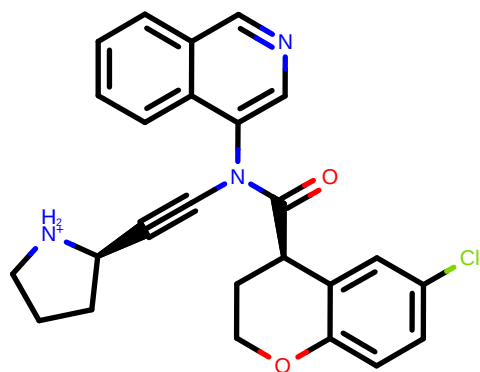
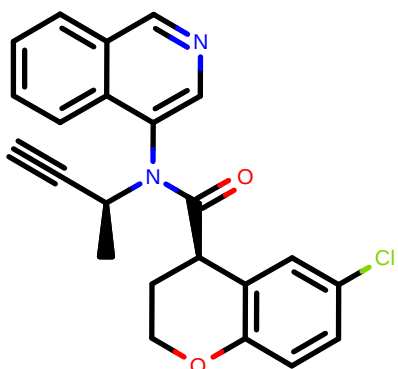


DAR-DIA-5ff57136-12_2



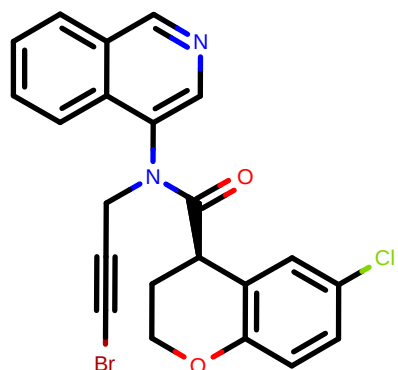
CID:	DAR-DIA-5ff57136-12_2
SMILES:	<chem>c1ccc2c(c1)cnc2N(C#C[C@H]3CCCC[NH2+])3C(=O)[C@@H]4CCOCc5ccc(cc5)Cl</chem>
RUN:	RUN95
DDG (kcal/mol):	-4.70
dDDG (kcal/mol):	0.21

DAR-DIA-5ff57136-16_1



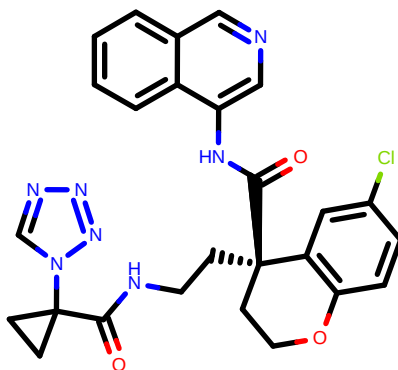
CID:	DAR-DIA-5ff57136-16_1
SMILES:	<chem>C[C@@H](C#C)N(c1cnc2c1cccc2)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl</chem>
RUN:	RUN165
DDG (kcal/mol):	-4.31
dDDG (kcal/mol):	0.15

DAR-DIA-5ff57136-17_1



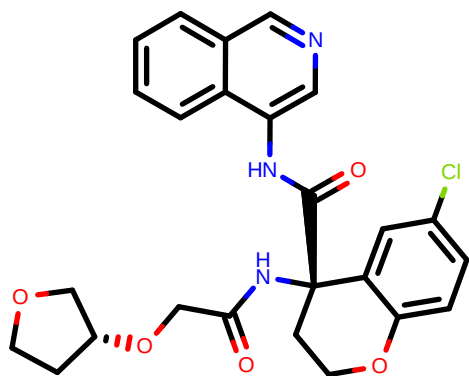
CID:	DAR-DIA-5ff57136-17_1
SMILES:	<chem>c1ccc2c(c1)cnc2N(CC#CBr)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl</chem>
RUN:	RUN69
DDG (kcal/mol):	-4.13
dDDG (kcal/mol):	0.15

EN300-263085_3_1



CID:	EN300-263085_3_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOCc4ccc(cc4)C)CCNC(=O)C5(C)C5n6cnm6</chem>
RUN:	RUN479
DDG (kcal/mol):	-4.13
dDDG (kcal/mol):	0.29

EN300-99391_1_1



CID: EN300-99391_1_1

SMILES:

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

RUN:

RUN1764

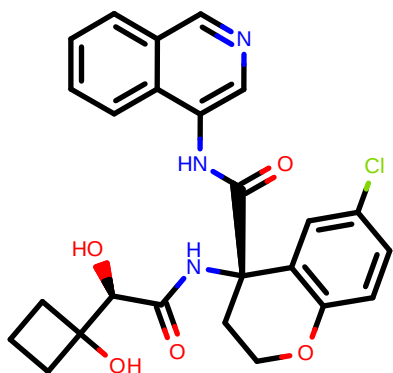
DDG (kcal/mol):

-4.03

dDDG (kcal/mol):

0.37

EN300-1073320_1_1



CID: EN300-1073320_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5(CCC5)O)O

RUN:

RUN1756

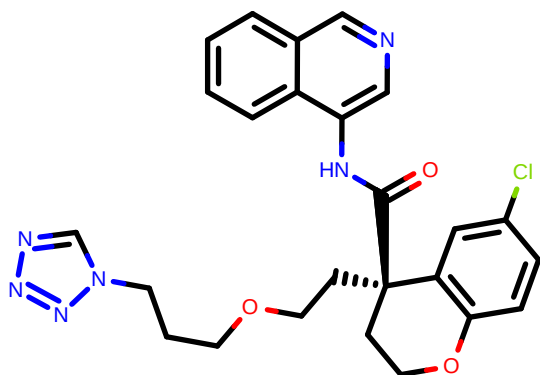
DDG (kcal/mol):

-3.92

dDDG (kcal/mol):

0.37

EN300-1696962_3_1



CID: EN300-1696962_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCN5cnnn5

RUN:

RUN409

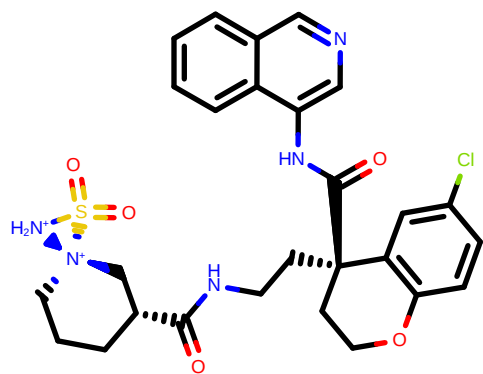
DDG (kcal/mol):

-3.77

dDDG (kcal/mol):

0.31

EN300-219496_3_1



CID: EN300-219496_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C(CCC5)N(S(=O)(=O)N)C6CCCCC6

RUN:

RUN1745

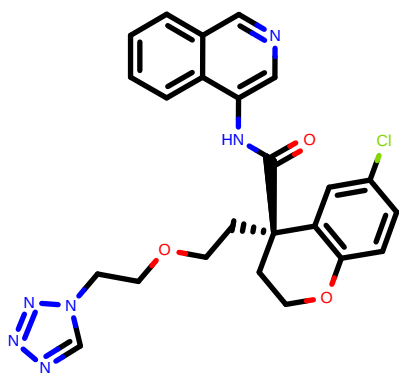
DDG (kcal/mol):

-3.76

dDDG (kcal/mol):

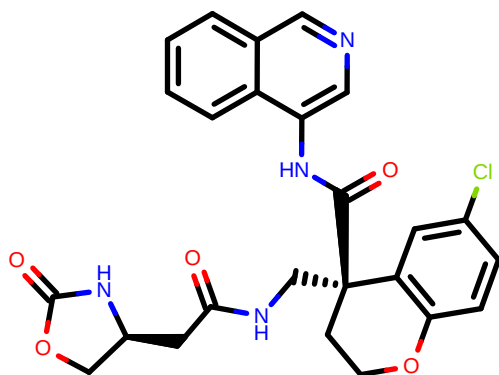
0.56

EN300-364679_3_1



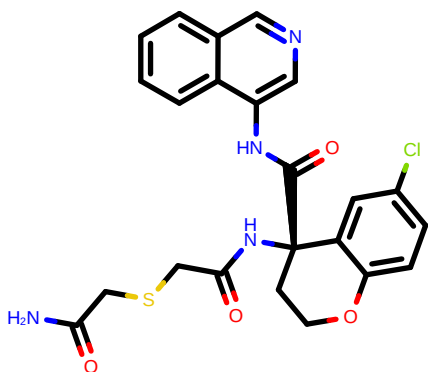
CID:	EN300-364679_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnnn5</chem>
RUN:	RUN297
DDG (kcal/mol):	-3.75
dDDG (kcal/mol):	0.29

EN300-1703852_2_1



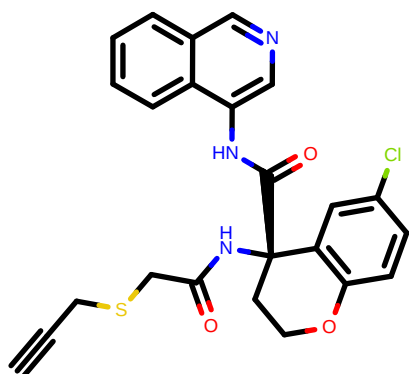
CID:	EN300-1703852_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@H]5COC(=O)N5</chem>
RUN:	RUN509
DDG (kcal/mol):	-3.70
dDDG (kcal/mol):	0.32

EN300-33513_1_1



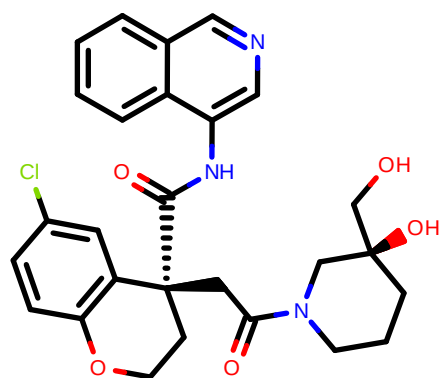
CID:	EN300-33513_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CSCC(=O)N</chem>
RUN:	RUN322
DDG (kcal/mol):	-3.66
dDDG (kcal/mol):	0.26

EN300-86878_1_1



CID:	EN300-86878_1_1
SMILES:	<chem>C#CCSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN585
DDG (kcal/mol):	-3.57
dDDG (kcal/mol):	0.24

EN300-251396_1_2



CID: EN300-251396_1_2

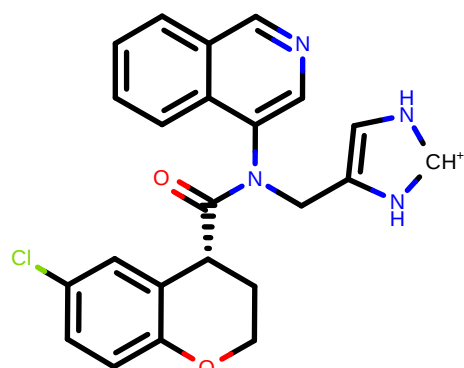
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC[C@](C5)(CO)O

RUN: RUN835

DDG (kcal/mol): -3.56

dDDG (kcal/mol): 0.52

ALP-UNI-44c99a80-2_1



CID: ALP-UNI-44c99a80-2_1

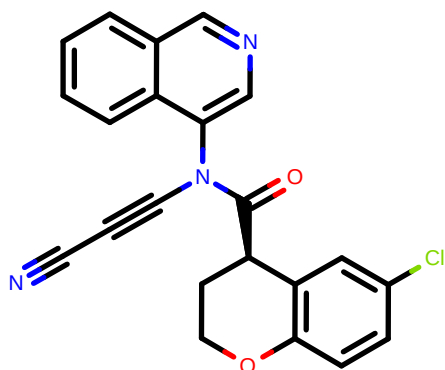
SMILES: c1ccc2c(c1)cncc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl

RUN: RUN251

DDG (kcal/mol): -3.56

dDDG (kcal/mol): 0.18

DAR-DIA-5ff57136-10_1



CID: DAR-DIA-5ff57136-10_1

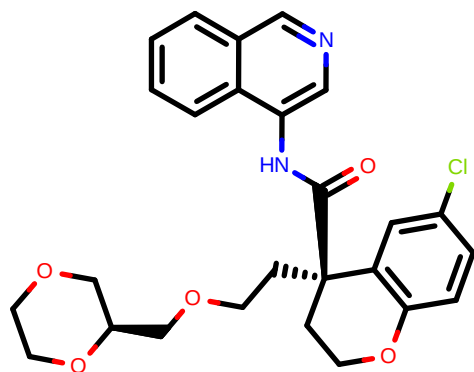
SMILES: c1ccc2c(c1)cncc2N(C#CC#N)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN126

DDG (kcal/mol): -3.55

dDDG (kcal/mol): 0.14

EN300-139167_3_1



CID: EN300-139167_3_1

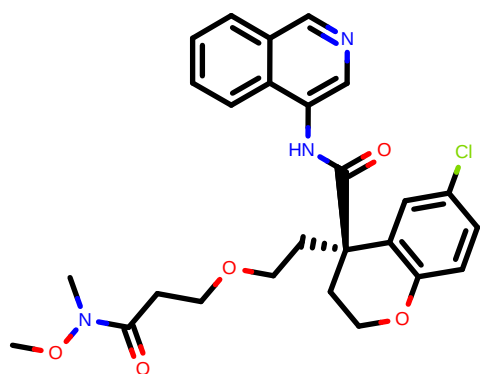
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@](C@H)5COC(CO)5

RUN: RUN656

DDG (kcal/mol): -3.54

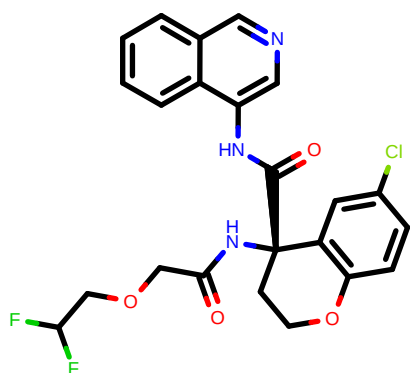
dDDG (kcal/mol): 0.31

EN300-174603_3_1



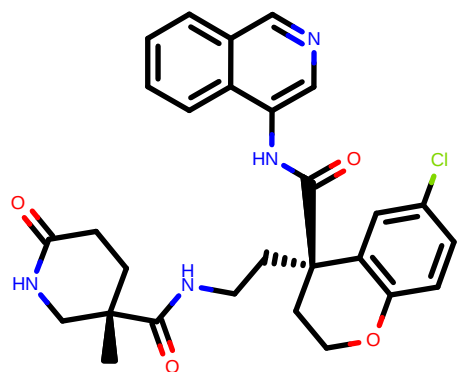
CID:	EN300-174603_3_1
SMILES:	<chem>CN(C(=O)CCOCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)OC</chem>
RUN:	RUN313
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.33

EN300-315792_1_1



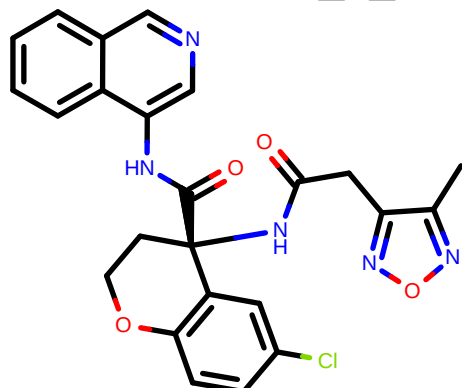
CID:	EN300-315792_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F</chem>
RUN:	RUN521
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.26

EN300-195924_3_1



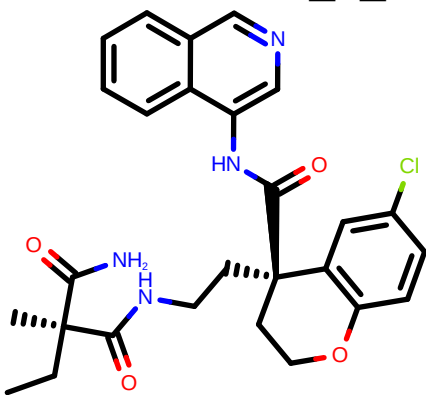
CID:	EN300-195924_3_1
SMILES:	<chem>C[C@@]1(CCC(=O)NC1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN906
DDG (kcal/mol):	-3.49
dDDG (kcal/mol):	0.40

EN300-254883_1_1



CID:	EN300-254883_1_1
SMILES:	<chem>Cc1c(non1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN1501
DDG (kcal/mol):	-3.44
dDDG (kcal/mol):	0.23

EN300-2908024_3_1



CID:

EN300-2908024_3_1

SMILES:

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

RUN:

RUN1354

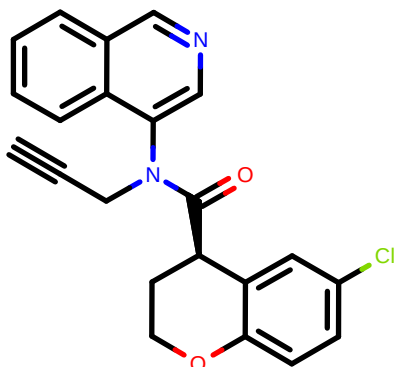
DDG (kcal/mol):

-3.44

dDDG (kcal/mol):

0.48

DAR-DIA-5ff57136-13_1



CID:

DAR-DIA-5ff57136-13_1

SMILES:

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

RUN:

RUN92

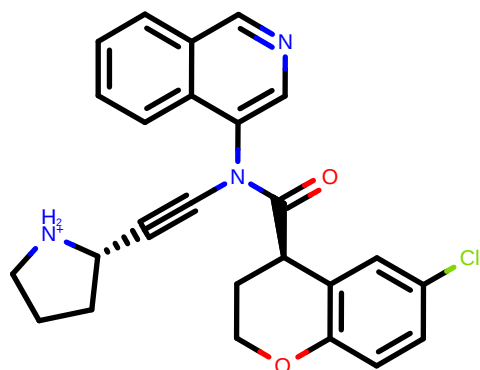
DDG (kcal/mol):

-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](C)4CCOc5c4cc(cc5)Cl

RUN:

RUN173

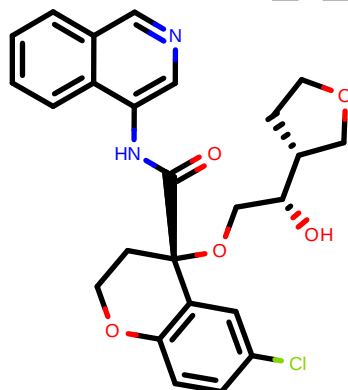
DDG (kcal/mol):

-3.41

dDDG (kcal/mol):

0.17

EN300-1911992_1_2



CID:

EN300-1911992_1_2

SMILES:

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

RUN:

RUN1751

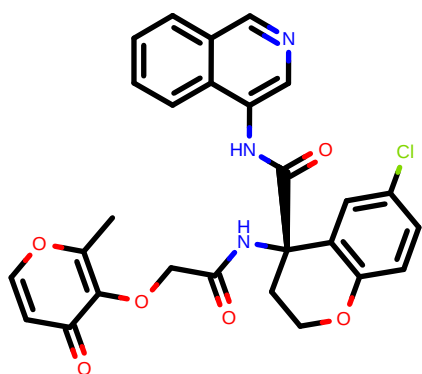
DDG (kcal/mol):

-3.40

dDDG (kcal/mol):

0.45

EN300-702714_1_1



CID: EN300-702714_1_1

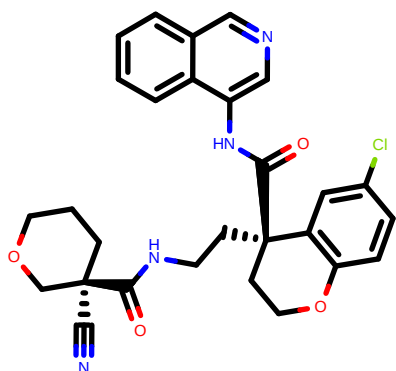
SMILES: Cc1c(c(=O)ccoc1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1341

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.26

EN300-301925_3_1



CID: EN300-301925_3_1

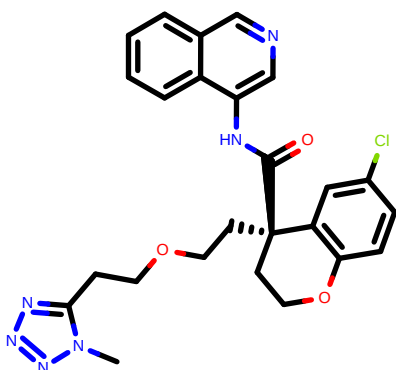
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN986

DDG (kcal/mol): -3.36

dDDG (kcal/mol): 0.35

EN300-365398_3_1



CID: EN300-365398_3_1

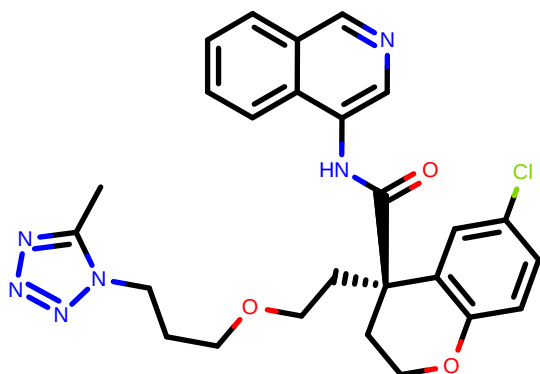
SMILES: Cn1c(nnn1)CCOCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN624

DDG (kcal/mol): -3.35

dDDG (kcal/mol): 0.36

EN300-197715_3_1



CID: EN300-197715_3_1

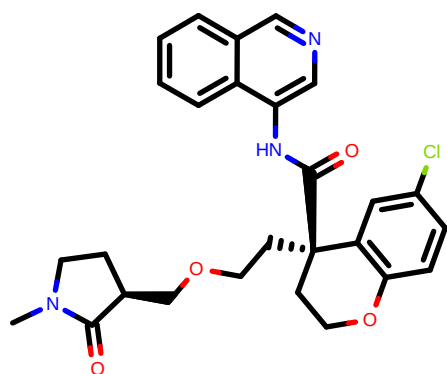
SMILES: Cc1nnnn1CCOCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN805

DDG (kcal/mol): -3.35

dDDG (kcal/mol): 0.31

EN300-260816_3_2



CID:

EN300-260816_3_2

SMILES:

CN1CC[C@H](C1=O)COC[C@]2(COC3C2CC(C3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN1060

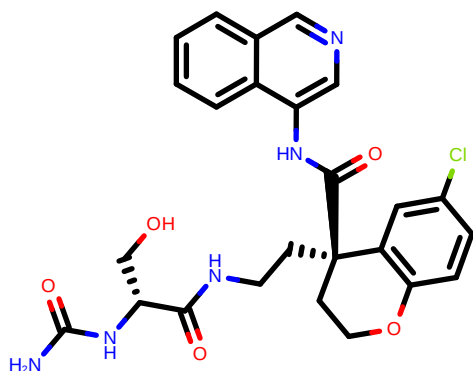
DDG (kcal/mol):

-3.28

dDDG (kcal/mol):

0.32

EN300-10170_3_1



CID:

EN300-10170_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@]3(COC4C3CC(C4)Cl)CCNC(=O)[C@H](CO)NC(=O)N

RUN:

RUN1066

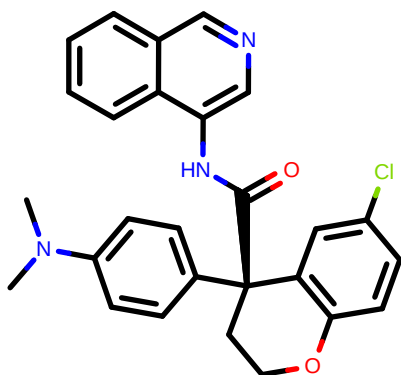
DDG (kcal/mol):

-3.22

dDDG (kcal/mol):

0.32

FRA-DIA-13af2da5-2_1



CID:

FRA-DIA-13af2da5-2_1

SMILES:

CN(C)c1ccc(cc1)[C@]2(COC3C2CC(C3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN168

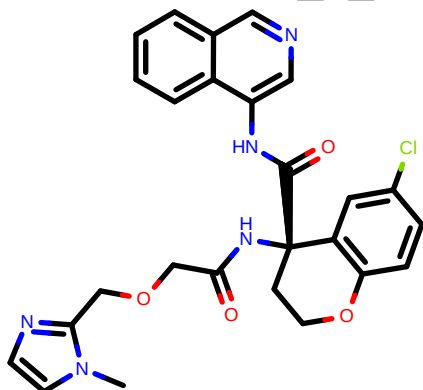
DDG (kcal/mol):

-3.22

dDDG (kcal/mol):

0.22

EN300-212341_1_1



CID:

EN300-212341_1_1

SMILES:

Cn1ccnc1COCC(=O)N[C@]2(COC3C2CC(C3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN482

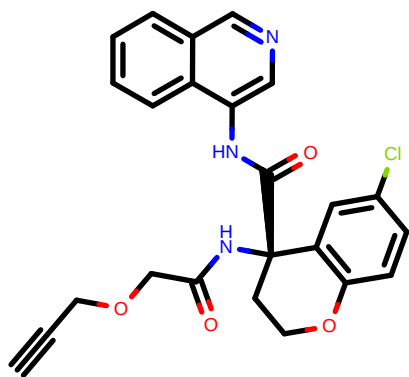
DDG (kcal/mol):

-3.21

dDDG (kcal/mol):

0.28

EN300-106432_1_1



CID: EN300-106432_1_1

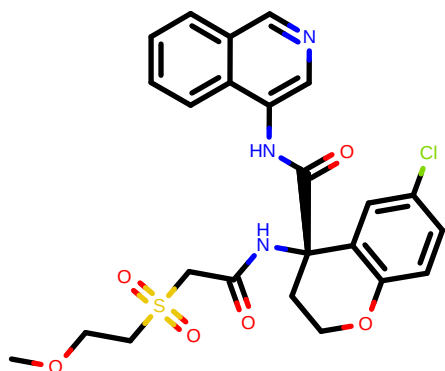
SMILES: C#CCOCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN450

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.20

EN300-39501_1_1



CID: EN300-39501_1_1

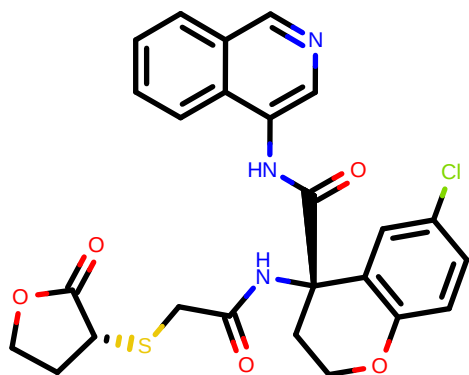
SMILES: COCCS(=O)(=O)CC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN609

DDG (kcal/mol): -3.14

dDDG (kcal/mol): 0.34

EN300-113218_1_1



CID: EN300-113218_1_1

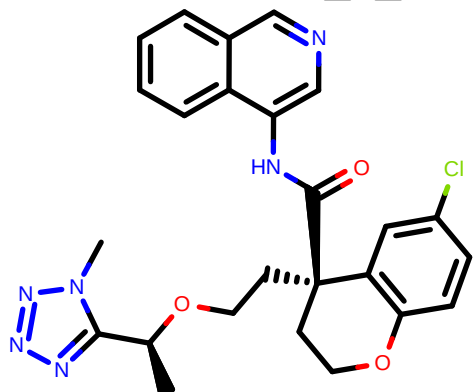
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@H]5CCOCC5=O

RUN: RUN1572

DDG (kcal/mol): -3.11

dDDG (kcal/mol): 0.36

EN300-173006_3_1



CID: EN300-173006_3_1

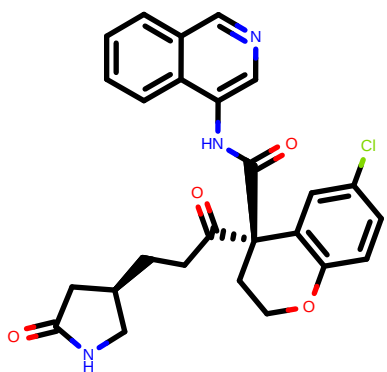
SMILES: C[C@@H](c1nnnn1C)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1124

DDG (kcal/mol): -3.09

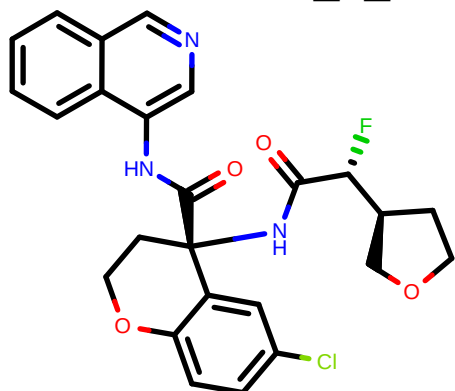
dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-21_1



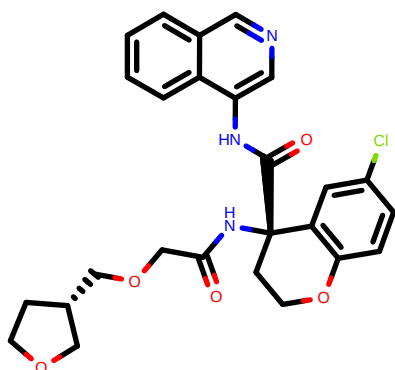
CID:	VLA-UCB-34f3ed0c-21_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NCS</chem>
RUN:	RUN27
DDG (kcal/mol):	-3.06
dDDG (kcal/mol):	0.38

EN300-783124_1_3



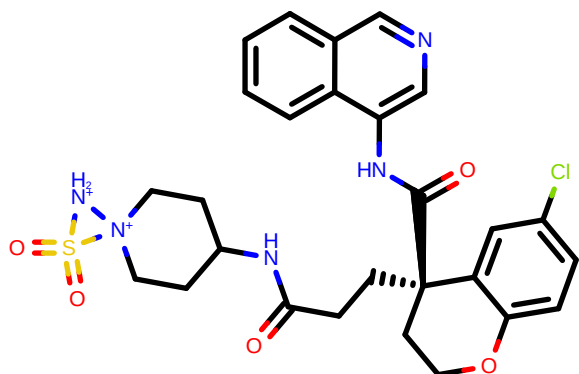
CID:	EN300-783124_1_3
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]([C@@H]5CCOC5)F</chem>
RUN:	RUN1285
DDG (kcal/mol):	-3.04
dDDG (kcal/mol):	0.24

EN300-80522_1_2



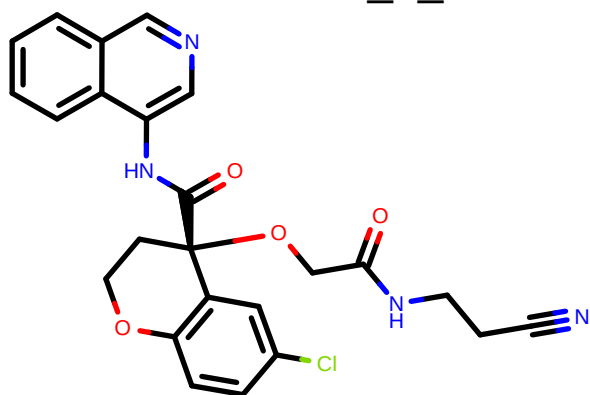
CID:	EN300-80522_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCOC5</chem>
RUN:	RUN1301
DDG (kcal/mol):	-3.01
dDDG (kcal/mol):	0.28

EN300-310398_2_1



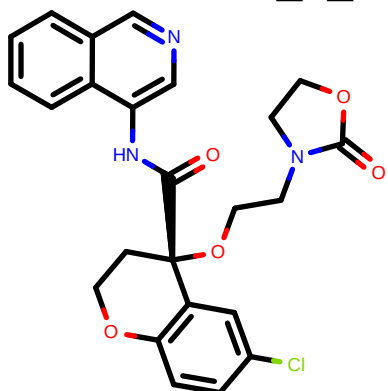
CID:	EN300-310398_2_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5CCN(CC5)S(=O)(=O)N</chem>
RUN:	RUN875
DDG (kcal/mol):	-2.97
dDDG (kcal/mol):	0.29

EN300-10895_1_1



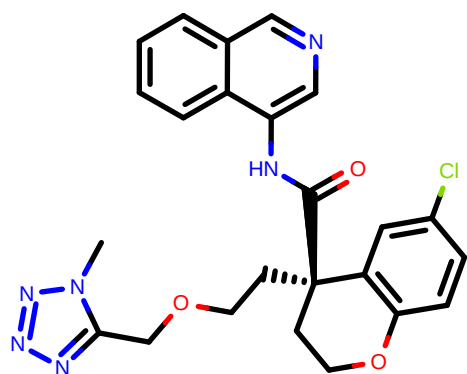
CID:	EN300-10895_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)NCCC#N</chem>
RUN:	RUN357
DDG (kcal/mol):	-2.97
dDDG (kcal/mol):	0.24

EN300-370967_1_1



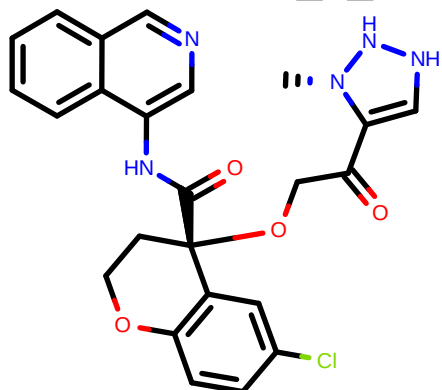
CID:	EN300-370967_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCCN5CCOC5=O</chem>
RUN:	RUN1647
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.25

EN300-62574_3_1



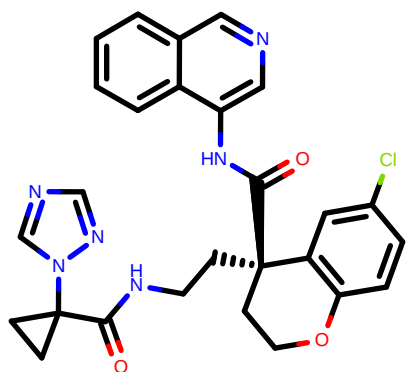
CID:	EN300-62574_3_1
SMILES:	<chem>Cn1c(nnn1)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1236
DDG (kcal/mol):	-2.93
dDDG (kcal/mol):	0.28

EN300-204936_1_1



CID:	EN300-204936_1_1
SMILES:	<chem>Cn1c(cnn1)C(=O)CO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN944
DDG (kcal/mol):	-2.92
dDDG (kcal/mol):	0.22

EN300-246440_3_1



CID: EN300-246440_3_1

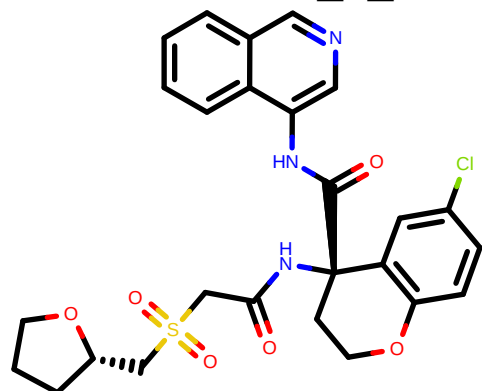
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCS)n6cncn6

RUN: RUN455

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.46

EN300-67023_1_1



CID: EN300-67023_1_1

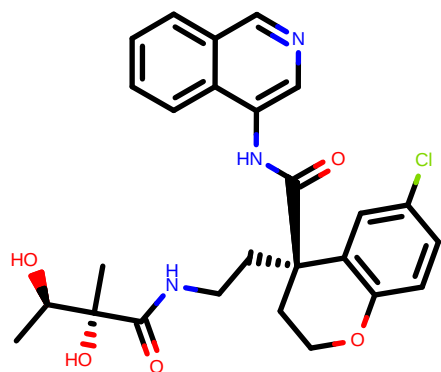
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C[C@H]5CCCCO5

RUN: RUN901

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.39

EN300-202922_3_2



CID: EN300-202922_3_2

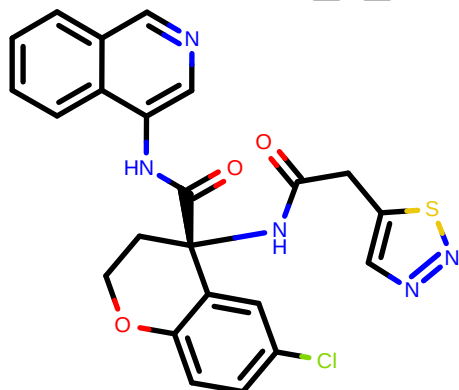
SMILES: C[C@H]([C@@])(C)(C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O)O

RUN: RUN1569

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.34

EN300-260152_1_1



CID: EN300-260152_1_1

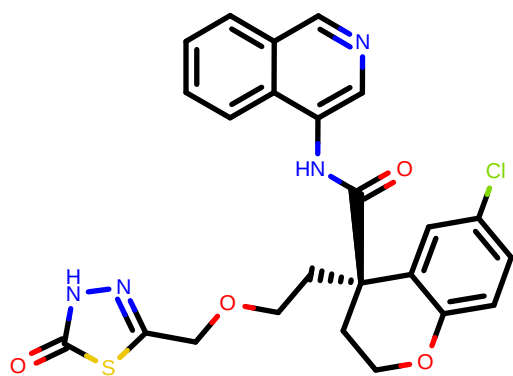
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnns5

RUN: RUN1205

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.21

EN300-171766_3_1



CID: EN300-171766_3_1

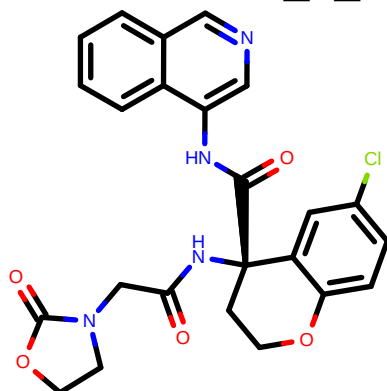
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5n[nH]c(=O)s5

RUN: RUN980

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.28

EN300-172179_1_1



CID: EN300-172179_1_1

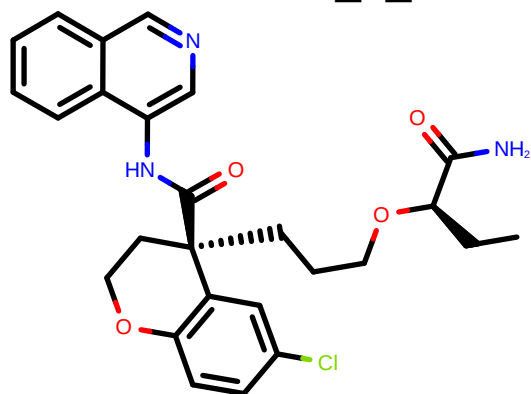
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCOC5=O

RUN: RUN1149

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.26

EN300-65839_4_2



CID: EN300-65839_4_2

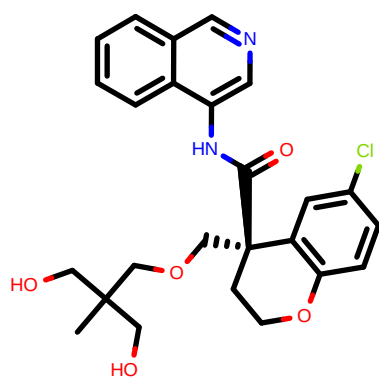
SMILES: CC[C@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN667

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.43

EN300-218116_2_1



CID: EN300-218116_2_1

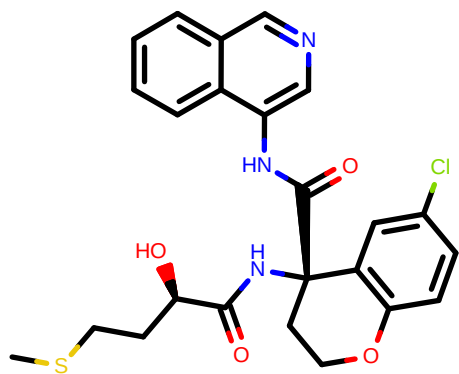
SMILES: CC(CO)(CO)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1430

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.37

EN300-103144_1_2



CID: EN300-103144_1_2

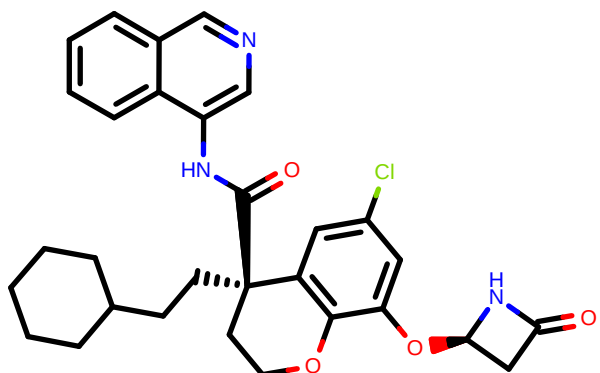
SMILES: CSCC[C@H](C(=O)N[C@@]1(COC2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN1453

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.33

VLA-UCB-50c39ae8-9_1



CID: VLA-UCB-50c39ae8-9_1

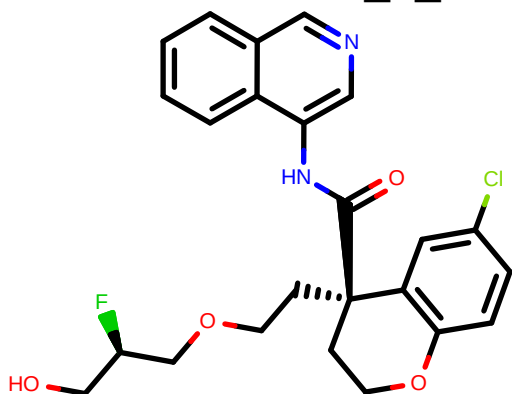
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC4c3cc(cc4O)[C@@H]5CC(=O)N5)C1)CCC6CCCCC6

RUN: RUN121

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.40

EN300-1600517_3_1



CID: EN300-1600517_3_1

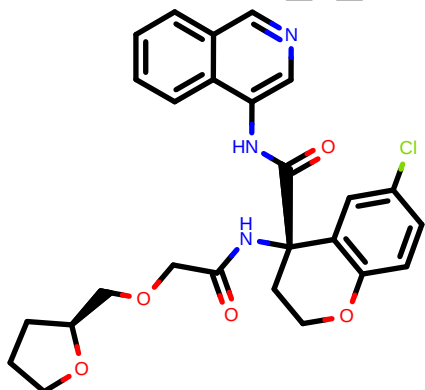
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC4c3cc(cc4)C)COC[C@H](CO)F

RUN: RUN1380

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.31

EN300-60033_1_1



CID: EN300-60033_1_1

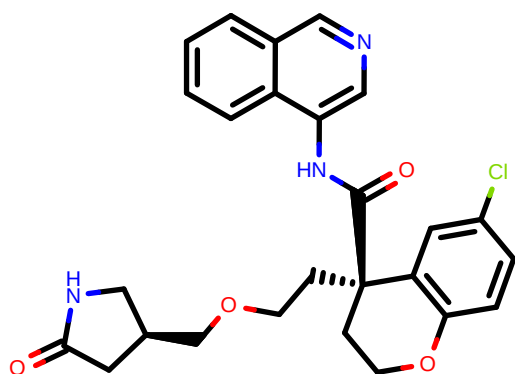
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC4c3cc(cc4)C)NC(=O)COC[C@H]5CCCO5

