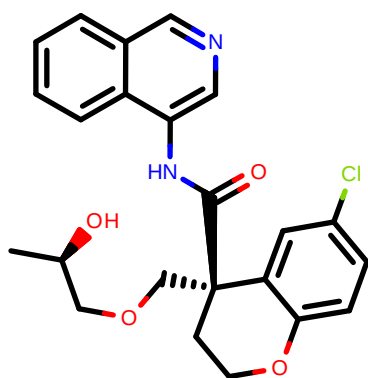
SMILES: Cn1cc(c(n1)CO)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5S(=O)(=O)N

RUN: RUN1400

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.29

EN300-185378_2_2



CID: EN300-185378_2_2

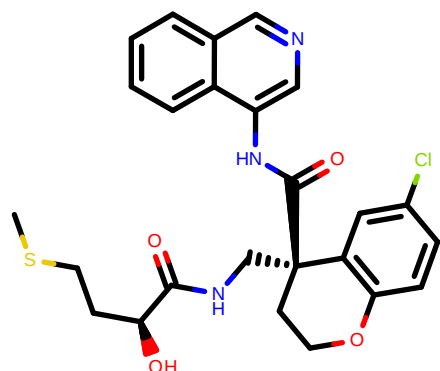
SMILES: C[C@H](COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN846

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-103144_2_1



CID: EN300-103144_2_1

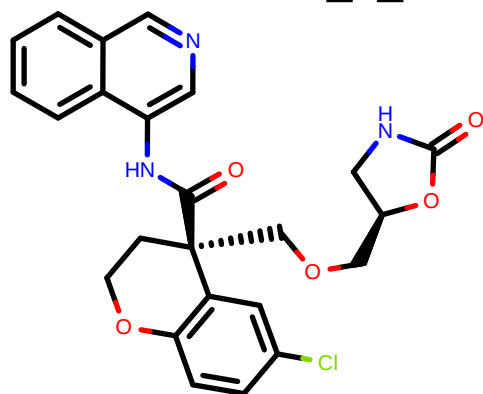
SMILES: CSCC[C@H](C(=O)NC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN770

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.35

EN300-203293_2_2



CID: EN300-203293_2_2

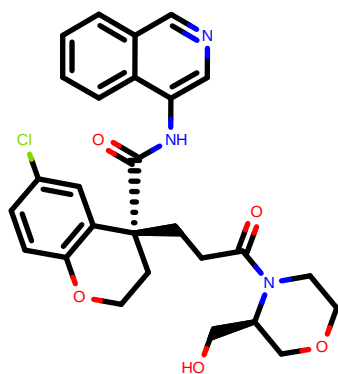
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CNC(=O)O5

RUN: RUN1637

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-154201_2_2



CID: EN300-154201_2_2

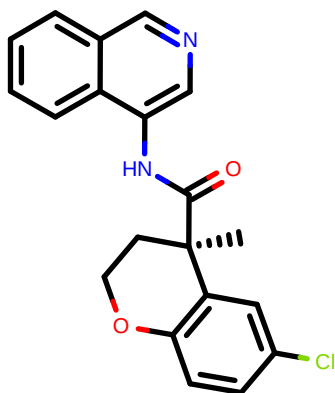
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@H]5CO

RUN: RUN1235

DDG (kcal/mol): -0.47

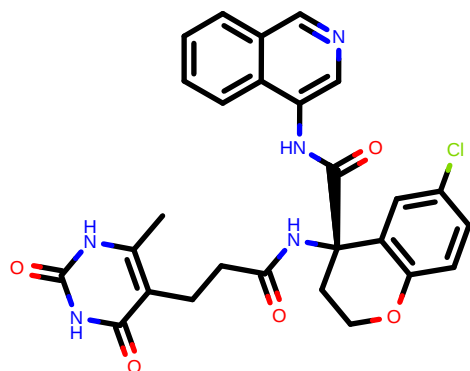
dDDG (kcal/mol): 0.28

EDJ-MED-e4b030d8-13_1



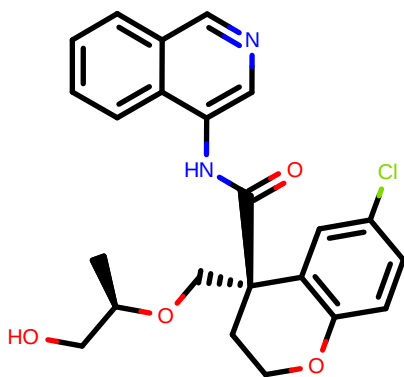
CID:	EDJ-MED-e4b030d8-13_1
SMILES:	<chem>C[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN8
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.11

EN300-25735_1_1



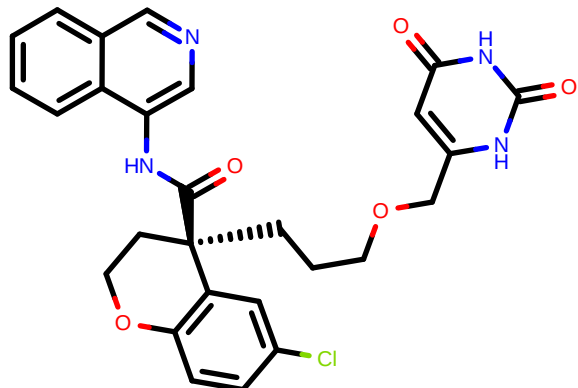
CID:	EN300-25735_1_1
SMILES:	<chem>Cc1c(c(=O)[nH]c(=O)[nH]1)CCC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN290
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.27

EN300-175186_2_2

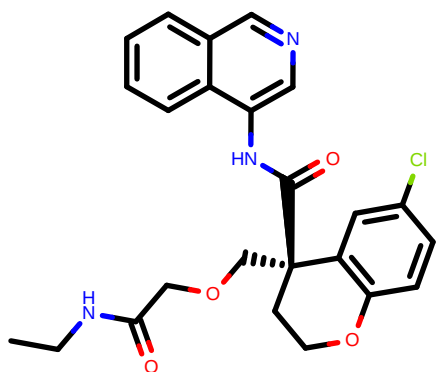


CID:	EN300-175186_2_2
SMILES:	<chem>C[C@H](CO)OC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN1390
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.27

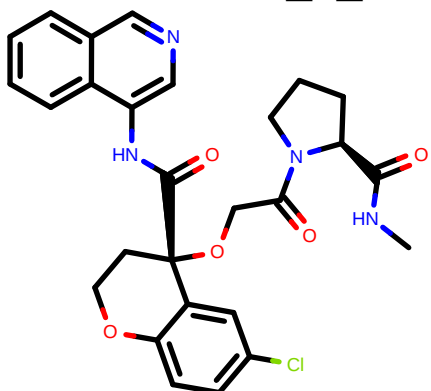
EN300-11300_4_1



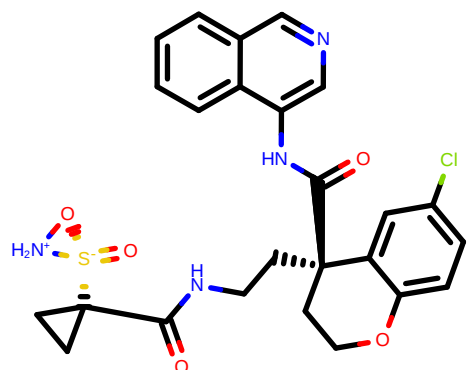
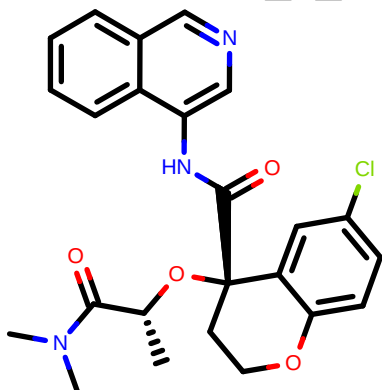
CID:	EN300-11300_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOCc5cc(=O)[nH]c(=O)[nH]5</chem>
RUN:	RUN1311
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.39



EN300-48902 1 1

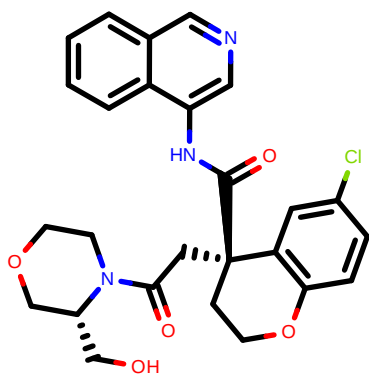


EN300-223741 3 1

EN300-14458 1 2

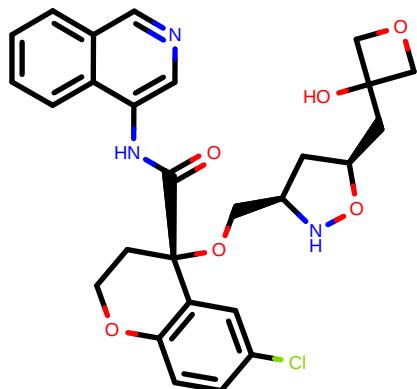
- 111 -

EN300-154201_1_2



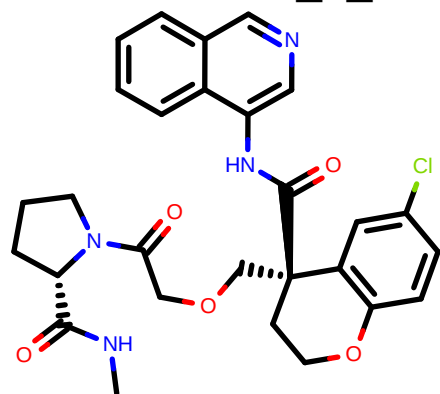
CID:	EN300-154201_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO</chem>
RUN:	RUN1194
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.32