RUN: RUN1541

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.27

EN300-246747_3_2



CID:

EN300-246747_3_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CCOC[C@H]5CC(=O)NCS

RUN:

RUN1044

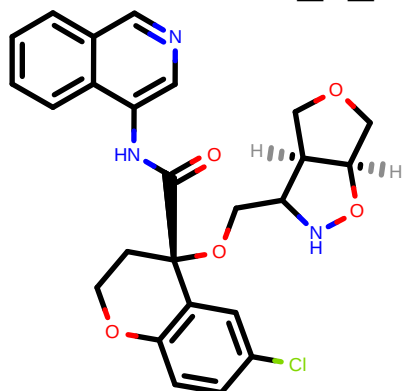
DDG (kcal/mol):

-2.79

dDDG (kcal/mol):

0.28

EN300-7436306_1_1



CID:

EN300-7436306_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)OCC5=NO[C@H]6[C@@H]5COC6

RUN:

RUN333

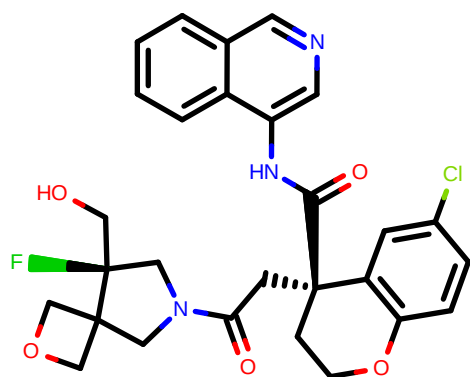
DDG (kcal/mol):

-2.79

dDDG (kcal/mol):

0.24

EN300-1719075_1_1



CID:

EN300-1719075_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CC(=O)N5C[C@](C6(C5)COC6)(CO)F

RUN:

RUN1034

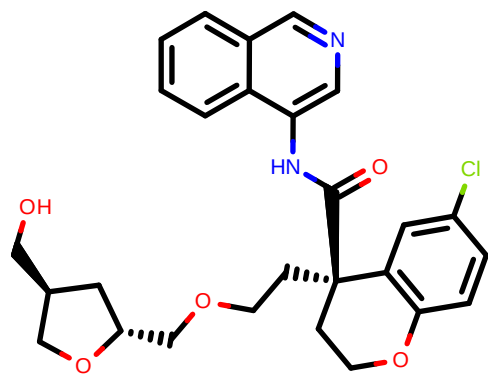
DDG (kcal/mol):

-2.78

dDDG (kcal/mol):

0.39

EN300-6494158_3_2



CID:

EN300-6494158_3_2

SMILES:

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

RUN:

RUN1004

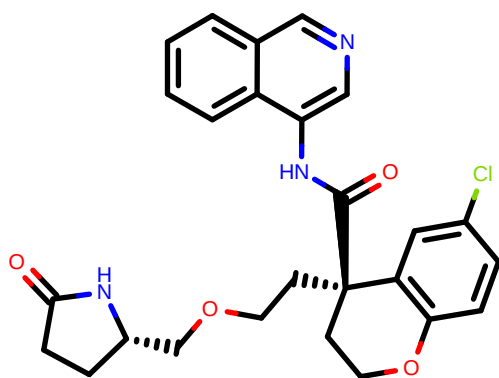
DDG (kcal/mol):

-2.77

dDDG (kcal/mol):

0.36

EN300-195756_3_1



CID:

EN300-195756_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCCC(=O)N5

RUN:

RUN868

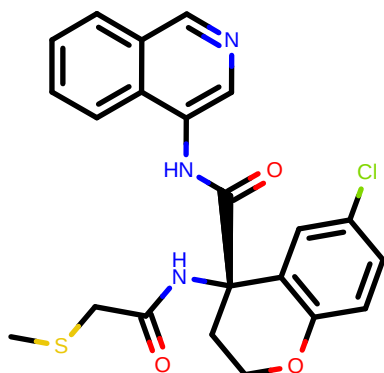
DDG (kcal/mol):

-2.75

dDDG (kcal/mol):

0.25

EN300-07879_1_1



CID:

EN300-07879_1_1

SMILES:

CSCC(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN:

RUN1061

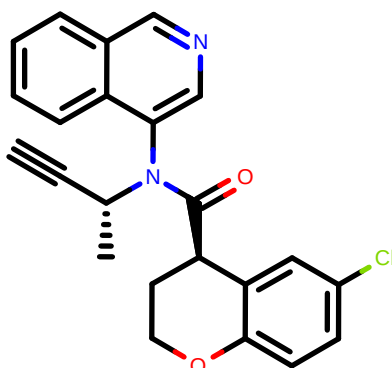
DDG (kcal/mol):

-2.74

dDDG (kcal/mol):

0.21

DAR-DIA-5ff57136-16_2



CID:

DAR-DIA-5ff57136-16_2

SMILES:

C[C@H](C#C)N(c1nccc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN:

RUN192

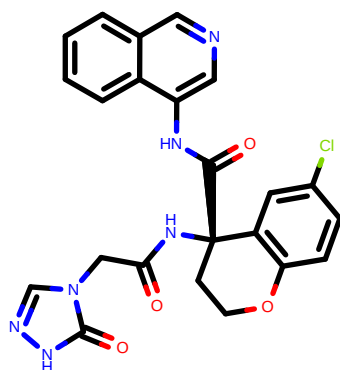
DDG (kcal/mol):

-2.73

dDDG (kcal/mol):

0.15

EN300-120820_1_1



CID:

EN300-120820_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cn[nH]c5=O

RUN:

RUN1325

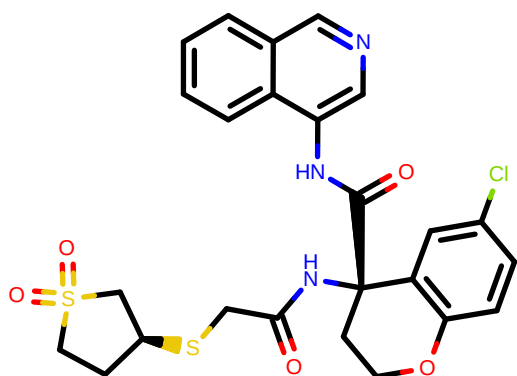
DDG (kcal/mol):

-2.72

dDDG (kcal/mol):

0.25

EN300-13890_1_2



CID: EN300-13890_1_2

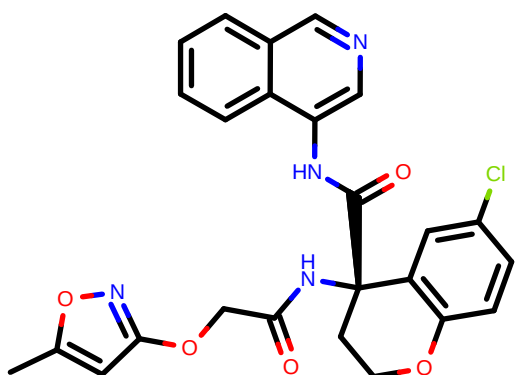
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@H]5CCS(=O)(=O)C5

RUN: RUN1093

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.31

EN300-12929_1_1



CID: EN300-12929_1_1

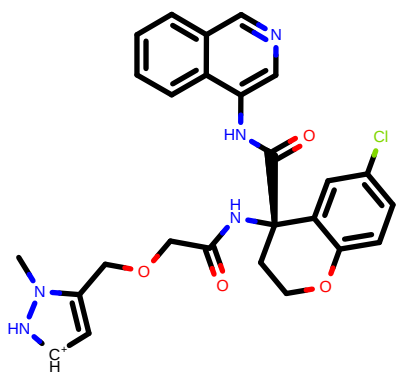
SMILES: Cc1cc(no1)OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1445

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.32

EN300-92472_1_1



CID: EN300-92472_1_1

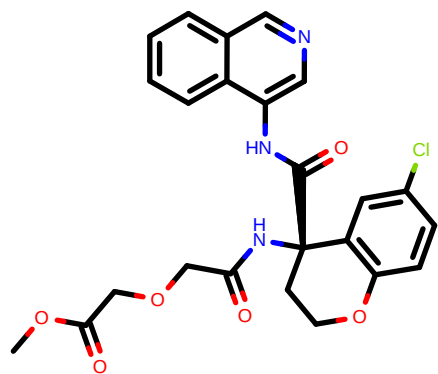
SMILES: Cn1c(ccn1)COCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN346

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.28

EN300-205635_1_1



CID: EN300-205635_1_1

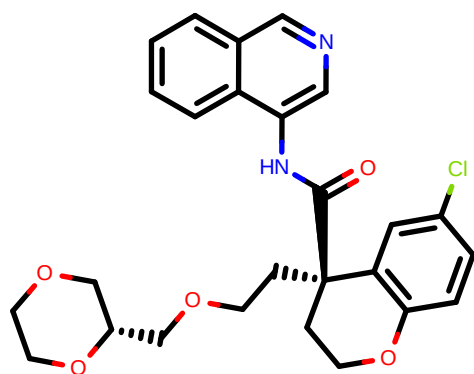
SMILES: COC(=O)COCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN402

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.24

EN300-139167_3_2



CID: EN300-139167_3_2

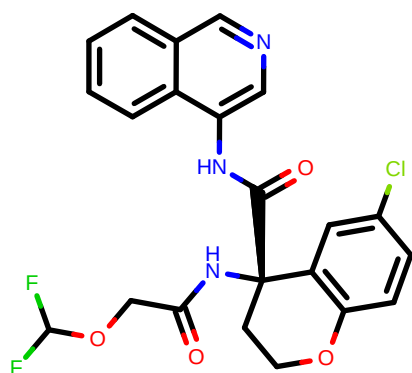
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H]5COC(CO5

RUN: RUN664

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.37

EN300-179091_1_1



CID: EN300-179091_1_1

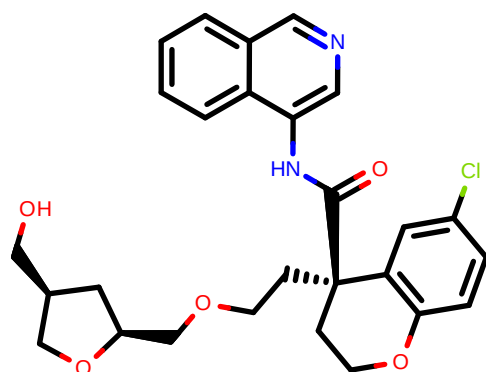
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)COC(F)(F)F

RUN: RUN1732

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.33

EN300-6494158_3_1



CID: EN300-6494158_3_1

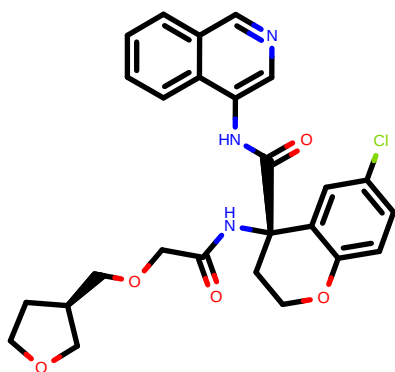
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H]5C[C@@H](CO5)CO

RUN: RUN528

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.28

EN300-80522_1_1



CID: EN300-80522_1_1

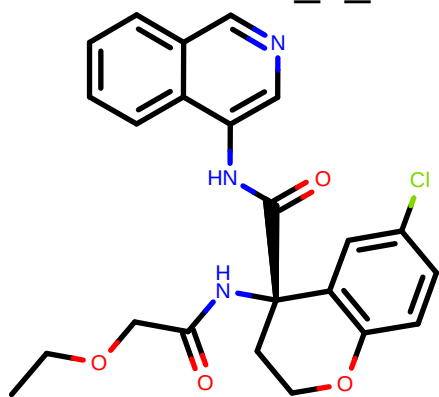
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)COC[C@@H]5COC(CO5

RUN: RUN1485

DDG (kcal/mol): -2.68

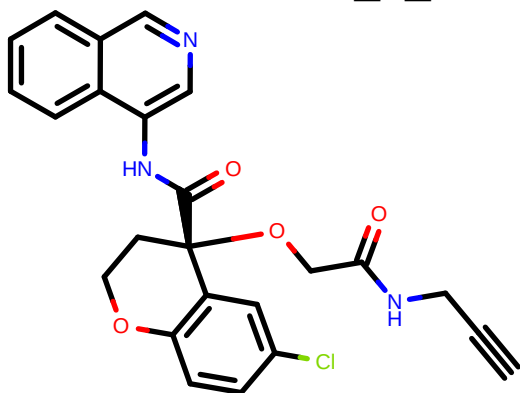
dDDG (kcal/mol): 0.27

EN300-21303_1_1



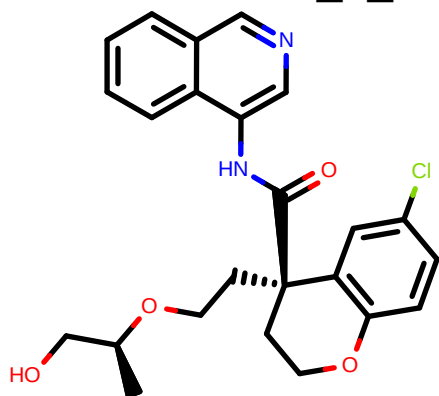
CID:	EN300-21303_1_1
SMILES:	<chem>CCOCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN354
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.26

EN300-1659582_1_1



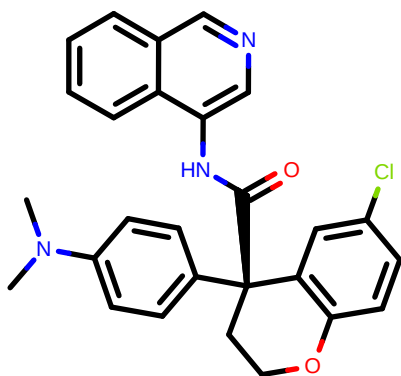
CID:	EN300-1659582_1_1
SMILES:	<chem>C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN453
DDG (kcal/mol):	-2.66
dDDG (kcal/mol):	0.21

EN300-175186_3_1



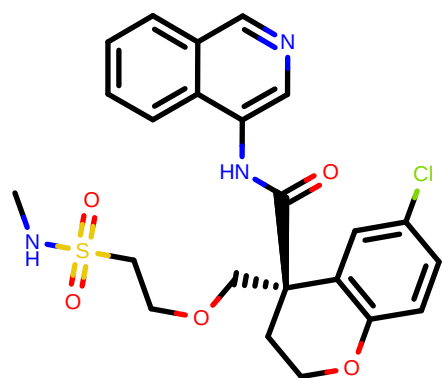
CID:	EN300-175186_3_1
SMILES:	<chem>C[C@@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1172
DDG (kcal/mol):	-2.66
dDDG (kcal/mol):	0.32

VLA-UCB-551c2366-1_1



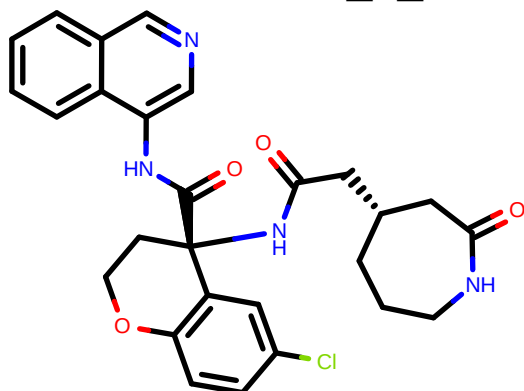
CID:	VLA-UCB-551c2366-1_1
SMILES:	<chem>CN(C)c1ccc(cc1)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN170
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.21

EN300-6482967_2_1



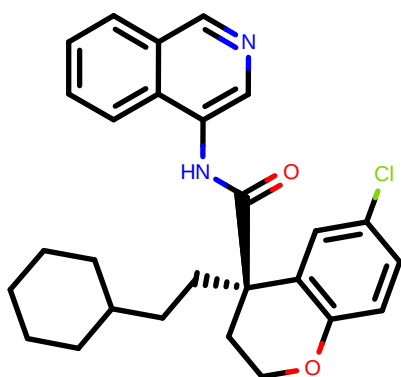
CID:	EN300-6482967_2_1
SMILES:	<chem>CNS(=O)(=O)CCOC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN650
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.37

EN300-195590_1_2



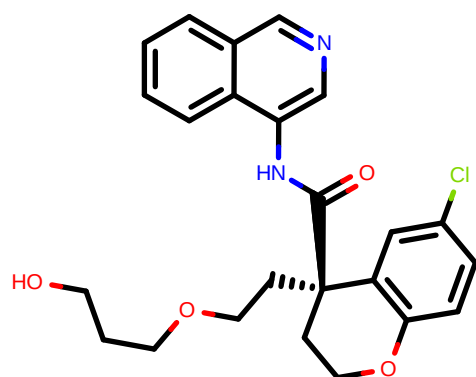
CID:	EN300-195590_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)C[H]5CCNC(=O)C5</chem>
RUN:	RUN743
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.37

DAR-DIA-6a508060-9_1



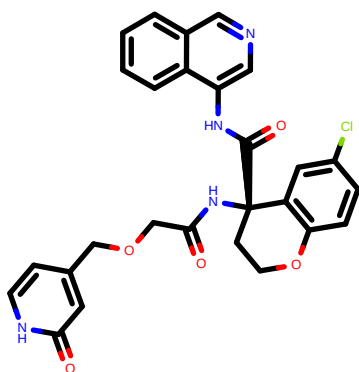
CID:	DAR-DIA-6a508060-9_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCCCCCCC5</chem>
RUN:	RUN142
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.31

EN300-221518_3_1



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

EN300-316258_1_1



CID: EN300-316258_1_1

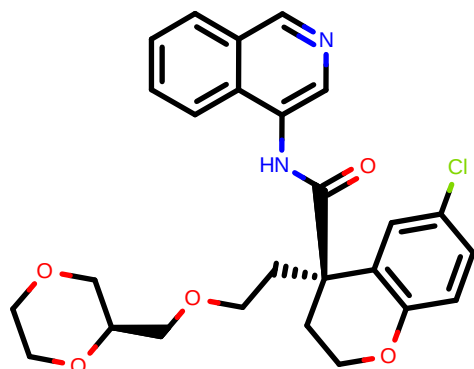
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)NC(=O)COCc5cc[nH]c(=O)c5

RUN: RUN617

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.31

EN300-139167_3_1



CID: EN300-139167_3_1

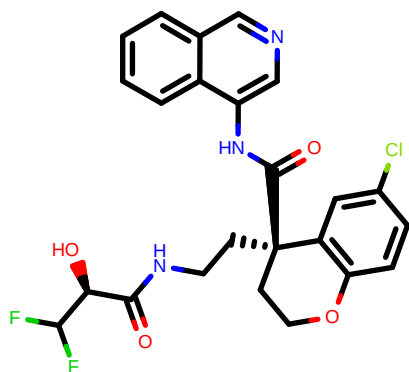
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN648

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.34

EN300-1932780_3_1



CID: EN300-1932780_3_1

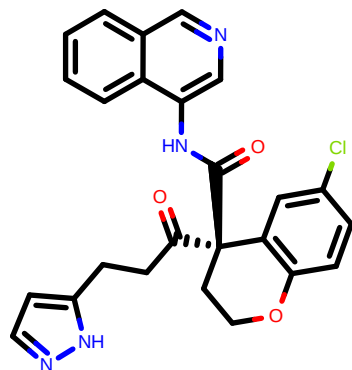
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C(F)F)O

RUN: RUN1418

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.29

VLA-UCB-34f3ed0c-8_1



CID: VLA-UCB-34f3ed0c-8_1

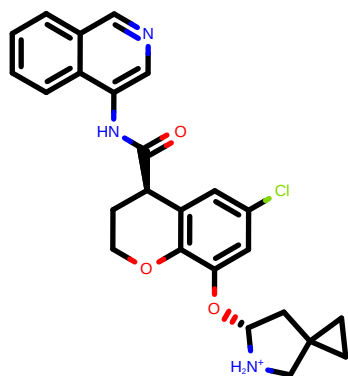
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]5

RUN: RUN76

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.25

DAR-DIA-23e5a6a0-4_1



CID:

DAR-DIA-23e5a6a0-4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4C3cc(cc4O)[C@@H]5CC6(CC6)C[NH2+][5]Cl

RUN:

RUN148

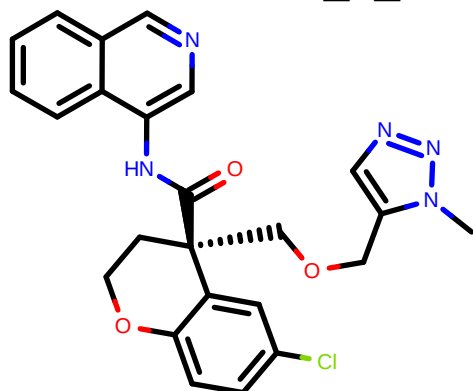
DDG (kcal/mol):

-2.56

dDDG (kcal/mol):

0.49

EN300-216673_2_1



CID:

EN300-216673_2_1

SMILES:

Cn1c(cnn1)COC[C@]2(C)C(=O)C3C2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN1350

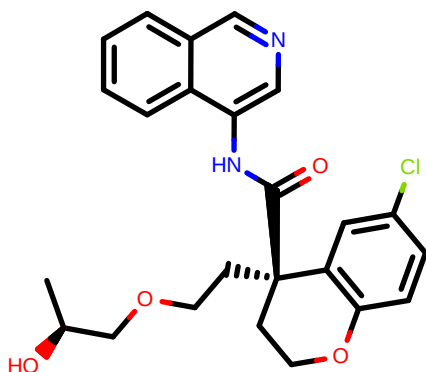
DDG (kcal/mol):

-2.55

dDDG (kcal/mol):

0.28

EN300-185378_3_1



CID:

EN300-185378_3_1

SMILES:

C[C@@H](COCC[C@]1(C)C(=O)C2C1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)O

RUN:

RUN1428

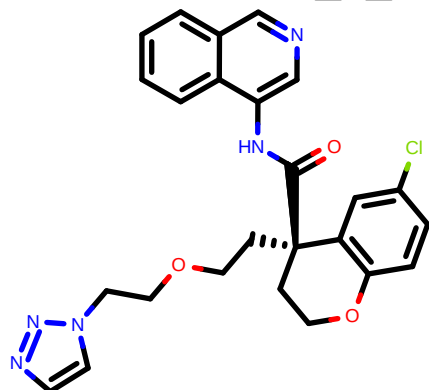
DDG (kcal/mol):

-2.55

dDDG (kcal/mol):

0.29

EN300-1715993_3_1



CID:

EN300-1715993_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4C3cc(cc4Cl)CCOCCn5ccnn5

RUN:

RUN1396

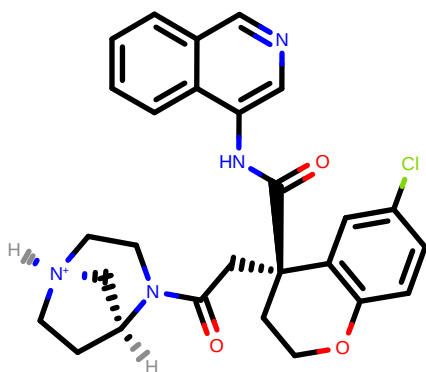
DDG (kcal/mol):

-2.53

dDDG (kcal/mol):

0.25

EN300-227218_1_1



CID:

EN300-227218_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[N@@H+]6CC[C@H]5C6

RUN:

RUN542

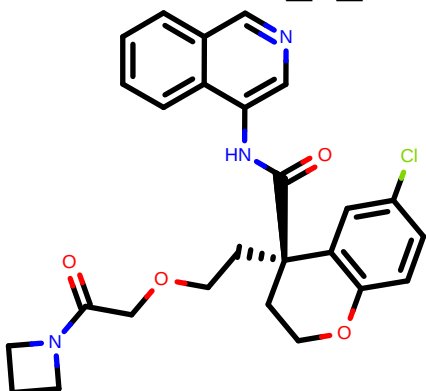
DDG (kcal/mol):

-2.52

dDDG (kcal/mol):

0.30

EN300-11195_3_1



CID:

EN300-11195_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N5CCCS5

RUN:

RUN1356

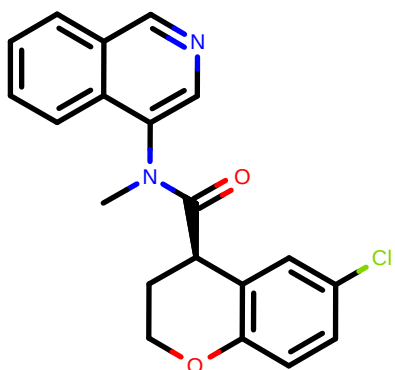
DDG (kcal/mol):

-2.52

dDDG (kcal/mol):

0.29

MAK-UNK-3875bbc8-2_1



CID:

MAK-UNK-3875bbc8-2_1

SMILES:

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

RUN:

RUN49

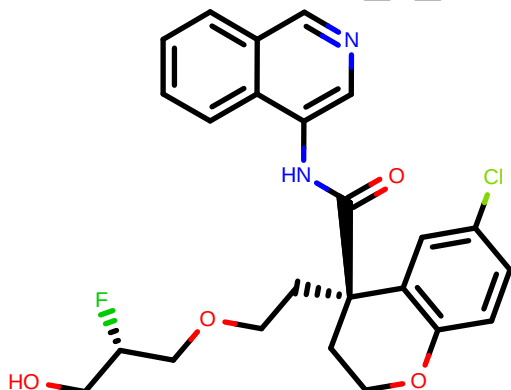
DDG (kcal/mol):

-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

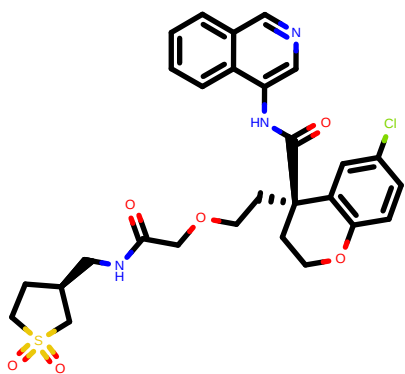
DDG (kcal/mol):

-2.51

dDDG (kcal/mol):

0.32

EN300-47606_3_1



CID:

EN300-47606_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@H](C)COC(=O)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N

RUN:

RUN1771

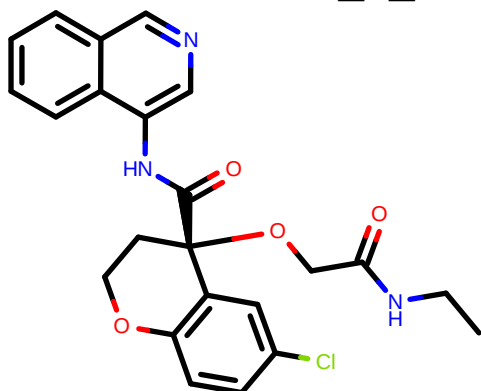
DDG (kcal/mol):

-2.50

dDDG (kcal/mol):

0.50

EN300-7003350_1_1



CID:

EN300-7003350_1_1

SMILES:

CCNC(=O)CO[C@H]1(C)COC(=O)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N

RUN:

RUN723

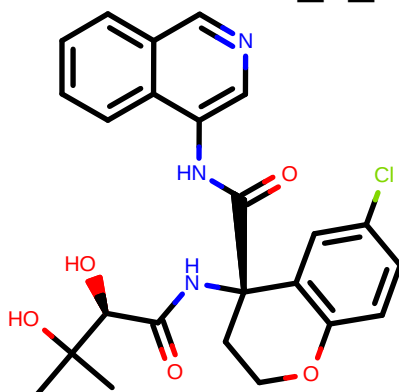
DDG (kcal/mol):

-2.50

dDDG (kcal/mol):

0.18

EN300-299532_1_2



CID:

EN300-299532_1_2

SMILES:

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

RUN:

RUN1644

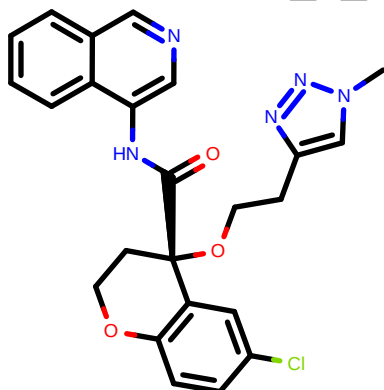
DDG (kcal/mol):

-2.50

dDDG (kcal/mol):

0.21

EN300-1600786_1_1



CID:

EN300-1600786_1_1

SMILES:

Cn1cc(nn1)CCO[C@H]2(C)COC(=O)C(=O)N[C@@H](C)C(=O)N[C@@H](C)C(=O)N

RUN:

RUN1032

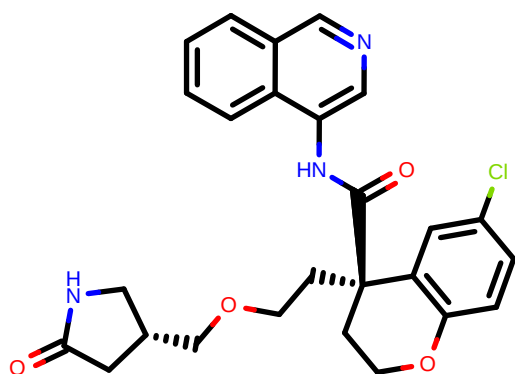
DDG (kcal/mol):

-2.50

dDDG (kcal/mol):

0.26

EN300-246747_3_1



CID: EN300-246747_3_1

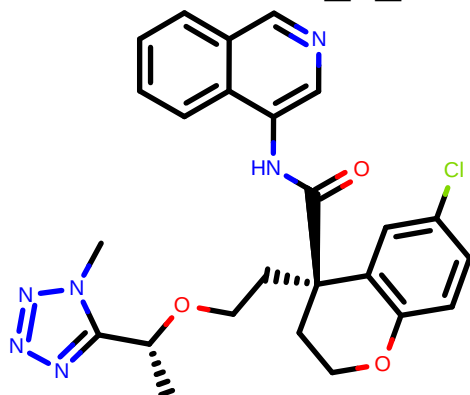
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CC(=O)NCS

RUN: RUN1212

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.26

EN300-173006_3_2



CID: EN300-173006_3_2

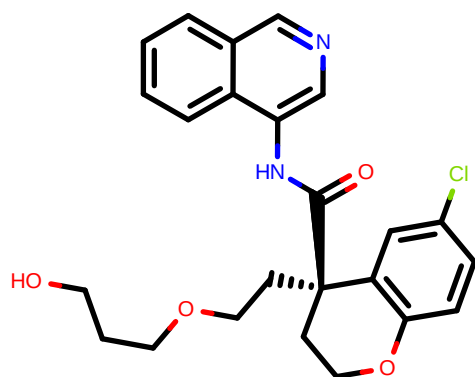
SMILES: C[C@@H](c1nnnn1C)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1715

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.31

EN300-221518_3_1



CID: EN300-221518_3_1

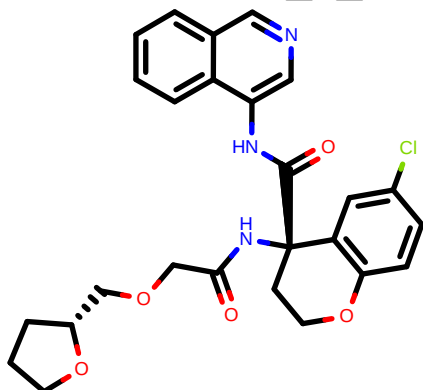
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCCO

RUN: RUN1412

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.23

EN300-60033_1_2



CID: EN300-60033_1_2

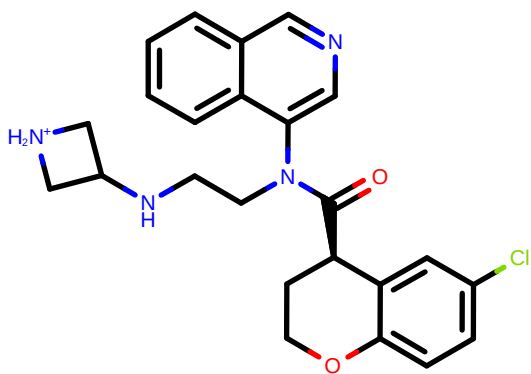
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCCO5

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(CN(C3C[NH2+](C3)C(=O)[C@@H](4CCOCc5c4cc(cc5)Cl

RUN:

RUN220

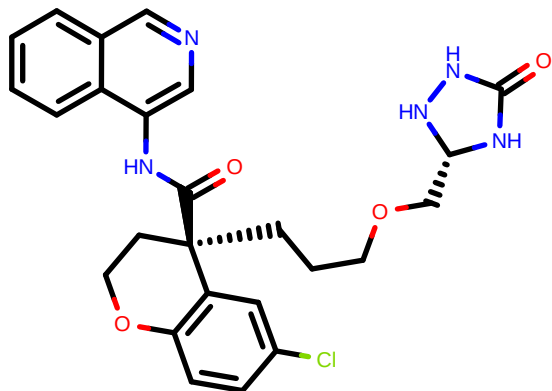
DDG (kcal/mol):

-2.47

dDDG (kcal/mol):

0.35

EN300-73772_4_1



CID:

EN300-73772_4_1

SMILES:

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

RUN:

RUN308

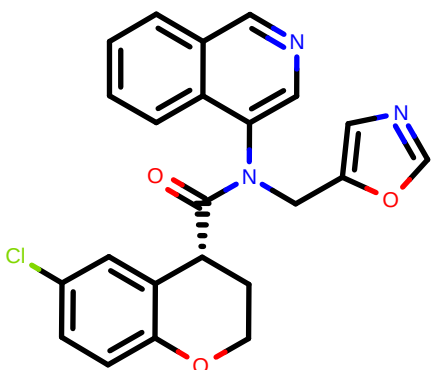
DDG (kcal/mol):

-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

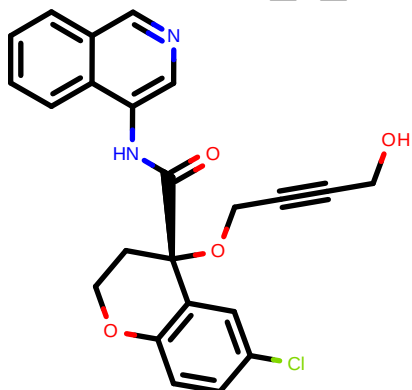
DDG (kcal/mol):

-2.45

dDDG (kcal/mol):

0.19

EN300-83766_1_1



CID:

EN300-83766_1_1

SMILES:

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

RUN:

RUN293

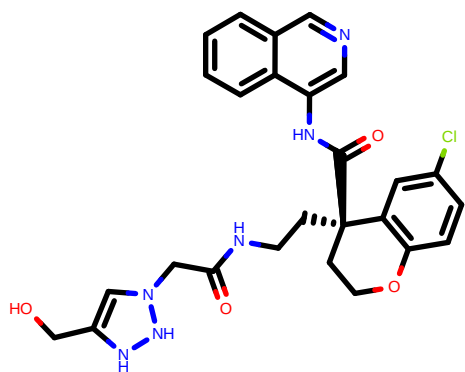
DDG (kcal/mol):

-2.44

dDDG (kcal/mol):

0.18

EN300-108236_3_1



CID:

EN300-108236_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)Cn5cc(n5)CO

RUN:

RUN803

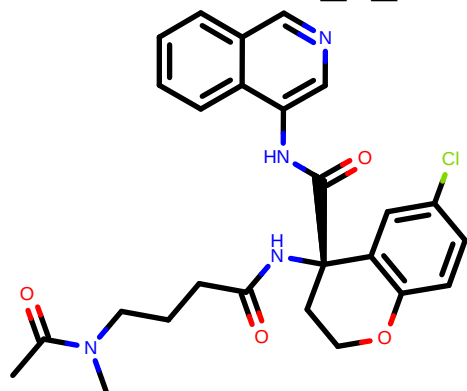
DDG (kcal/mol):

-2.43

dDDG (kcal/mol):

0.31

EN300-128750_1_1



CID:

EN300-128750_1_1

SMILES:

CC(=O)N(C)CCCC(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3cccc4

RUN:

RUN1604

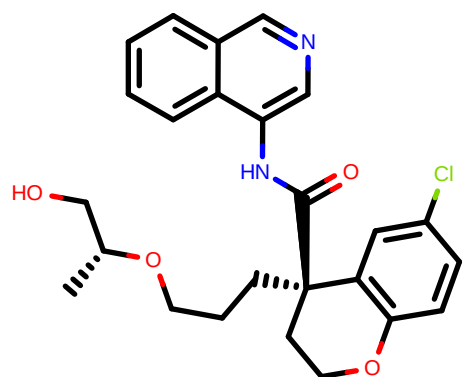
DDG (kcal/mol):

-2.43

dDDG (kcal/mol):

0.30

EN300-175186_4_2



CID:

EN300-175186_4_2

SMILES:

C[C@H](CO)OCCC[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3cccc4

RUN:

RUN460

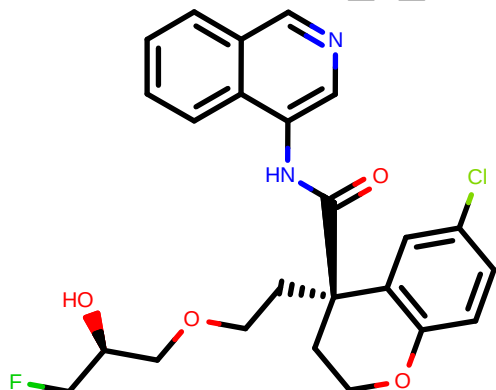
DDG (kcal/mol):

-2.42

dDDG (kcal/mol):

0.30

EN300-1968342_3_1



CID:

EN300-1968342_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCOC[C@@H](CF)O

RUN:

RUN916

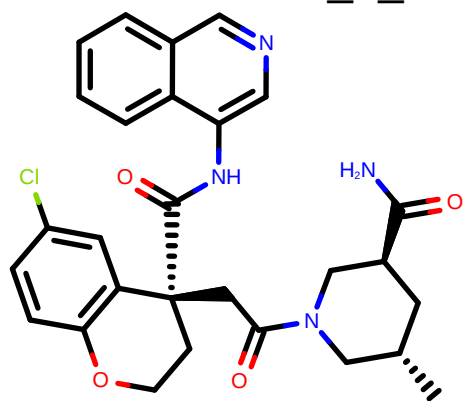
DDG (kcal/mol):

-2.42

dDDG (kcal/mol):

0.36

EN300-1724086_1_2



CID:

EN300-1724086_1_2

SMILES:

C[C@H]1C[C@H](CN(C1)C(=O)C[C@H]2(CCOc3c2cc(c3)C)C(=O)Nc4nc5c6cccc5)C(=O)N

RUN:

RUN423

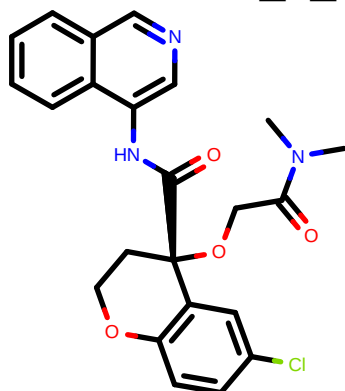
DDG (kcal/mol):

-2.41

dDDG (kcal/mol):

0.32

EN300-216063_1_1



CID:

EN300-216063_1_1

SMILES:

CN(C)C(=O)CO[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nc4c3cccc4

RUN:

RUN777

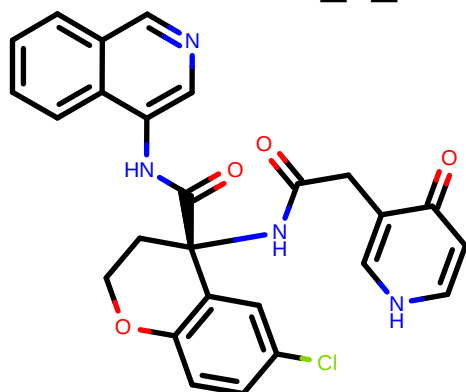
DDG (kcal/mol):

-2.41

dDDG (kcal/mol):

0.23

EN300-205486_1_1



CID:

EN300-205486_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]ccc5=O

RUN:

RUN1724

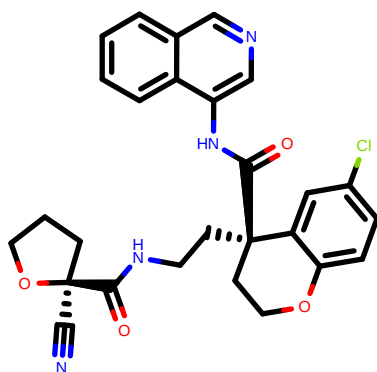
DDG (kcal/mol):

-2.39

dDDG (kcal/mol):

0.31

EN300-3710141_3_1



CID:

EN300-3710141_3_1

SMILES:

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

RUN:

RUN1002

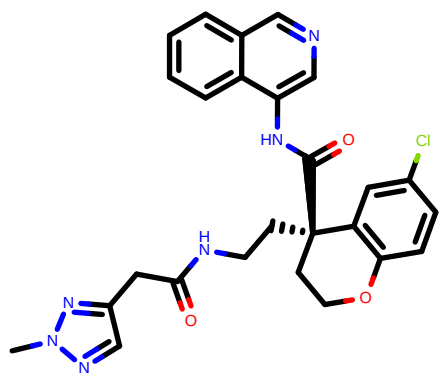
DDG (kcal/mol):

-2.39

dDDG (kcal/mol):

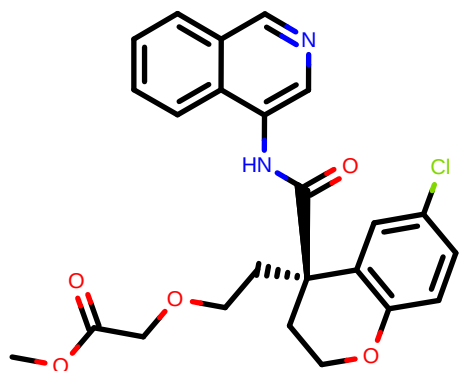
0.30

EN300-755161_3_1



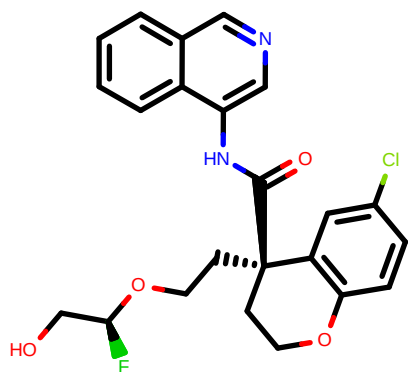
CID:	EN300-755161_3_1
SMILES:	<chem>Cn1ncc(n1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1378
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.34

EN300-19700_3_1



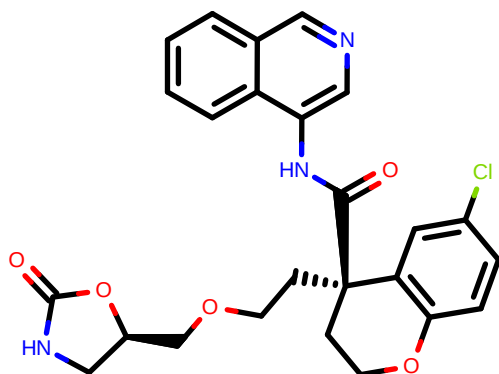
CID:	EN300-19700_3_1
SMILES:	<chem>COC(=O)COCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1571
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.24

EN300-861925_3_2



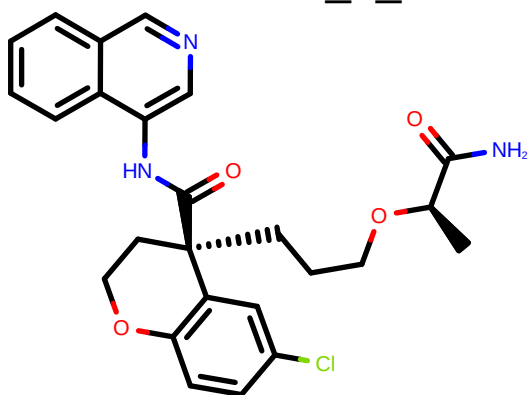
CID:	EN300-861925_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCO[C@H](CO)F</chem>
RUN:	RUN1372
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.26

EN300-203293_3_2



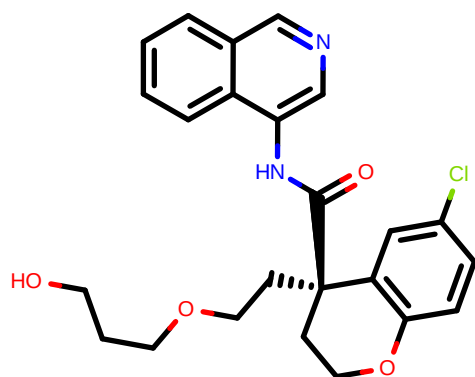
CID:	EN300-203293_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC[C@H]5CNC(=O)O5</chem>
RUN:	RUN742
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.26

EN300-17381_4_2



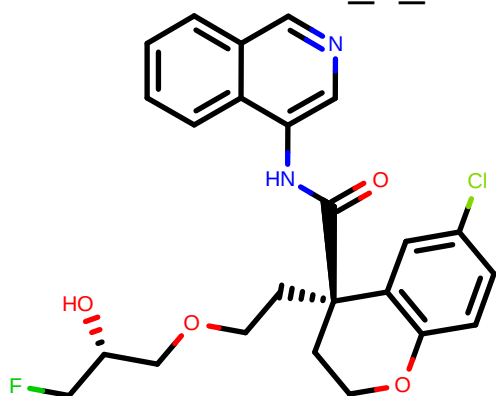
CID:	EN300-17381_4_2
SMILES:	<chem>C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN388
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.23

EN300-221518_3_1



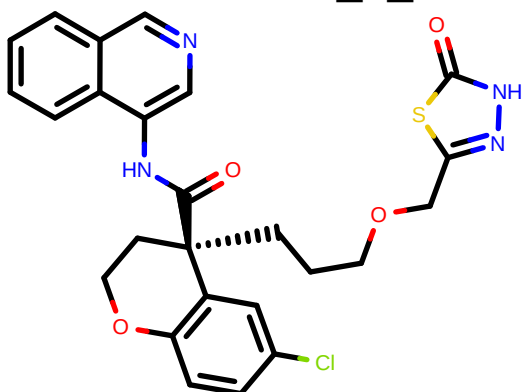
CID:	EN300-221518_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCCO</chem>
RUN:	RUN1420
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.24

EN300-1968342_3_2



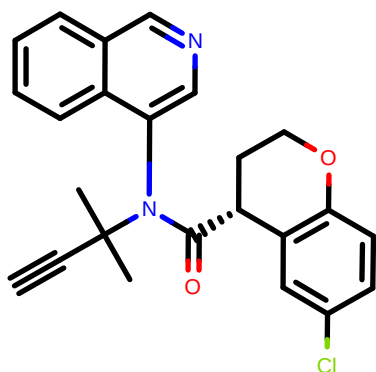
CID:	EN300-1968342_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O</chem>
RUN:	RUN1548
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.36

EN300-171766_4_1



CID:	EN300-171766_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5n[nH]c(=O)s5</chem>
RUN:	RUN292
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.27

DAR-DIA-5ff57136-14_1



CID:

DAR-DIA-5ff57136-14_1

SMILES:

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

RUN:

RUN127

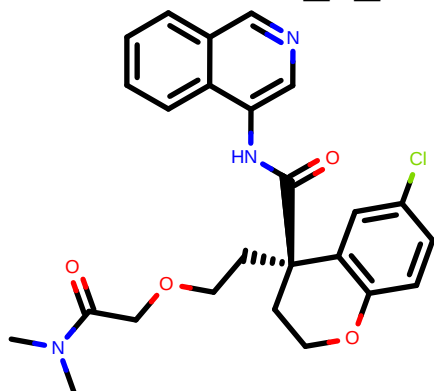
DDG (kcal/mol):

-2.34

dDDG (kcal/mol):

0.20

EN300-216063_3_1



CID:

EN300-216063_3_1

SMILES:

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

RUN:

RUN1468

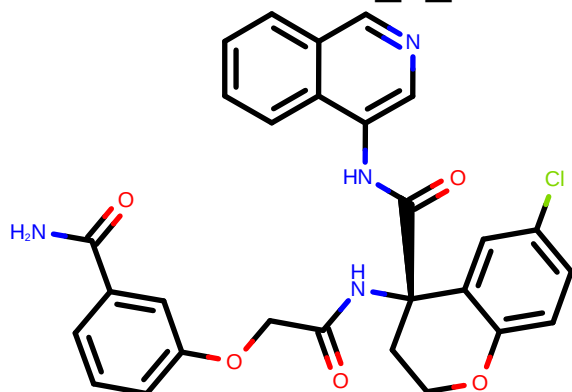
DDG (kcal/mol):

-2.33

dDDG (kcal/mol):

0.22

EN300-51736_1_1



CID:

EN300-51736_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H](3(CCOc4c3cc(cc4)Cl)NC(=O)COc5cccc(c5)C(=O)N

RUN:

RUN370

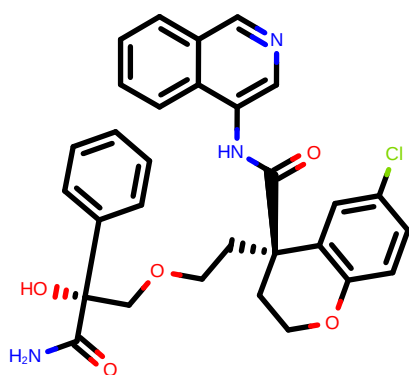
DDG (kcal/mol):

-2.33

dDDG (kcal/mol):

0.30

EN300-248526_3_1



CID:

EN300-248526_3_1

SMILES:

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

RUN:

RUN703

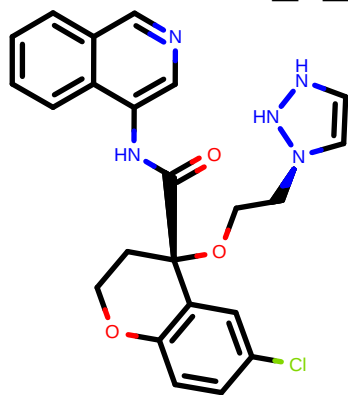
DDG (kcal/mol):

-2.33

dDDG (kcal/mol):

0.55

EN300-1715993_1_1



CID: EN300-1715993_1_1

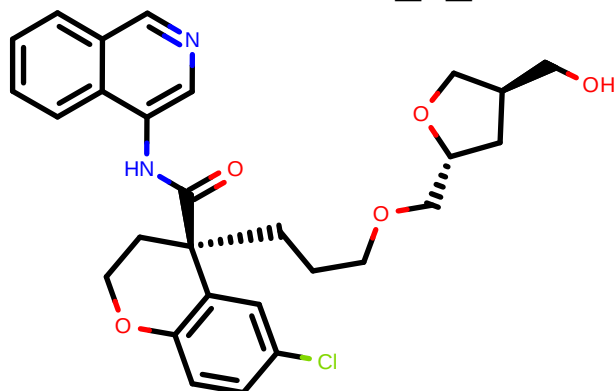
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5ccnn5

RUN: RUN1424

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.19

EN300-6494158_4_2



CID: EN300-6494158_4_2

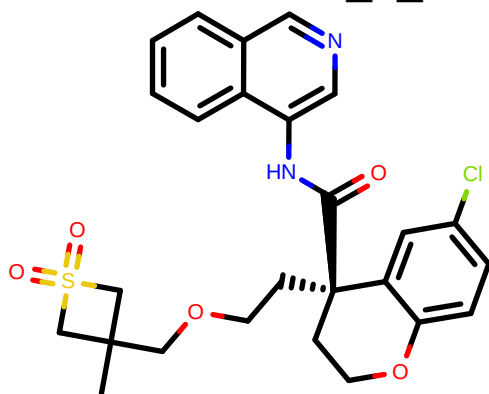
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5C[C@@H](CO)CO

RUN: RUN571

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.50

EN300-1705754_3_1



CID: EN300-1705754_3_1

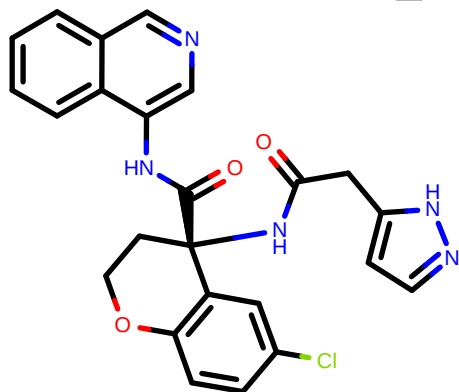
SMILES: CC1(CS(=O)(=O)C1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccs5

RUN: RUN417

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.32

VLA-UCB-34f3ed0c-4_1



CID: VLA-UCB-34f3ed0c-4_1

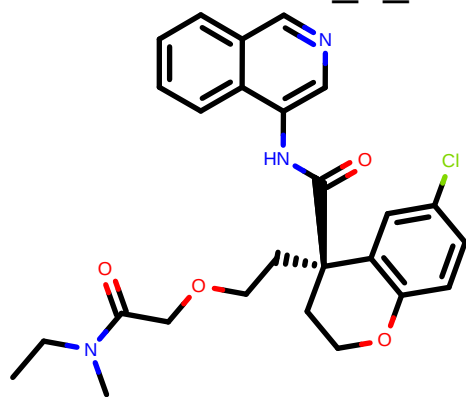
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cc[nH]5

RUN: RUN266

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.23

EN300-1253122_3_1



CID: EN300-1253122_3_1

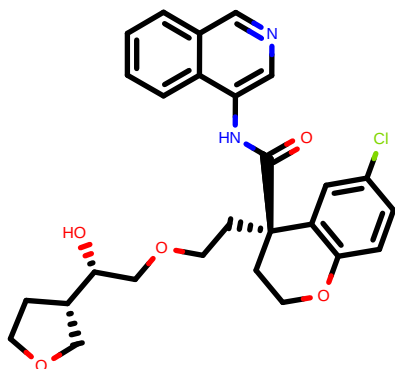
SMILES: CCN(C)C(=O)COC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN576

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.28

EN300-1911992_3_4



CID: EN300-1911992_3_4

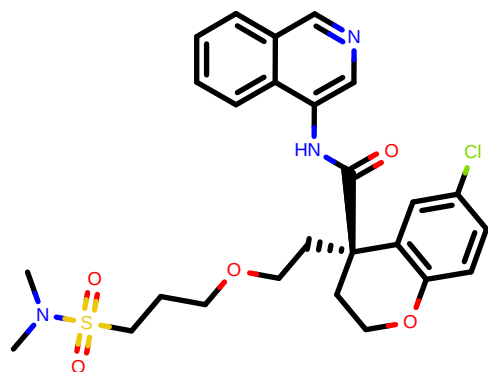
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(COC4c3cc(cc4)Cl)CCOC[C@H]([C@H]5CCOC5)O

RUN: RUN449

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.36

EN300-66432_3_1



CID: EN300-66432_3_1

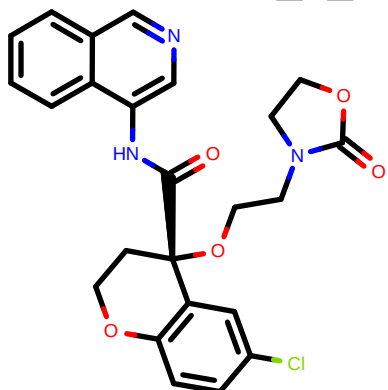
SMILES: CN(C)S(=O)(=O)CCCOC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN441

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.38

EN300-370967_1_1



CID: EN300-370967_1_1

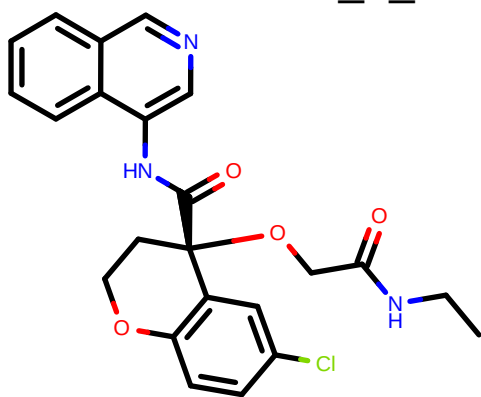
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(COC4c3cc(cc4)Cl)OCCN5CCOC5=O

RUN: RUN1655

DDG (kcal/mol): -2.30

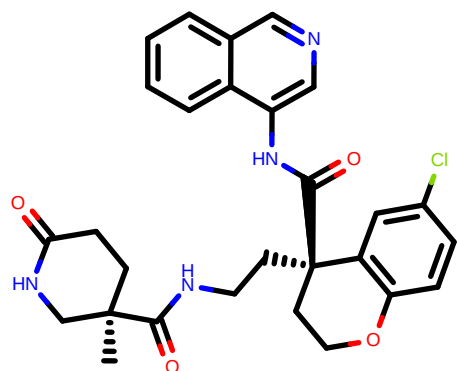
dDDG (kcal/mol): 0.27

EN300-7003350_1_1



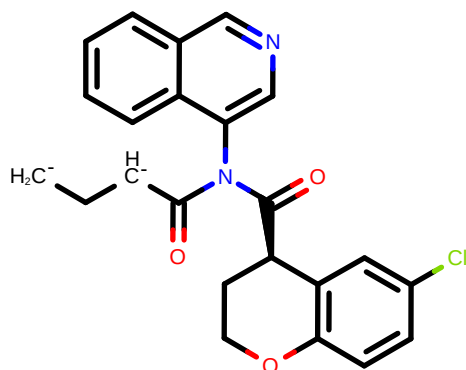
CID:	EN300-7003350_1_1
SMILES:	<chem>CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN738
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.20

EN300-195924_3_2



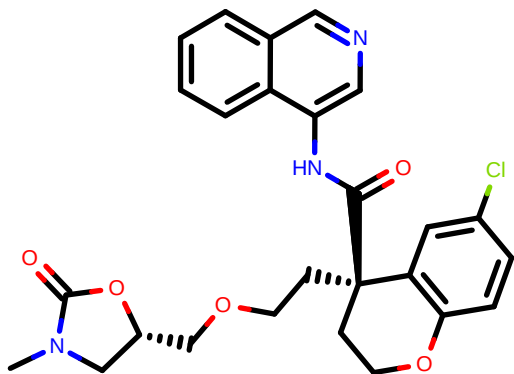
CID:	EN300-195924_3_2
SMILES:	<chem>Cl[C@]1(CCC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1530
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.33

DAR-DIA-5ff57136-11_1



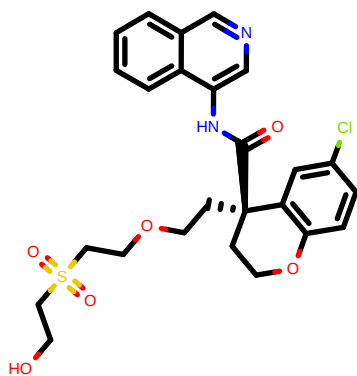
CID:	DAR-DIA-5ff57136-11_1
SMILES:	<chem>C=C=CC(=O)N(c1ncc2c1cccc2)C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN221
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.19

EN300-222969_3_2



CID:	EN300-222969_3_2
SMILES:	<chem>CN1C[C@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN457
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.31

EN300-7463171_3_1



CID:

EN300-7463171_3_1

SMILES:

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

RUN:

RUN813

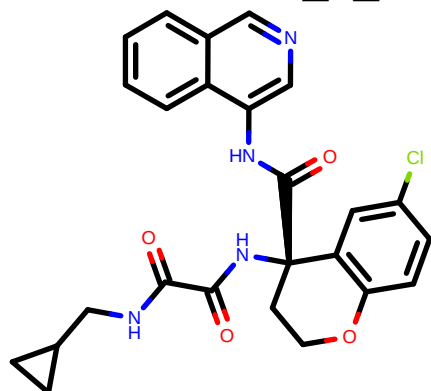
DDG (kcal/mol):

-2.27

dDDG (kcal/mol):

0.64

EN300-173216_1_1



CID:

EN300-173216_1_1

SMILES:

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

RUN:

RUN1716

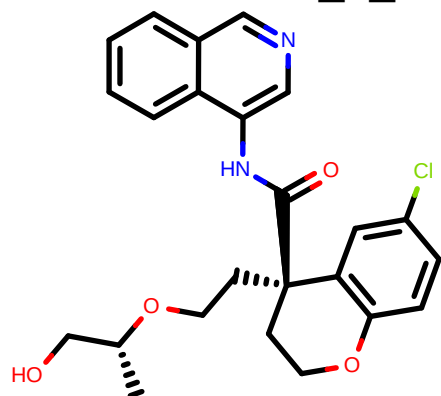
DDG (kcal/mol):

-2.27

dDDG (kcal/mol):

0.22

EN300-175186_3_2



CID:

EN300-175186_3_2

SMILES:

C[C@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1364

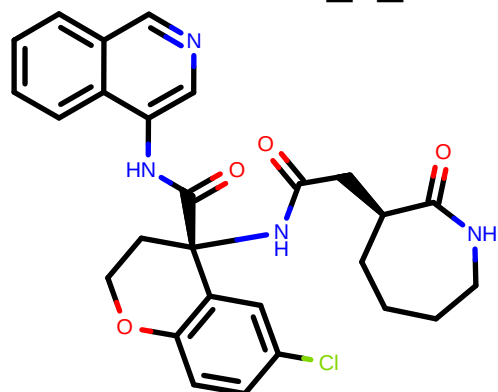
DDG (kcal/mol):

-2.25

dDDG (kcal/mol):

0.25

EN300-198633_1_1



CID:

EN300-198633_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5C5CCNC5=O

RUN:

RUN1045

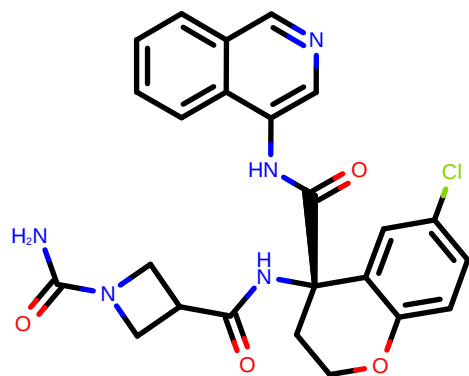
DDG (kcal/mol):

-2.24

dDDG (kcal/mol):

0.30

EN300-1248250_1_1



CID:

EN300-1248250_1_1

SMILES:

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

RUN:

RUN1293

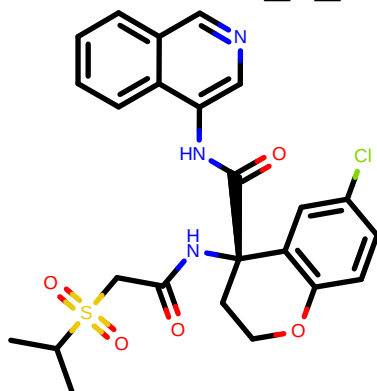
DDG (kcal/mol):

-2.24

dDDG (kcal/mol):

0.24

EN300-51028_1_1



CID:

EN300-51028_1_1

SMILES:

CC(C)S(=O)(=O)CC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4

RUN:

RUN941

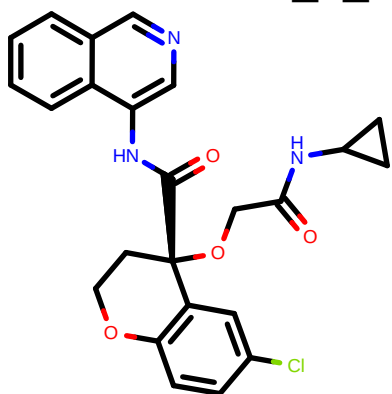
DDG (kcal/mol):

-2.24

dDDG (kcal/mol):

0.27

EN300-1253178_1_1



CID:

EN300-1253178_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN:

RUN620

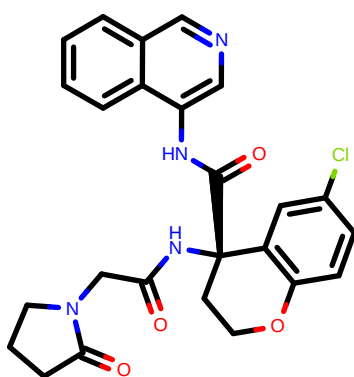
DDG (kcal/mol):

-2.24

dDDG (kcal/mol):

0.26

EN300-11934_1_1



CID:

EN300-11934_1_1

SMILES:

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

RUN:

RUN1405

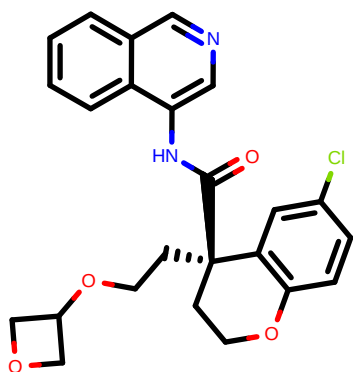
DDG (kcal/mol):

-2.24

dDDG (kcal/mol):

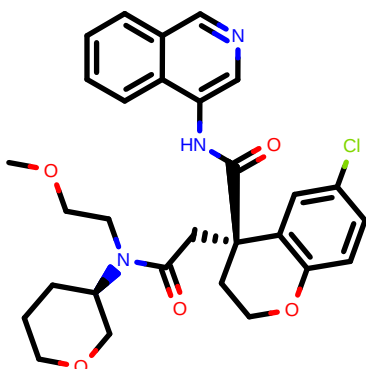
0.24

EN300-317082_3_1



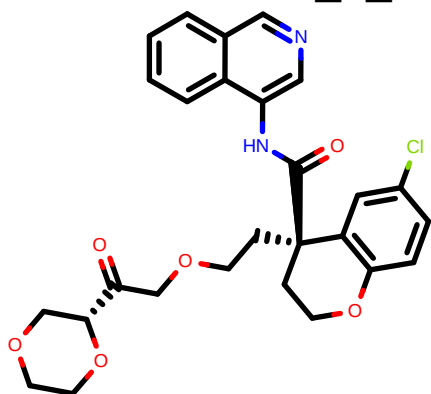
CID:	EN300-317082_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5COC5</chem>
RUN:	RUN1340
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.21

JAG-UCB-706446eb-5_1



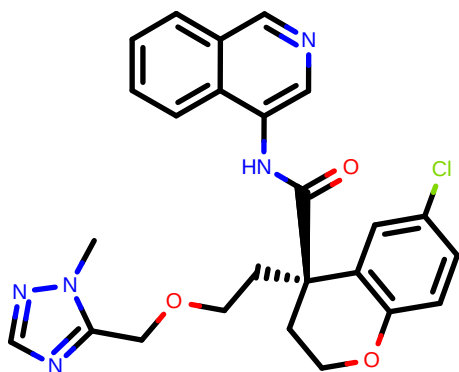
CID:	JAG-UCB-706446eb-5_1
SMILES:	<chem>COCN([C@@H]1CCCOC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN264
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.27

EN300-6238494_3_2



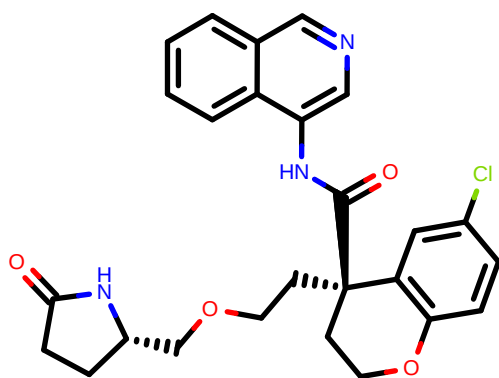
CID:	EN300-6238494_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)[C@H]5COCOC5</chem>
RUN:	RUN1076
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.33

EN300-87334_3_1



CID:	EN300-87334_3_1
SMILES:	<chem>Cn1c(ncn1)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1300
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.27

EN300-264301_3_1



CID: EN300-264301_3_1

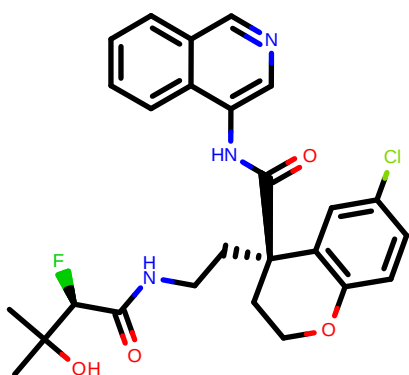
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCC(=O)N5

RUN: RUN860

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.25

EN300-264744_3_2



CID: EN300-264744_3_2

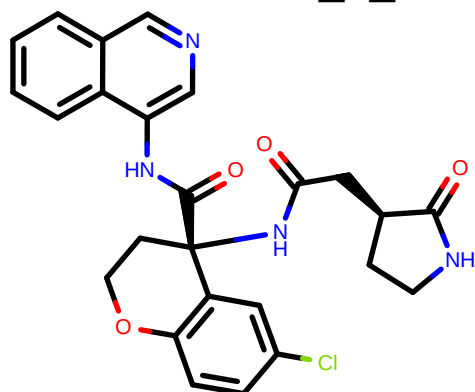
SMILES: CC(C)[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4F)O

RUN: RUN1338

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.30

EN300-343474_1_1



CID: EN300-343474_1_1

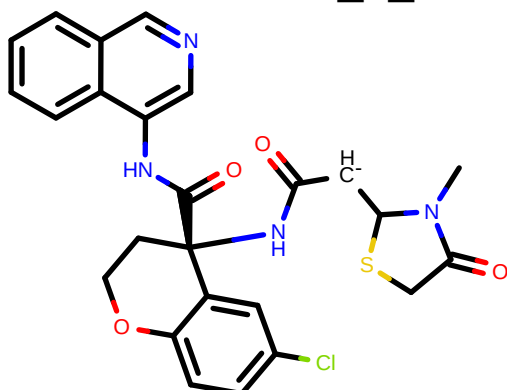
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCNC5=O

RUN: RUN673

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.29

EN300-143564_1_2



CID: EN300-143564_1_2

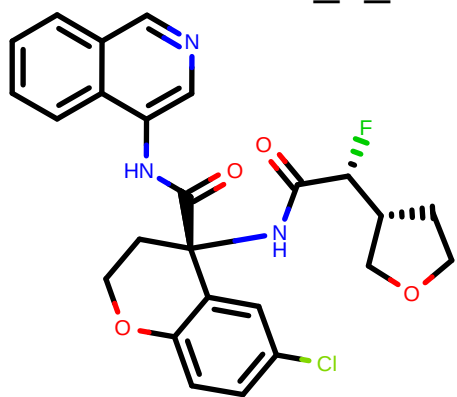
SMILES: CN1C(=O)CS/C1=C/C(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN529

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.22

EN300-783124_1_1



CID: EN300-783124_1_1

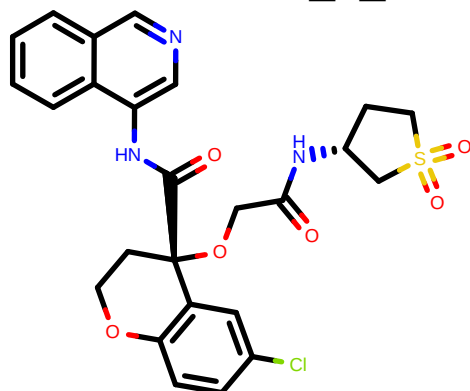
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4C3CC(Cc4)C)NC(=O)[C@H]([C@@H]5CCOC5)F

RUN: RUN1469

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.23

EN300-05512_1_1



CID: EN300-05512_1_1

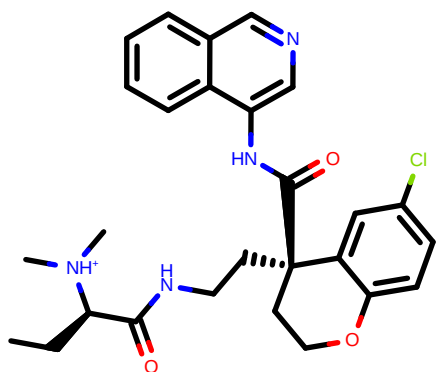
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4C3CC(Cc4)C)OCC(=O)N[C@@H]5CCS(=O)(=O)C5

RUN: RUN421

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.41

EN300-110012_3_2



CID: EN300-110012_3_2

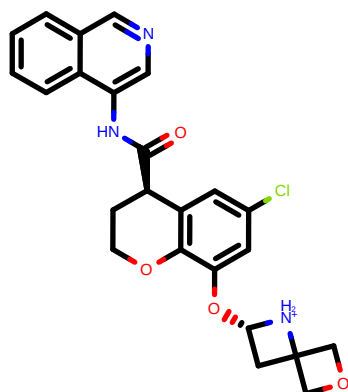
SMILES: CC[C@H](C(=O)NCC[C@]1(CCOC2C1CC(Cc2)C)C(=O)Nc3ncnc4c3cccc4)(NH+)(C)C

RUN: RUN654

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.42

DAR-DIA-23e5a6a0-3_2



CID: DAR-DIA-23e5a6a0-3_2

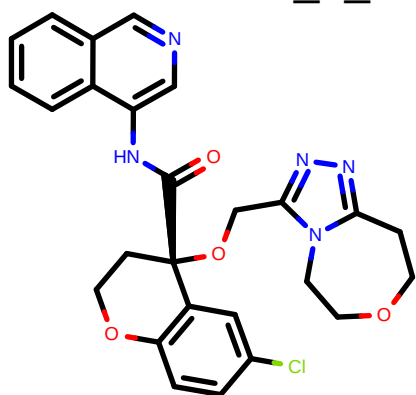
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4C3CC(Cc4)C)[C@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN91

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.30

EN300-310888_1_1



CID: EN300-310888_1_1

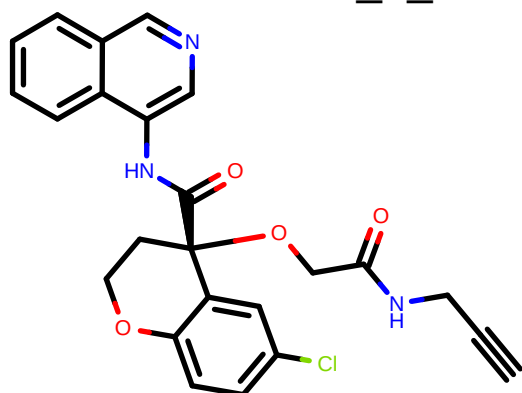
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5nnnc6n5CCOC6

RUN: RUN1048

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.29

EN300-1659582_1_1



CID: EN300-1659582_1_1

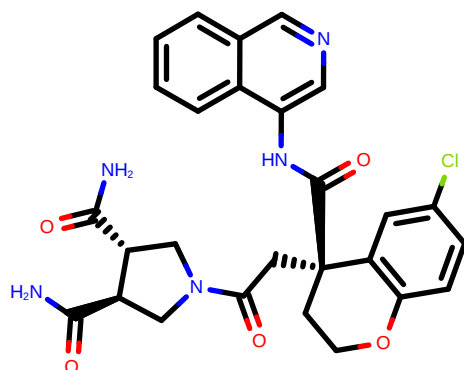
SMILES: C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3cccc4

RUN: RUN461

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.26

EN300-7444316_1_1



CID: EN300-7444316_1_1

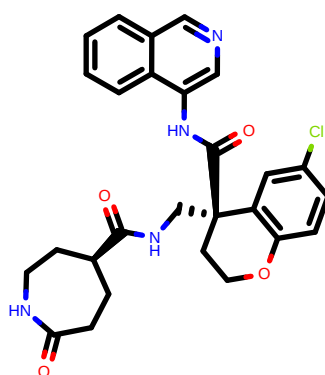
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@H](C[C@@H](C5)Cl=O)N[C@@H]6C(=O)N[C@@H]6C(=O)N

RUN: RUN1402

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.53

EN300-152337_2_2



CID: EN300-152337_2_2

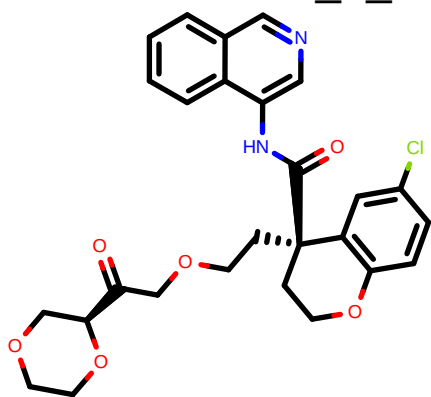
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCC(=O)NC5

RUN: RUN310

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.38

EN300-6238494_3_1



CID: EN300-6238494_3_1

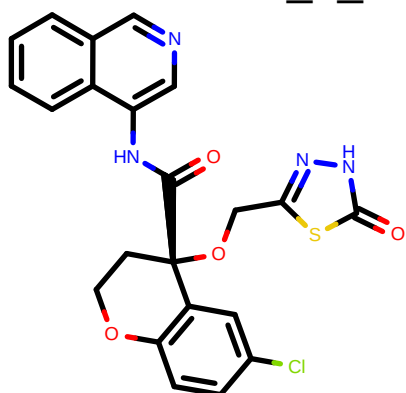
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)C[C@@H]5COCCO5

RUN: RUN940

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.32

EN300-171766_1_1



CID: EN300-171766_1_1

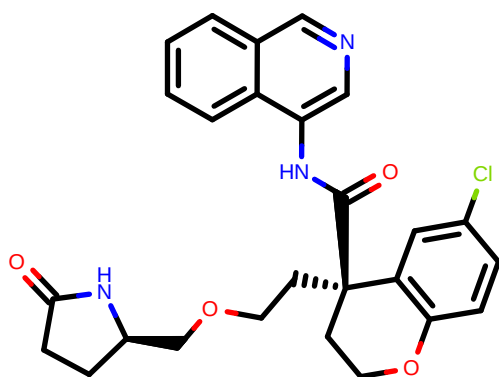
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5n[nH]c(=O)s5

RUN: RUN636

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.22

EN300-195756_3_2



CID: EN300-195756_3_2

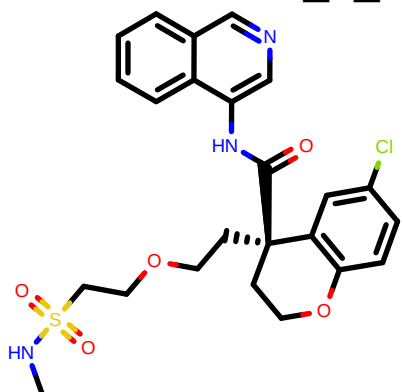
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCCC(=O)N5

RUN: RUN1084

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.24

EN300-6482967_3_1



CID: EN300-6482967_3_1

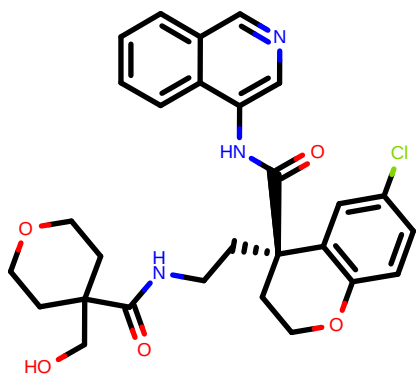
SMILES: CNS(=O)(=O)CCOCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN329

DDG (kcal/mol): -2.16

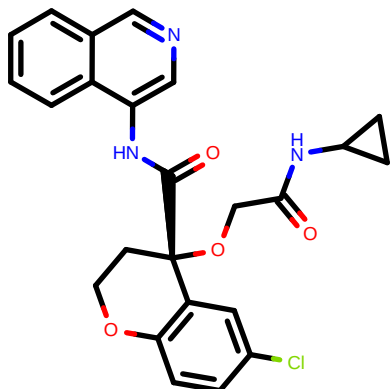
dDDG (kcal/mol): 0.33

EN300-244909_3_1



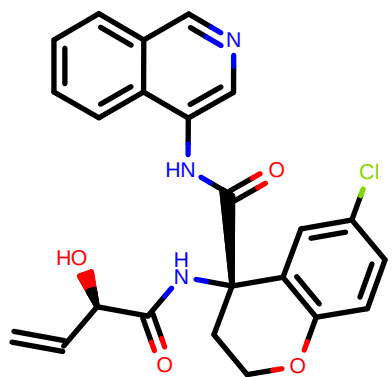
CID:	EN300-244909_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCOCC5)CO</chem>
RUN:	RUN1138
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.37

EN300-1253178_1_1



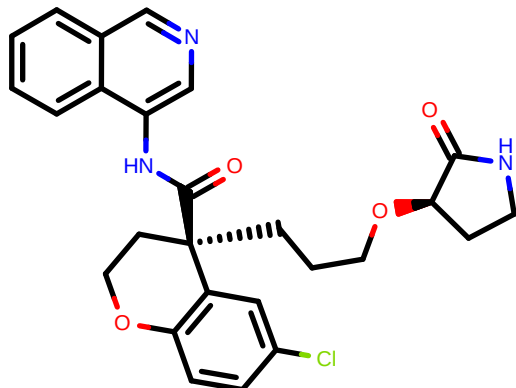
CID:	EN300-1253178_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5</chem>
RUN:	RUN628
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.20

EN300-181492_1_2



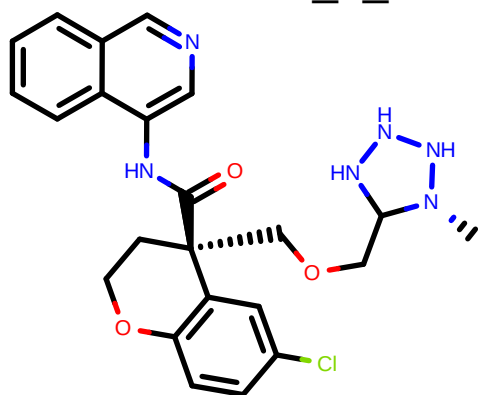
CID:	EN300-181492_1_2
SMILES:	<chem>C=C[C@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)O</chem>
RUN:	RUN1165
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.29

EN300-6736413_4_1



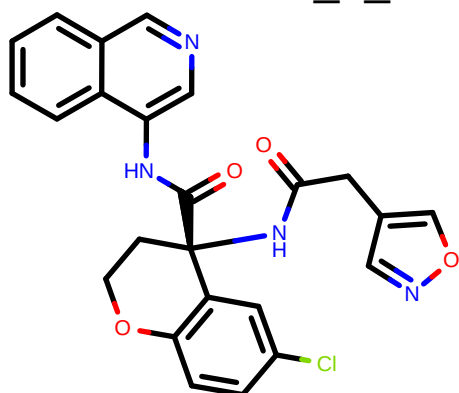
CID:	EN300-6736413_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O</chem>
RUN:	RUN983
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.34

EN300-62574_2_1



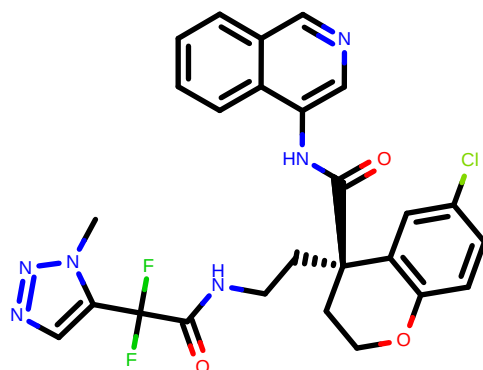
CID:	EN300-62574_2_1
SMILES:	<chem>Cn1c(nnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1102
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.28

EN300-315963_1_1



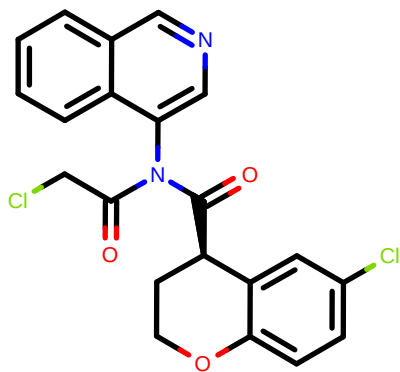
CID:	EN300-315963_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnoc5</chem>
RUN:	RUN1077
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.24

EN300-1726073_3_1



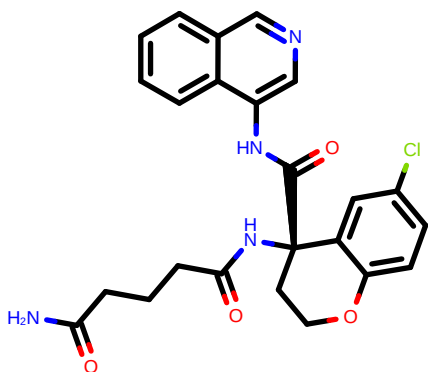
CID:	EN300-1726073_3_1
SMILES:	<chem>Cn1c(cnn1)C(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(F)F</chem>
RUN:	RUN1705
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.32

VLA-UCB-50c39ae8-6_1



CID:	VLA-UCB-50c39ae8-6_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN122
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.18

EN300-59478_1_1



CID: EN300-59478_1_1

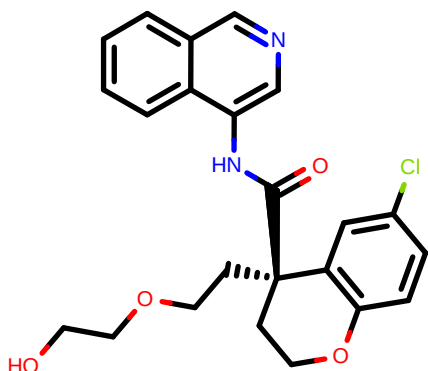
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN790

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.31

EN300-21258_3_1



CID: EN300-21258_3_1

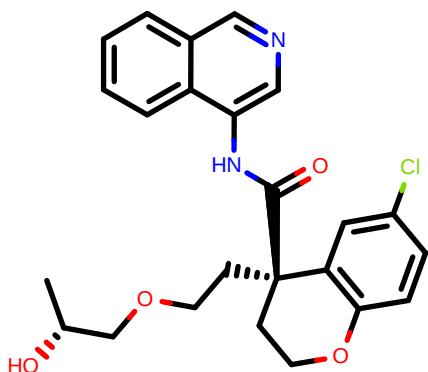
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)O

RUN: RUN1516

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.26

EN300-185378_3_2



CID: EN300-185378_3_2

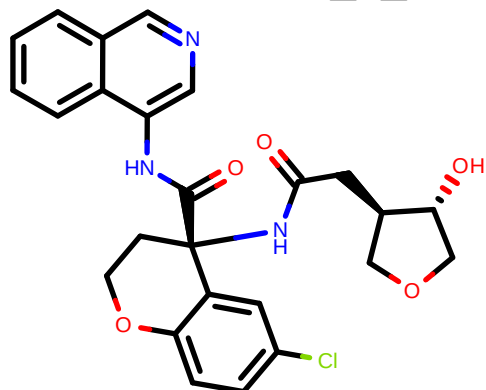
SMILES: C[C@H](COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccc4)O