EN300-7457160_1_1



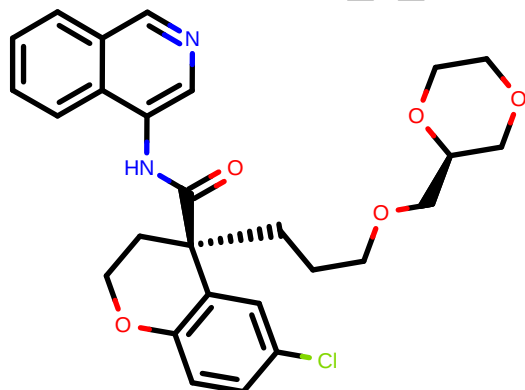
CID:	EN300-7457160_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)OCC5=NO[C@H](C5)CC5(COC6)O</chem>
RUN:	RUN1496
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.30

EN300-48902_2_1



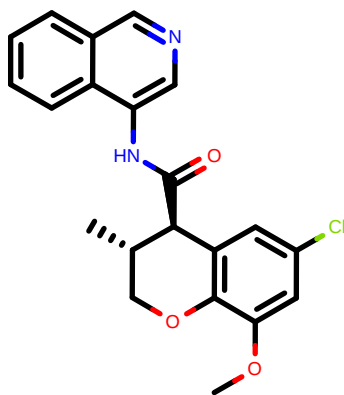
CID:	EN300-48902_2_1
SMILES:	<chem>CNC(=O)[C@@H]1CCCN1C(=O)COC[C@]2(C(COC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5</chem>
RUN:	RUN697
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.37

EN300-139167_4_1



CID:	EN300-139167_4_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCOC[C@H]5COC(CO5</chem>
RUN:	RUN508
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.45

DAR-DIA-0d514e7d-1_1



CID:

DAR-DIA-0d514e7d-1_1

SMILES:

C[C@H]1COc2c(cc2OC)C1[C@@H]1C(=O)Nc3ncc4c3ccc4

RUN:

RUN79

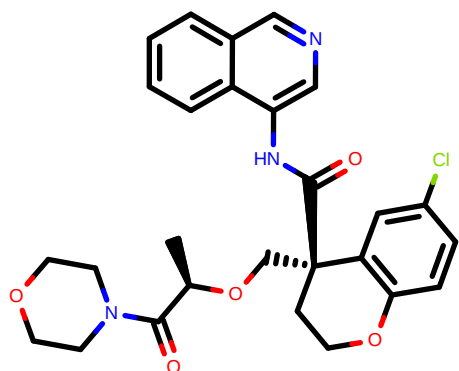
DDG (kcal/mol):

-0.43

dDDG (kcal/mol):

0.13

EN300-05754_2_2



CID:

EN300-05754_2_2

SMILES:

C[C@H](C(=O)N1CCOCC1)OC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN:

RUN1757

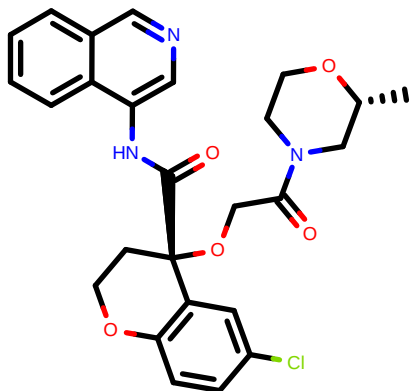
DDG (kcal/mol):

-0.42

dDDG (kcal/mol):

0.37

EN300-25572_1_1



CID:

EN300-25572_1_1

SMILES:

C[C@H]1CN(CCO1)C(=O)CO[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4ccc5

RUN:

RUN572

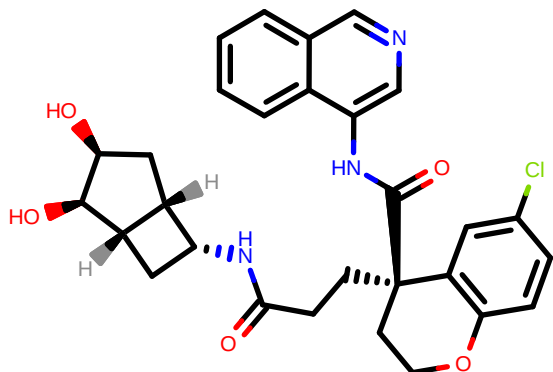
DDG (kcal/mol):

-0.41

dDDG (kcal/mol):

0.31

EN300-6736851_2_1



CID:

EN300-6736851_2_1

SMILES:

c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H]5C[C@H](C)[C@@H]6C[C@H](C)[C@@H]6O

RUN:

RUN1099

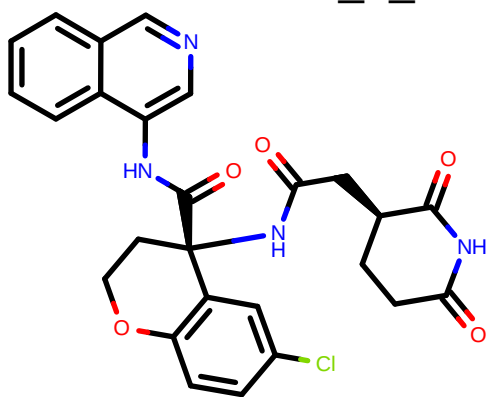
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.35

EN300-3451857_1_1



CID:

EN300-3451857_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)NC5=O

RUN:

RUN1085

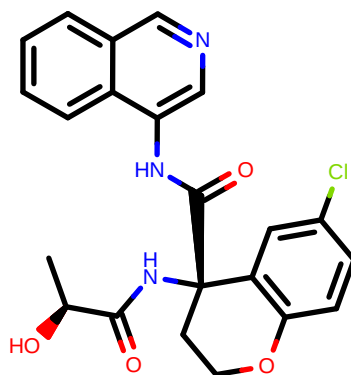
DDG (kcal/mol):

-0.39

dDDG (kcal/mol):

0.26

EN300-19542_1_1



CID:

EN300-19542_1_1

SMILES:

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

RUN:

RUN1213

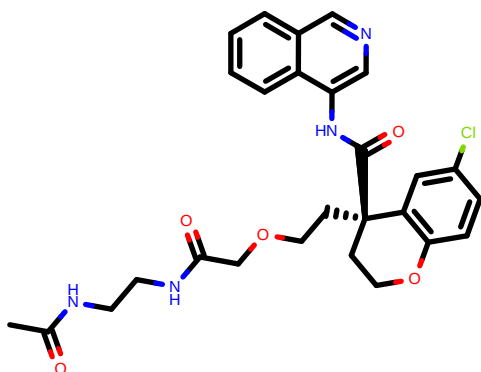
DDG (kcal/mol):

-0.38

dDDG (kcal/mol):

0.23

EN300-23129_3_1



CID:

EN300-23129_3_1

SMILES:

CC(=O)NCCNC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN:

RUN1316

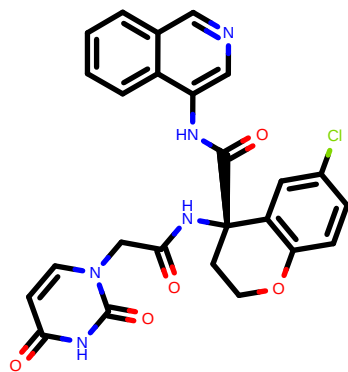
DDG (kcal/mol):

-0.38

dDDG (kcal/mol):

0.27

EN300-13287_1_1



CID:

EN300-13287_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccc(=O)[nH]c5=O

RUN:

RUN601

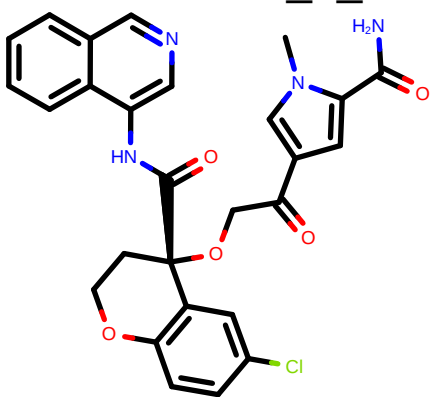
DDG (kcal/mol):

-0.38

dDDG (kcal/mol):

0.30

EN300-35592_1_1



CID:

EN300-35592_1_1

SMILES:

Cn1cc(cc1C(=O)N)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN:

RUN1016

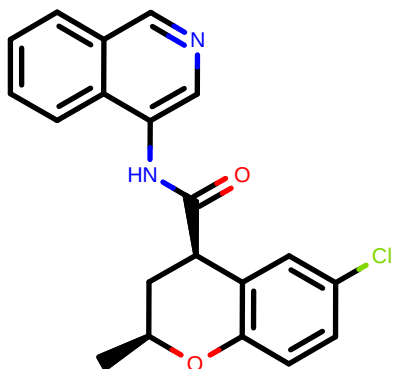
DDG (kcal/mol):

-0.37

dDDG (kcal/mol):

0.33

EDJ-MED-e4b030d8-3_1



CID:

EDJ-MED-e4b030d8-3_1

SMILES:

C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncoc4c3ccccc4

RUN:

RUN22

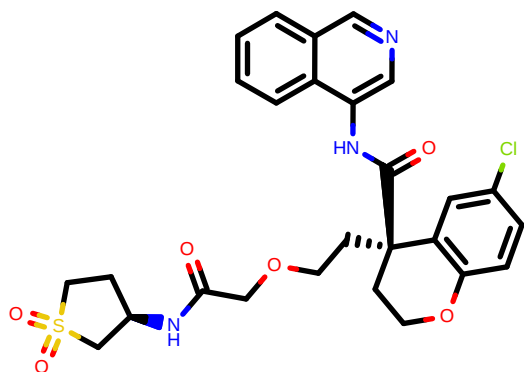
DDG (kcal/mol):

-0.37

dDDG (kcal/mol):

0.10

EN300-05512_3_1



CID:

EN300-05512_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@@H]5SCCS(=O)(=O)C5

RUN:

RUN1196

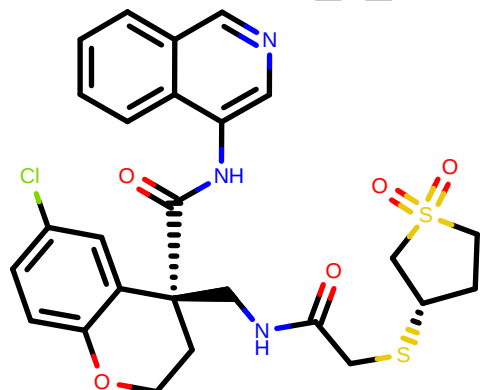
DDG (kcal/mol):

-0.36

dDDG (kcal/mol):

0.36

EN300-13890_2_2



CID:

EN300-13890_2_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS[C@@H]5SCCS(=O)(=O)C5

RUN:

RUN1313

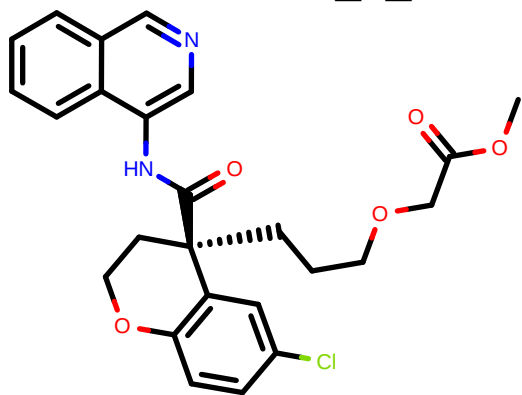
DDG (kcal/mol):

-0.36

dDDG (kcal/mol):

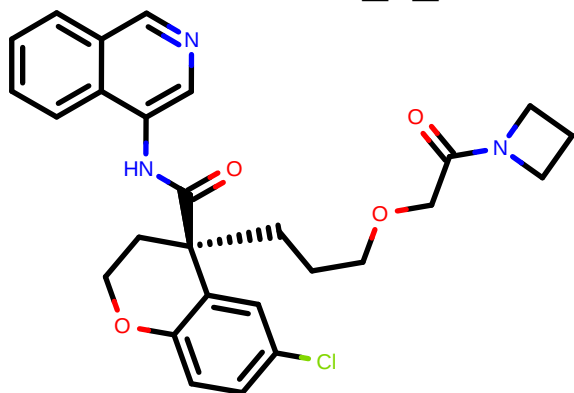
0.36

EN300-19700_4_1



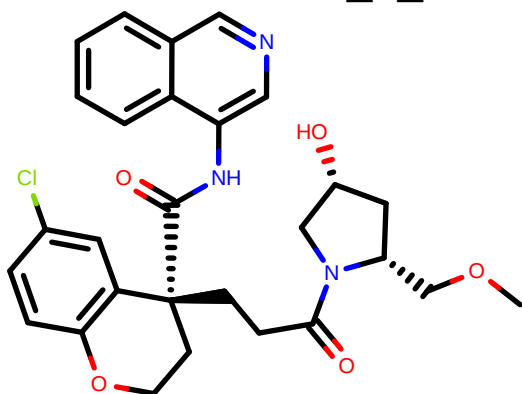
CID:	EN300-19700_4_1
SMILES:	<chem>COC(=O)COCC[C@]1(COC(=O)C1Cc2cc(Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN420
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.32

EN300-11195_4_1



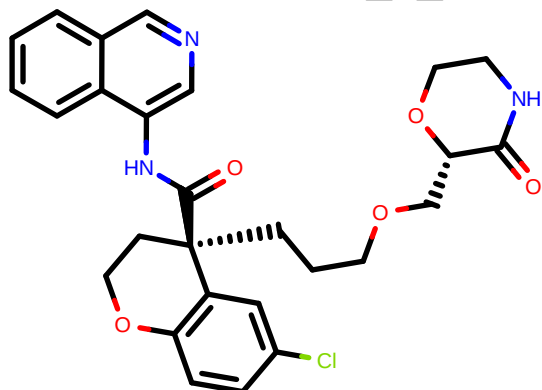
CID:	EN300-11195_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCCC5</chem>
RUN:	RUN1255
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.30

EN300-263601_2_1



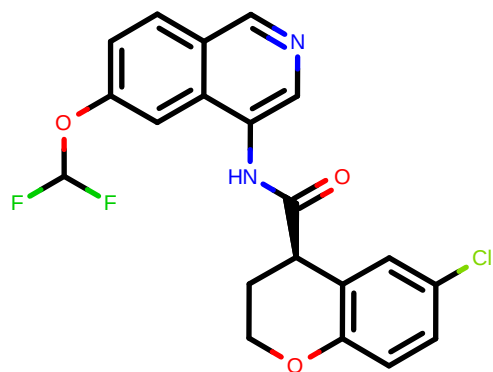
CID:	EN300-263601_2_1
SMILES:	<chem>COC[C@H]1C[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O</chem>
RUN:	RUN1698
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.36

EN300-1706036_4_2



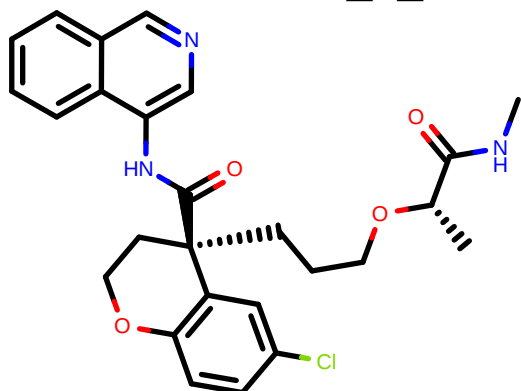
CID:	EN300-1706036_4_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C(=O)NCCO5</chem>
RUN:	RUN1407
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.33

BEN-DND-c852c98b-6_1



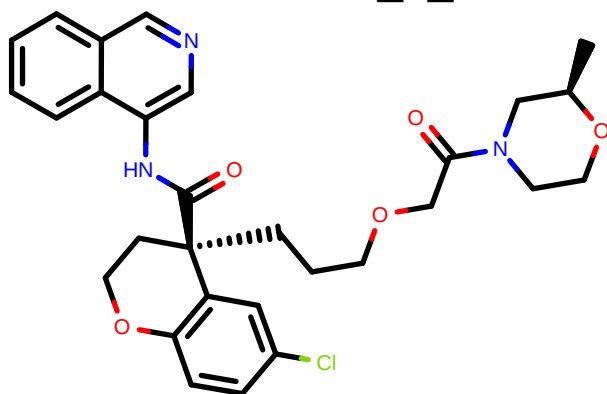
CID:	BEN-DND-c852c98b-6_1
SMILES:	<chem>c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN53
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.07

EN300-211482_4_1



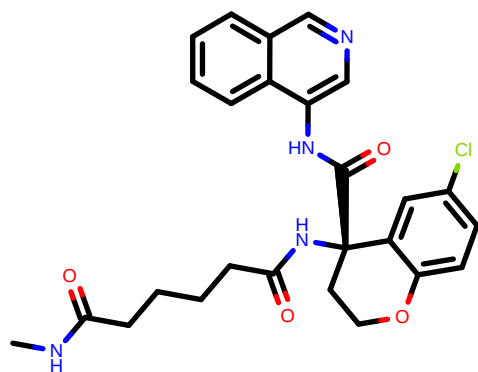
CID:	EN300-211482_4_1
SMILES:	<chem>C[C@@H](C(=O)NC)OCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1023
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.34

EN300-25572_4_1



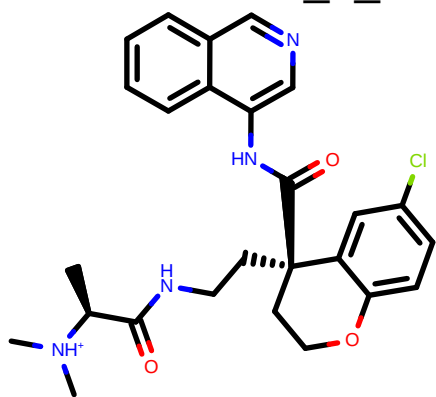
CID:	EN300-25572_4_1
SMILES:	<chem>C[C@@H]1CN(CCO1)C(=O)OCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN999
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.38

EN300-154693_1_1



CID:	EN300-154693_1_1
SMILES:	<chem>CNC(=O)CCCCC(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1021
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.33

EN300-306495_3_1



CID:

EN300-306495_3_1

SMILES:

C[C@@H](C(=O)N)C[C@]1(C)C(=O)C2=CC(=CC=C2)C1C(=O)Nc3ncnc4c3ccccc4)[NH+](C)C

RUN:

RUN287

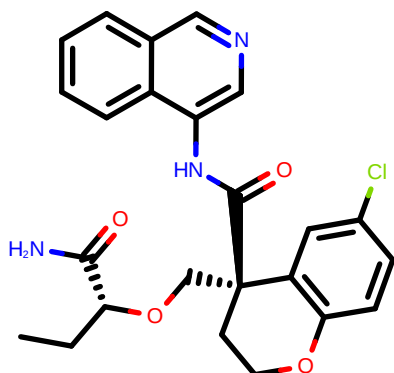
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

0.36

EN300-65839_2_2



CID:

EN300-65839_2_2

SMILES:

CC[C@H](C(=O)N)OC[C@]1(C)C(=O)C2=CC(=CC=C2)C1C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN926

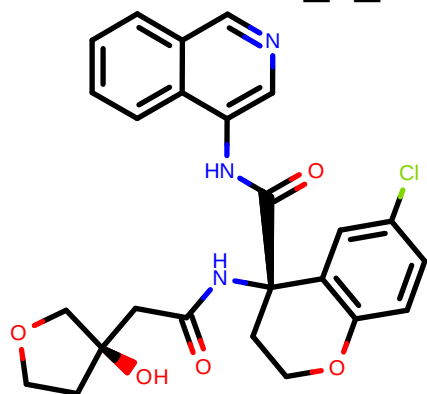
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