RUN: RUN1643

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.24

EN300-1708882_1_1



CID: EN300-1708882_1_1

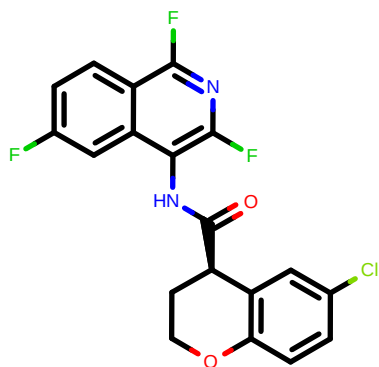
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5COC[C@H]5O

RUN: RUN751

DDG (kcal/mol): -2.10

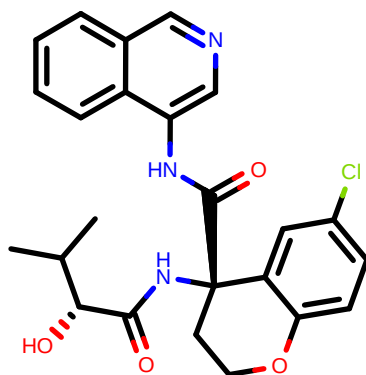
dDDG (kcal/mol): 0.25

JOH-SUS-a69c159d-7_1



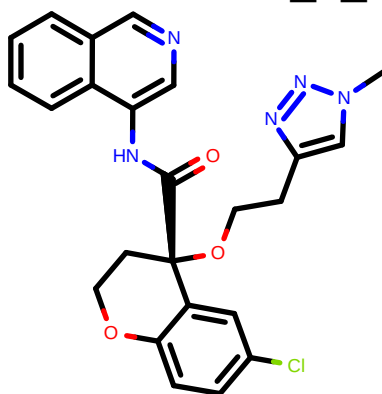
CID:	JOH-SUS-a69c159d-7_1
SMILES:	<chem>c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN71
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.06

EN300-115017_1_1



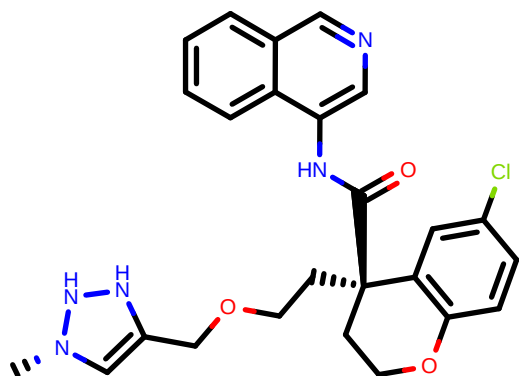
CID:	EN300-115017_1_1
SMILES:	<chem>CC(C)[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O</chem>
RUN:	RUN458
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.24

EN300-1600786_1_1



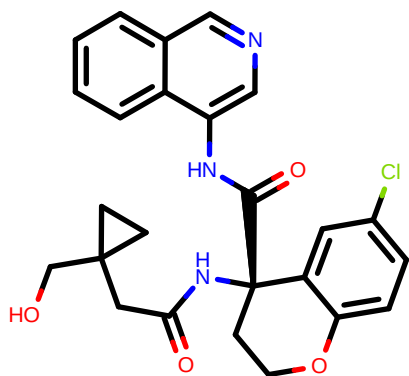
CID:	EN300-1600786_1_1
SMILES:	<chem>Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1024
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.22

EN300-120282_3_1



CID:	EN300-120282_3_1
SMILES:	<chem>Cn1cc(nn1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1324
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.26

EN300-107048_1_1



CID: EN300-107048_1_1

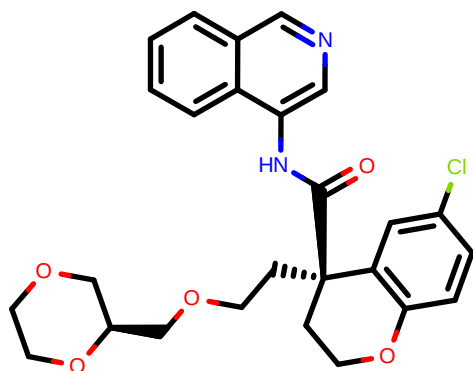
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)NC(=O)CC5(CC5)CO

RUN: RUN418

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.25

EN300-139167_3_1



CID: EN300-139167_3_1

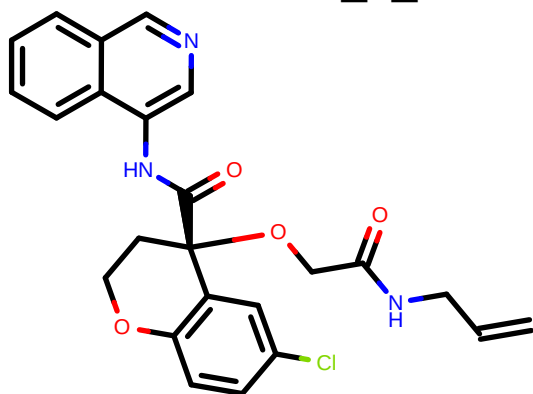
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5COCCO5

RUN: RUN640

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.37

EN300-17184_1_1



CID: EN300-17184_1_1

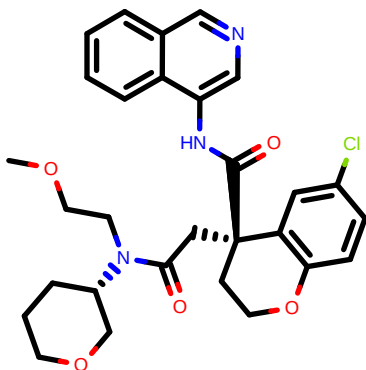
SMILES: C=CCNC(=O)CO[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN445

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.19

JAG-UCB-706446eb-5_2



CID: JAG-UCB-706446eb-5_2

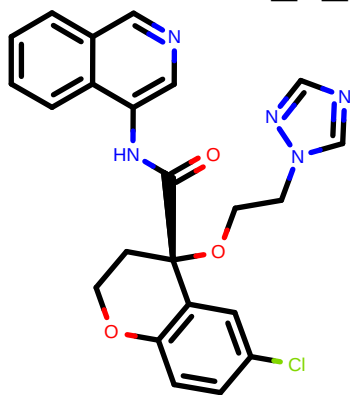
SMILES: COCCN([C@@H]1CCCOC1)C(=O)C[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN265

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.30

EN300-6255179_1_1



CID: EN300-6255179_1_1

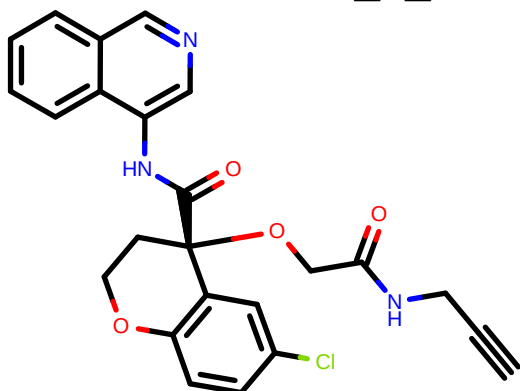
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnc5

RUN: RUN1088

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.19

EN300-1659582_1_1



CID: EN300-1659582_1_1

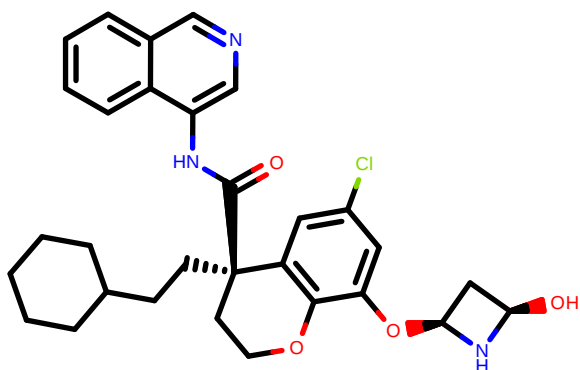
SMILES: C#CCNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN469

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.18

VLA-UCB-50c39ae8-9_2



CID: VLA-UCB-50c39ae8-9_2

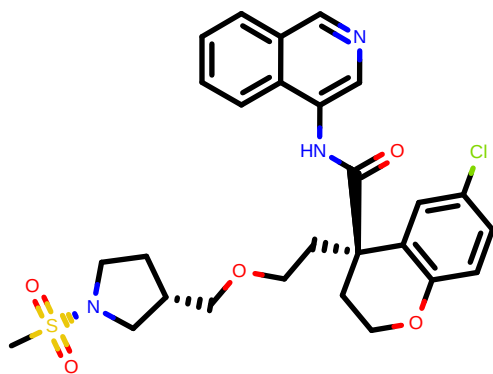
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[C@H]5CC(=O)N5)Cl)CC6CCCCC6

RUN: RUN124

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.30

EN300-261986_3_1



CID: EN300-261986_3_1

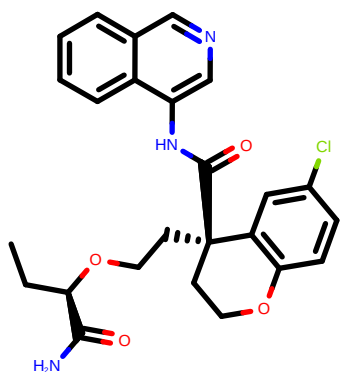
SMILES: CS(=O)(=O)N1CC[C@@H]1CC[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN465

DDG (kcal/mol): -2.03

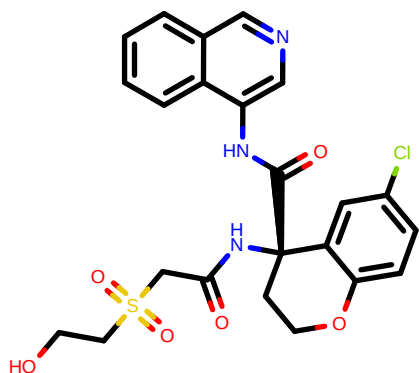
dDDG (kcal/mol): 0.36

EN300-65839_3_2



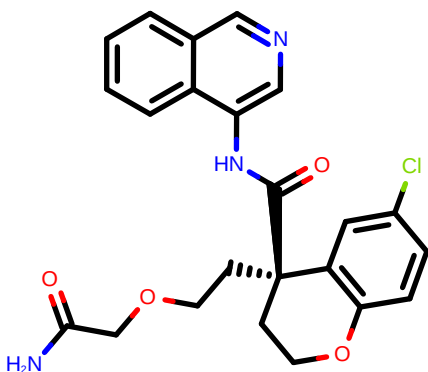
CID:	EN300-65839_3_2
SMILES:	<chem>CC[C@H](C(=O)N)OCC[C@]1(COC(=O)Cc2cc(Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1699
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.33

EN300-4293814_1_1



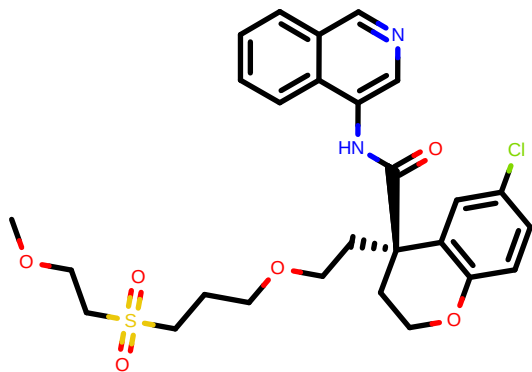
CID:	EN300-4293814_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(Cl)C(=O)N)C(=O)CS(=O)(=O)CCO</chem>
RUN:	RUN466
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.48

EN300-18249_3_1



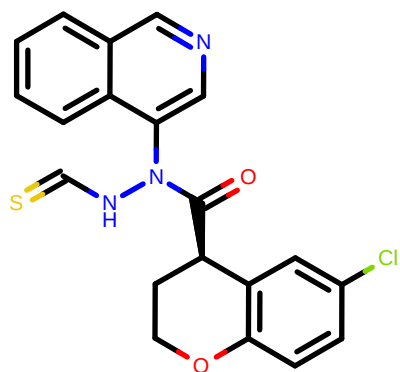
CID:	EN300-18249_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(Cl)C(=O)N)C(=O)OCC(=O)N</chem>
RUN:	RUN1564
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.20

EN300-62857_3_1



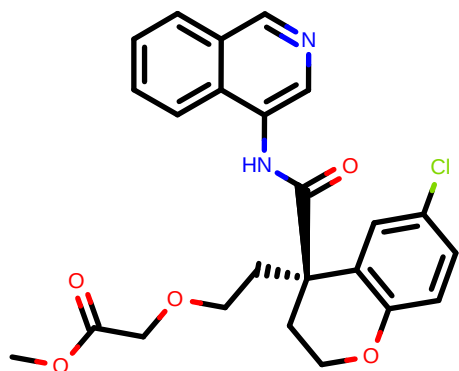
CID:	EN300-62857_3_1
SMILES:	<chem>COCCS(=O)(=O)CCCOC[C@]1(CCOc2c1cc(Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN608
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.48

DAR-DIA-5ff57136-18_1



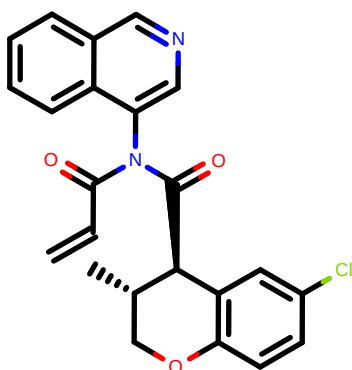
CID:	DAR-DIA-5ff57136-18_1
SMILES:	<chem>c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOCc4c3cc(cc4)Cl)N=C=S</chem>
RUN:	RUN101
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.13

EN300-19700_3_1



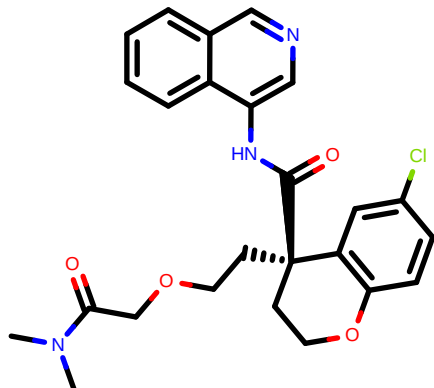
CID:	EN300-19700_3_1
SMILES:	<chem>COC(=O)COCC[C@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1579
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.21

DAR-DIA-5ff57136-2_1



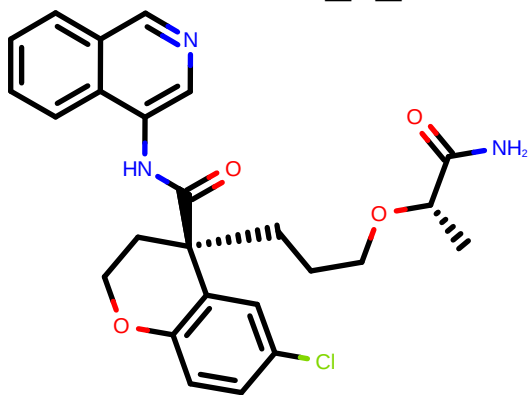
CID:	DAR-DIA-5ff57136-2_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl</chem>
RUN:	RUN134
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.17

EN300-216063_3_1



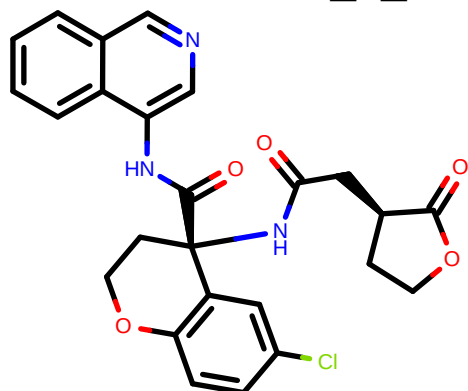
CID:	EN300-216063_3_1
SMILES:	<chem>CN(C)C(=O)COCC[C@H]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1476
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.28

EN300-17381_4_1



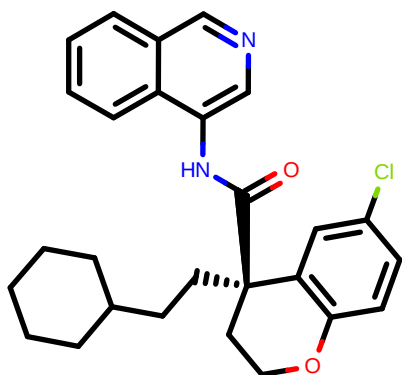
CID:	EN300-17381_4_1
SMILES:	<chem>C[C@@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4</chem>
RUN:	RUN1071
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.34

EN300-1072972_1_1



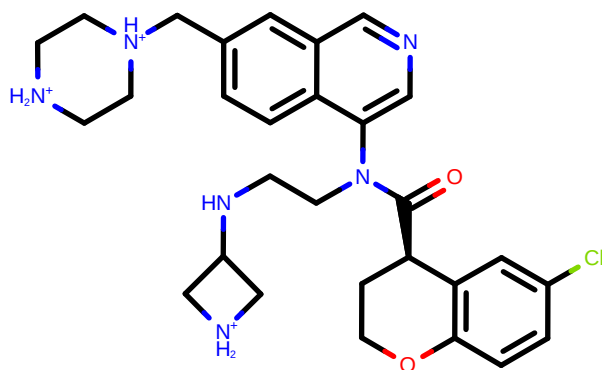
CID:	EN300-1072972_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCOC5=O</chem>
RUN:	RUN1133
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.26

VLA-UCB-50c39ae8-10_1



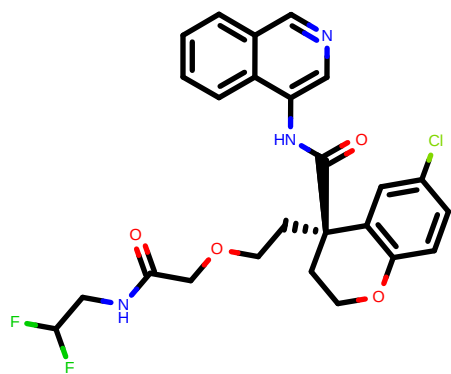
CID:	VLA-UCB-50c39ae8-10_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCCCCC5</chem>
RUN:	RUN141
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.25

MAK-UNK-83e0a0b4-2_1



CID:	MAK-UNK-83e0a0b4-2_1
SMILES:	<chem>c1cc2cc(c1CN3CC[NH2+])CC3]cncc2N(CCNc4c1cc(cc4)Cl)C(=O)[C@@H]5CCOC5c6ccccc6Cl</chem>
RUN:	RUN34
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.50

EN300-120586_3_1



CID: EN300-120586_3_1

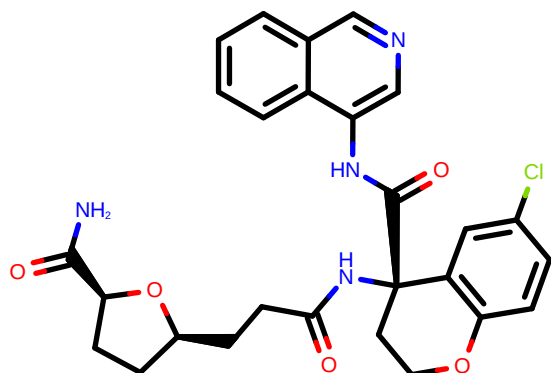
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCC(F)F

RUN: RUN369

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.30

EN300-364992_1_1



CID: EN300-364992_1_1

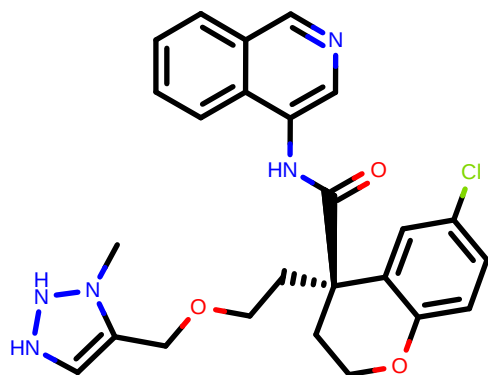
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC[C@H]5O

RUN: RUN696

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.38

EN300-216673_3_1



CID: EN300-216673_3_1

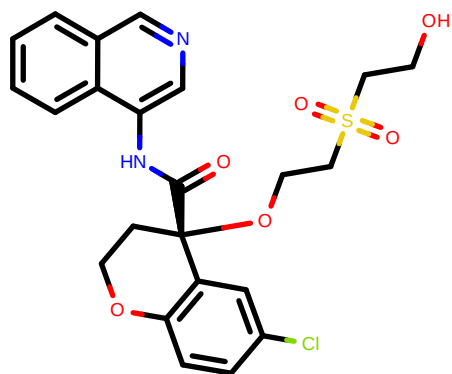
SMILES: Cn1c(cnn1)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1180

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.31

EN300-7463171_1_1



CID: EN300-7463171_1_1

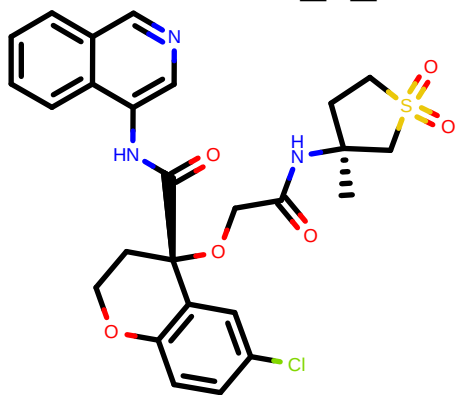
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCO

RUN: RUN612

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.48

EN300-10414_1_1



CID: EN300-10414_1_1

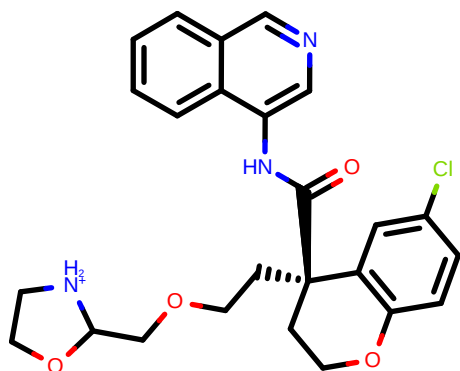
SMILES: C[C@@]1([C](=O)(=O)C1)NC(=O)CO[C@]2(CCOC3C2CC(C3)Cl)C(=O)Nc4nc5c4ccccc5

RUN: RUN437

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.35

EN300-317555_3_1



CID: EN300-317555_3_1

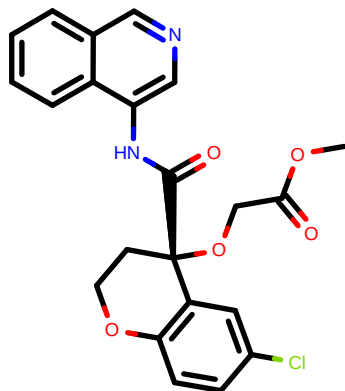
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4C3CC(C4)Cl)CCOCC5=NCCO5

RUN: RUN797

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.27

EN300-19700_1_1



CID: EN300-19700_1_1

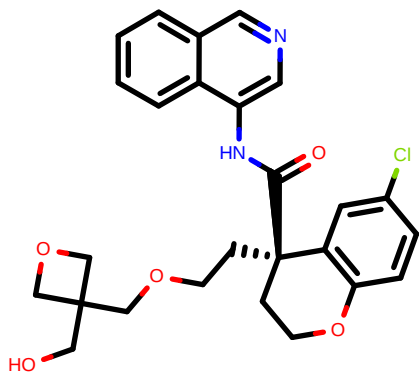
SMILES: COC(=O)CO[C@]1([C](O)C2C1CC(C2)Cl)C(=O)Nc3nc4c3ccccc4

RUN: RUN373

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.18

EN300-102347_3_1



CID: EN300-102347_3_1

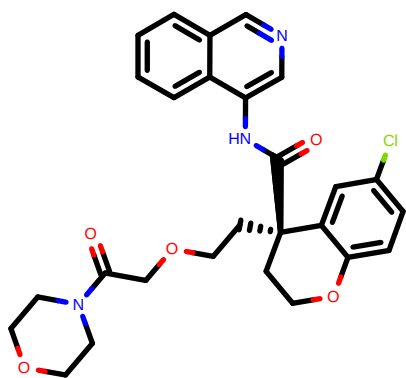
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4C3CC(C4)Cl)CCOCC5(COC5)CO

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)C)CCOCC(=O)N5CCOCC5

RUN:

RUN829

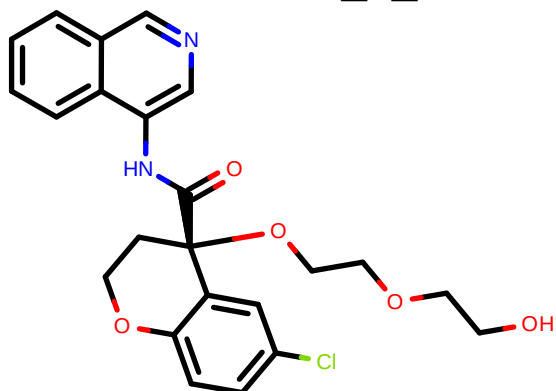
DDG (kcal/mol):

-1.94

dDDG (kcal/mol):

0.31

EN300-52467_1_1



CID:

EN300-52467_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCCOCCO

RUN:

RUN912

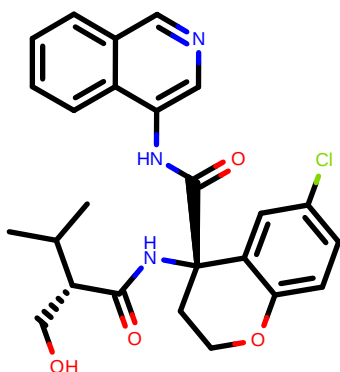
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

0.25

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

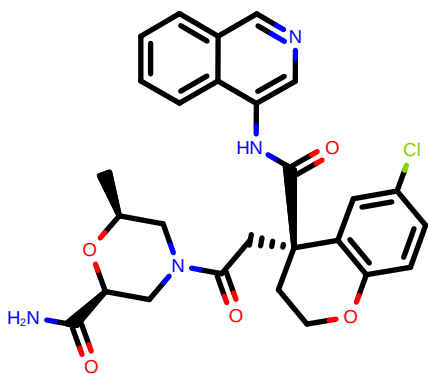
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

0.24

EN300-295905_1_4



CID:

EN300-295905_1_4

SMILES:

C[C@@H]1CN(C[C@@H](O1)C(=O)N)C(=O)C[C@@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN:

RUN733

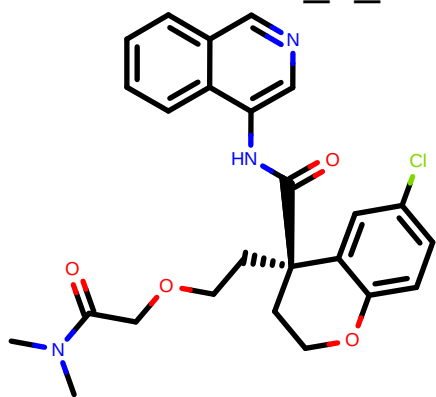
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

0.30

EN300-216063_3_1



CID:

EN300-216063_3_1

SMILES:

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

RUN:

RUN1460

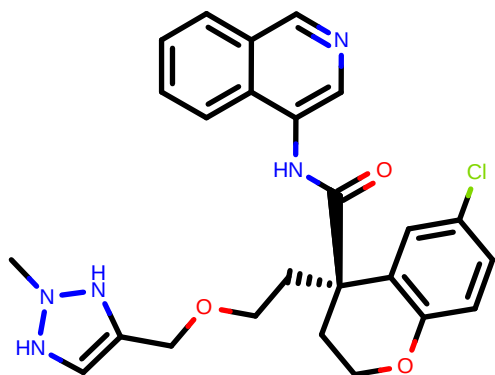
DDG (kcal/mol):

-1.93

dDDG (kcal/mol):

0.27

EN300-219020_3_1



CID:

EN300-219020_3_1

SMILES:

Cn1ncc(n1)COCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN1635

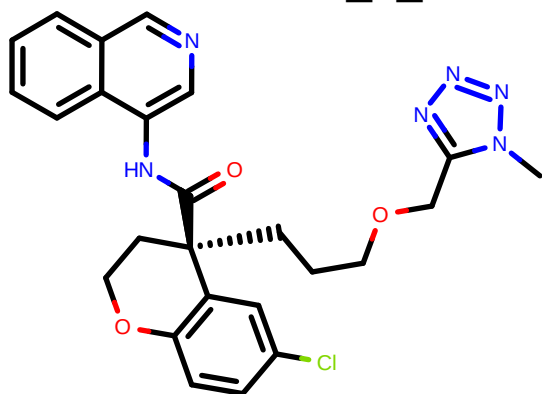
DDG (kcal/mol):

-1.92

dDDG (kcal/mol):

0.24

EN300-62574_4_1



CID:

EN300-62574_4_1

SMILES:

Cn1c(nnn1)COCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN332

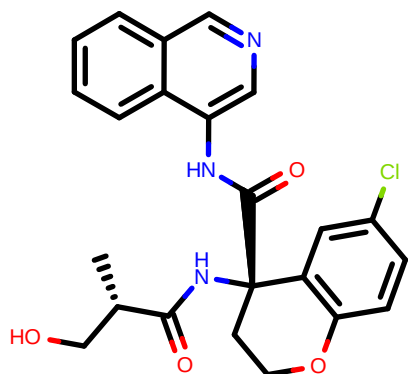
DDG (kcal/mol):

-1.91

dDDG (kcal/mol):

0.39

EN300-55072_1_1



CID:

EN300-55072_1_1

SMILES:

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

RUN:

RUN1381

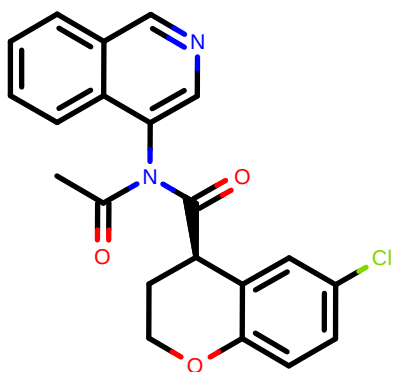
DDG (kcal/mol):

-1.91

dDDG (kcal/mol):

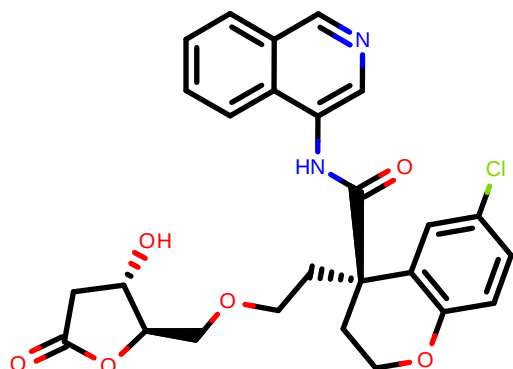
0.26

VLA-UCB-50c39ae8-1_1



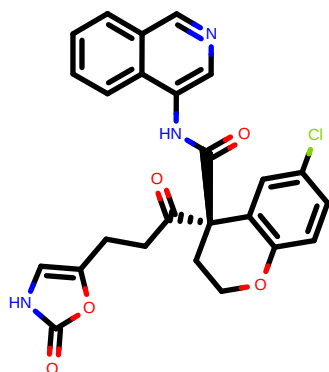
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	<chem>CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN94
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.13

EN300-6487407_3_1



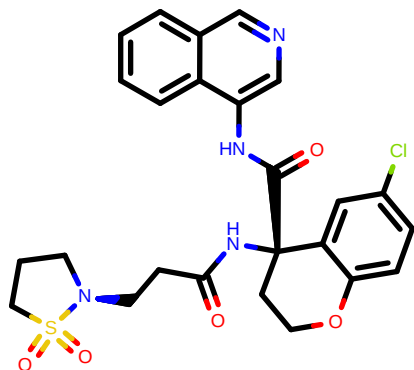
CID:	EN300-6487407_3_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC[C@@H]5[C@@H](CC(=O)O5)O</chem>
RUN:	RUN433
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.38

VLA-UCB-34f3ed0c-9_1



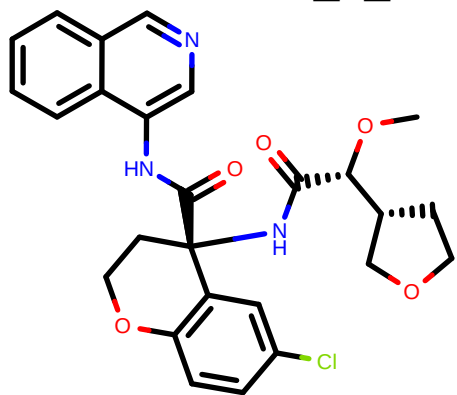
CID:	VLA-UCB-34f3ed0c-9_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5</chem>
RUN:	RUN72
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.33

EN300-44873_1_1



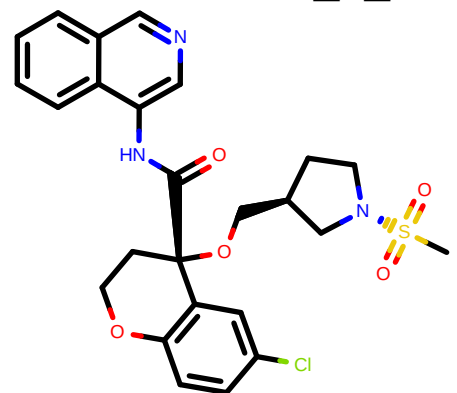
CID:	EN300-44873_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)CC[N@@]5CCCS5(=O)=O</chem>
RUN:	RUN506
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.40

EN300-298552_1_2



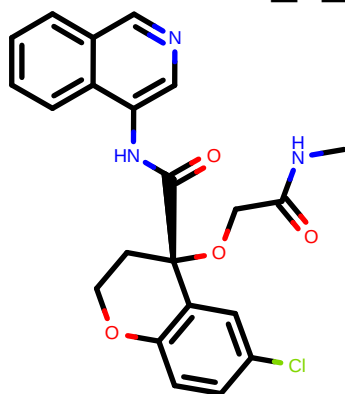
CID:	EN300-298552_1_2
SMILES:	<chem>CO[C@H]([C@@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1373
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.24

EN300-261986_1_1



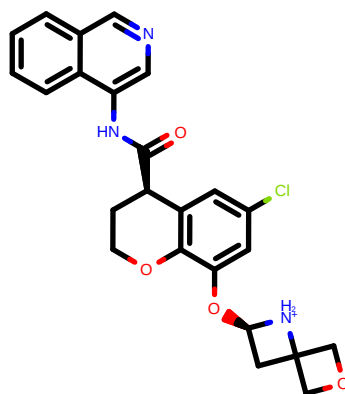
CID:	EN300-261986_1_1
SMILES:	<chem>CS(=O)(=O)N[C@@]1CC[C@H](C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN524
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.29

EN300-2977549_1_1



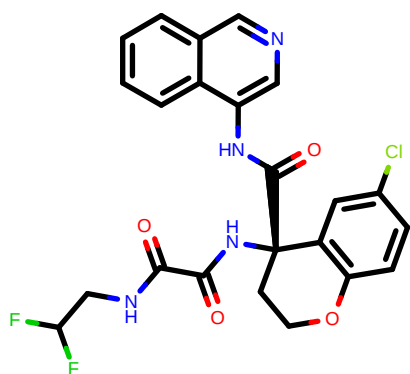
CID:	EN300-2977549_1_1
SMILES:	<chem>CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN1072
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.17

DAR-DIA-23e5a6a0-3_1



CID:	DAR-DIA-23e5a6a0-3_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@@H]5CC6([NH2+][5])COC6)Cl</chem>
RUN:	RUN110
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.31

EN300-128277_1_1



CID: EN300-128277_1_1

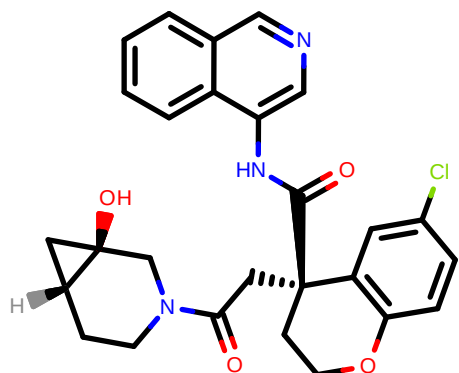
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NCC(F)F

RUN: RUN1157

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.24

EN300-1267093_1_1



CID: EN300-1267093_1_1

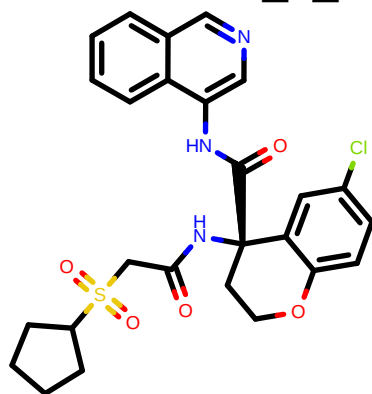
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N6CC[C@H]6[C@@]3(C)O

RUN: RUN1282

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.33

EN300-42154_1_1



CID: EN300-42154_1_1

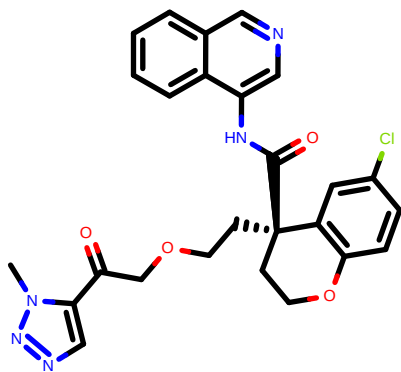
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C5CCCC5

RUN: RUN877

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.32

EN300-204936_3_1



CID: EN300-204936_3_1

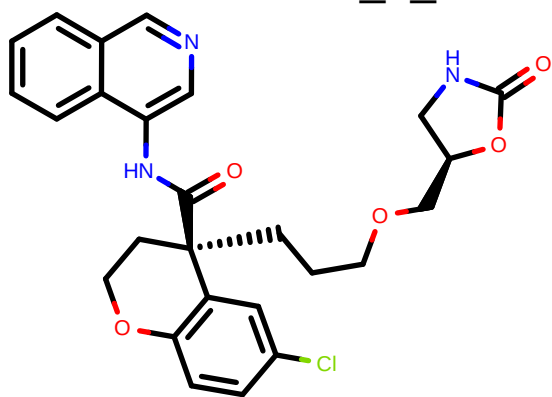
SMILES: Cn1c(cnn1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cc5

RUN: RUN345

DDG (kcal/mol): -1.87

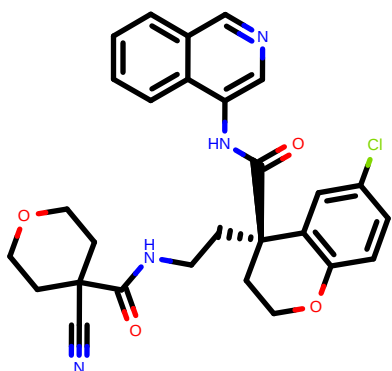
dDDG (kcal/mol): 0.29

EN300-203293_4_2



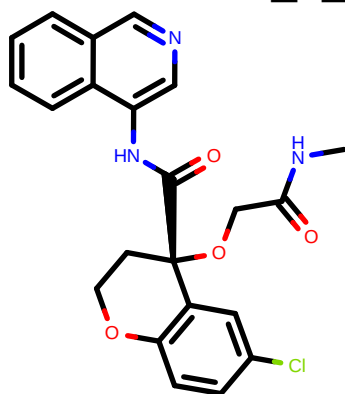
CID:	EN300-203293_4_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CNC(=O)O5</chem>
RUN:	RUN1215
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.44

EN300-74089_3_1



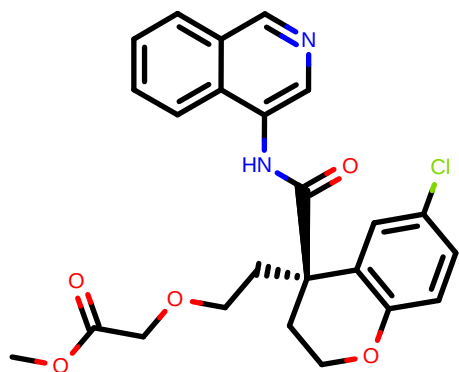
CID:	EN300-74089_3_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCOCC5)C#N</chem>
RUN:	RUN439
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.37

EN300-2977549_1_1



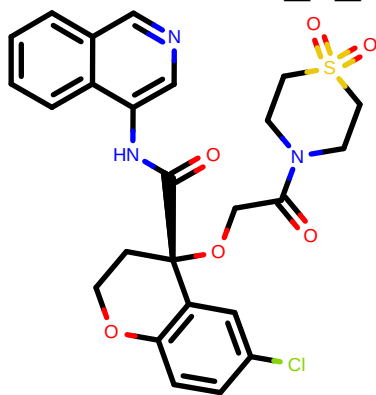
CID:	EN300-2977549_1_1
SMILES:	<chem>CNC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4</chem>
RUN:	RUN1064
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.18

EN300-19700_3_1



CID:	EN300-19700_3_1
SMILES:	<chem>COC(=O)COCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4</chem>
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

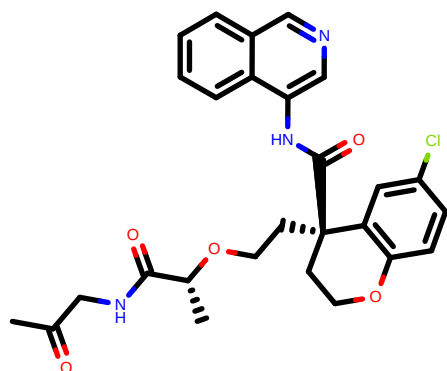
DDG (kcal/mol):

-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)Nc3nccc4c3ccc4

RUN:

RUN1691

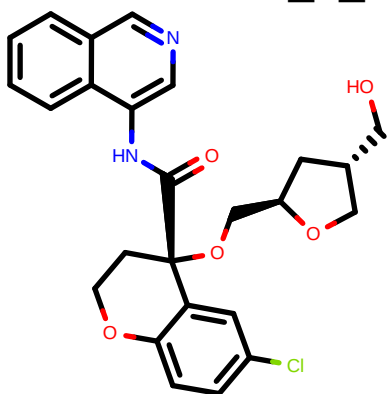
DDG (kcal/mol):

-1.85

dDDG (kcal/mol):

0.30

EN300-6494158_1_2



CID:

EN300-6494158_1_2

SMILES:

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

RUN:

RUN864

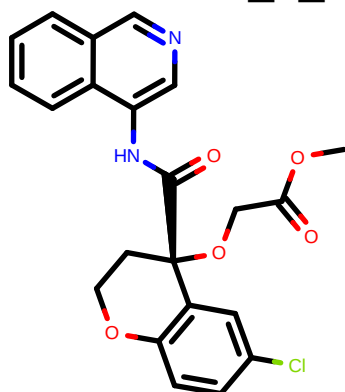
DDG (kcal/mol):

-1.85

dDDG (kcal/mol):

0.32

EN300-19700_1_1



CID:

EN300-19700_1_1

SMILES:

COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccc4

RUN:

RUN381

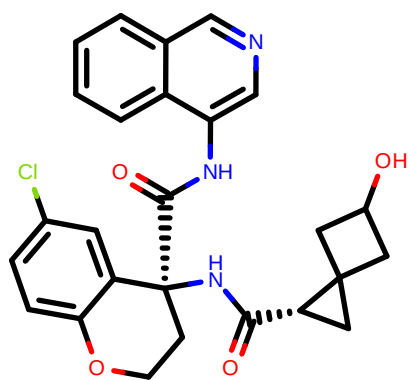
DDG (kcal/mol):