0.31

EN300-360157_1_1



CID:

EN300-360157_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(=O)C4=CC(=CC=C4)C1C(=O)Nc5cncnc5C(=O)C[C@]6(C)C(=O)C5O

RUN:

RUN766

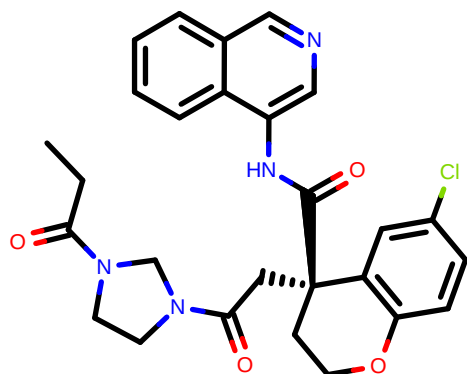
DDG (kcal/mol):

-0.32

dDDG (kcal/mol):

0.34

EN300-257790_1_1



CID:

EN300-257790_1_1

SMILES:

CCC(=O)N1CCN(C1)C(=O)C[C@]2(C)C(=O)C3=CC(=CC=C3)C1C(=O)Nc4cncnc4C(=O)C5C(=O)C5

RUN:

RUN1625

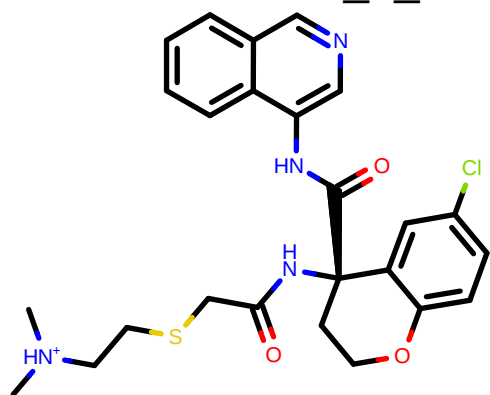
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.27

EN300-1708620_1_1



CID:

EN300-1708620_1_1

SMILES:

C[NH+](C)CCSCC(=O)N[C@]1(C)CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1101

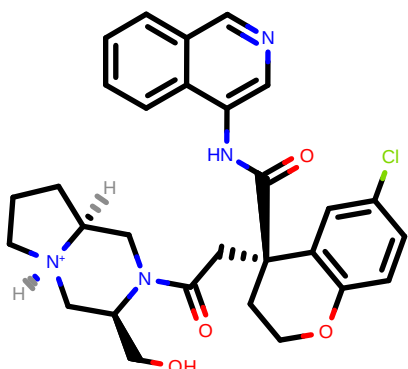
DDG (kcal/mol):

-0.31

dDDG (kcal/mol):

0.34

EN300-365281_1_1



CID:

EN300-365281_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@H](C)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CC[C@H](C)N6[C@H]5C

RUN:

RUN311

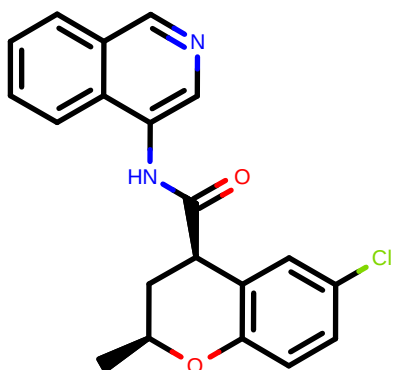
DDG (kcal/mol):

-0.30

dDDG (kcal/mol):

0.34

ALP-POS-d3acb8cc-1_1



CID:

ALP-POS-d3acb8cc-1_1

SMILES:

C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN23

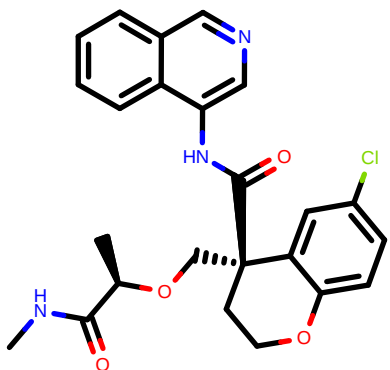
DDG (kcal/mol):

-0.30

dDDG (kcal/mol):

0.10

EN300-211482_2_2



CID:

EN300-211482_2_2

SMILES:

C[C@H](C(=O)NC)OC[C@]1(C)CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1534

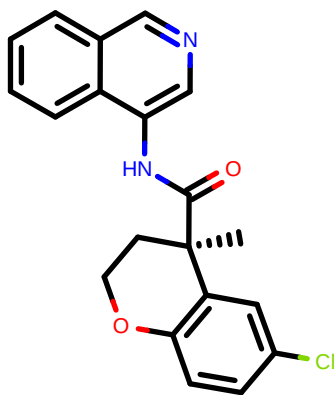
DDG (kcal/mol):

-0.29

dDDG (kcal/mol):

0.33

DAR-DIA-6a508060-10_2



CID:

DAR-DIA-6a508060-10_2

SMILES:

C[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN9

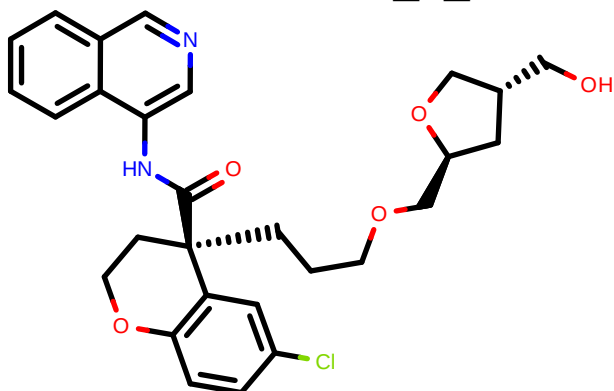
DDG (kcal/mol):

-0.29

dDDG (kcal/mol):

0.12

EN300-6494158_4_3



CID:

EN300-6494158_4_3

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5C[C@H](CO)CO5

RUN:

RUN792

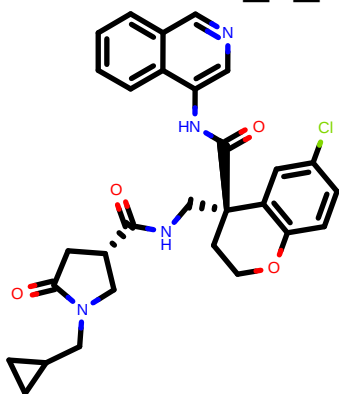
DDG (kcal/mol):

-0.29

dDDG (kcal/mol):

0.40

EN300-31969_2_2



CID:

EN300-31969_2_2

SMILES:

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

RUN:

RUN708

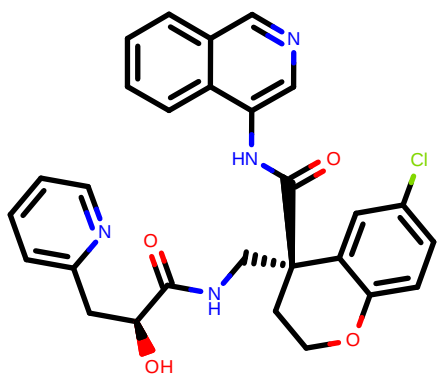
DDG (kcal/mol):

-0.29

dDDG (kcal/mol):

0.31

EN300-6762327_2_2



CID:

EN300-6762327_2_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5c5ccccc5)O5

RUN:

RUN1137

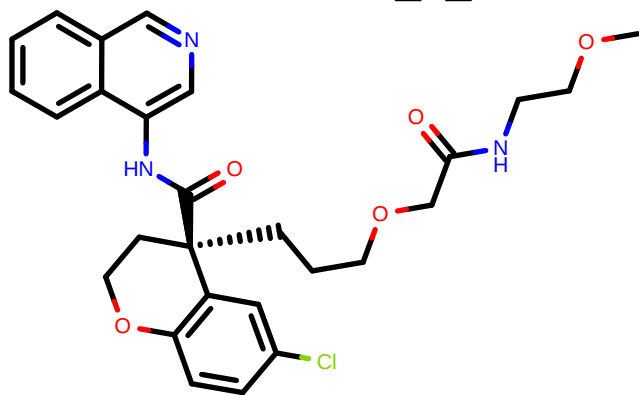
DDG (kcal/mol):

-0.29

dDDG (kcal/mol):

0.33

EN300-02015_4_1



CID: EN300-02015_4_1

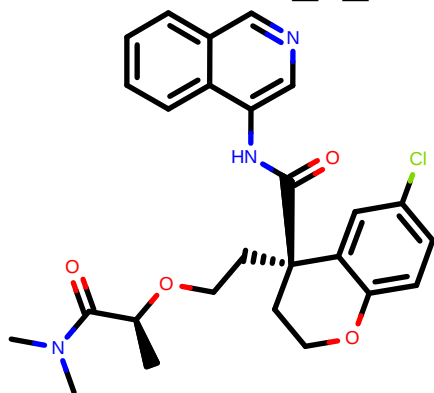
SMILES: COCCNC(=O)COC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN1646

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.39

EN300-14458_3_1



CID: EN300-14458_3_1

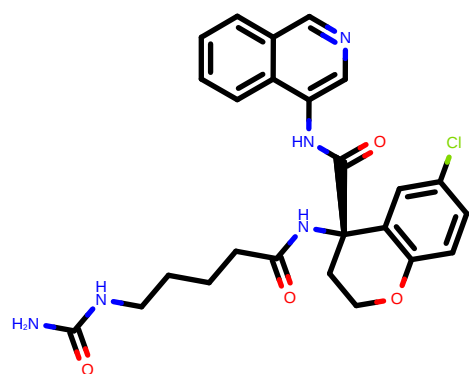
SMILES: C[C@@H](C(=O)N(C)C)OC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN1524

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.32

EN300-13499_1_1



CID: EN300-13499_1_1

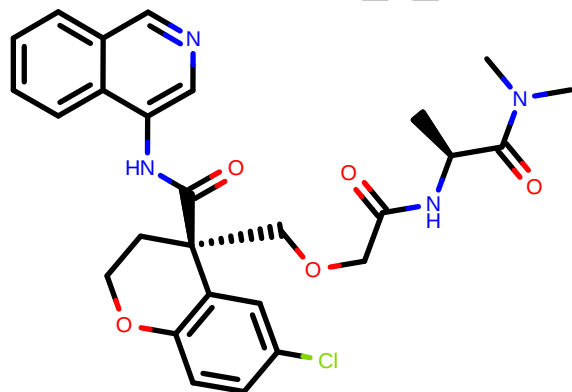
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(COC4c3cc(cc4)Cl)NC(=O)CCCCNC(=O)N

RUN: RUN720

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.30

EN300-47657_2_1



CID: EN300-47657_2_1

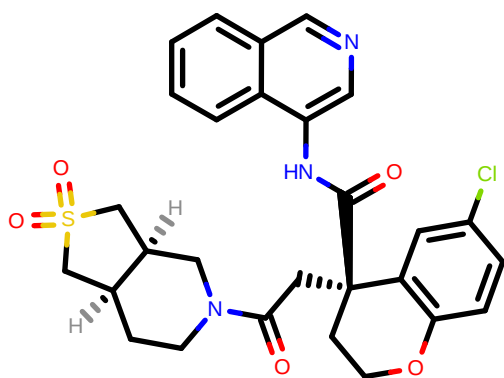
SMILES: C[C@@H](C(=O)N(C)C)NC(=O)COC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN530

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.29

EN300-365993_1_4



CID: EN300-365993_1_4

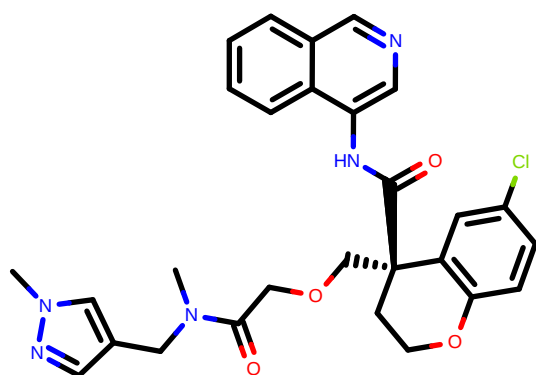
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C(COC(=O)C(=O)C)CC(=O)N8CC[C@H]6C5(=O)[C@H](C)[C@H]6C5

RUN: RUN842

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.40

EN300-65978_2_1



CID: EN300-65978_2_1

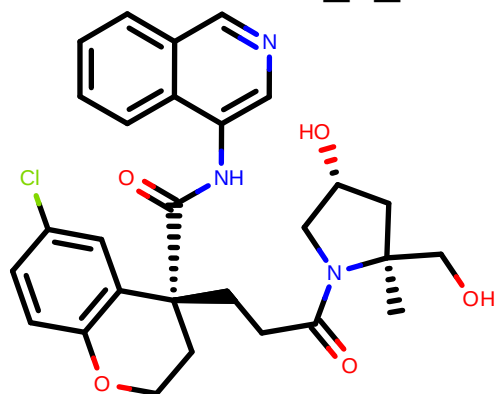
SMILES: Cn1cc(cn1)CN(C)C(=O)COC[C@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5

RUN: RUN1310

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.37

EN300-307336_2_4



CID: EN300-307336_2_4

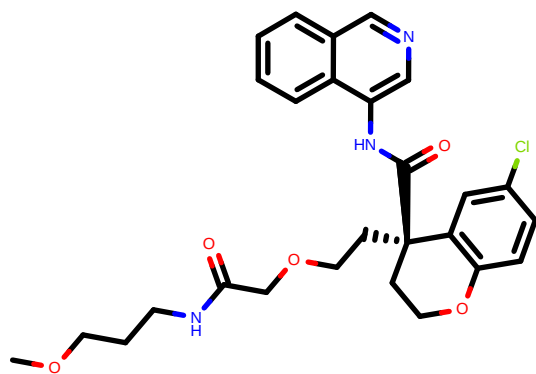
SMILES: C[C@H]1[C][C@H](CN1C(=O)CC[C@H]2(CCOc3c2cc(cc3)C)C(=O)Nc4nccc5c4cccc5O)CO

RUN: RUN304

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.31

EN300-04492_3_1



CID: EN300-04492_3_1

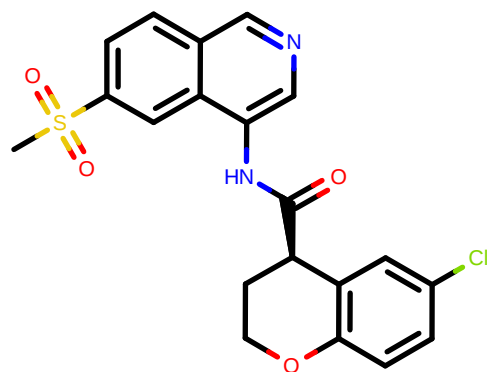
SMILES: COCCCN(C(=O)COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN1651

DDG (kcal/mol): -0.23

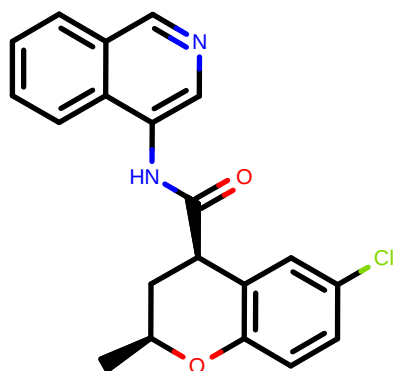
dDDG (kcal/mol): 0.32

BEN-DND-c852c98b-5_1



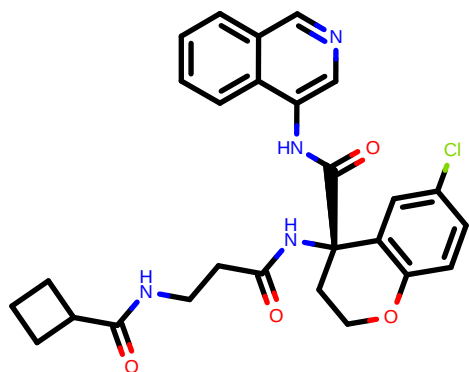
CID:	BEN-DND-c852c98b-5_1
SMILES:	<chem>CS(=O)(=O)c1ccc2ncnc(c2c1)NC(=O)[C@@H]3CCOCc4cc(cc4)Cl</chem>
RUN:	RUN54
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.08

MAT-POS-8a69d52e-1_4



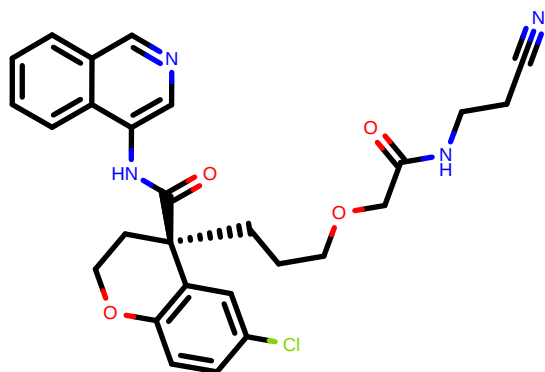
CID:	MAT-POS-8a69d52e-1_4
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN21
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.09

EN300-62449_1_1



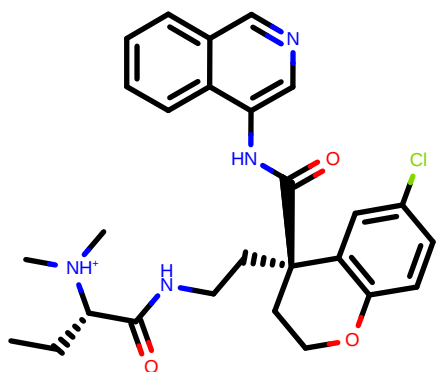
CID:	EN300-62449_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5CCCC5</chem>
RUN:	RUN314
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.29

EN300-10895_4_1



CID:	EN300-10895_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCCCC#N</chem>
RUN:	RUN1766
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.47

EN300-223964_3_1



CID:

EN300-223964_3_1

SMILES:

CC[C@H](C)(=O)NCC[C@]1(C)C(=O)C2C1CC(C2)C(=O)Nc3ncnc4c3ccoc4)NH+](C)C

RUN:

RUN590

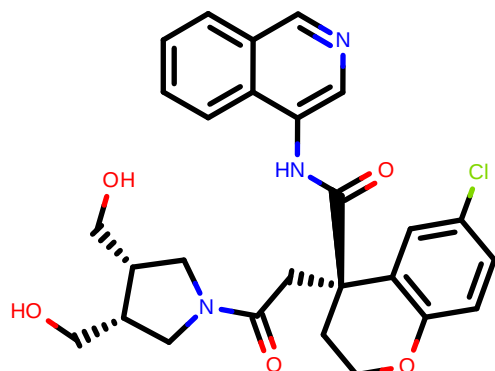
DDG (kcal/mol):

-0.21

dDDG (kcal/mol):

0.46

EN300-333677_1_1



CID:

EN300-333677_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@]3(C)C(=O)C4C3CC(C4)C(=O)N5C[C@@H](C)[C@@H](C)C5CO

RUN:

RUN550

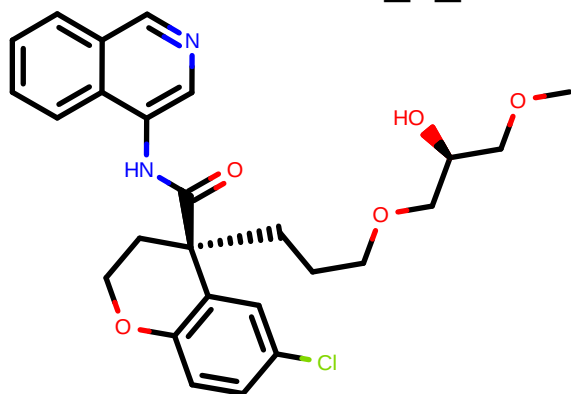
DDG (kcal/mol):

-0.20

dDDG (kcal/mol):

0.30

EN300-1915260_4_1



CID:

EN300-1915260_4_1

SMILES:

COC[C@H](C)(COCC[C@]1(C)C(=O)C2C1CC(C2)C(=O)Nc3ncnc4c3ccoc4)O

RUN:

RUN714

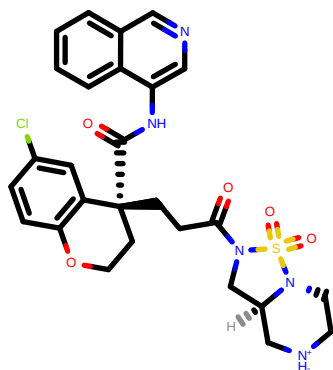
DDG (kcal/mol):

-0.20

dDDG (kcal/mol):

0.41

EN300-717233_2_1



CID:

EN300-717233_2_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@]3(C)C(=O)C4C3CC(C4)C(=O)N5C[C@@H](C)[C@@H](C)C5CO

RUN:

RUN1754

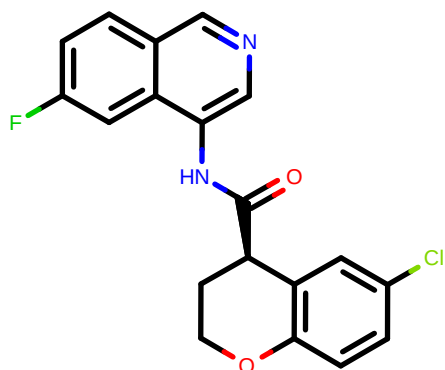
DDG (kcal/mol):

-0.20

dDDG (kcal/mol):

0.47

ALP-POS-696356e4-1_1



CID:

ALP-POS-696356e4-1_1

SMILES:

c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN:

RUN20

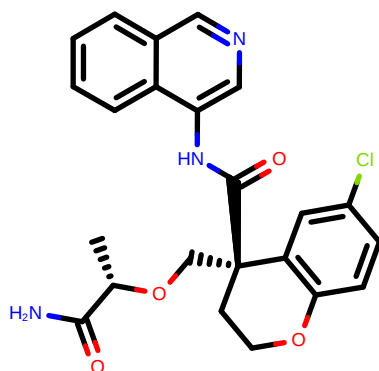
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.04

EN300-17381_2_1



CID:

EN300-17381_2_1

SMILES:

C[C@@H](C(=O)N)OC[C@]1(C)COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN878

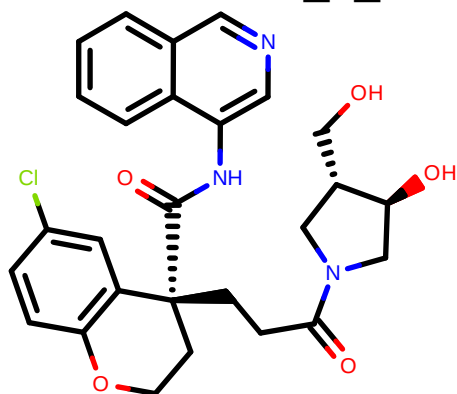
DDG (kcal/mol):

-0.19

dDDG (kcal/mol):

0.27

EN300-248521_2_3



CID:

EN300-248521_2_3

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(C)COC4c3cc(cc4)C)CCC(=O)N[C@@H]5C[C@H](C5)O)CO

RUN:

RUN296

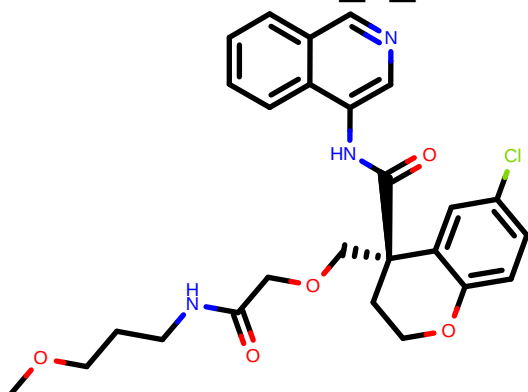
DDG (kcal/mol):

-0.18

dDDG (kcal/mol):

0.26

EN300-04492_2_1



CID:

EN300-04492_2_1

SMILES:

COCCCN(C(=O)COC[C@]1(C)COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1398

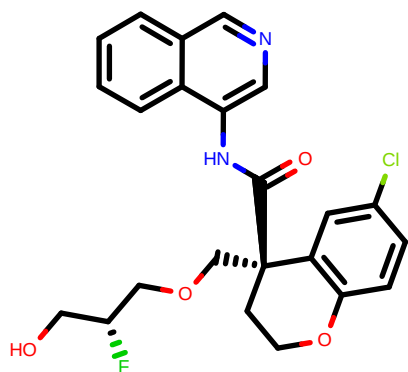
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.32

EN300-1600517_2_1



CID:

EN300-1600517_2_1

SMILES:

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

RUN:

RUN1262

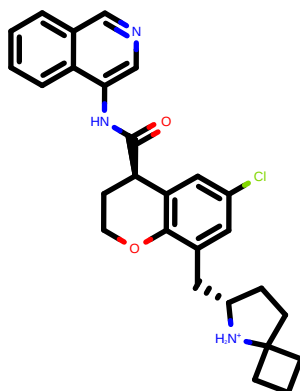
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.29

DAR-DIA-23e5a6a0-6_1



CID:

DAR-DIA-23e5a6a0-6_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C[C@H]5CCCC6([NH2+][5])CCC6)Cl

RUN:

RUN132

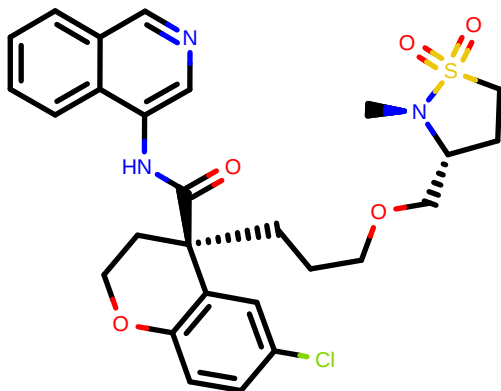
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

0.30

EN300-393148_4_2



CID:

EN300-393148_4_2

SMILES:

C[N+]([C@H]1C[C@H](CCS1(=O)=O)COCC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN:

RUN745

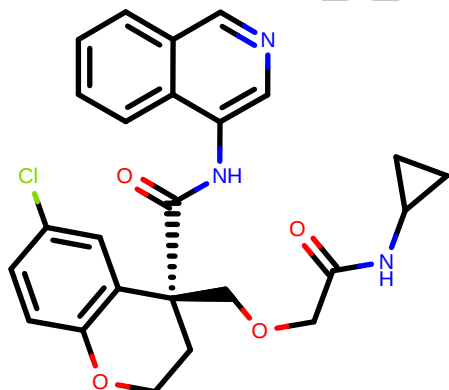
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

0.31

EN300-1253178_2_1



CID:

EN300-1253178_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CCC5

RUN:

RUN1094

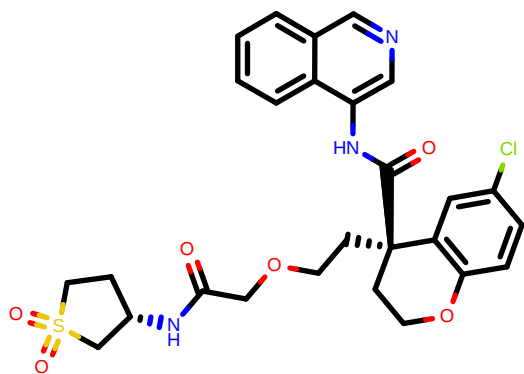
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

0.23

EN300-05512_3_2



CID: EN300-05512_3_2

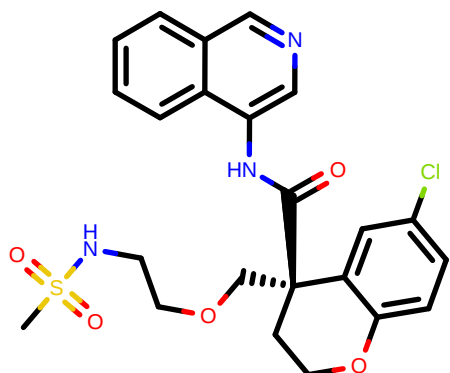
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@H]5CCS(=O)(=O)C5

RUN: RUN1276

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.33

EN300-1238839_2_1



CID: EN300-1238839_2_1

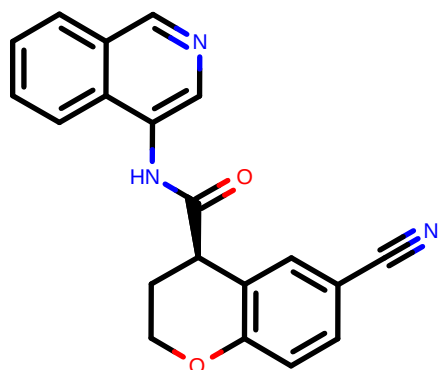
SMILES: CS(=O)(=O)NCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN283