-1.84

dDDG (kcal/mol):

0.20

EN300-1717166_1_2



CID: EN300-1717166_1_2

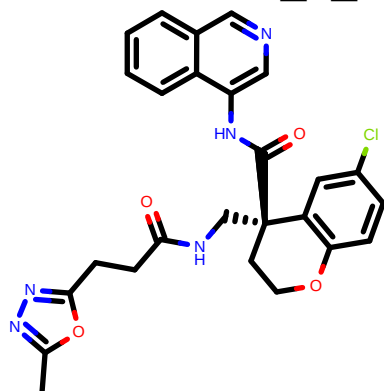
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC56CC(C6)O

RUN: RUN861

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.29

EN300-304662_2_1



CID: EN300-304662_2_1

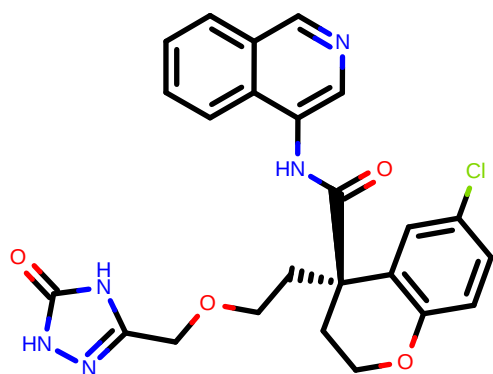
SMILES: Cc1nnc(o1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1273

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.26

EN300-73772_3_1



CID: EN300-73772_3_1

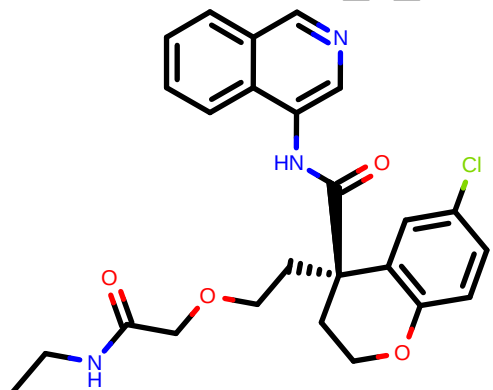
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]n5

RUN: RUN1308

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.27

EN300-7003350_3_1



CID: EN300-7003350_3_1

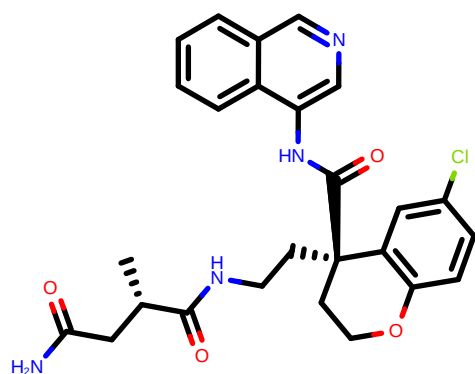
SMILES: CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1484

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.27

EN300-202757_3_1



CID: EN300-202757_3_1

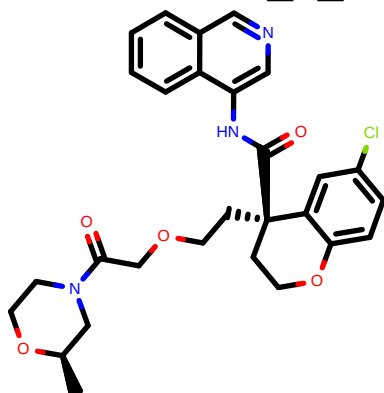
SMILES: C[C@@H](CC(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1442

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.35

EN300-25572_3_1



CID: EN300-25572_3_1

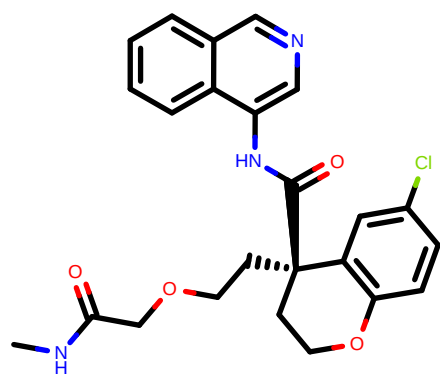
SMILES: C[C@@H]1CN(CCO1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1292

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.35

EN300-2977549_3_1



CID: EN300-2977549_3_1

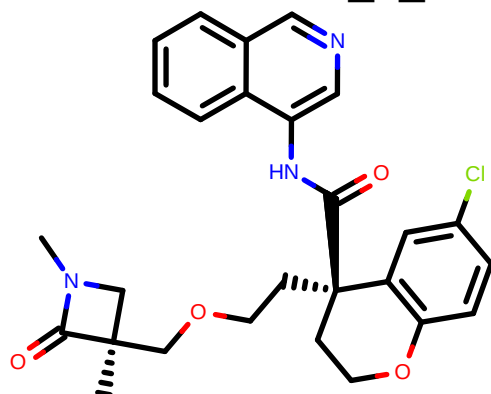
SMILES: CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1747

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.35

EN300-1273362_3_2



CID: EN300-1273362_3_2

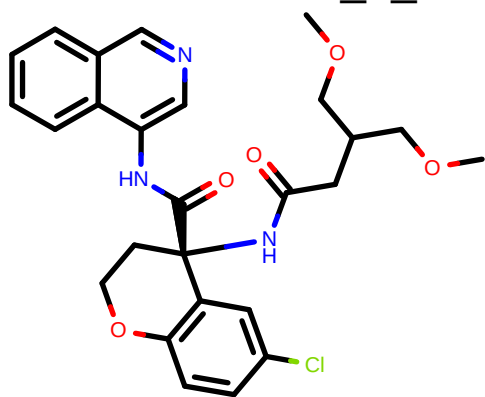
SMILES: C[C@]1(CN(C1=O)C)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN305

DDG (kcal/mol): -1.82

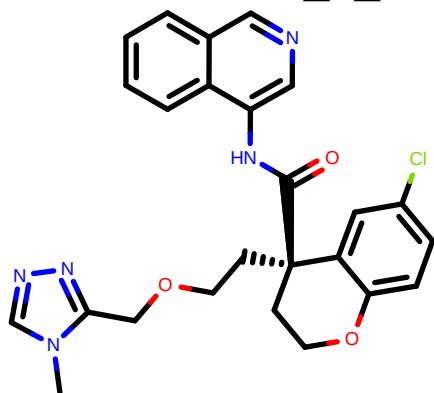
dDDG (kcal/mol): 0.32

EN300-7102031_1_1



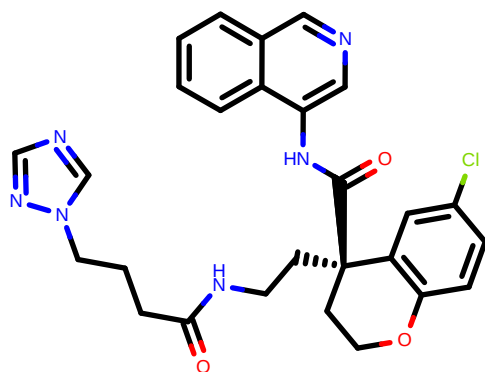
CID:	EN300-7102031_1_1
SMILES:	<chem>COCC(CC(=O)N[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)COC</chem>
RUN:	RUN758
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.28

EN300-113112_3_1



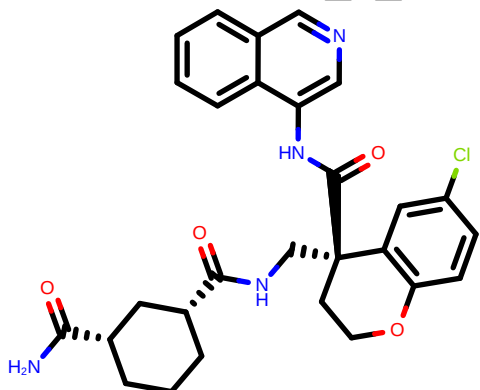
CID:	EN300-113112_3_1
SMILES:	<chem>Cn1cnnc1COCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1723
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.24

EN300-316216_3_1



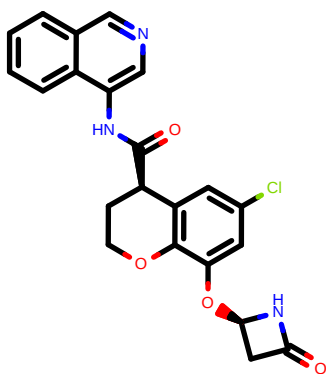
CID:	EN300-316216_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)CCC5cncc5</chem>
RUN:	RUN748
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.37

EN300-90142_2_1



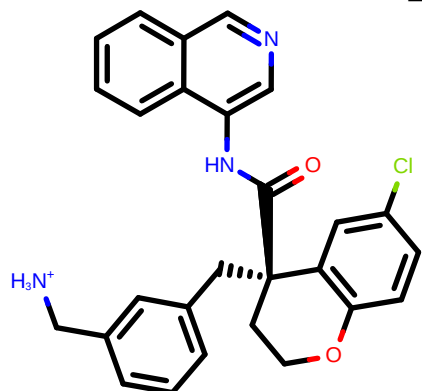
CID:	EN300-90142_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CNC(=O)C[C@@H]5CCCC[C@@H](C5)C(=O)N</chem>
RUN:	RUN406
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.24

VLA-UCB-50c39ae8-8_1



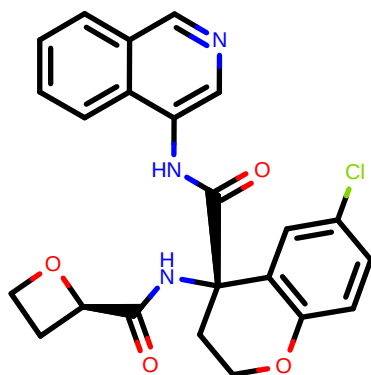
CID:	VLA-UCB-50c39ae8-8_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5Cl</chem>
RUN:	RUN104
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.20

JAG-UCB-706446eb-8_1



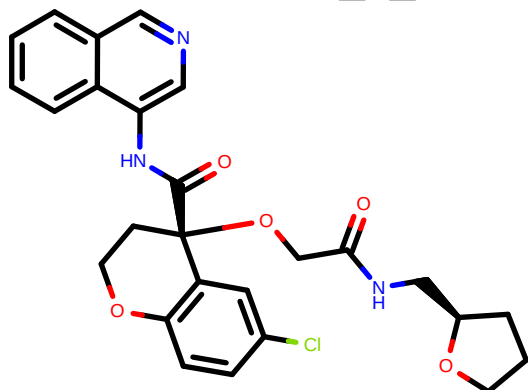
CID:	JAG-UCB-706446eb-8_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)Cc5ccccc5)[C@H]3N3+</chem>
RUN:	RUN140
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.30

EN300-85760_1_2



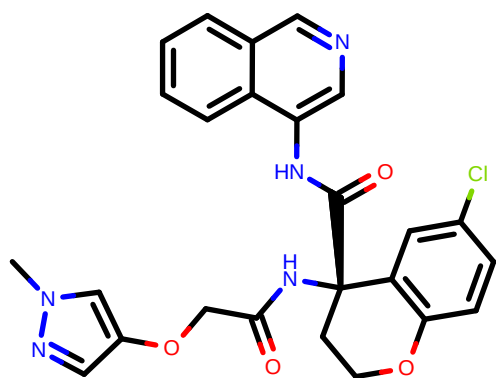
CID:	EN300-85760_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)NC(=O)[C@H]5CCOC5</chem>
RUN:	RUN909
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.25

EN300-01527_1_2



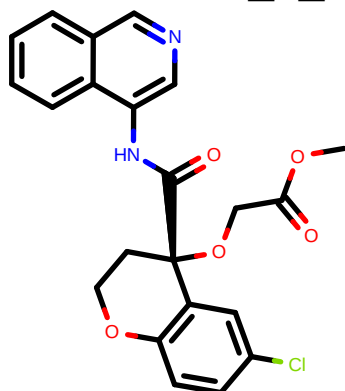
CID:	EN300-01527_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)OCC(=O)NC[C@H]5CCCC5</chem>
RUN:	RUN1719
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.27

EN300-201553_1_1



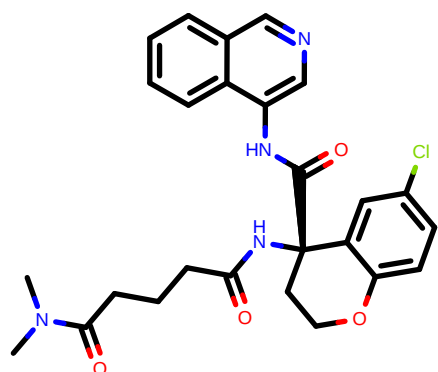
CID:	EN300-201553_1_1
SMILES:	<chem>Cn1cc(cn1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN806
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.28

EN300-19700_1_1



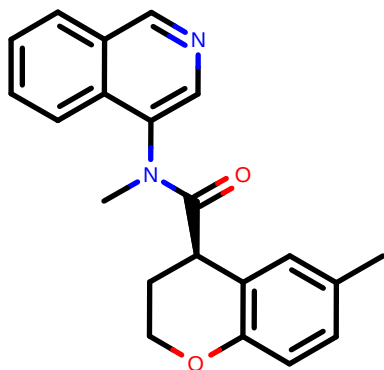
CID:	EN300-19700_1_1
SMILES:	<chem>COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN389
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.18

EN300-69215_1_1



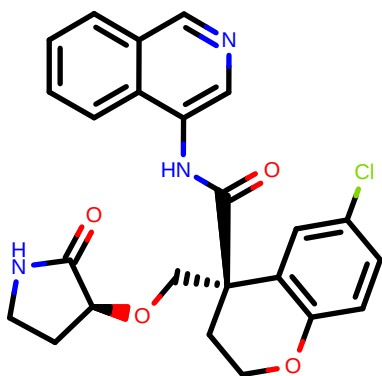
CID:	EN300-69215_1_1
SMILES:	<chem>CN(C)C(=O)CCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN274
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.33

MAK-UNK-3875bbc8-1_1



CID:	MAK-UNK-3875bbc8-1_1
SMILES:	<chem>Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)c3cncc4c3cccc4</chem>
RUN:	RUN32
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.11

EN300-6736413_2_2



CID: EN300-6736413_2_2

SMILES:

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

RUN:

RUN1182

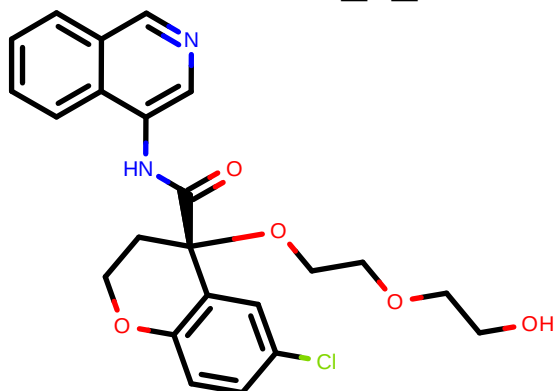
DDG (kcal/mol):

-1.79

dDDG (kcal/mol):

0.25

EN300-52467_1_1



CID: EN300-52467_1_1

SMILES:

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

RUN:

RUN904

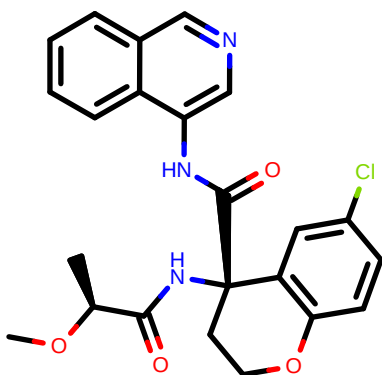
DDG (kcal/mol):

-1.79

dDDG (kcal/mol):

0.25

EN300-258477_1_1



CID: EN300-258477_1_1

SMILES:

C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)OC

RUN:

RUN774

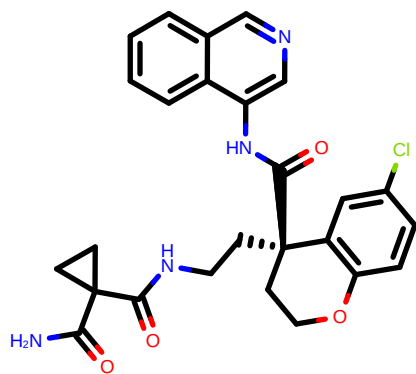
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.24

EN300-69070_3_1



CID: EN300-69070_3_1

SMILES:

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

RUN:

RUN890

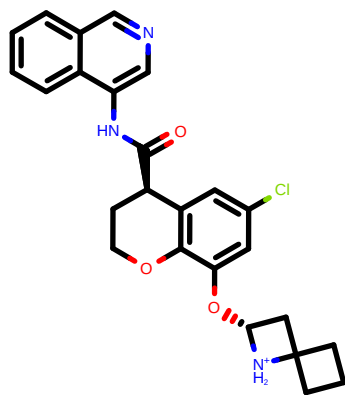
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.30

DAR-DIA-23e5a6a0-2_1



CID:

DAR-DIA-23e5a6a0-2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOC4c3cc(cc4O)[C@@H]5CC6([NH2+][5])CC6)Cl

RUN:

RUN81

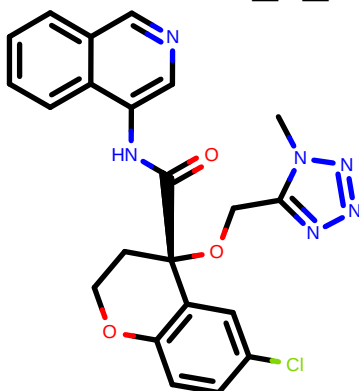
DDG (kcal/mol):

-1.78

dDDG (kcal/mol):

0.58

EN300-62574_1_1



CID:

EN300-62574_1_1

SMILES:

Cn1c(nnn1)CO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN:

RUN1240

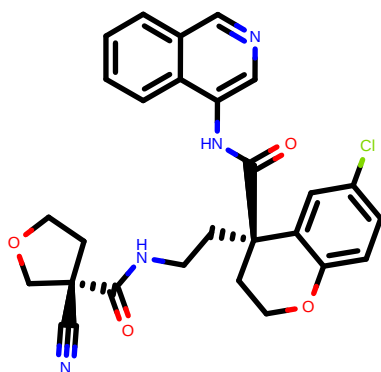
DDG (kcal/mol):

-1.77

dDDG (kcal/mol):

0.22

EN300-261210_3_2



CID:

EN300-261210_3_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOC5)C#N

RUN:

RUN898

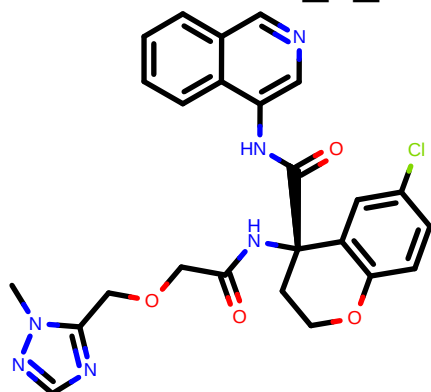
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

0.31

EN300-213358_1_1



CID:

EN300-213358_1_1

SMILES:

Cn1c(ncn1)COCC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN:

RUN569

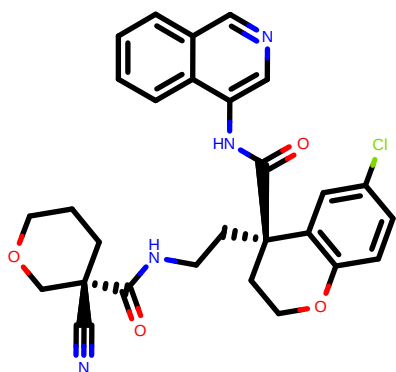
DDG (kcal/mol):

-1.76

dDDG (kcal/mol):

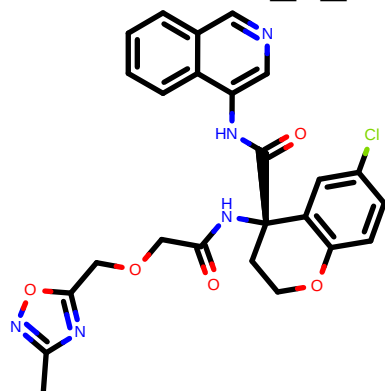
0.36

EN300-301925_3_2



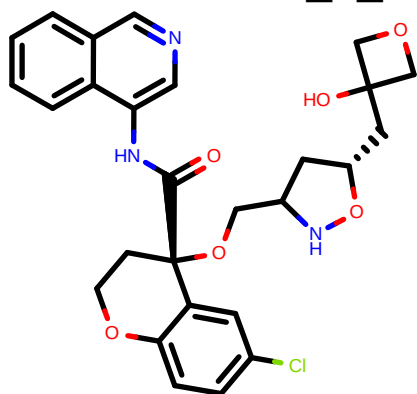
CID:	EN300-301925_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCOC5)C#N</chem>
RUN:	RUN1426
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.24

EN300-77006_1_1



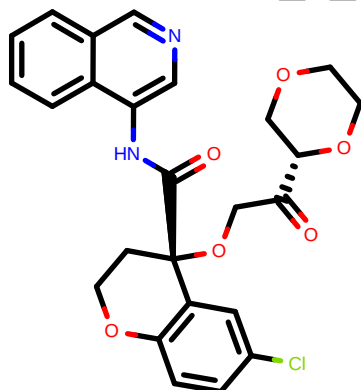
CID:	EN300-77006_1_1
SMILES:	<chem>Cc1nc(on1)COC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN965
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.29

EN300-7457160_1_2



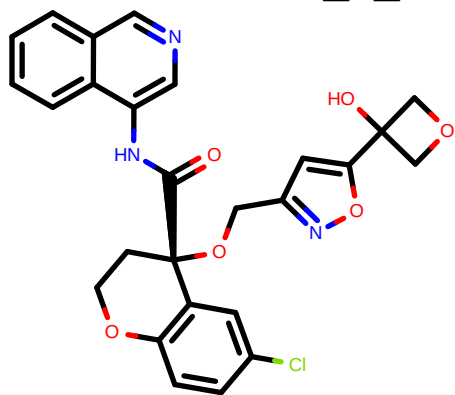
CID:	EN300-7457160_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC(=O)N[C@@H](C5)C6(COC6)O</chem>
RUN:	RUN801
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.34

EN300-6238494_1_1



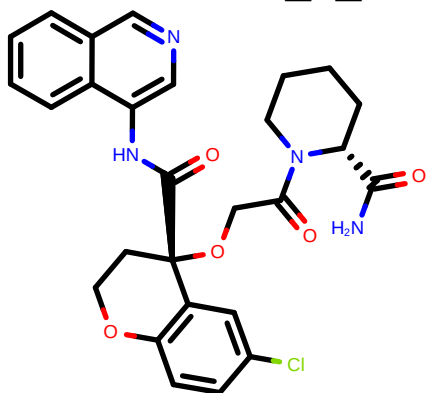
CID:	EN300-6238494_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COC(=O)C5</chem>
RUN:	RUN301
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.30

EN300-7457159_1_1



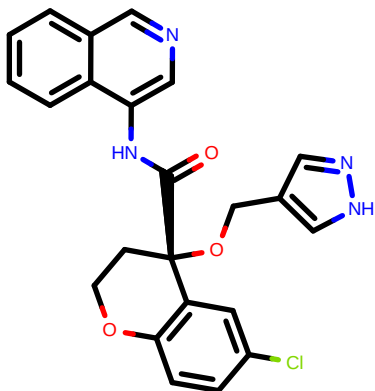
CID:	EN300-7457159_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cc(on5)C6(COC6)O</chem>
RUN:	RUN1248
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.28

EN300-22879_1_1



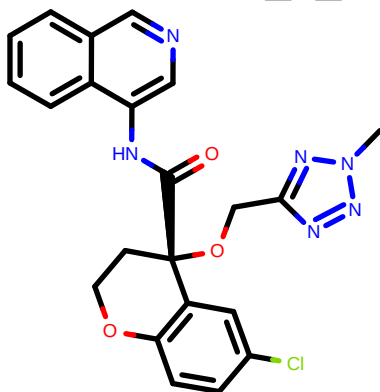
CID:	EN300-22879_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@@H]5C(=O)N</chem>
RUN:	RUN1687
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.29

EDJ-MED-28ec730d-4_1



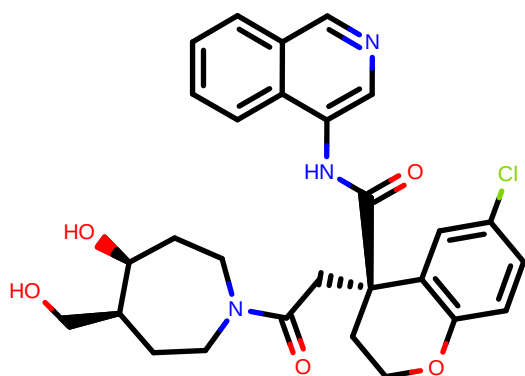
CID:	EDJ-MED-28ec730d-4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5</chem>
RUN:	RUN65
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.20

EN300-90225_1_1



CID:	EN300-90225_1_1
SMILES:	<chem>Cn1nc(nn1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1216
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.21

EN300-7353672_1_4



CID: EN300-7353672_1_4

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc(c4)C)CC(=O)N5C[C@@H](C@H)(C5)OCCO

RUN:

RUN303

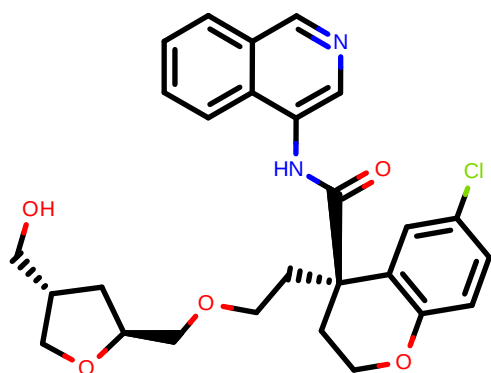
DDG (kcal/mol):

-1.73

dDDG (kcal/mol):

0.49

EN300-6494158_3_3



CID: EN300-6494158_3_3

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc(c4)C)CCOC[C@@H]5C[C@@H](C5)CO

RUN:

RUN505

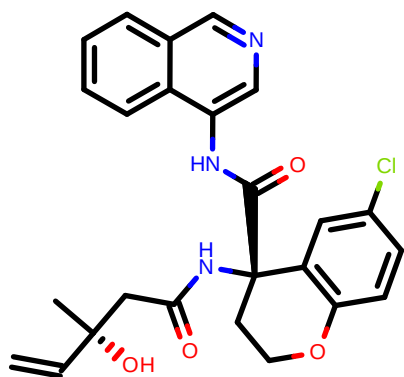
DDG (kcal/mol):

-1.73

dDDG (kcal/mol):

0.33

EN300-181938_1_1



CID: EN300-181938_1_1

SMILES:

C[C@@H](CC(=O)N[C@@H]1[C@@H](COCc2cc1cc(c2)C)C(=O)Nc3cnc4c3cccc4)(C=C)O

RUN:

RUN933

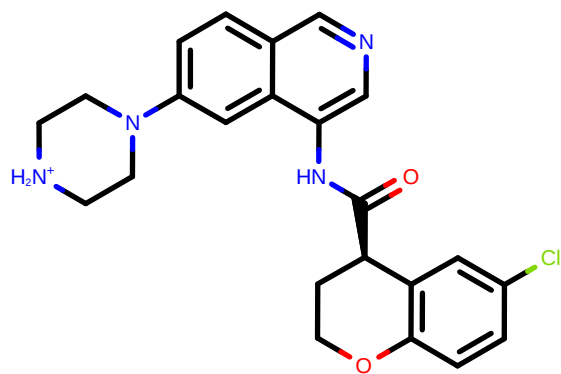
DDG (kcal/mol):

-1.73

dDDG (kcal/mol):

0.24

MAK-UNK-8be7dca9-4_1



CID: MAK-UNK-8be7dca9-4_1

SMILES:

c1cc2cncnc2c2cc1N3CC[NH2+](CC3)NC(=O)[C@@H]4CCOCc5cc(cc5)Cl

RUN:

RUN56

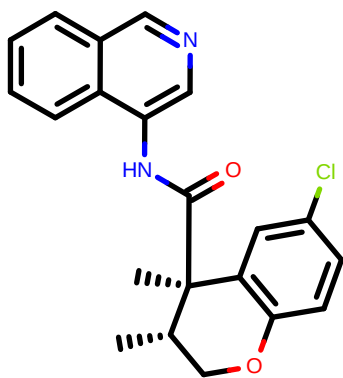
DDG (kcal/mol):

-1.73

dDDG (kcal/mol):

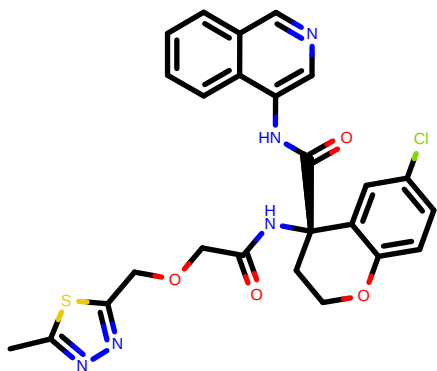
0.09

DAR-DIA-0d514e7d-28_1



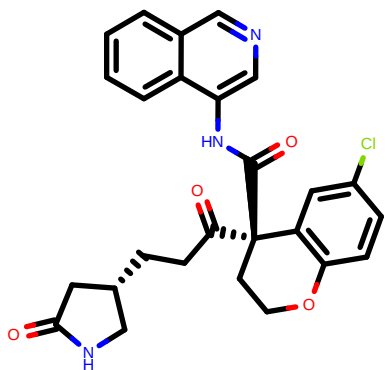
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	<chem>C[C@H]1COC2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN6
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.10

EN300-206870_1_1



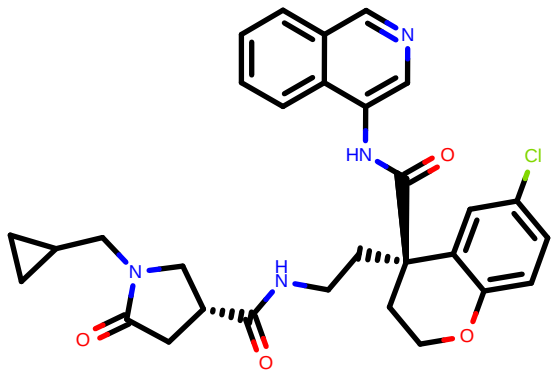
CID:	EN300-206870_1_1
SMILES:	<chem>Cc1nnc(s1)COC(=O)N[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN845
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.27

VLA-UCB-34f3ed0c-21_2



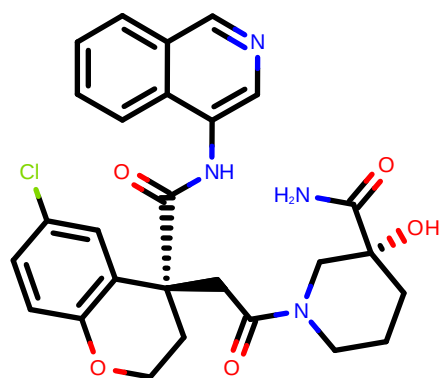
CID:	VLA-UCB-34f3ed0c-21_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOC4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NCS</chem>
RUN:	RUN0
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.32

EN300-31969_3_1



CID:	EN300-31969_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOC4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)N[C@]5(C)COC6C</chem>
RUN:	RUN1266
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.34

EN300-210553_1_1



CID: EN300-210553_1_1

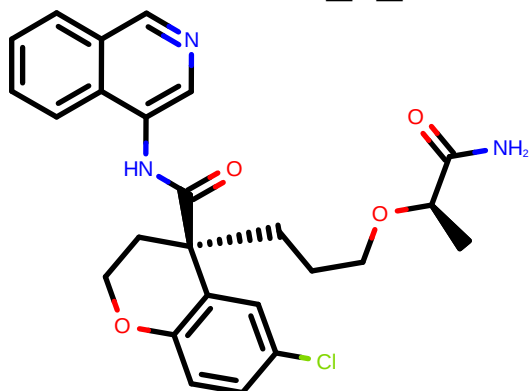
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)CC(=O)N5CCC[C@@](C5)(C(=O)N)O

RUN: RUN1498

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.44

EN300-17381_4_2



CID: EN300-17381_4_2

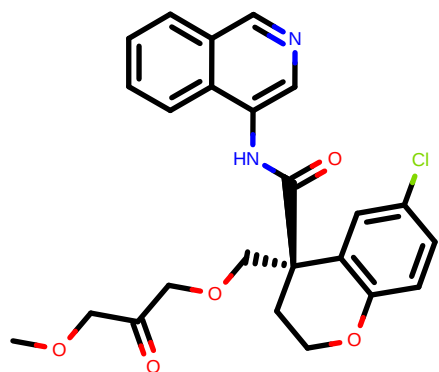
SMILES: C[C@H](C(=O)N)OCCC[C@@]1(CCCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN380

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.27

EN300-125140_2_1



CID: EN300-125140_2_1

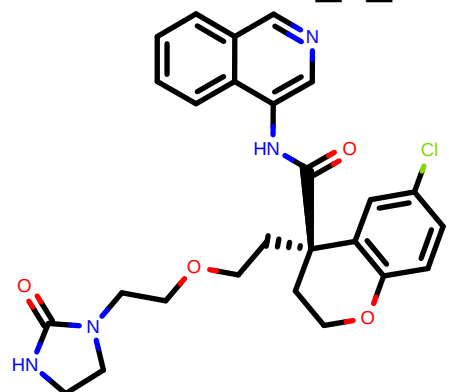
SMILES: COCC(=O)COC[C@@]1(CCCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN918

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.35

EN300-214800_3_1



CID: EN300-214800_3_1

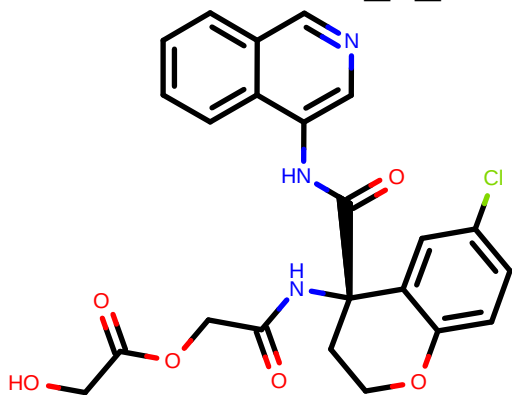
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)CCOCCN5CCNC5=O

RUN: RUN972

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.32

EN300-7459916_1_1



CID: EN300-7459916_1_1

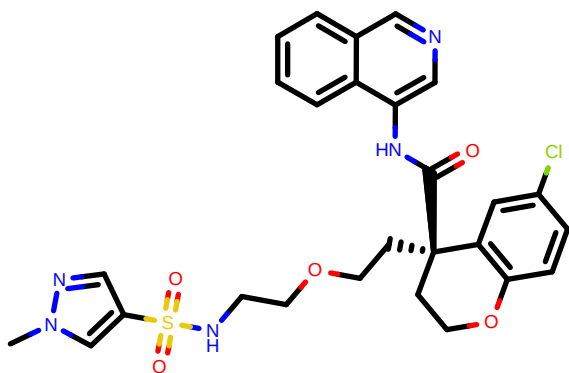
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(=O)CO

RUN: RUN1660

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.30

EN300-95598_3_1



CID: EN300-95598_3_1

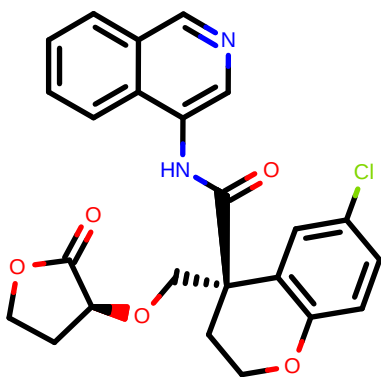
SMILES: Cn1cc(en1)S(=O)(=O)NCCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1532

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.50

EN300-20496_2_2



CID: EN300-20496_2_2

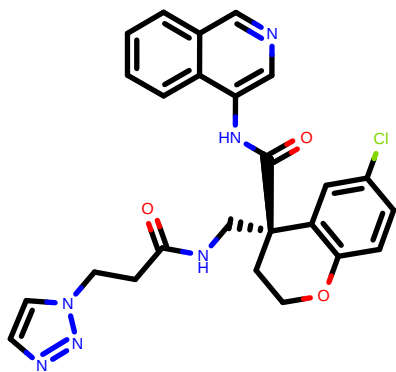
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCOC5=O

RUN: RUN1166

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.22

EN300-28871_2_1



CID: EN300-28871_2_1

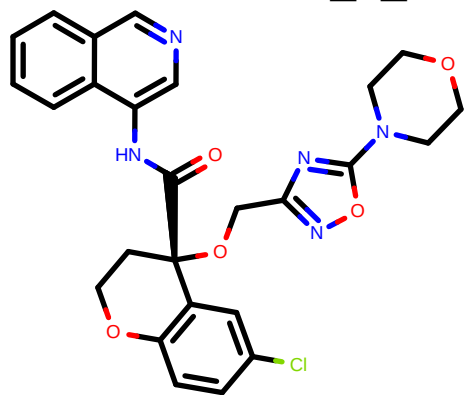
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5ccnn5

RUN: RUN597

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.20

EN300-1608590_1_1



CID: EN300-1608590_1_1

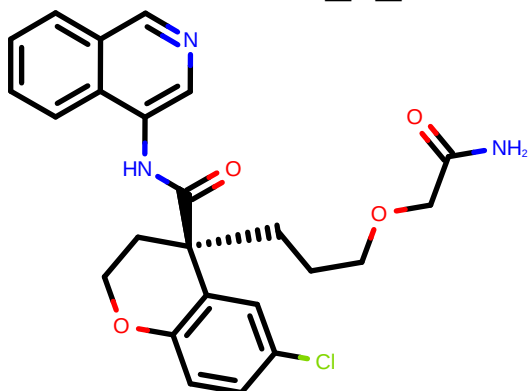
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(on5)N6CCOCC6

RUN: RUN1615

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.26

EN300-18249_4_1



CID: EN300-18249_4_1

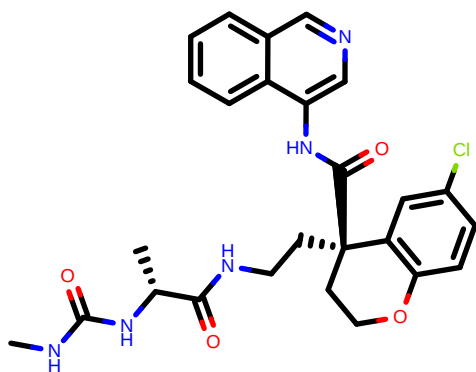
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC(=O)N

RUN: RUN276

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.23

EN300-2958082_3_1



CID: EN300-2958082_3_1

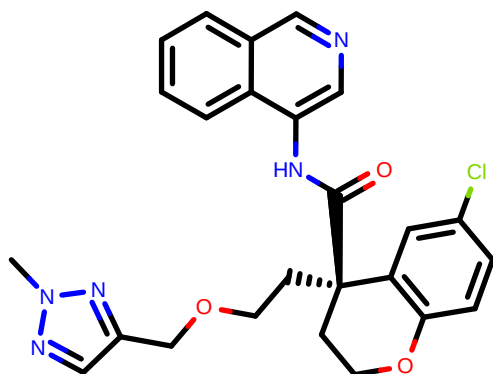
SMILES: C[C@@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)N

RUN: RUN1018

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.32

EN300-219020_3_1



CID: EN300-219020_3_1

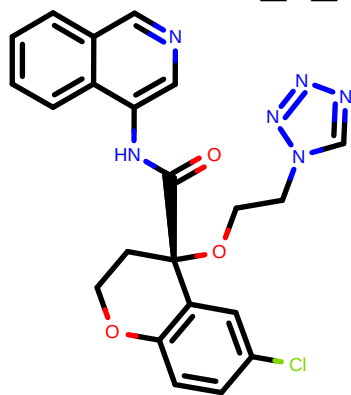
SMILES: Cn1ncc(n1)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1627

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.30

EN300-364679_1_1



CID:

EN300-364679_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5nnn5

RUN:

RUN1408

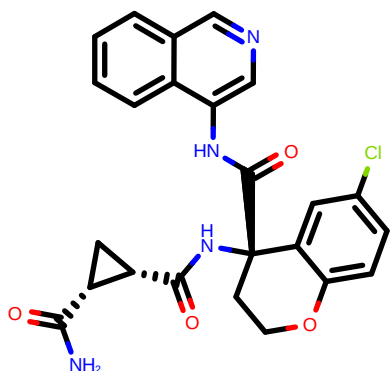
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.22

EN300-331941_1_1



CID:

EN300-331941_1_1

SMILES:

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

RUN:

RUN1580

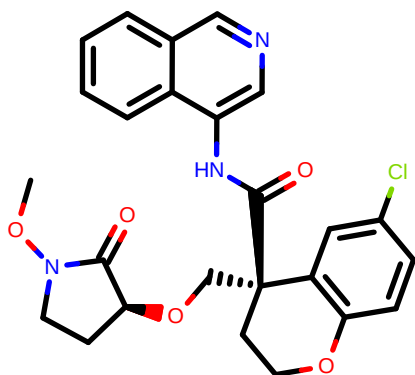
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.32

EN300-302058_2_1



CID:

EN300-302058_2_1

SMILES:

CO1CC[C@H](C1=O)OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN:

RUN1629

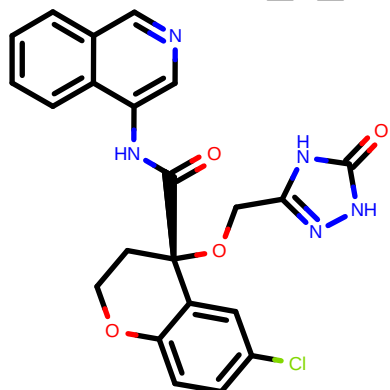
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

0.29

EN300-73772_1_1



CID:

EN300-73772_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5[nH]c(=O)[nH]n5

RUN:

RUN1040

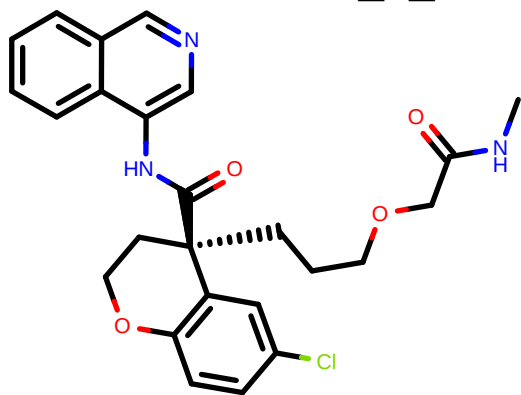
DDG (kcal/mol):

-1.66

dDDG (kcal/mol):