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.39

DAR-DIA-6a508060-3_1



CID: DAR-DIA-6a508060-3_1

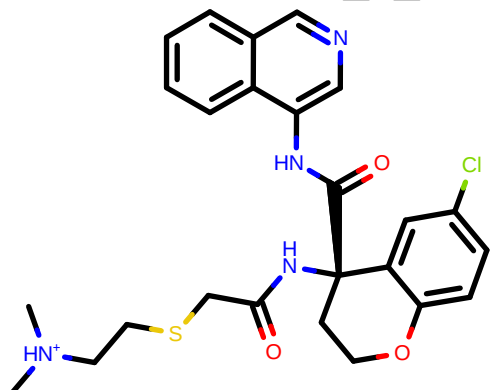
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCCOc4c3cc(cc4)C#N

RUN: RUN26

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.05

EN300-1708620_1_1



CID: EN300-1708620_1_1

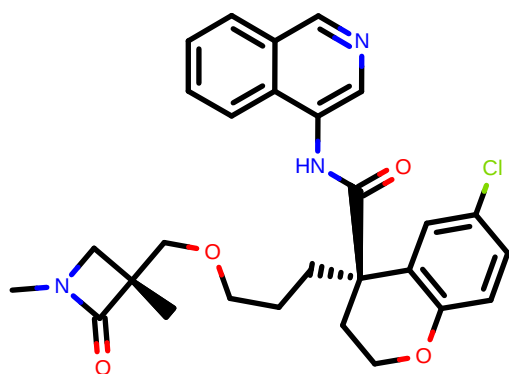
SMILES: C[NH+](C)CCSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1109

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.39

EN300-1273362_4_1



CID: EN300-1273362_4_1

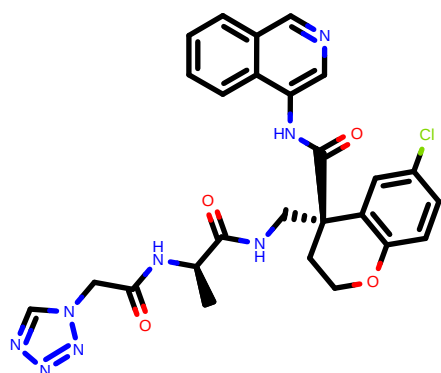
SMILES: C[C@@]1(CN(C1=O)C)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN1471

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.46

EN300-649743_2_1



CID: EN300-649743_2_1

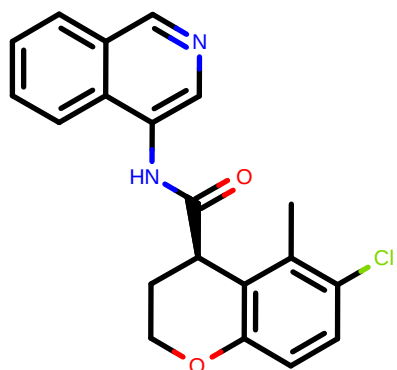
SMILES: C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3ccccc4)NC(=O)Cn5cnm5

RUN: RUN1161

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.41

EDJ-MED-e4b030d8-8_1



CID: EDJ-MED-e4b030d8-8_1

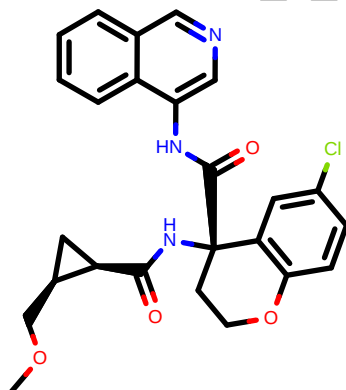
SMILES: Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3ccccc4)Cl

RUN: RUN44

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.07

EN300-705381_1_1



CID: EN300-705381_1_1

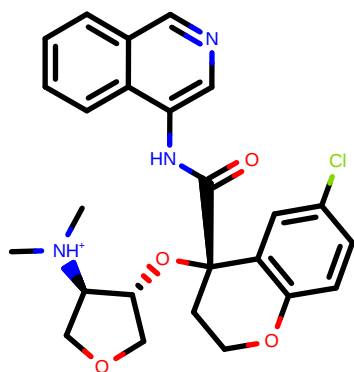
SMILES: COC[C@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN1692

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.26

EN300-2723070_1_3



CID: EN300-2723070_1_3

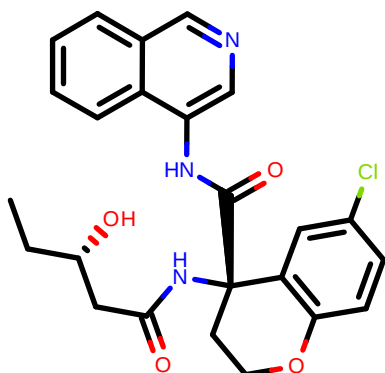
SMILES: C[NH+](C)[C@@H]1COC[C@H]1O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1336

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.32

EN300-224741_1_1



CID: EN300-224741_1_1

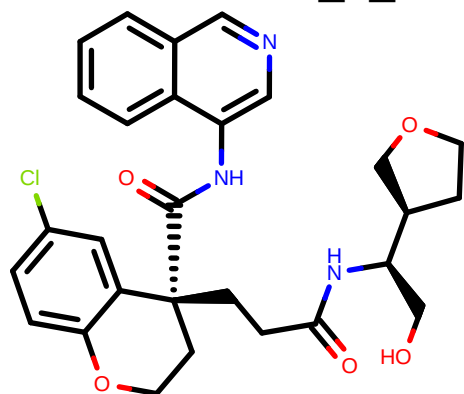
SMILES: CC[C@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN1125

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.24

EN300-104493_2_2



CID: EN300-104493_2_2

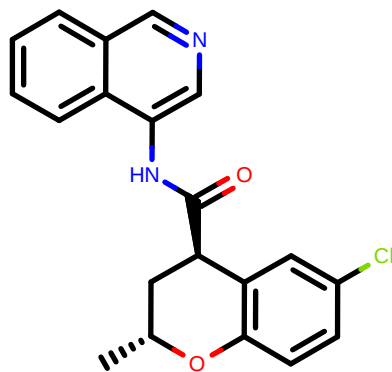
SMILES: c1ccc2c(c1)ncc2N[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)[C@@H]5COC(=O)C5

RUN: RUN1339

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.35

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

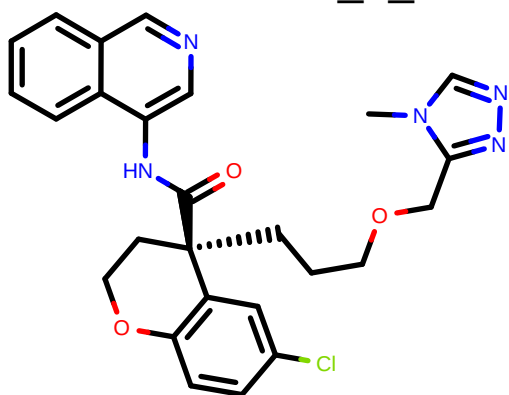
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN38

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.05

EN300-113112_4_1



CID: EN300-113112_4_1

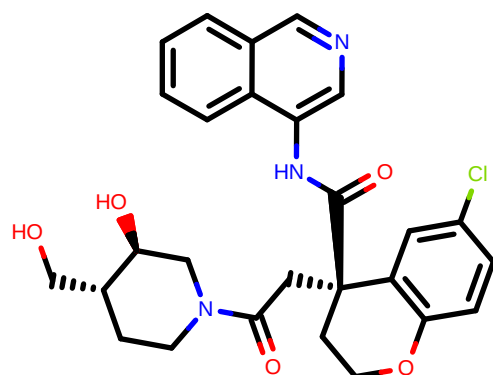
SMILES: Cn1ennc1COCCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN824

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.37

EN300-95639_1_3



CID: EN300-95639_1_3

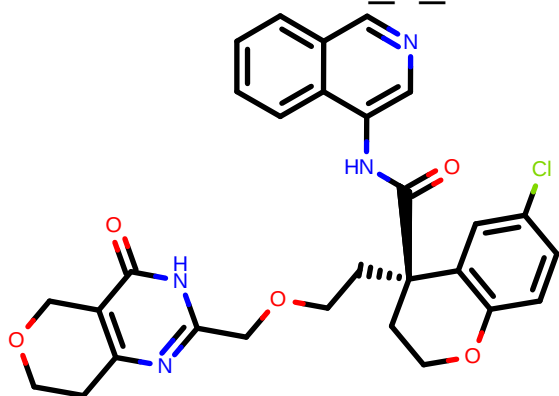
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]3[C@H](C5)OCCO

RUN: RUN447

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.40

EN300-343103_3_1



CID: EN300-343103_3_1

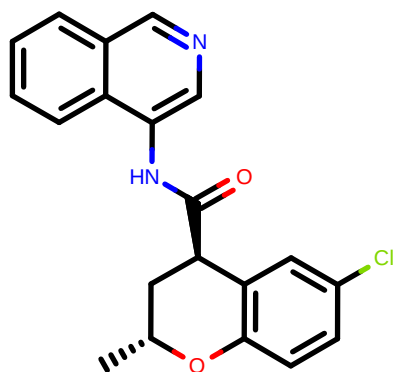
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)c6c(n5)CCOC6

RUN: RUN1779

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.56

MAT-POS-8a69d52e-1_3



CID: MAT-POS-8a69d52e-1_3

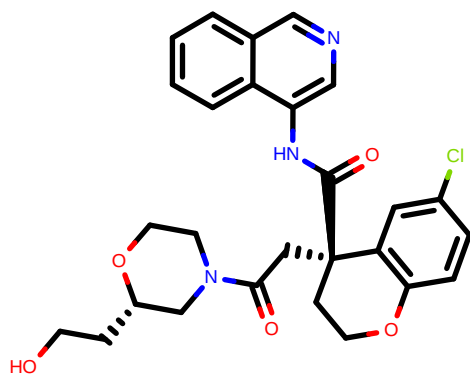
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN37

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.04

EN300-102007_1_2



CID:

EN300-102007_1_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CCO

RUN:

RUN693

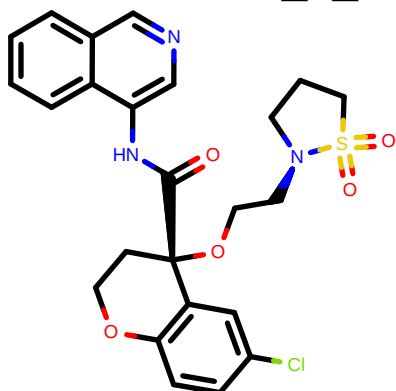
DDG (kcal/mol):

-0.10

dDDG (kcal/mol):

0.44

EN300-114134_1_1



CID:

EN300-114134_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@]5CCCCS(=O)=O

RUN:

RUN856

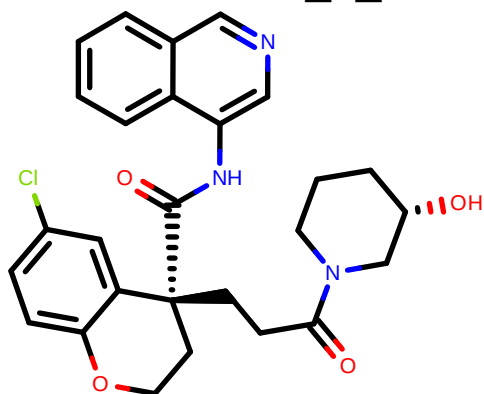
DDG (kcal/mol):

-0.09

dDDG (kcal/mol):

0.27

EN300-20284_2_1



CID:

EN300-20284_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCC[C@H](C5)O

RUN:

RUN796

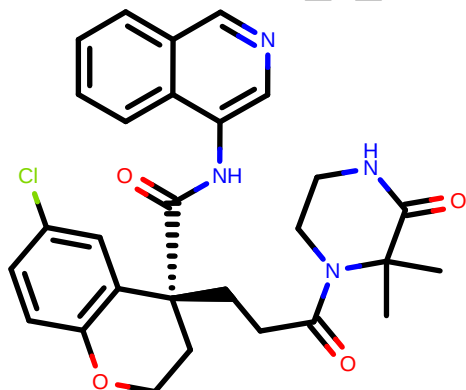
DDG (kcal/mol):

-0.09

dDDG (kcal/mol):

0.27

EN300-68882_2_1



CID:

EN300-68882_2_1

SMILES:

CC1(C(=O)NCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5)C

RUN:

RUN804

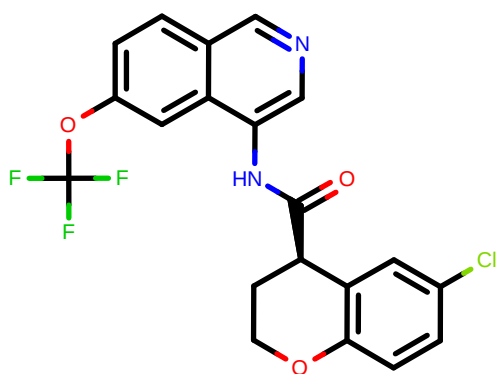
DDG (kcal/mol):

-0.09

dDDG (kcal/mol):

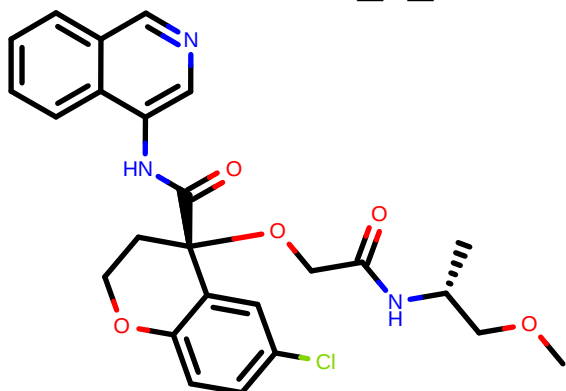
0.35

BEN-DND-c852c98b-2_1



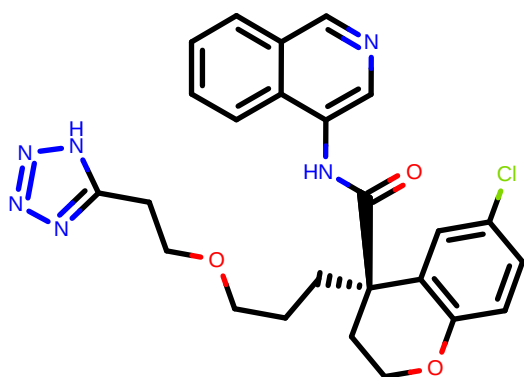
CID:	BEN-DND-c852c98b-2_1
SMILES:	<chem>c1cc2cncc(c2cc1OC(F)(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN61
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.07

EN300-02067_1_2



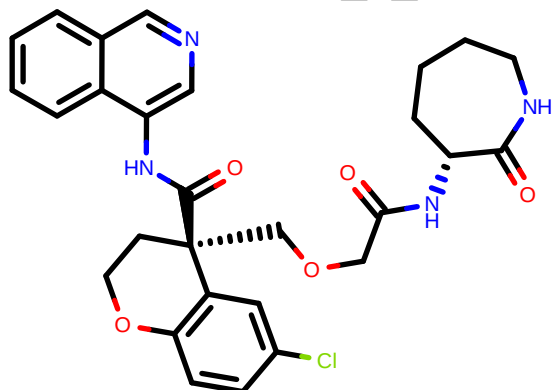
CID:	EN300-02067_1_2
SMILES:	<chem>C[C@H](COC)NC(=O)CO[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1192
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.24

EN300-183231_4_1

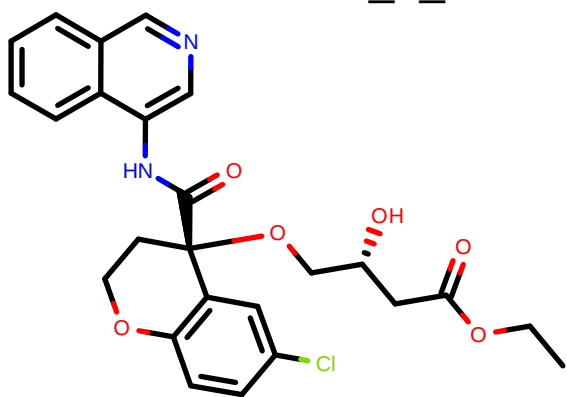


CID:	EN300-183231_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOCCc5n[nH]n5</chem>
RUN:	RUN1782
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.57

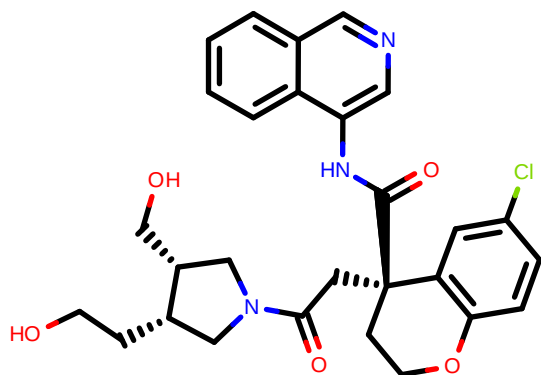
EN300-37195_2_1



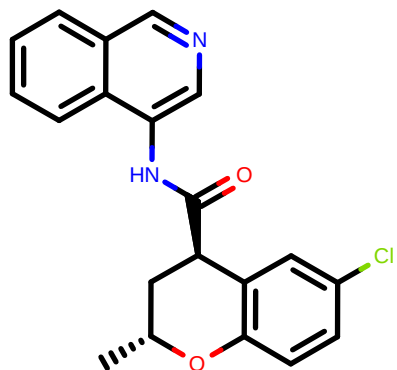
CID:	EN300-37195_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COCC(=O)N[C@@H]5CCCCNC5=O</chem>
RUN:	RUN443
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.30



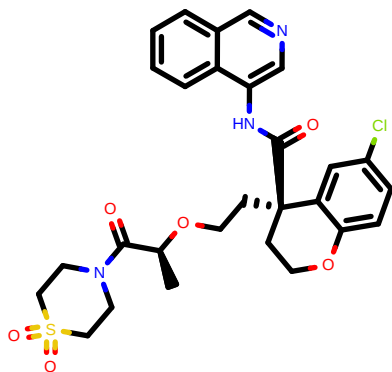
EN300-1425608_1_1



EDJ-MED-e4b030d8-2_1

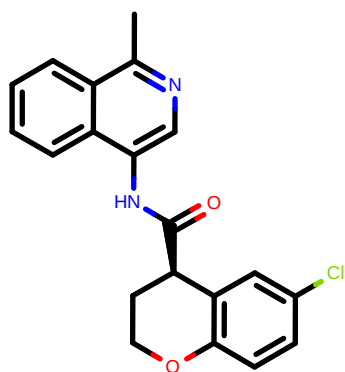


EN300-1265949_3_1



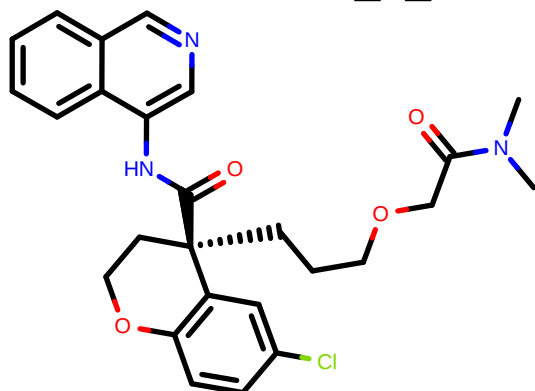
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ADA-UCB-dc2b944c-12_1



CID:	ADA-UCB-dc2b944c-12_1
SMILES:	<chem>Cc1c2ccccc2c(c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN64
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.08

EN300-216063_4_1



CID:	EN300-216063_4_1
SMILES:	<chem>CN(C)C(=O)COCC[C@]1(C)C(Cc2cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN635
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.32