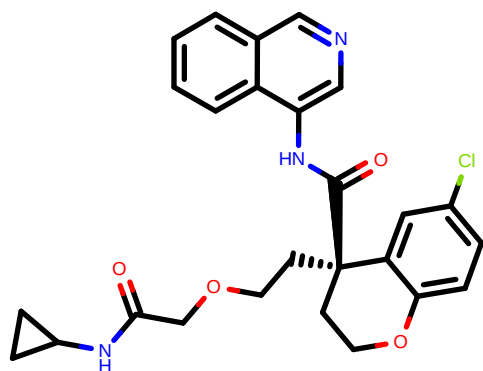
0.25

EN300-2977549_4_1



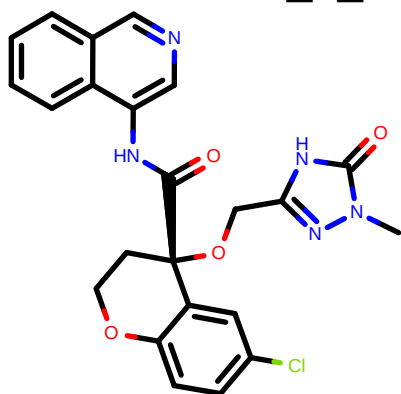
CID:	EN300-2977549_4_1
SMILES:	<chem>CNC(=O)COC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN619
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.30

EN300-1253178_3_1



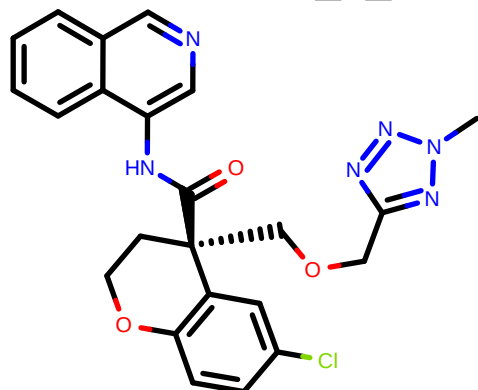
CID:	EN300-1253178_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(COC4c3cc(cc4)Cl)CCOC(=O)NC5CC5</chem>
RUN:	RUN1675
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.25

EN300-124918_1_1



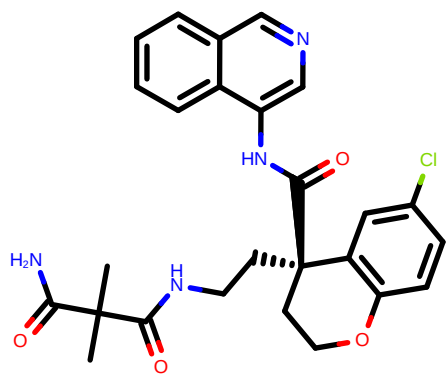
CID:	EN300-124918_1_1
SMILES:	<chem>Cn1c(=O)[nH]c(n1)CO[C@]2(C)C(COC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN684
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.20

EN300-90225_2_1



CID:	EN300-90225_2_1
SMILES:	<chem>Cn1nc(nn1)COC[C@]2(C)C(COC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1717
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.25

EN300-182913_3_1



CID: EN300-182913_3_1

SMILES:

CC(C)(C(=O)N)C(=O)NCC[C@]1(C)C(=O)C2C1CC(C2)C(=O)Nc3ccc4c3ccc4

RUN:

RUN1649

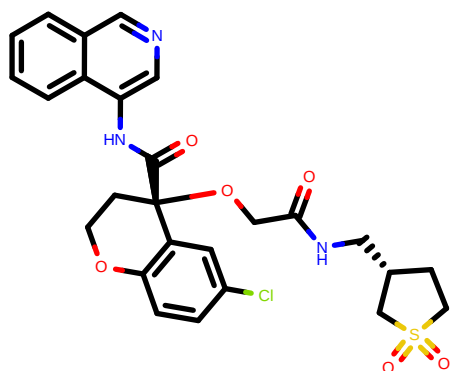
DDG (kcal/mol):

-1.64

dDDG (kcal/mol):

0.31

EN300-47606_1_1



CID: EN300-47606_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4C3CC(C4)C(=O)NCC[C@H]5SCCS(=O)(=O)C5

RUN:

RUN1639

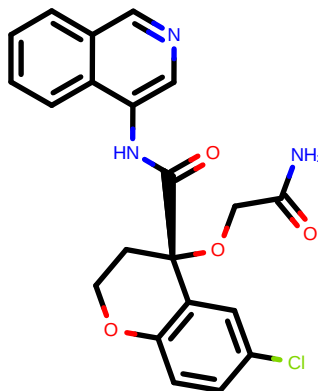
DDG (kcal/mol):

-1.64

dDDG (kcal/mol):

0.27

EN300-18249_1_1



CID: EN300-18249_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4C3CC(C4)C(=O)NCC[C@H]5SCCS(=O)(=O)C5

RUN:

RUN1128

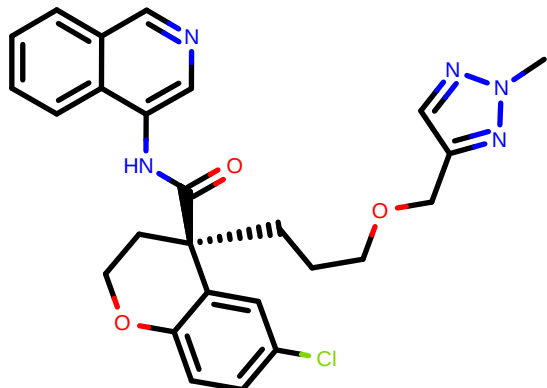
DDG (kcal/mol):

-1.64

dDDG (kcal/mol):

0.16

EN300-219020_4_1



CID: EN300-219020_4_1

SMILES:

Cn1ncc(n1)COC[C@]2(C)C(=O)C3C2CC(C3)C(=O)Nc4cnc5c4cccc5

RUN:

RUN547

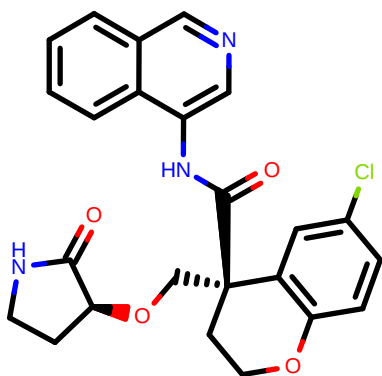
DDG (kcal/mol):

-1.64

dDDG (kcal/mol):

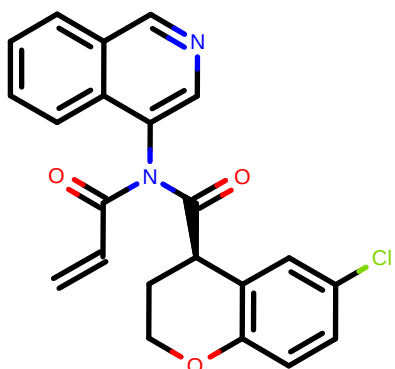
0.32

EN300-6736413_2_2



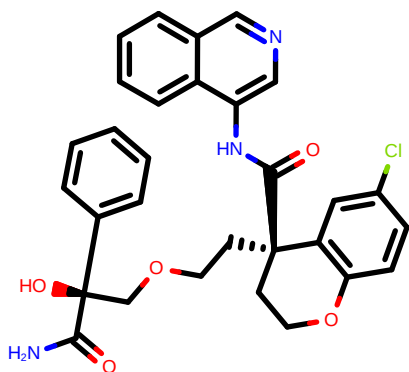
CID:	EN300-6736413_2_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O</chem>
RUN:	RUN1174
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.20

VLA-UCB-50c39ae8-7_1



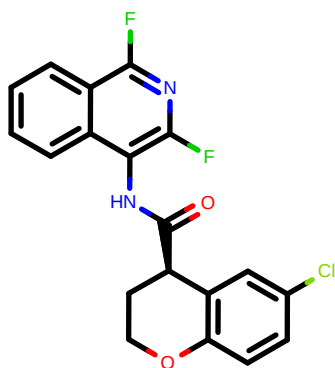
CID:	VLA-UCB-50c39ae8-7_1
SMILES:	<chem>C=CC(=O)N(c1ncnc2c1cccc2)C(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)</chem>
RUN:	RUN147
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.18

EN300-248526_3_2



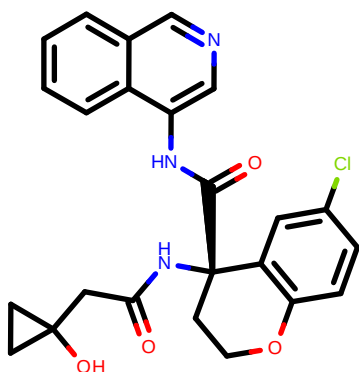
CID:	EN300-248526_3_2
SMILES:	<chem>c1ccc(cc1)[C@H](COCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)(C(=O)N)O</chem>
RUN:	RUN600
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.34

JOH-SUS-a69c159d-6_1



CID:	JOH-SUS-a69c159d-6_1
SMILES:	<chem>c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)</chem>
RUN:	RUN70
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.06

EN300-207873_1_1



CID: EN300-207873_1_1

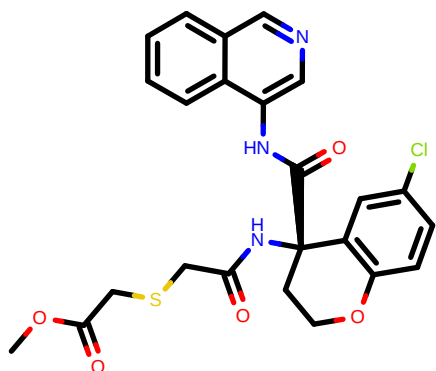
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CC5)O

RUN: RUN338

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.22

EN300-135060_1_1



CID: EN300-135060_1_1

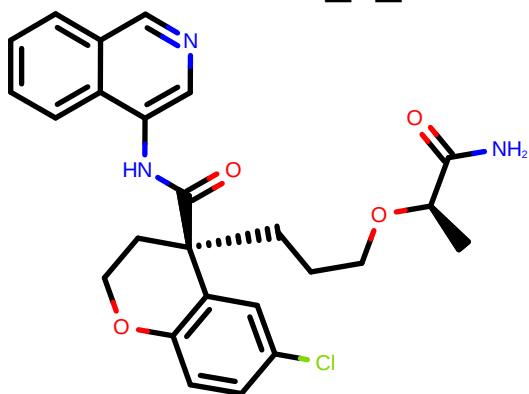
SMILES: COC(=O)CSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN330

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.31

EN300-17381_4_2



CID: EN300-17381_4_2

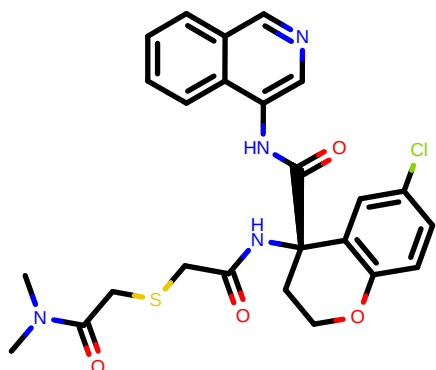
SMILES: C[C@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN396

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.28

EN300-12139_1_1



CID: EN300-12139_1_1

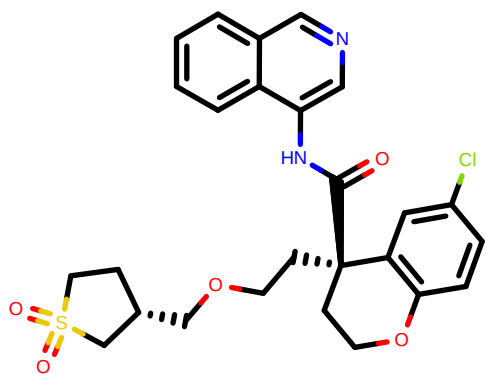
SMILES: CN(C)C(=O)CSCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

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)C)CCOC[C@H]5CCS(=O)(=O)C5

RUN:

RUN1252

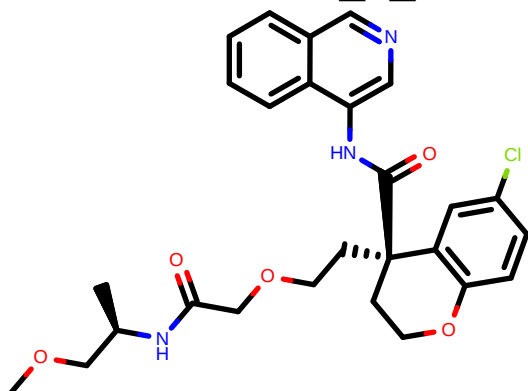
DDG (kcal/mol):

-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)C)C(=O)Nc3ncoc4c3ccc4

RUN:

RUN711

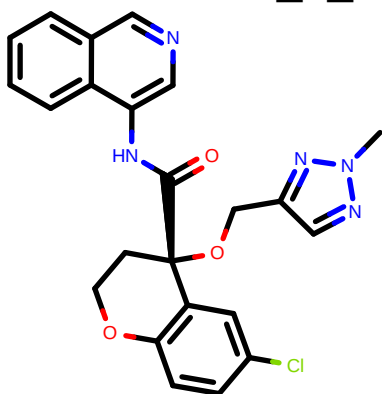
DDG (kcal/mol):

-1.62

dDDG (kcal/mol):

0.34

EN300-219020_1_1



CID:

EN300-219020_1_1

SMILES:

Cn1nc(n1)CO[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cnc5c4cccc5

RUN:

RUN833

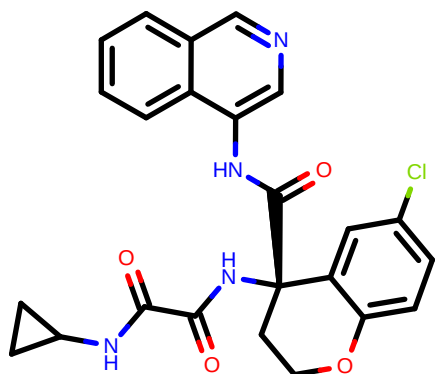
DDG (kcal/mol):

-1.61

dDDG (kcal/mol):

0.21

EN300-78135_1_1



CID:

EN300-78135_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NC5CC5

RUN:

RUN1700

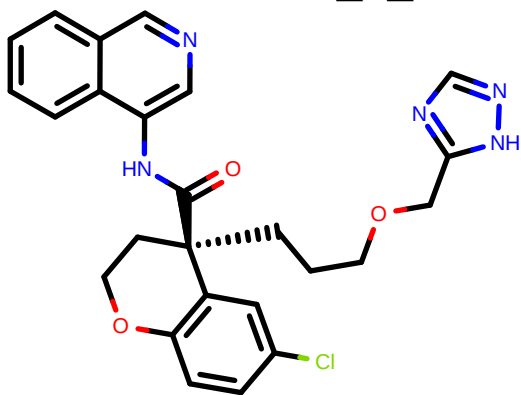
DDG (kcal/mol):

-1.61

dDDG (kcal/mol):

0.23

EN300-306316_4_1



CID: EN300-306316_4_1

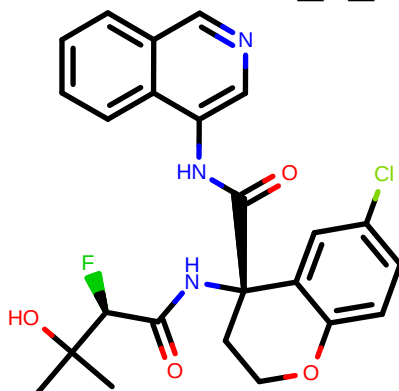
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOCOC5[nH]jncn5

RUN: RUN284

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.24

EN300-264744_1_2



CID: EN300-264744_1_2

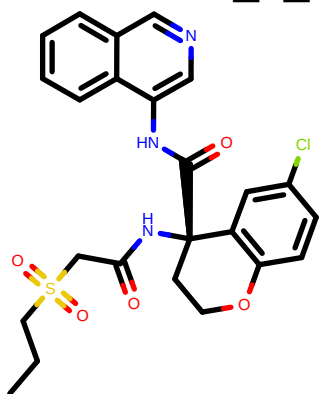
SMILES: CC(C)[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4)F)O

RUN: RUN1413

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.22

EN300-52325_1_1



CID: EN300-52325_1_1

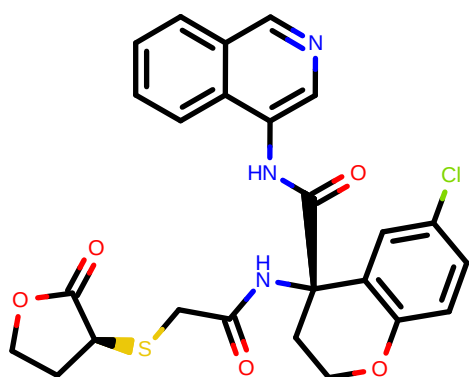
SMILES: CCCS(=O)(=O)CC(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN1309

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.36

EN300-113218_1_2



CID: EN300-113218_1_2

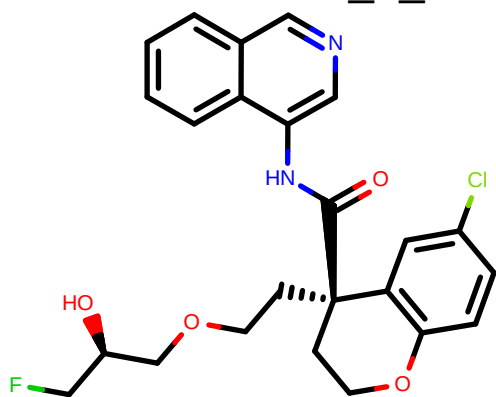
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)CS[C@@H]5CCOC5=O

RUN: RUN513

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.26

EN300-1968342_3_1



CID:

EN300-1968342_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4ccc(cc4)C)CCOC[C@@H](CF)O

RUN:

RUN908

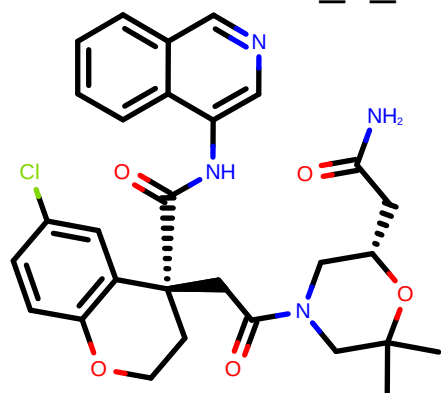
DDG (kcal/mol):

-1.60

dDDG (kcal/mol):

0.38

EN300-6488034_1_1



CID:

EN300-6488034_1_1

SMILES:

CC1CN(C[C@@H](O1)CC(=O)N[C@@H]2C(=O)C(=O)C(=O)C(=O)C(=O)Nc3ccc4c3ccccc4

RUN:

RUN874

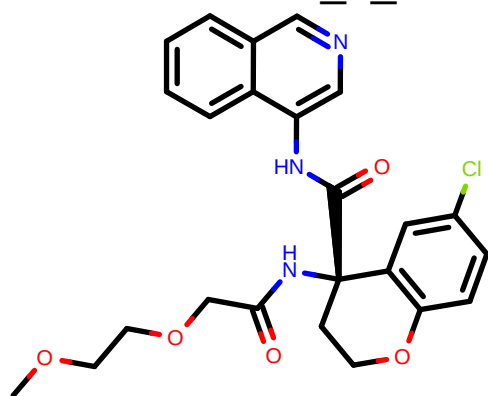
DDG (kcal/mol):

-1.60

dDDG (kcal/mol):

0.38

EN300-20375_1_1



CID:

EN300-20375_1_1

SMILES:

COCOCOC(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4

RUN:

RUN1117

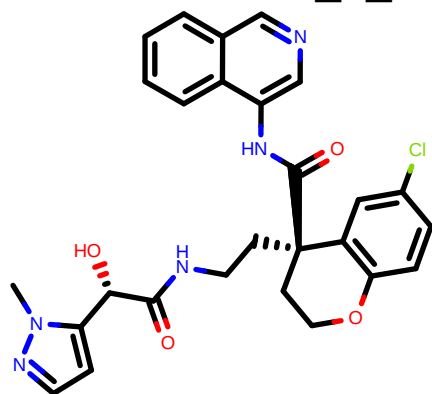
DDG (kcal/mol):

-1.60

dDDG (kcal/mol):

0.26

EN300-6473273_3_1



CID:

EN300-6473273_3_1

SMILES:

Cn1c(ccn1)[C@@H](C(=O)NCC[C@@H]2(CCOc3cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5)O

RUN:

RUN1689

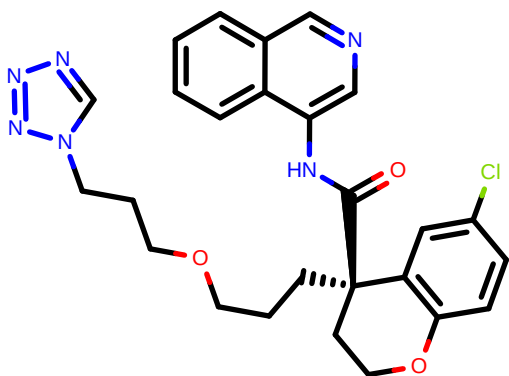
DDG (kcal/mol):

-1.59

dDDG (kcal/mol):

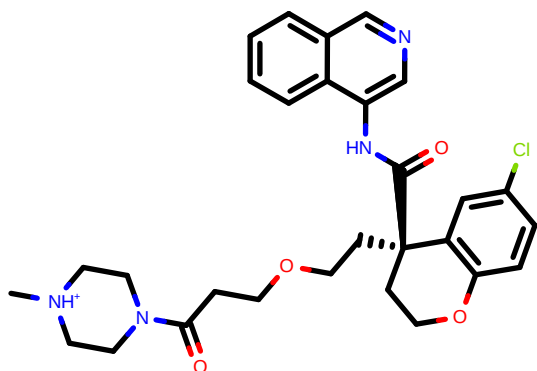
0.42

EN300-1696962_4_1



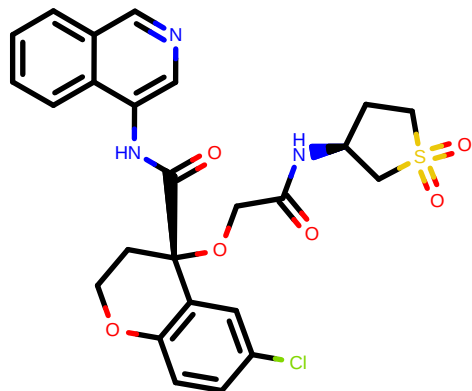
CID:	EN300-1696962_4_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCN5cnnn5</chem>
RUN:	RUN1063
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.41

EN300-178293_3_1



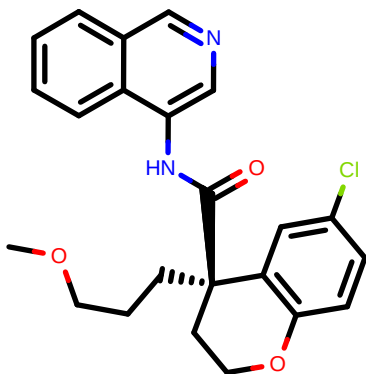
CID:	EN300-178293_3_1
SMILES:	<chem>C[NH+]1CCN(CC1)C(=O)CCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN844
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.57

EN300-05512_1_2



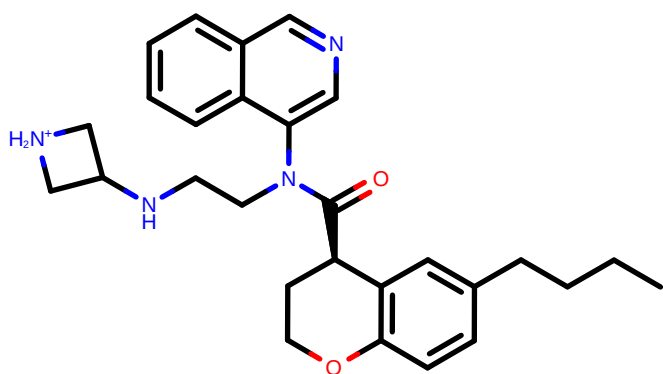
CID:	EN300-05512_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@H]5SCCS(=O)(=O)C5</chem>
RUN:	RUN349
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.33

EDJ-MED-28ec730d-1_1



CID:	EDJ-MED-28ec730d-1_1
SMILES:	<chem>COCCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4</chem>
RUN:	RUN62
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.26

MAK-UNK-83e0a0b4-4_1



CID:

MAK-UNK-83e0a0b4-4_1

SMILES:

CCCC1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCN3CC[NH2+](C3)c4cncc5c4cccc5

RUN:

RUN238

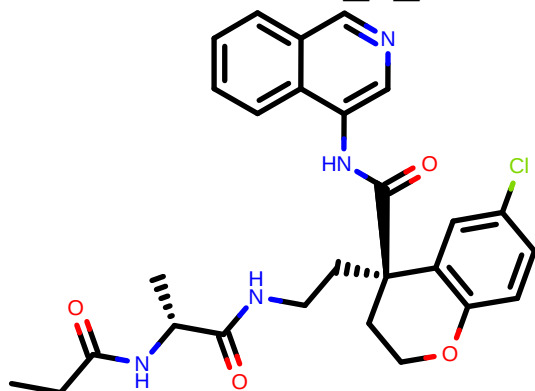
DDG (kcal/mol):

-1.58

dDDG (kcal/mol):

0.42

EN300-31148_3_2



CID:

EN300-31148_3_2

SMILES:

CCC(=O)N[C@@H](C)[C@H](C)C(=O)NCC[C@]1(C)C(=O)C2=CC(=C(C=C2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1162

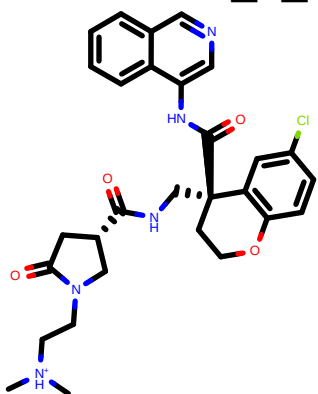
DDG (kcal/mol):

-1.57

dDDG (kcal/mol):

0.40

EN300-51735_2_2



CID:

EN300-51735_2_2

SMILES:

C[NH+](C)CCN1C[C@H](C)[C@H](C)C(=O)NCC[C@]2(C)C(=O)C3=CC(=C(C=C3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN645

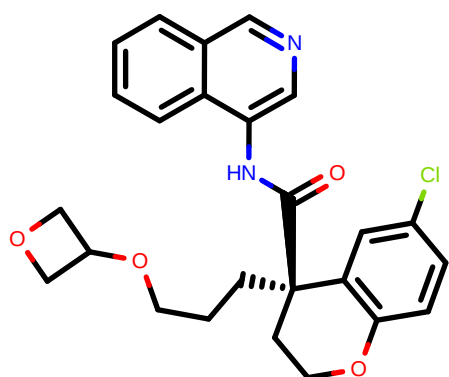
DDG (kcal/mol):

-1.57

dDDG (kcal/mol):

0.34

EN300-317082_4_1



CID:

EN300-317082_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4=CC(=C(C=C4)Cl)CCCC5COC5

RUN:

RUN1303

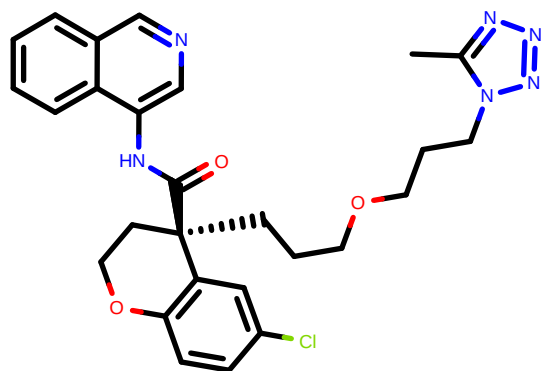
DDG (kcal/mol):

-1.57

dDDG (kcal/mol):

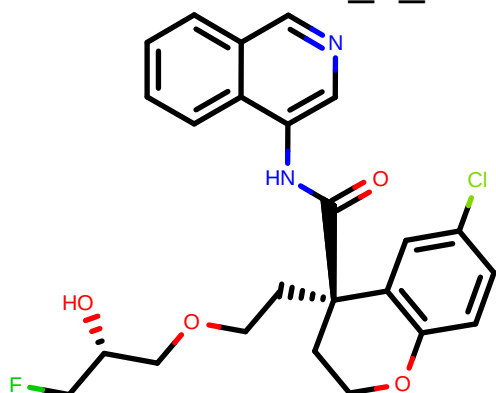
0.25

EN300-197715_4_1



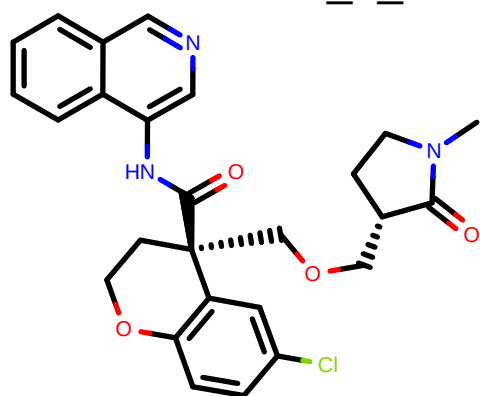
CID:	EN300-197715_4_1
SMILES:	<chem>Cc1nnnn1CCCOCCCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1543
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.33

EN300-1968342_3_2



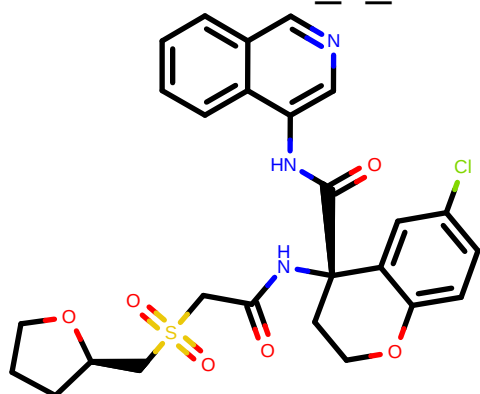
CID:	EN300-1968342_3_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCOC[C@H](CF)O</chem>
RUN:	RUN1556
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.35

EN300-260816_2_2



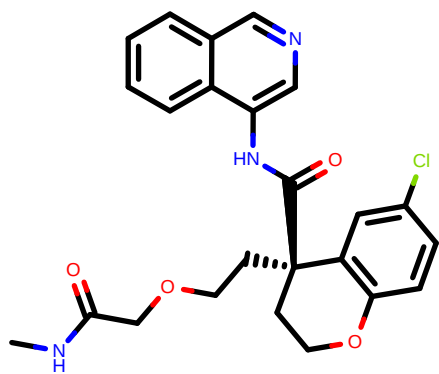
CID:	EN300-260816_2_2
SMILES:	<chem>CN1CC[C@H](C1=O)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN331
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.30

EN300-67023_1_2



CID:	EN300-67023_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C[C@H]5CCCCO5</chem>
RUN:	RUN704
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.35

EN300-2977549_3_1



CID: EN300-2977549_3_1

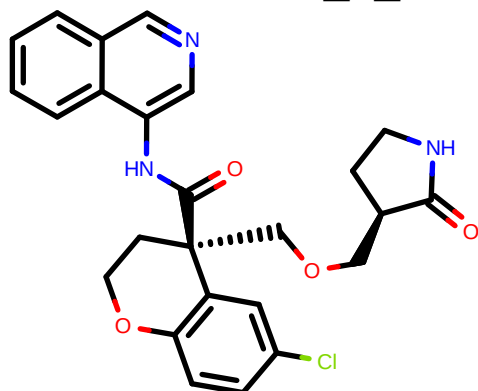
SMILES: CNC(=O)COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1739

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.31

EN300-246248_2_2



CID: EN300-246248_2_2

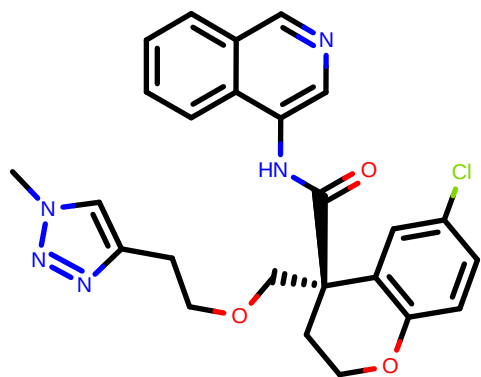
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)COC[C@H]5CCNC5=O

RUN: RUN998

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.29

EN300-1600786_2_1



CID: EN300-1600786_2_1

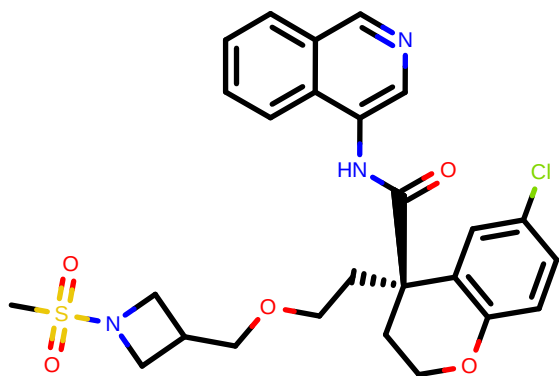
SMILES: Cn1cc(nn1)COC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1781

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.39

EN300-302290_3_1



CID: EN300-302290_3_1

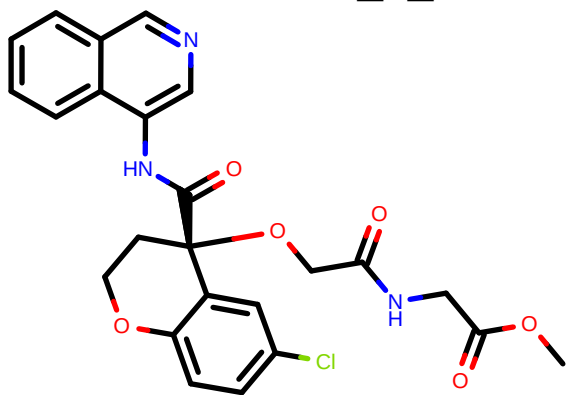
SMILES: CS(=O)(=O)N1CC(C1)COC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1220

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.36

EN300-04409_1_1



CID: EN300-04409_1_1

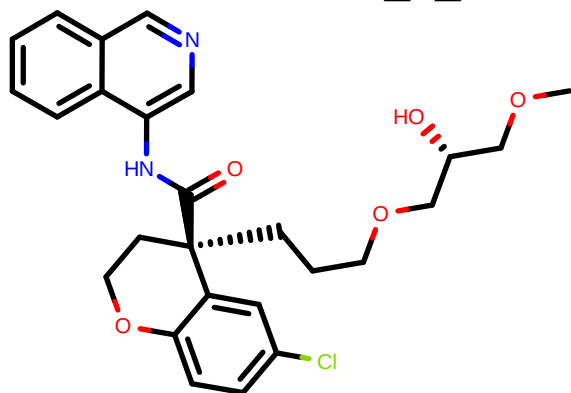
SMILES: COC(=O)CNC(=O)CO[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1583

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.28

EN300-1915260_4_2



CID: EN300-1915260_4_2

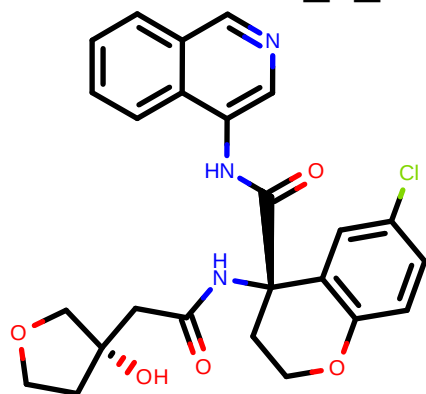
SMILES: COC[C@H](COCCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)O

RUN: RUN579

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.43

EN300-360157_1_2



CID: EN300-360157_1_2

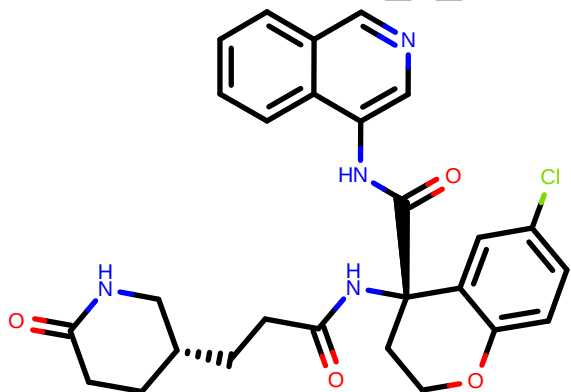
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@]5(CCOCS)O

RUN: RUN657

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.26

EN300-1215738_1_1



CID: EN300-1215738_1_1

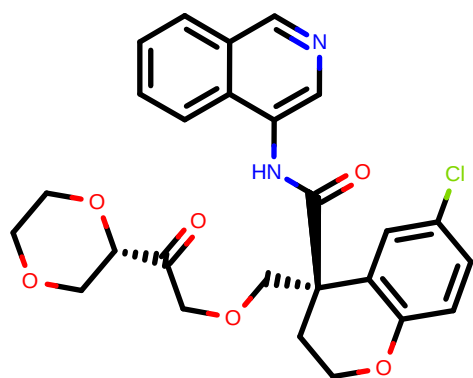
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@]5H5CCC(=O)NCS

RUN: RUN973

DDG (kcal/mol): -1.55

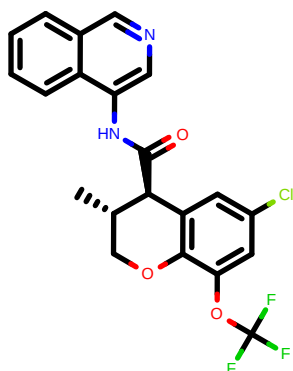
dDDG (kcal/mol): 0.39

EN300-6238494_2_1



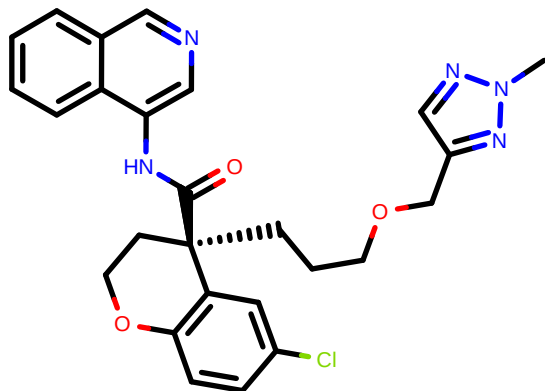
CID:	EN300-6238494_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)[C@@H]5COC(=O)C5</chem>
RUN:	RUN759
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-18_1



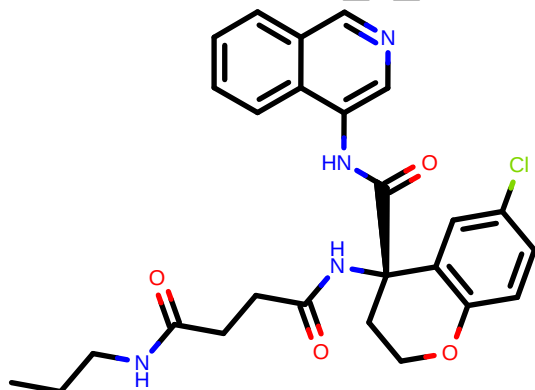
CID:	DAR-DIA-0d514e7d-18_1
SMILES:	<chem>C[C@H]1COC2C(Cc2OC(F)(F)F)Cl)[C@@H]1C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN123
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.14

EN300-219020_4_1



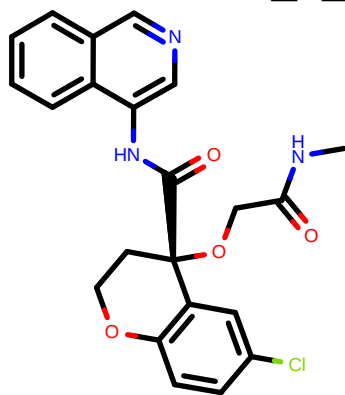
CID:	EN300-219020_4_1
SMILES:	<chem>Cn1ncc(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN555
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.36

EN300-68740_1_1



CID:	EN300-68740_1_1
SMILES:	<chem>CCCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
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(COC(=O)Cc2cc(Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1056

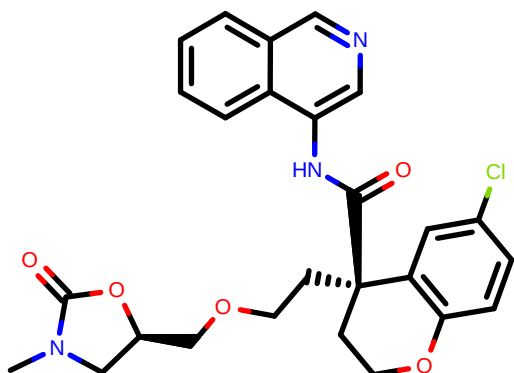
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.21

EN300-222969_3_1



CID:

EN300-222969_3_1

SMILES:

CN1C[C@@H](OC1=O)COC[C@]2(COC(=O)Cc3cc(Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN727

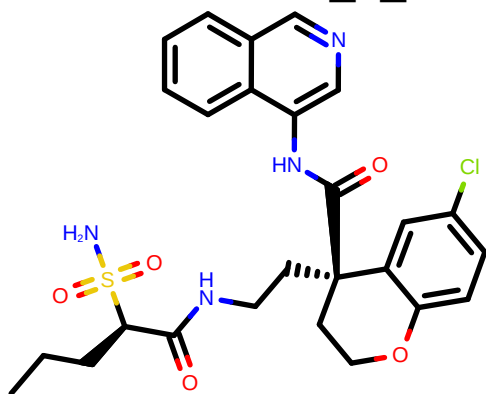
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.31

EN300-206592_3_2



CID:

EN300-206592_3_2

SMILES:

CCC[C@H](C(=O)NCC[C@]1(COC(=O)Cc2cc(Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N

RUN:

RUN518

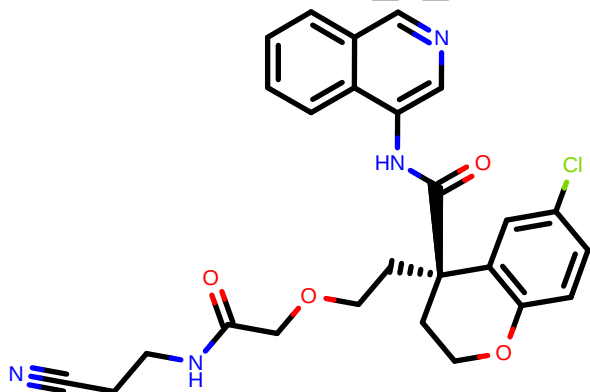
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.47

EN300-10895_3_1



CID:

EN300-10895_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC(=O)Cc4cc(Cl)C(=O)Nc5cncc6c5cccc6

RUN:

RUN757

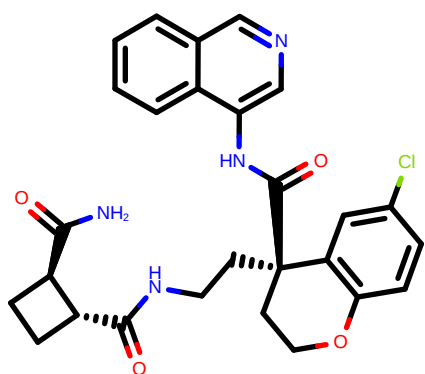
DDG (kcal/mol):

-1.54

dDDG (kcal/mol):

0.34

EN300-217107_3_3



CID:

EN300-217107_3_3

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@H]3[C@@H](CCOC4c3cc(cc4)C)CCOC(C(=O)[C@H]5CC[C@H]5C(=O)N

RUN:

RUN503

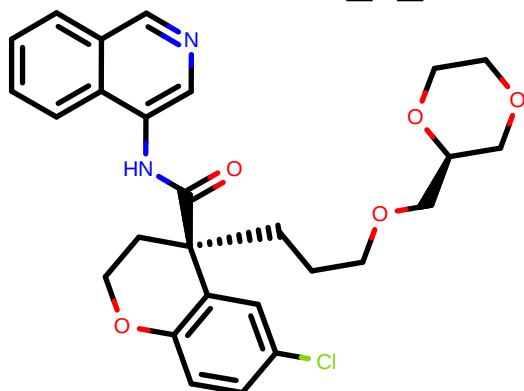
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.32

EN300-139167_4_1



CID:

EN300-139167_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@H]3[C@@H](CCOC4c3cc(cc4)C)CCOC(C(=O)[C@H]5CCOC5

RUN:

RUN515

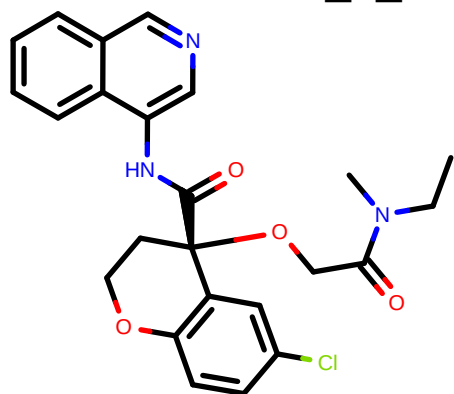
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.31

EN300-1253122_1_1



CID:

EN300-1253122_1_1

SMILES:

CCN(C)C(=O)CO[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN556

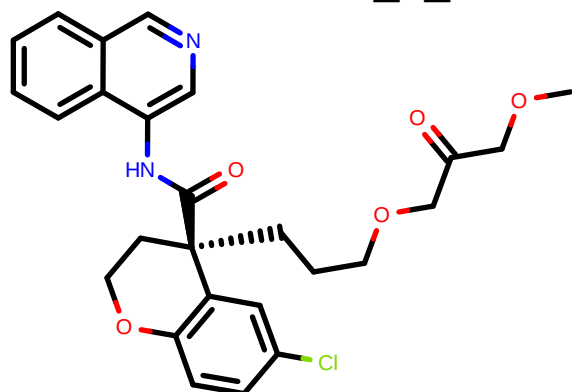
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.23

EN300-125140_4_1



CID:

EN300-125140_4_1

SMILES:

COCC(=O)COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN659

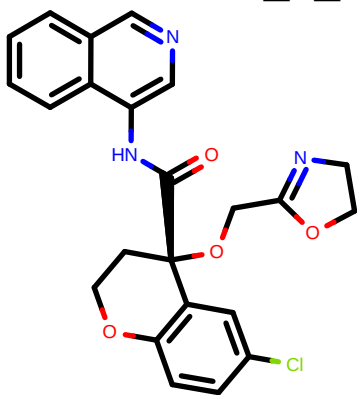
DDG (kcal/mol):

-1.53

dDDG (kcal/mol):

0.33

EN300-317555_1_1



CID: EN300-317555_1_1

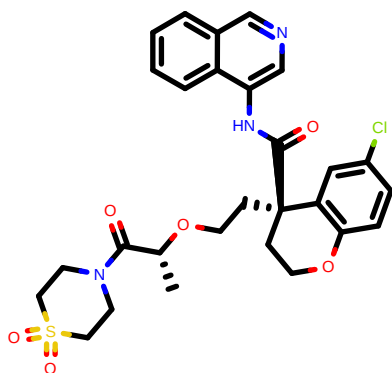
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5

RUN: RUN397

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.22

EN300-1265949_3_2



CID: EN300-1265949_3_2

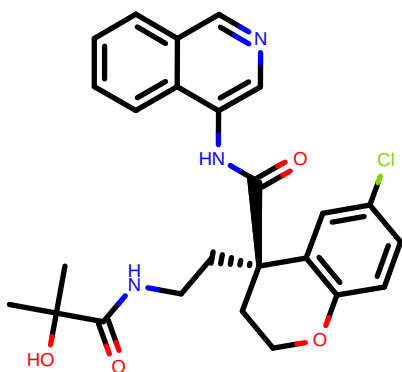
SMILES: C[C@H](C(=O)N1CCS(=O)(=O)CC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5

RUN: RUN1436

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.50

EN300-59285_3_1



CID: EN300-59285_3_1

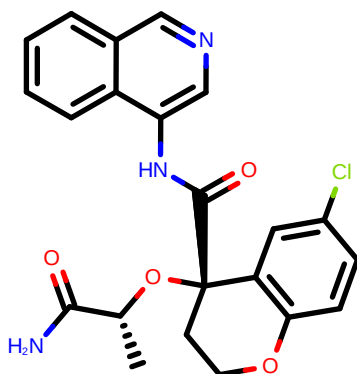
SMILES: CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4)O

RUN: RUN1482

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-17381_1_2



CID: EN300-17381_1_2

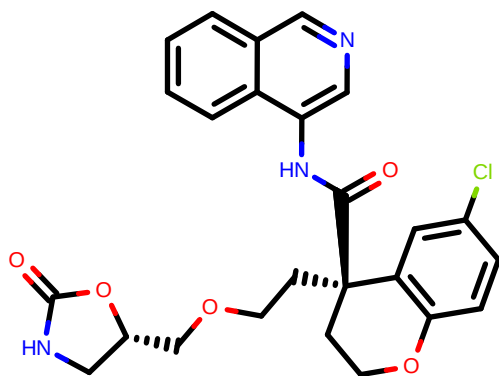
SMILES: C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN809

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.20

EN300-203293_3_1



CID:

EN300-203293_3_1

SMILES:

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

RUN:

RUN425

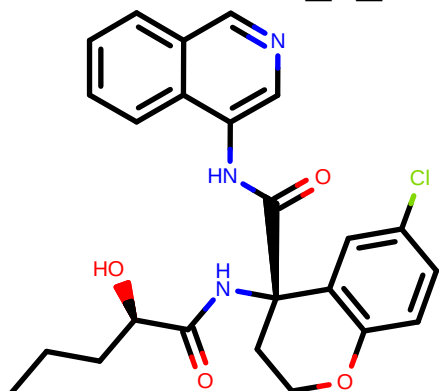
DDG (kcal/mol):

-1.52

dDDG (kcal/mol):

0.29

EN300-219531_1_2



CID:

EN300-219531_1_2

SMILES:

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

RUN:

RUN1676

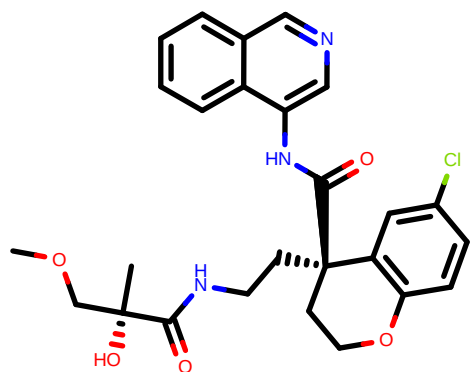
DDG (kcal/mol):

-1.52

dDDG (kcal/mol):

0.32

EN300-76841_3_2



CID:

EN300-76841_3_2

SMILES:

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

RUN:

RUN614

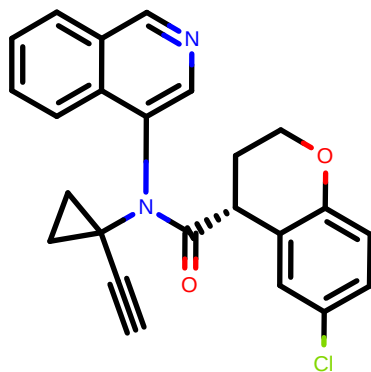
DDG (kcal/mol):

-1.52

dDDG (kcal/mol):

0.43

DAR-DIA-5ff57136-15_1



CID:

DAR-DIA-5ff57136-15_1

SMILES:

C#CC1(CC1)N(c2cnc3c2cccc3)C(=O)[C@H]4CCOC5c4cc(cc5)Cl

RUN:

RUN198

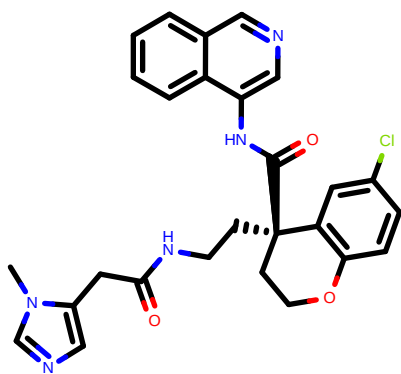
DDG (kcal/mol):

-1.52

dDDG (kcal/mol):

0.16

EN300-152418_3_1



CID: EN300-152418_3_1

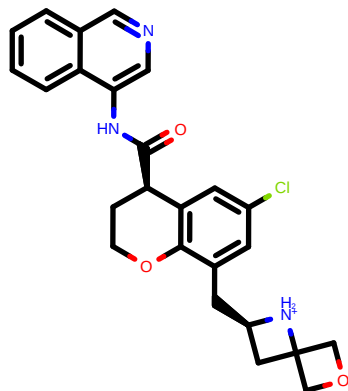
SMILES: Cn1cncc1CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1170

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.33

DAR-DIA-23e5a6a0-8_1



CID: DAR-DIA-23e5a6a0-8_1

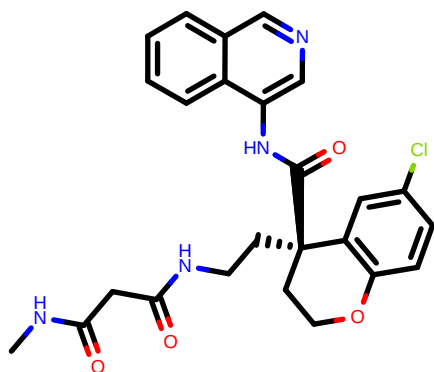
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4)C[C@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN222

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.26

EN300-128463_3_1



CID: EN300-128463_3_1

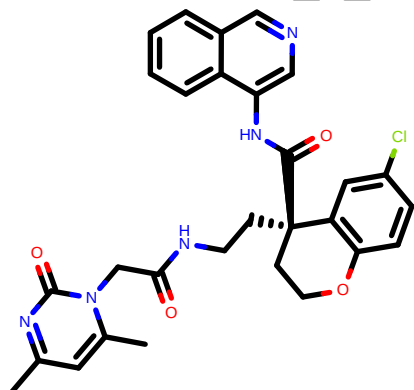
SMILES: CNC(=O)CC(=O)NCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1090

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.35

EN300-137191_3_1



CID: EN300-137191_3_1

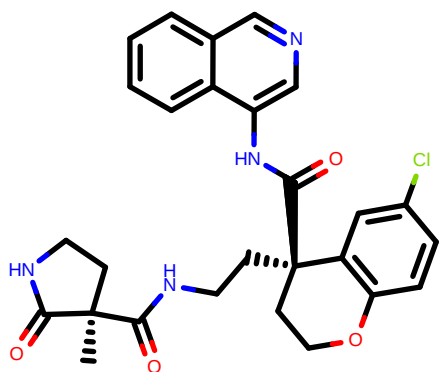
SMILES: Cc1cc(n(c(=O)n1)CC(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C

RUN: RUN1609

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.41

EN300-207959_3_2



CID: EN300-207959_3_2

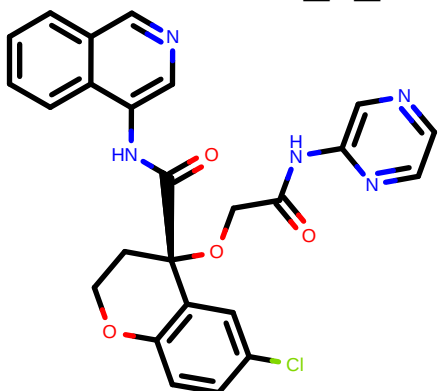
SMILES: C[C@]1(CCN(C1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN1729

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.64

EN300-105267_1_1



CID: EN300-105267_1_1

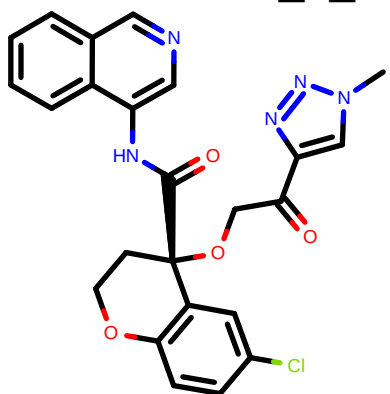
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5ccccn5

RUN: RUN676

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-263153_1_1



CID: EN300-263153_1_1

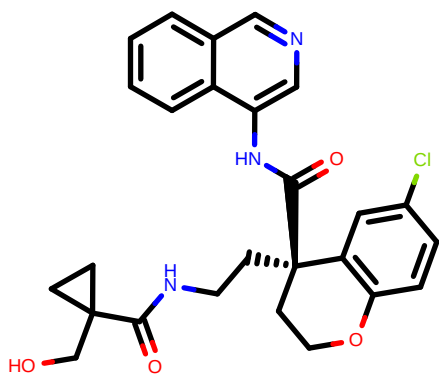
SMILES: Cn1cc(nn1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN1464

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.29

EN300-146174_3_1



CID: EN300-146174_3_1

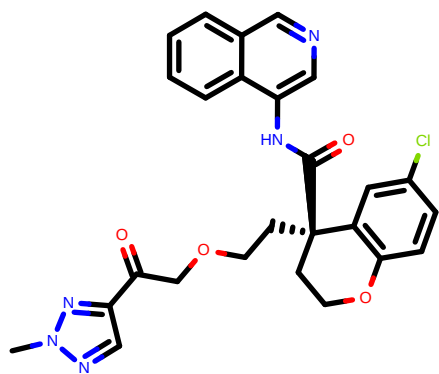
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(C)C5CO

RUN: RUN882

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.33

EN300-204935_3_1



CID:

EN300-204935_3_1

SMILES:

Cn1ccc(n1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN688

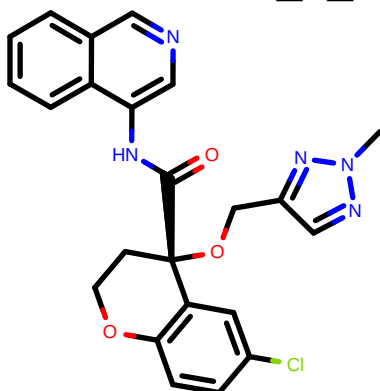
DDG (kcal/mol):

-1.50

dDDG (kcal/mol):

0.34

EN300-219020_1_1



CID:

EN300-219020_1_1

SMILES:

Cn1ccc(n1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN840

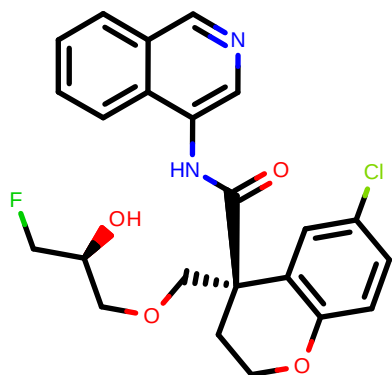
DDG (kcal/mol):

-1.49

dDDG (kcal/mol):

0.22

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:

RUN483

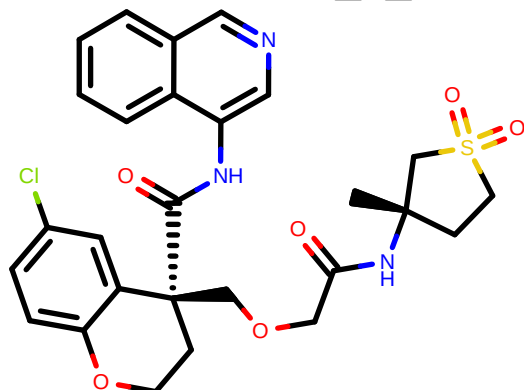
DDG (kcal/mol):

-1.49

dDDG (kcal/mol):

0.32

EN300-10414_2_1



CID:

EN300-10414_2_1

SMILES:

C[C@@]1(CCS(=O)(=O)C1)NC(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN634

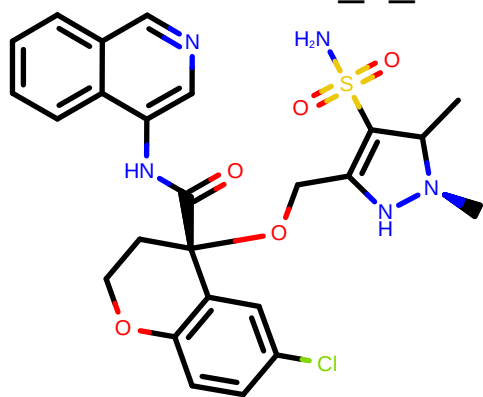
DDG (kcal/mol):

-1.49

dDDG (kcal/mol):

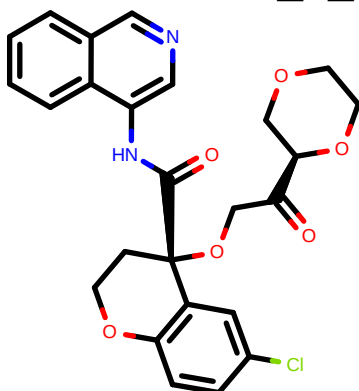
0.33

EN300-1629199_1_1



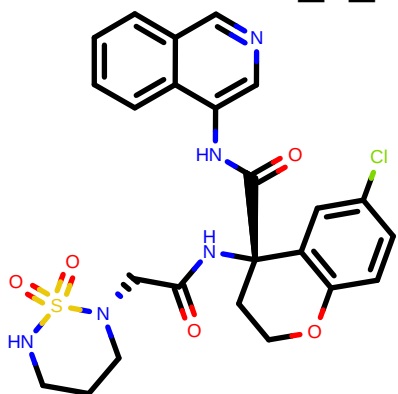
CID:	EN300-1629199_1_1
SMILES:	<chem>Cc1c(c(m1C)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)N</chem>
RUN:	RUN1520
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.30

EN300-6238494_1_2



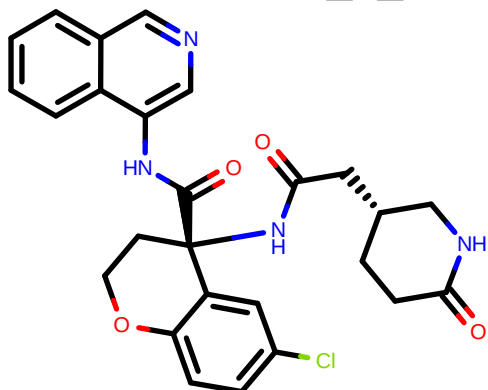
CID:	EN300-6238494_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5COCCO5</chem>
RUN:	RUN309
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.30

EN300-4726186_1_1



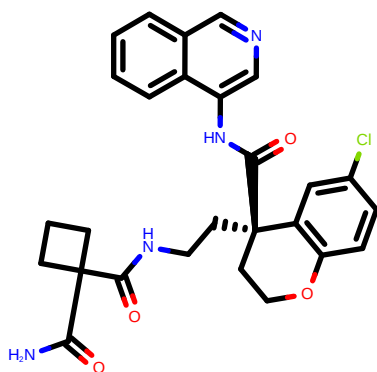
CID:	EN300-4726186_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[N@@]5CCCCN5(=O)=O</chem>
RUN:	RUN917
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.52

EN300-246992_1_2



CID:	EN300-246992_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCC(=O)NC5</chem>
RUN:	RUN474
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.24

EN300-68747_3_1



CID: EN300-68747_3_1

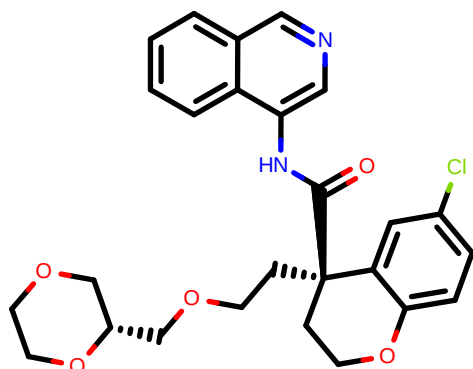
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)C(=O)N

RUN: RUN1330

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.34

EN300-139167_3_2



CID: EN300-139167_3_2

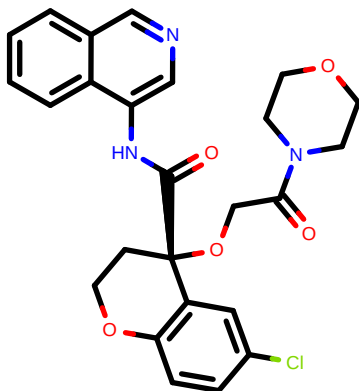
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCCO5

RUN: RUN680

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.31

EN300-1241327_1_1



CID: EN300-1241327_1_1

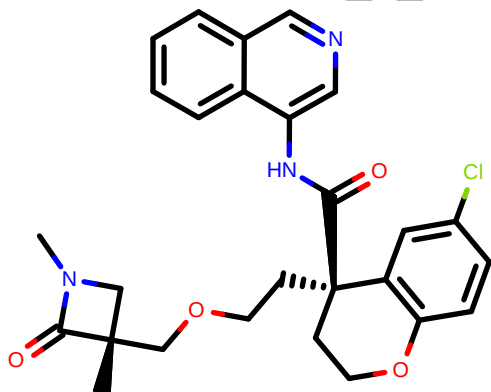
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5COCCO5

RUN: RUN532

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.30

EN300-1273362_3_1



CID: EN300-1273362_3_1

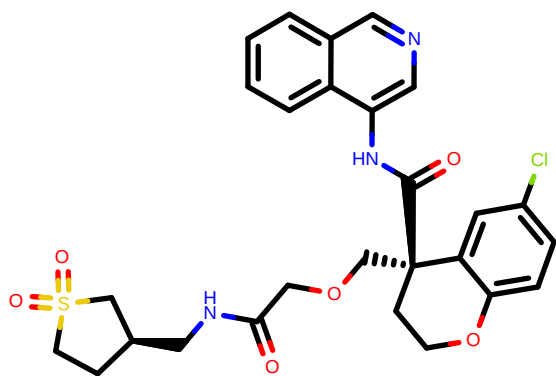
SMILES: C[C@@]1(CN(C1=O)C)COCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN401

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.38

EN300-47606_2_2



CID: EN300-47606_2_2

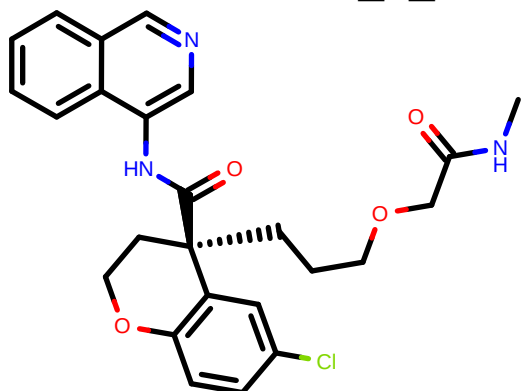
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@H]5SCC5(=O)(=O)C5

RUN: RUN1765

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.53

EN300-2977549_4_1



CID: EN300-2977549_4_1

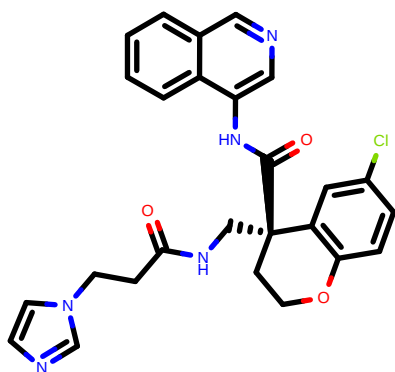
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN611

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.30

EN300-75342_2_1



CID: EN300-75342_2_1

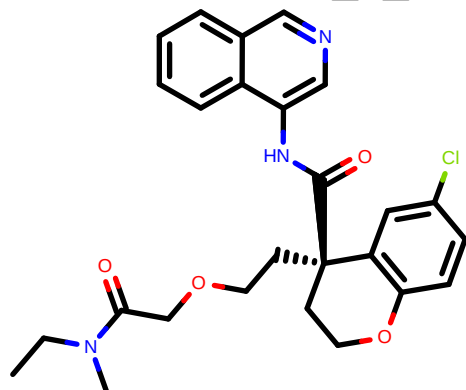
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5scnc5

RUN: RUN724

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-1253122_3_1



CID: EN300-1253122_3_1

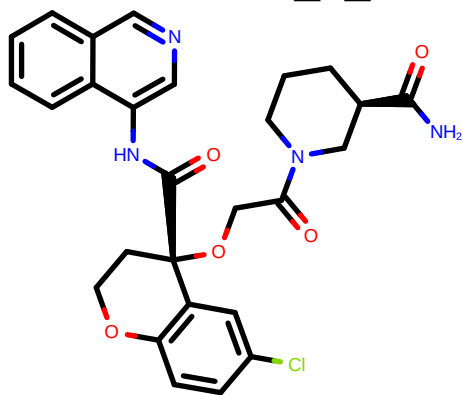
SMILES: CCN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN584

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.26

EN300-22880_1_2



CID: EN300-22880_1_2

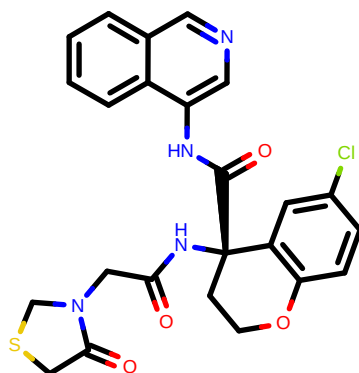
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@H](C5)C(=O)N

RUN: RUN880

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.29

EN300-10747_1_1



CID: EN300-10747_1_1

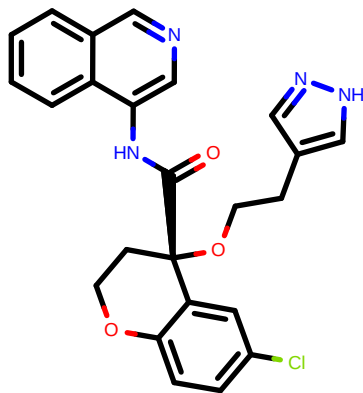
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5SCCSC5=O

RUN: RUN1317

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EDJ-MED-28ec730d-5_1



CID: EDJ-MED-28ec730d-5_1

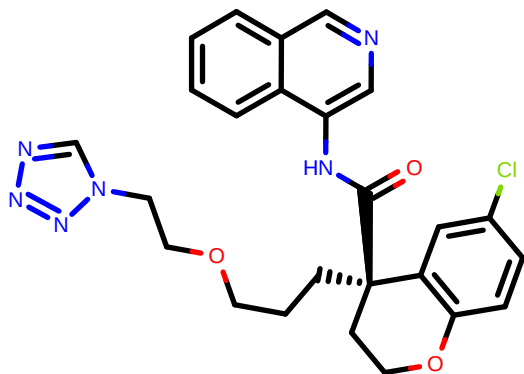
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5

RUN: RUN31

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.24

EN300-364679_4_1



CID: EN300-364679_4_1

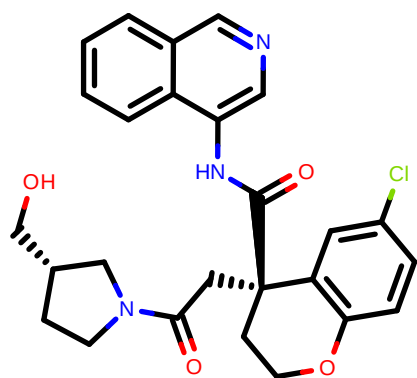
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCCn5cnnn5

RUN: RUN1750

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.40

EN300-88131_1_1



CID: EN300-88131_1_1

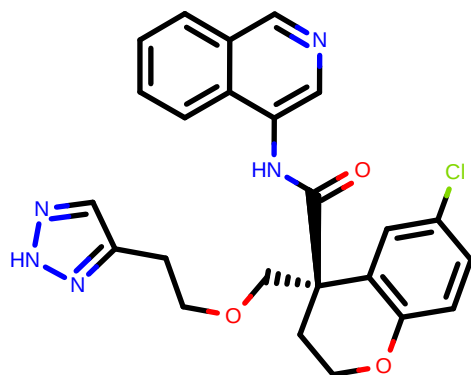
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN1466

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.24

EN300-222357_2_1



CID: EN300-222357_2_1

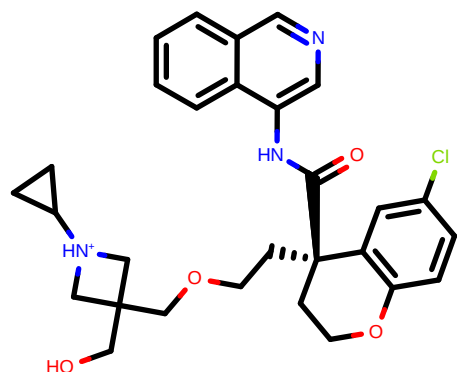
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cn[nH]n5

RUN: RUN990

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.29

EN300-6735421_3_1



CID: EN300-6735421_3_1

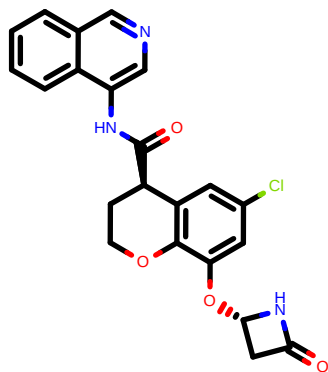
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5(C)[NH+](C5)C6CC6)CO

RUN: RUN497

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.53

VLA-UCB-50c39ae8-8_2



CID: VLA-UCB-50c39ae8-8_2

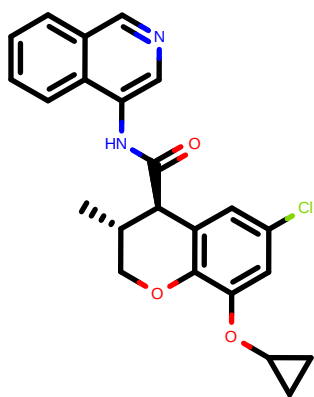
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CC(=O)N5)Cl

RUN: RUN107

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.19

DAR-DIA-0d514e7d-6_1



CID:

DAR-DIA-0d514e7d-6_1

SMILES:

C[C@H]1COC2c(cc2OC3CC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN:

RUN105

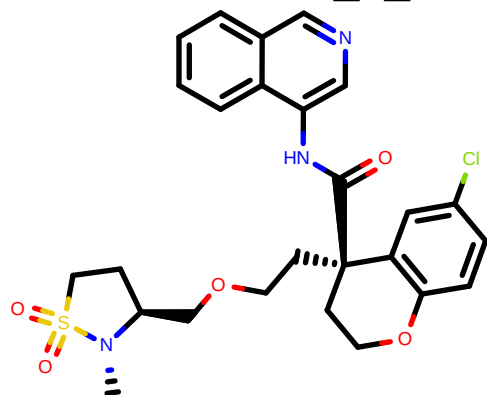
DDG (kcal/mol):

-1.44

dDDG (kcal/mol):

0.17

EN300-393148_3_1



CID:

EN300-393148_3_1

SMILES:

C[N@]1[C@@H](CCS1(=O)=O)COC[C@]2(COC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN385

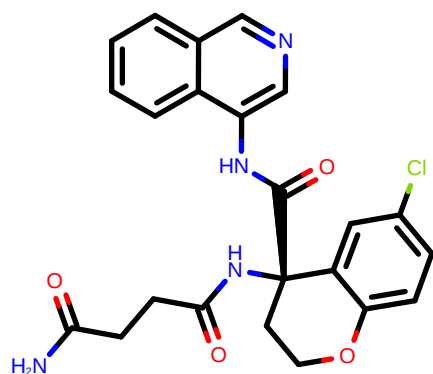
DDG (kcal/mol):

-1.44

dDDG (kcal/mol):

0.29

EN300-178515_1_1



CID:

EN300-178515_1_1

SMILES:

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

RUN:

RUN641

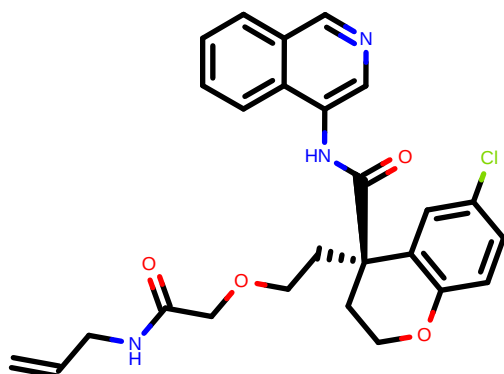
DDG (kcal/mol):

-1.43

dDDG (kcal/mol):

0.22

EN300-17184_3_1



CID:

EN300-17184_3_1

SMILES:

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

RUN:

RUN560

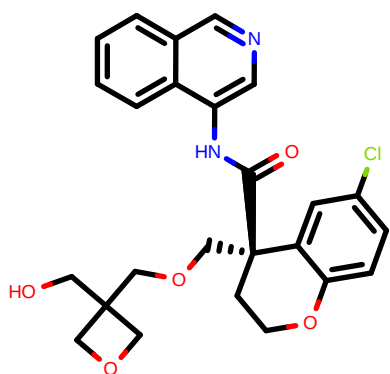
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.26

EN300-102347_2_1



CID:

EN300-102347_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(C5(COC5)CO

RUN:

RUN1478

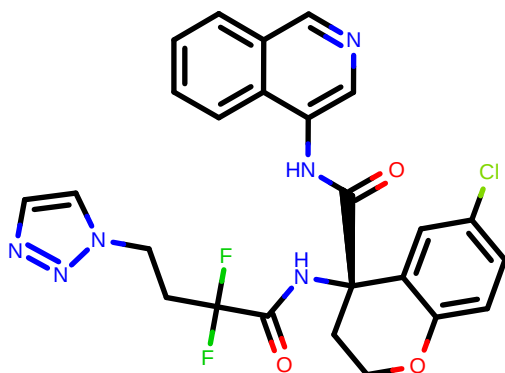
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.26

EN300-6474220_1_1



CID:

EN300-6474220_1_1

SMILES:

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

RUN:

RUN1461

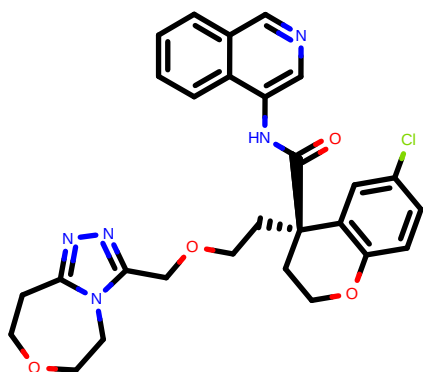
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.27

EN300-310888_3_1



CID:

EN300-310888_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(C5n[nH]5)COC(C6

RUN:

RUN1619

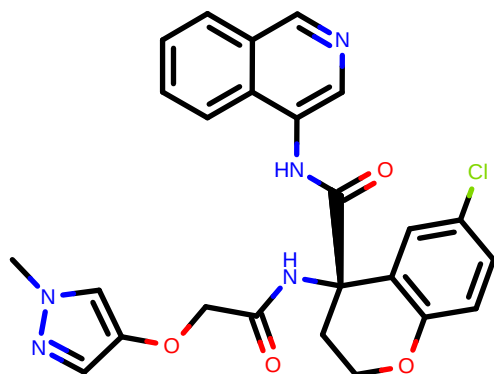
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.37

EN300-201553_1_1



CID:

EN300-201553_1_1

SMILES:

Cn1cc(c[n1])OCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN814

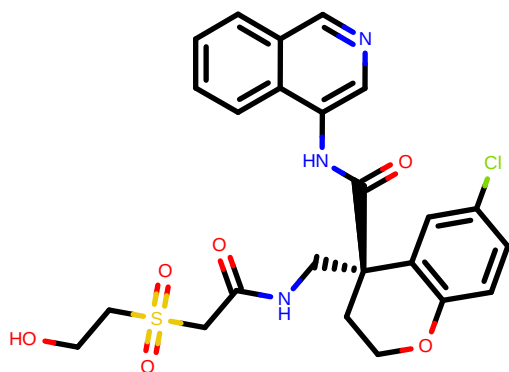
DDG (kcal/mol):

-1.42

dDDG (kcal/mol):

0.25

EN300-4293814_2_1



CID: EN300-4293814_2_1

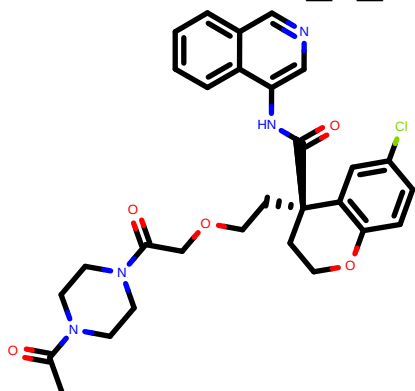
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS(=O)(=O)CCO

RUN: RUN398

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.64

EN300-1724771_3_1



CID: EN300-1724771_3_1

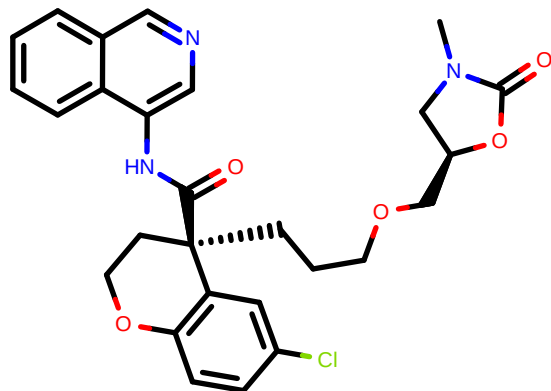
SMILES: CC(=O)N1CCN(CC1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1595

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.36

EN300-222969_4_1



CID: EN300-222969_4_1

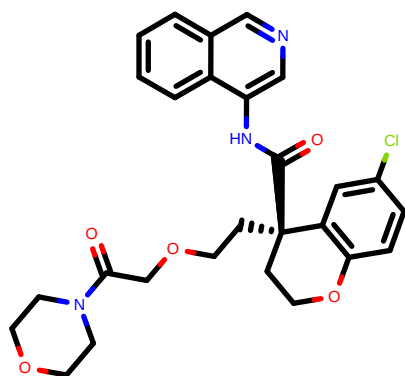
SMILES: CN1C[C@@H](OC1=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1375

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.53

EN300-1241327_3_1



CID: EN300-1241327_3_1

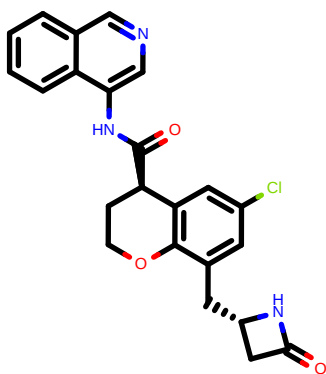
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCOCC5

RUN: RUN821

DDG (kcal/mol): -1.40

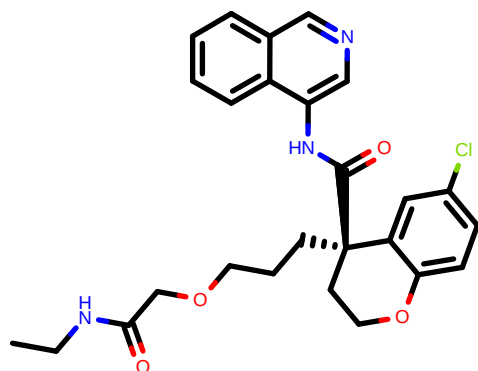
dDDG (kcal/mol): 0.28

DAR-DIA-6a508060-5_3



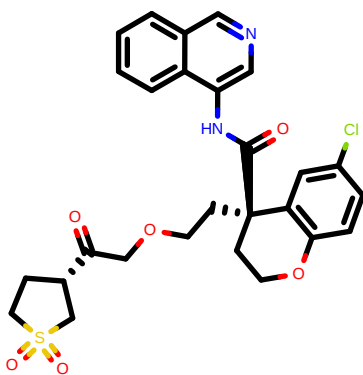
CID:	DAR-DIA-6a508060-5_3
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC(=O)N5)Cl</chem>
RUN:	RUN218
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.16

EN300-7003350_4_1



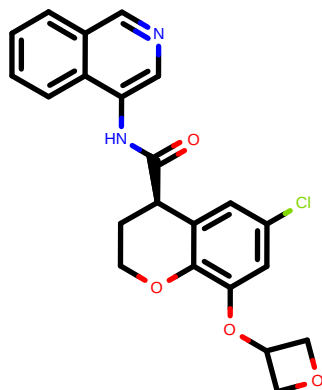
CID:	EN300-7003350_4_1
SMILES:	<chem>CCNC(=O)COCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN1047
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.31

EN300-226314_3_2



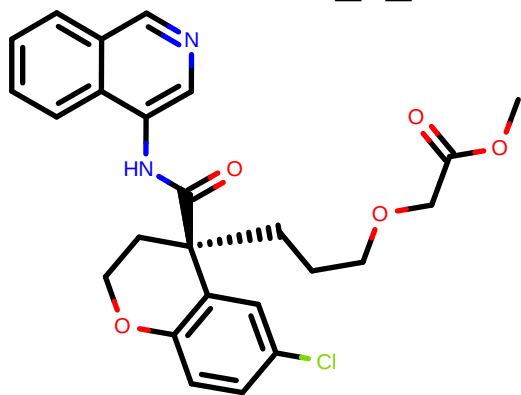
CID:	EN300-226314_3_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@H]5SCS(=O)(=O)C5</chem>
RUN:	RUN1332
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.36

EDJ-MED-e4b030d8-4_1



CID:	EDJ-MED-e4b030d8-4_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4OC5COC5)Cl</chem>
RUN:	RUN150
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.21

EN300-19700_4_1



CID:

EN300-19700_4_1

SMILES:

COC(=O)COCC[C@]1(C)C(COC2C1CC(C2)Cl)C(=O)Nc3ncc4c3cccc4

RUN:

RUN428

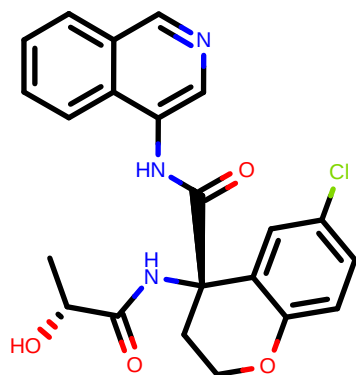
DDG (kcal/mol):

-1.40

dDDG (kcal/mol):

0.29

EN300-77464_1_1



CID:

EN300-77464_1_1

SMILES:

C[C@H](C(=O)N[C@]1(C)C(COC2C1CC(C2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN:

RUN1397

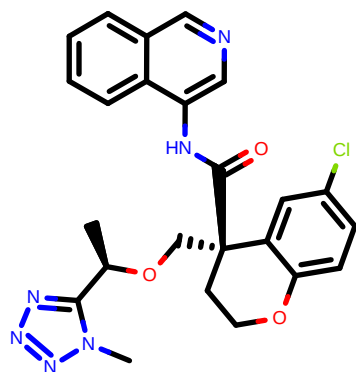
DDG (kcal/mol):

-1.39

dDDG (kcal/mol):

0.24

EN300-173006_2_2



CID:

EN300-173006_2_2

SMILES:

C[C@H](c1nnnn1C)OC[C@]2(C)C(COC3C2CC(C3)Cl)C(=O)Nc4ncc5c4cccc5

RUN:

RUN1502

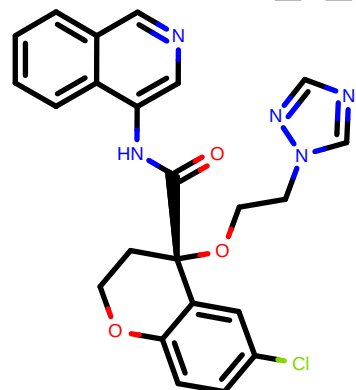
DDG (kcal/mol):

-1.39

dDDG (kcal/mol):

0.33

EN300-6255179_1_1



CID:

EN300-6255179_1_1

SMILES:

c1ccc2c(c1)ncc2NC(=O)[C@@]3(C)C(COC4C3CC(C4)Cl)OCCn5cncn5

RUN:

RUN1096

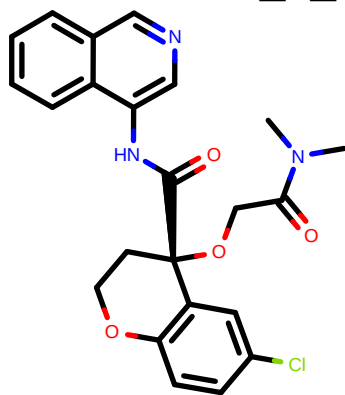
DDG (kcal/mol):

-1.39

dDDG (kcal/mol):

0.25

EN300-216063_1_1



CID: EN300-216063_1_1

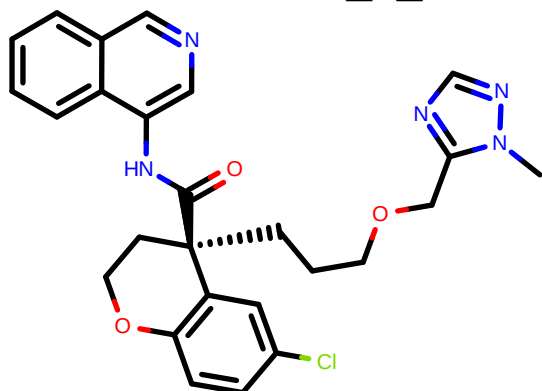
SMILES: CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN785

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.23

EN300-87334_4_1



CID: EN300-87334_4_1

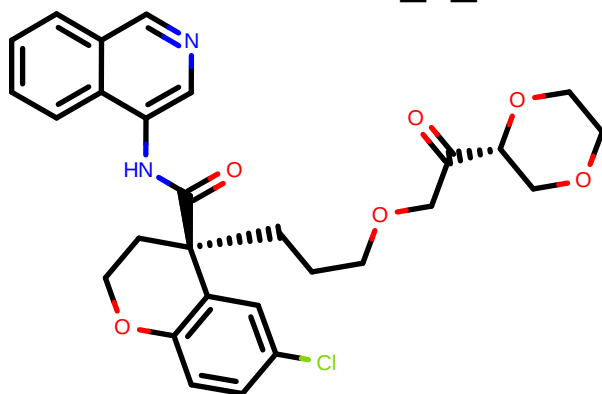
SMILES: Cn1c(ncn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN324

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.31

EN300-6238494_4_2



CID: EN300-6238494_4_2

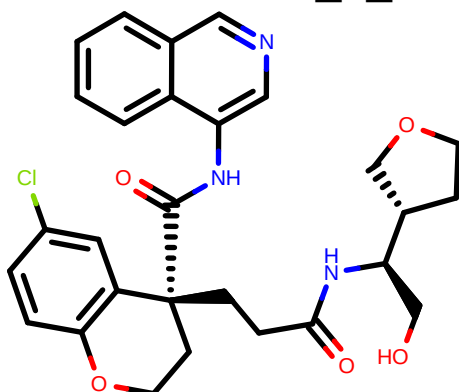
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC(=O)[C@H]5COCOC5

RUN: RUN1127

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.29

EN300-104493_2_4



CID: EN300-104493_2_4

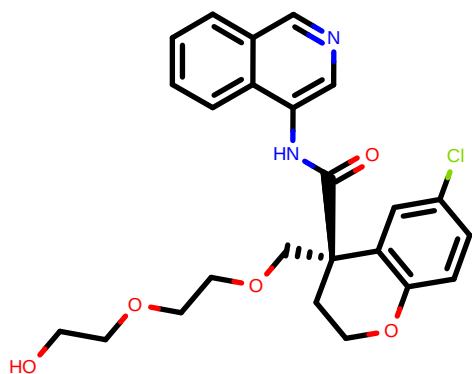
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H](CO)[C@H]5COCOC5

RUN: RUN987

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.34

EN300-52467_2_1



CID:

EN300-52467_2_1

SMILES:

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

RUN:

RUN1589

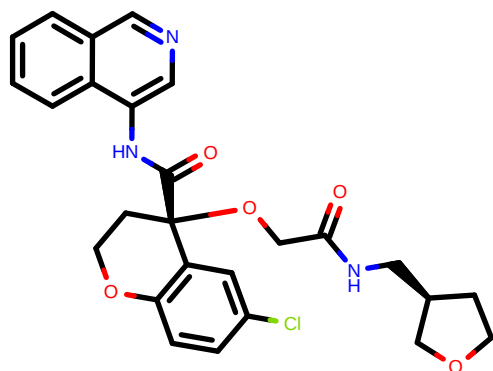
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.26

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

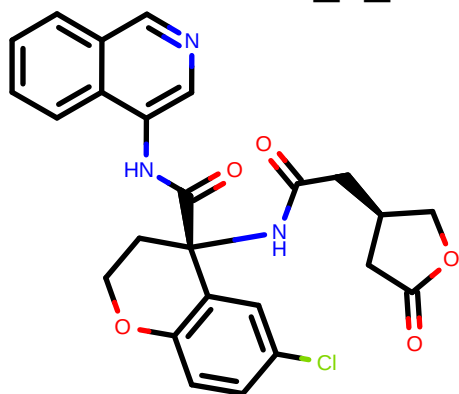
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.26

EN300-109535_1_1



CID:

EN300-109535_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)OC5

RUN:

RUN1245

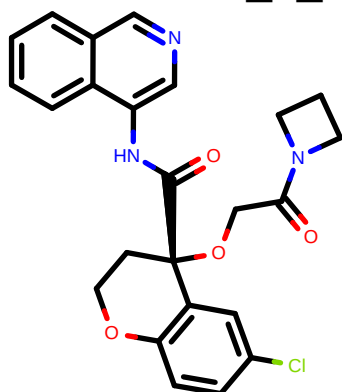
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.29

EN300-11195_1_1



CID:

EN300-11195_1_1

SMILES:

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

RUN:

RUN588

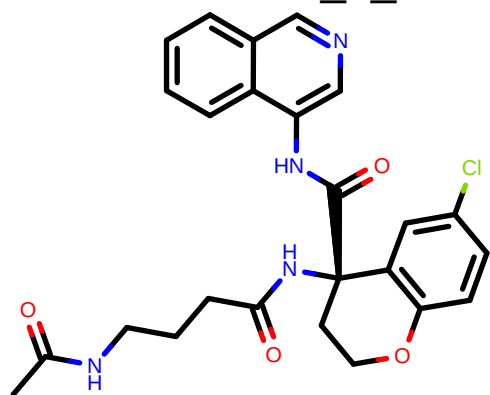
DDG (kcal/mol):

-1.38

dDDG (kcal/mol):

0.20

EN300-18564_1_1



CID:

EN300-18564_1_1

SMILES:

CC(=O)NCCCC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN498

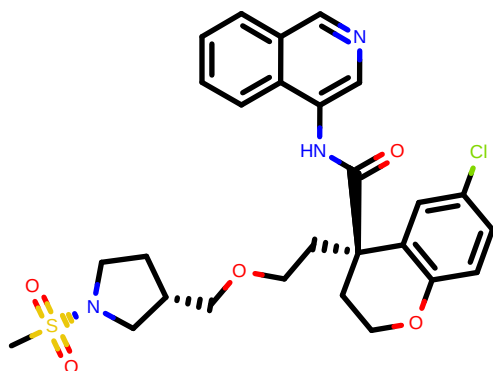
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.25

EN300-261986_3_1



CID:

EN300-261986_3_1

SMILES:

CS(=O)(=O)N1CC[C@H]1CC[C@@H]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN473

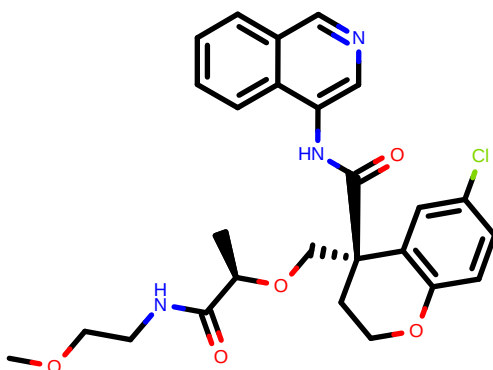
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.36

EN300-23317_2_2



CID:

EN300-23317_2_2

SMILES:

C[C@H](C(=O)NCCOC)OC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN610

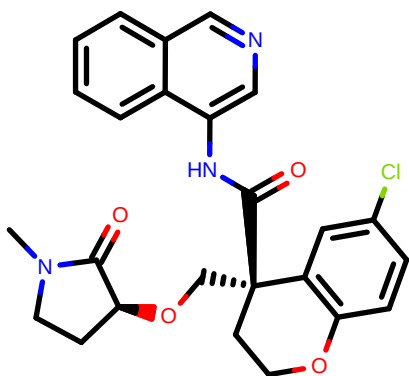
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.48

EN300-98648_2_1



CID:

EN300-98648_2_1

SMILES:

CN1CC[C@H]1C(=O)OC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN1685

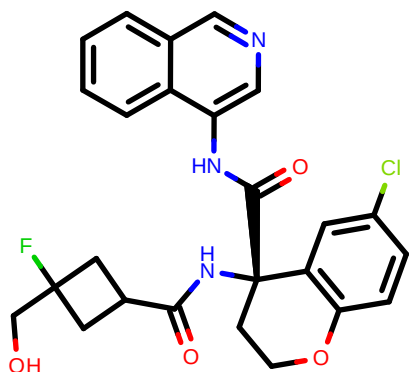
DDG (kcal/mol):

-1.37

dDDG (kcal/mol):

0.27

EN300-6746890_1_1



CID:

EN300-6746890_1_1

SMILES:

c1cc2c(c(nc2)NC(=O)[C@@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@H]5C[C@@](C5)(F)CO)cc1

RUN:

RUN1596

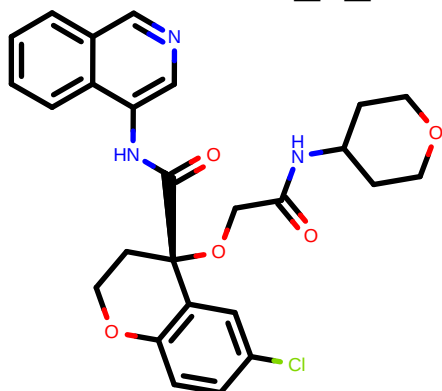
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.25

EN300-67573_1_1



CID:

EN300-67573_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)OCC(=O)NC5COCC5

RUN:

RUN1184

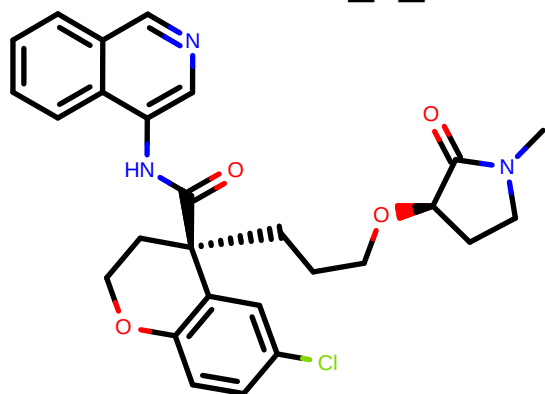
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.23

EN300-98648_4_2



CID:

EN300-98648_4_2

SMILES:

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

RUN:

RUN1678

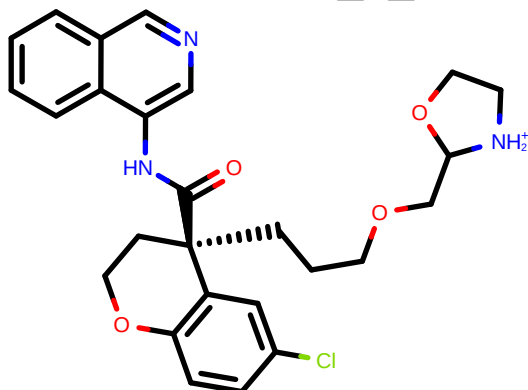
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.32

EN300-317555_4_1



CID:

EN300-317555_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5

RUN:

RUN500

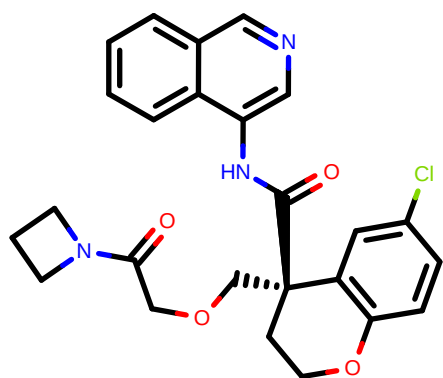
DDG (kcal/mol):

-1.36

dDDG (kcal/mol):

0.27

EN300-11195_2_1



CID: EN300-11195_2_1

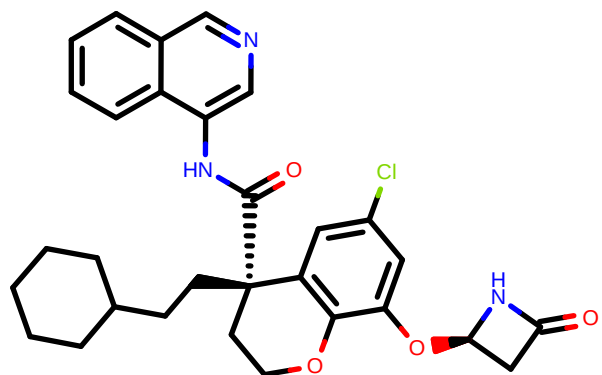
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC5

RUN: RUN1142

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.23

VLA-UCB-05e51b3f-12_1



CID: VLA-UCB-05e51b3f-12_1

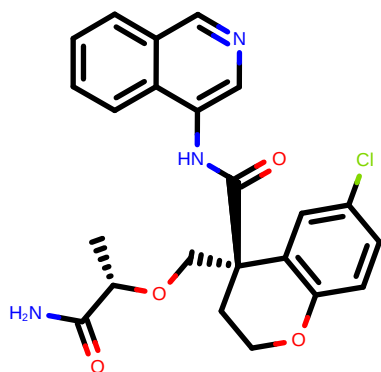
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)Cl)COC6CCCCC6

RUN: RUN241

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.32

EN300-17381_2_1



CID: EN300-17381_2_1

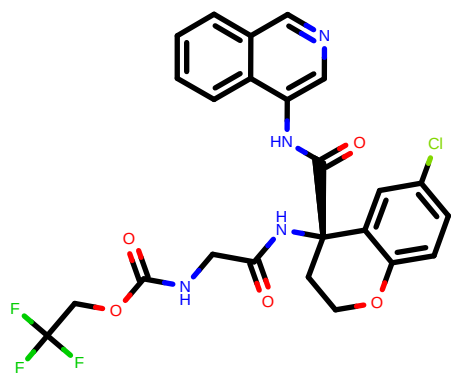
SMILES: C[C@@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN894

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-50488_1_1



CID: EN300-50488_1_1

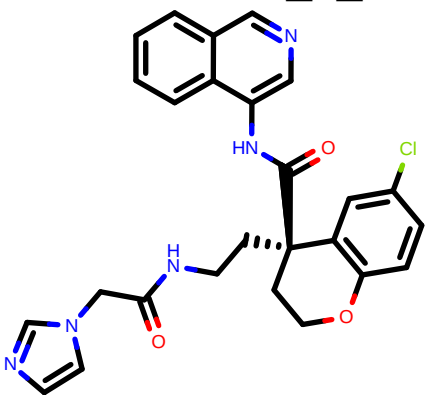
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)OCC(F)(F)F

RUN: RUN1005

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.27

EN300-38979_3_1



CID:

EN300-38979_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ccnc5

RUN:

RUN1386

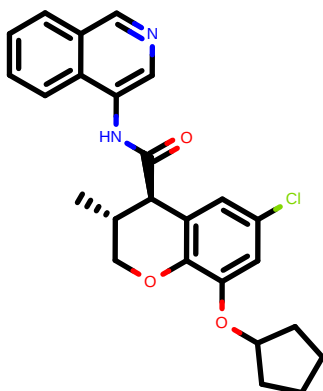
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.30

DAR-DIA-0d514e7d-4_1



CID:

DAR-DIA-0d514e7d-4_1

SMILES:

C[C@H]1COC2c(cc2OC3CCCC3)C[C@@H]1C(=O)Nc4cnc5c4cccc5

RUN:

RUN93

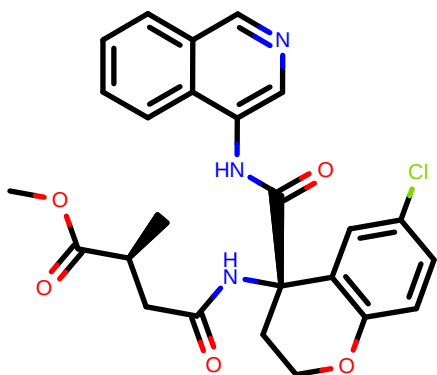
DDG (kcal/mol):

-1.35

dDDG (kcal/mol):

0.26

EN300-108413_1_1



CID:

EN300-108413_1_1

SMILES:

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

RUN:

RUN1517

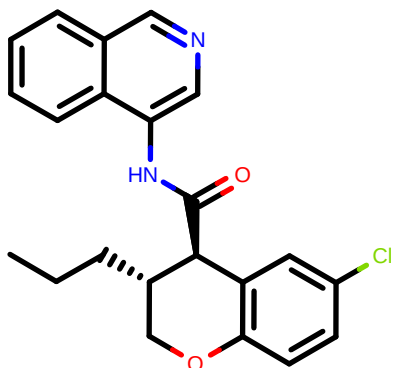
DDG (kcal/mol):

-1.34

dDDG (kcal/mol):

0.29

EDJ-MED-e4b030d8-6_1



CID:

EDJ-MED-e4b030d8-6_1

SMILES:

CCC[C@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cnc4c3cccc4)Cl

RUN:

RUN7

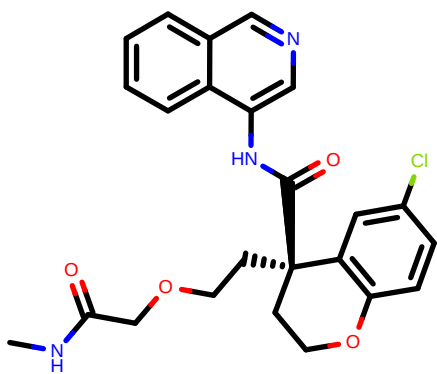
DDG (kcal/mol):

-1.34

dDDG (kcal/mol):

0.11

EN300-2977549_3_1



CID: EN300-2977549_3_1

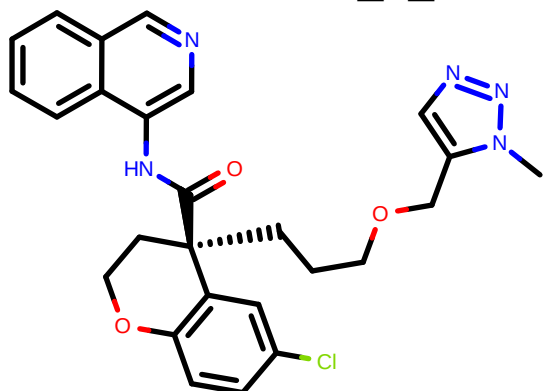
SMILES: CNC(=O)COCC[C@]1(COC(=O)Cc2cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1755

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.27

EN300-216673_4_1



CID: EN300-216673_4_1

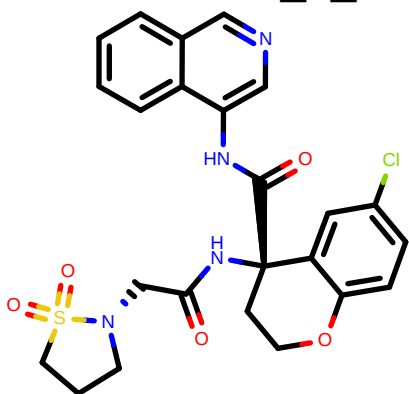
SMILES: Cn1c(cnn1)COC[C@]2(COC(=O)Cc3cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN300

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.31

EN300-43206_1_1



CID: EN300-43206_1_1

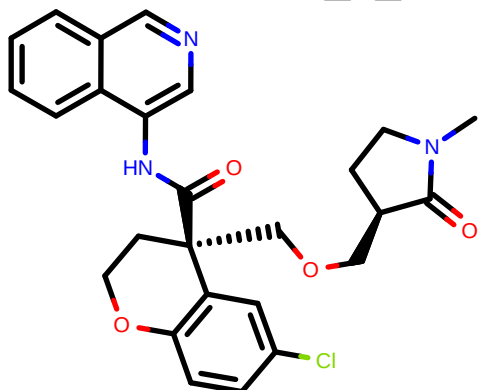
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC(=O)Cc4cc(cc4)Cl)NC(=O)C[N@]5CCCC5(=O)=O

RUN: RUN1636

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.35

EN300-260816_2_1



CID: EN300-260816_2_1

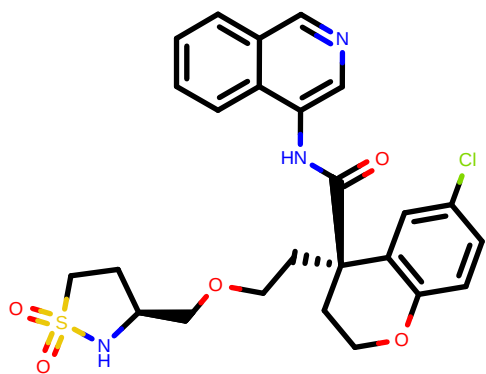
SMILES: CN1CC[C@@H](C1=O)COC[C@]2(COC(=O)Cc3cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1669

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.29

EN300-1699871_3_1



CID: EN300-1699871_3_1

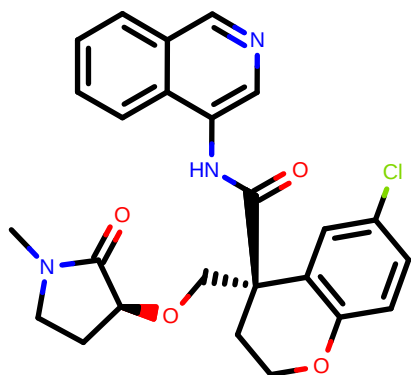
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5SCCS(=O)(=O)N5

RUN: RUN1140

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.34

EN300-98648_2_1



CID: EN300-98648_2_1

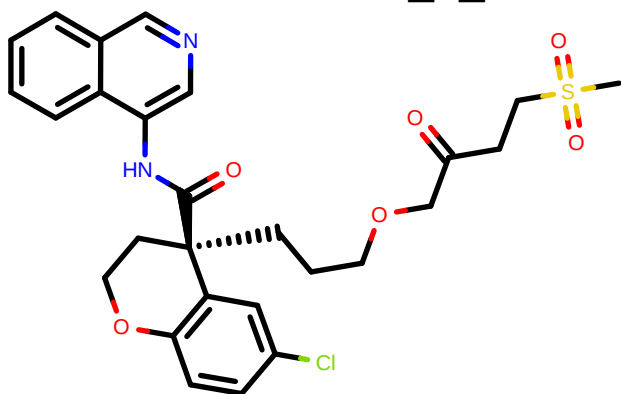
SMILES: CN1CC[C@@H](C1=O)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4ccccc5

RUN: RUN1693

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.26

EN300-1988306_4_1



CID: EN300-1988306_4_1

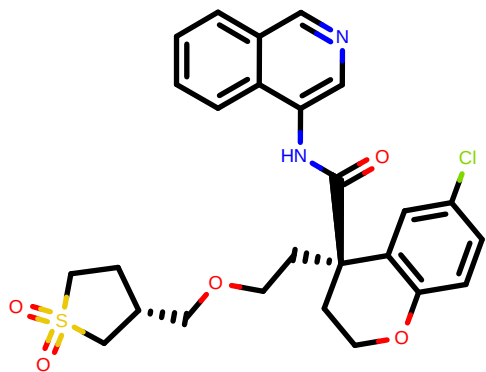
SMILES: CS(=O)(=O)CCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4

RUN: RUN1638

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.43

EN300-1448603_3_2



CID: EN300-1448603_3_2

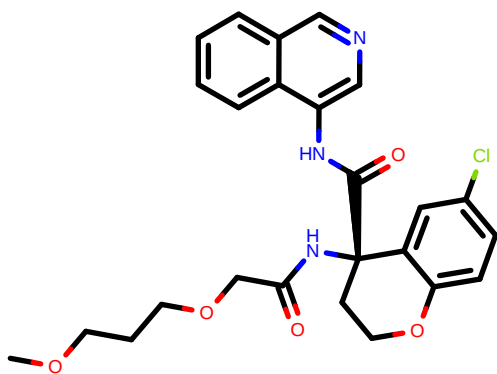
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN1244

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.40

EN300-125769_1_1



CID: EN300-125769_1_1

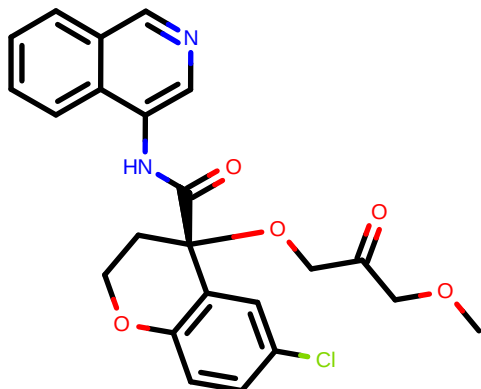
SMILES: COCCCCOC(=O)N[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1365

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.31

EN300-125140_1_1



CID: EN300-125140_1_1

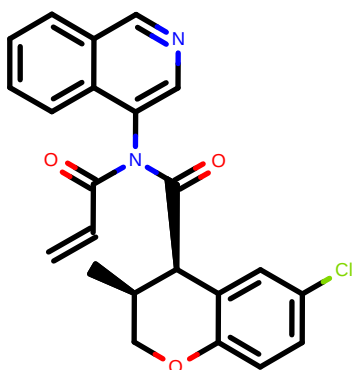
SMILES: COCC(=O)CO[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN405

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

DAR-DIA-5ff57136-1_1



CID: DAR-DIA-5ff57136-1_1

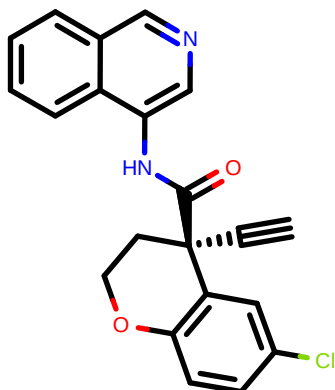
SMILES: C[C@@H]1COC2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl

RUN: RUN243

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.23

PET-UNK-29afea89-1_1



CID: PET-UNK-29afea89-1_1

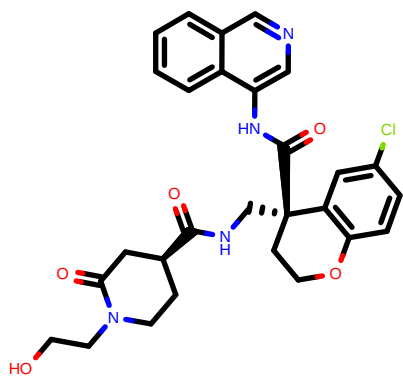
SMILES: C#C[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN40

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.10

EN300-1723663_2_2



CID:

EN300-1723663_2_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@H]5CCN(C(=O)C5)CCO

RUN:

RUN358

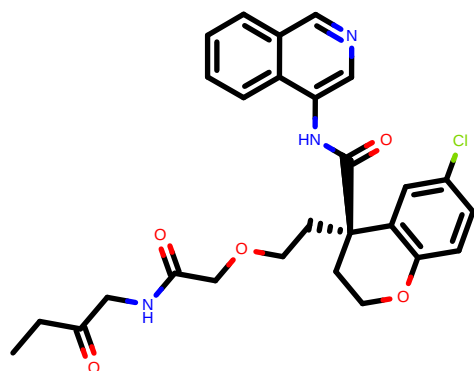
DDG (kcal/mol):

-1.31

dDDG (kcal/mol):

0.34

EN300-132624_3_1



CID:

EN300-132624_3_1

SMILES:

CCC(=O)CNC(=O)COC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3ccoc4

RUN:

RUN948

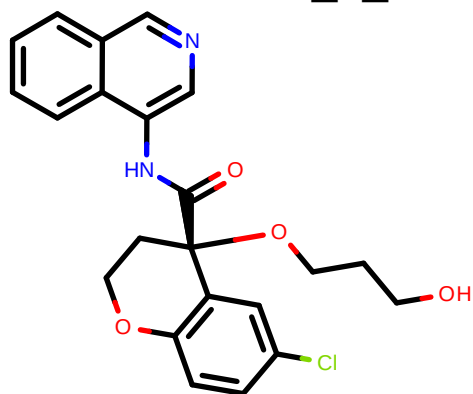
DDG (kcal/mol):

-1.30

dDDG (kcal/mol):

0.32

EN300-221518_1_1



CID:

EN300-221518_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CCCCO

RUN:

RUN1000

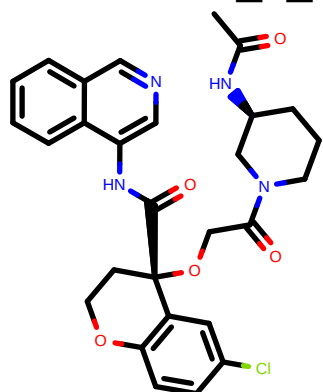
DDG (kcal/mol):

-1.29

dDDG (kcal/mol):

0.20

EN300-48886_1_2



CID:

EN300-48886_1_2

SMILES:

CC(=O)N[C@H]1CCCN(C1)C(=O)CO[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccccc5

RUN:

RUN1416

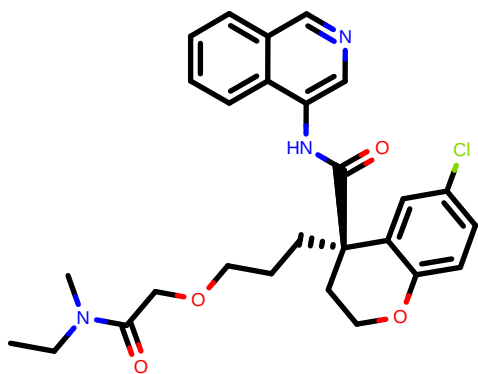
DDG (kcal/mol):

-1.29

dDDG (kcal/mol):

0.28

EN300-1253122_4_1



CID: EN300-1253122_4_1

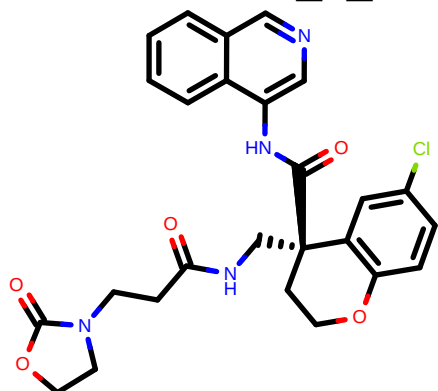
SMILES: CCN(C)C(=O)COCC[C@@]1(COC(=O)Cc2cc(C)C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN691

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.33

EN300-53918_2_1



CID: EN300-53918_2_1

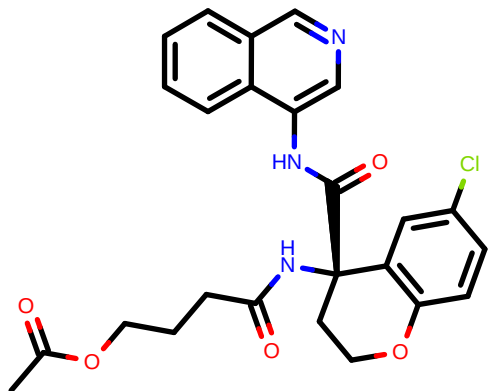
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC(=O)Cc4cc(C)C)CNC(=O)CCN5CCCC5=O

RUN: RUN685

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.33

EN300-1696058_1_1



CID: EN300-1696058_1_1

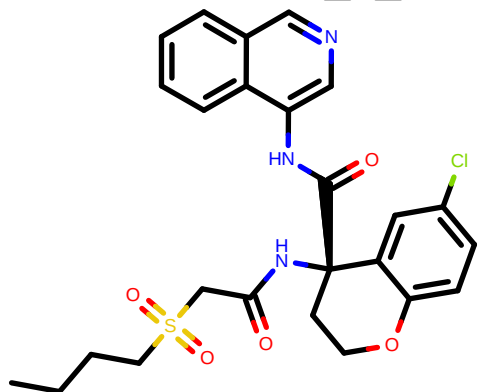
SMILES: CC(=O)OCCCC(=O)N[C@@]1(COC(=O)Cc2cc(C)C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN394

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

EN300-686903_1_1



CID: EN300-686903_1_1

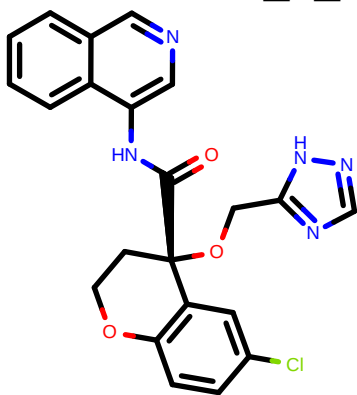
SMILES: CCCCS(=O)(=O)CC(=O)N[C@@]1(COC(=O)Cc2cc(C)C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN712

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.41

EN300-306316_1_1



CID: EN300-306316_1_1

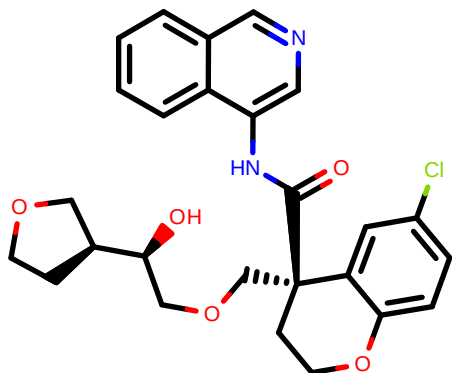
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5[nH]ncn5

RUN: RUN668

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.23

EN300-1911992_2_3



CID: EN300-1911992_2_3

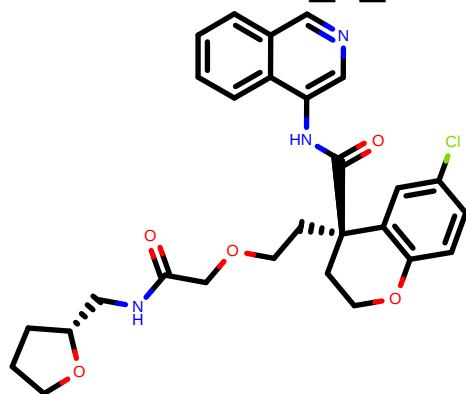
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC@H5COC(C)O

RUN: RUN1278

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.32

EN300-01527_3_2



CID: EN300-01527_3_2

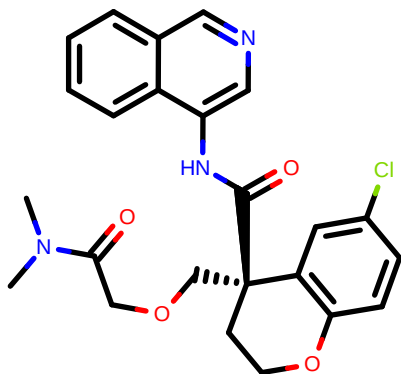
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@H]5CCCCO5

RUN: RUN964

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.35

EN300-216063_2_1



CID: EN300-216063_2_1

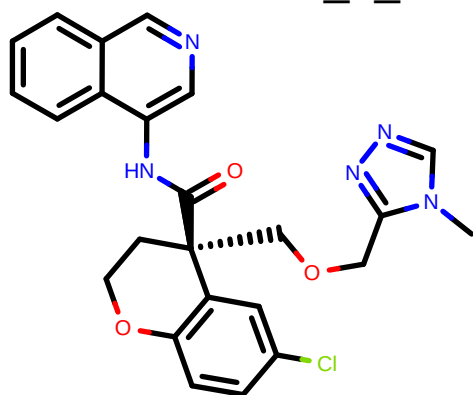
SMILES: CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1190

DDG (kcal/mol): -1.28

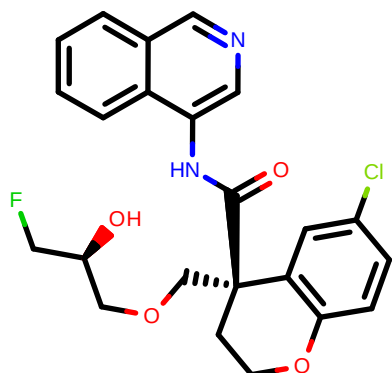
dDDG (kcal/mol): 0.27

EN300-113112_2_1



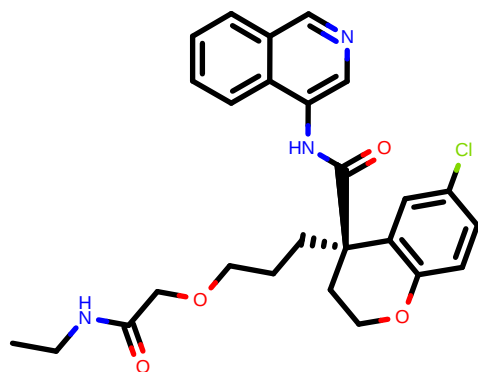
CID:	EN300-113112_2_1
SMILES:	<chem>Cn1cnnc1COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1438
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.23

EN300-1968342_2_1



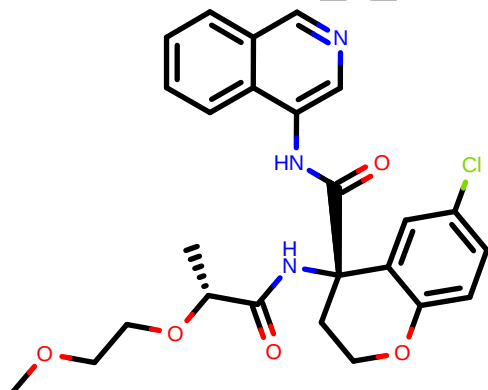
CID:	EN300-1968342_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COC[C@H](CF)O</chem>
RUN:	RUN491
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.35

EN300-7003350_4_1



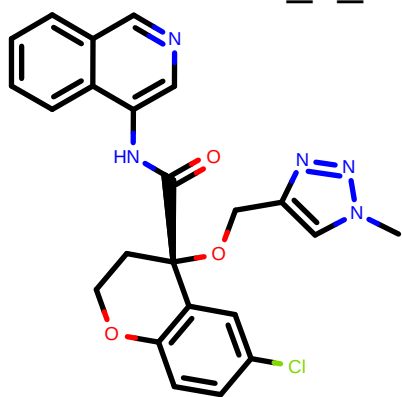
CID:	EN300-7003350_4_1
SMILES:	<chem>CCNC(=O)COC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1031
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.31

EN300-77359_1_2



CID:	EN300-77359_1_2
SMILES:	<chem>C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OCCOC</chem>
RUN:	RUN1333
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.27

EN300-120282_1_1



CID: EN300-120282_1_1

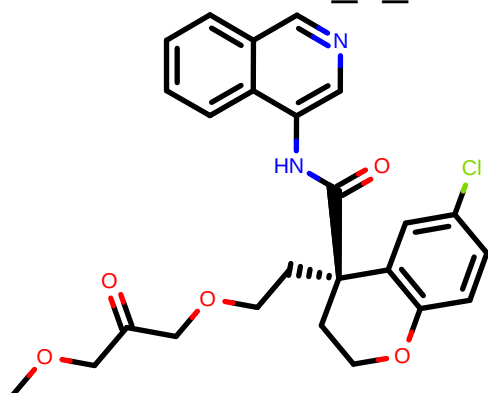
SMILES: Cn1cc(nn1)CO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN485

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.21

EN300-125140_3_1



CID: EN300-125140_3_1

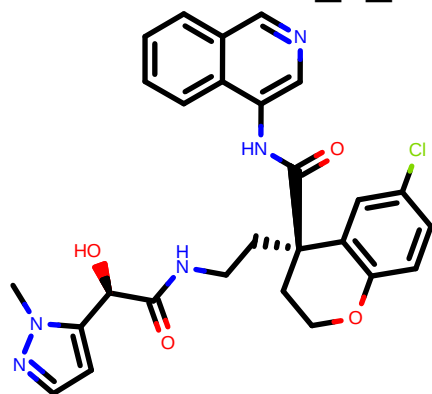
SMILES: COCC(=O)COCC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN735

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.27

EN300-6473273_3_2



CID: EN300-6473273_3_2

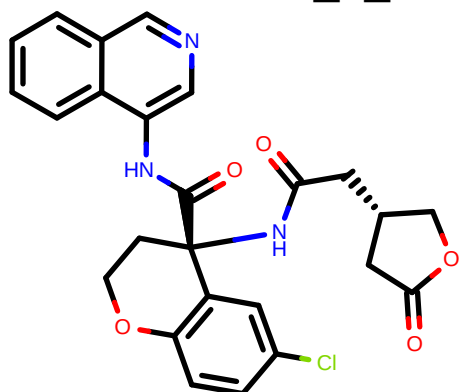
SMILES: Cn1c(cn1)[C@H](C(=O)NCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN1114

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.36

EN300-109535_1_2



CID: EN300-109535_1_2

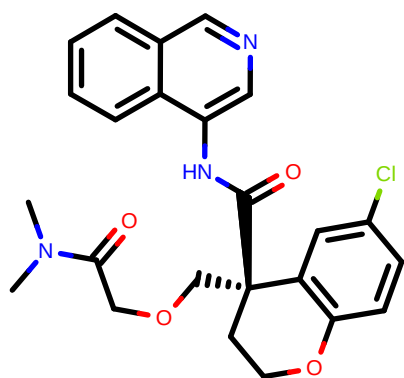
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)OC5

RUN: RUN869

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.26

EN300-216063_2_1



CID: EN300-216063_2_1

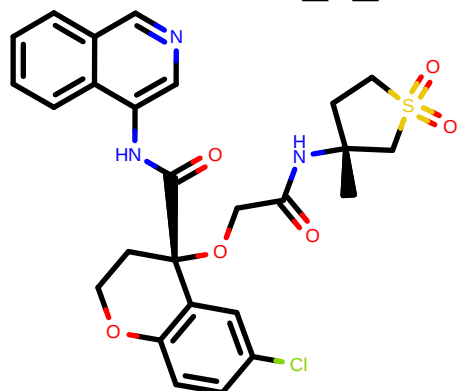
SMILES: CN(C)C(=O)COC[C@]1(C)C(=O)C2C1C(C2)C(=O)Nc3ccc4c3ccccc4

RUN: RUN1206

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.24

EN300-10414_1_2



CID: EN300-10414_1_2

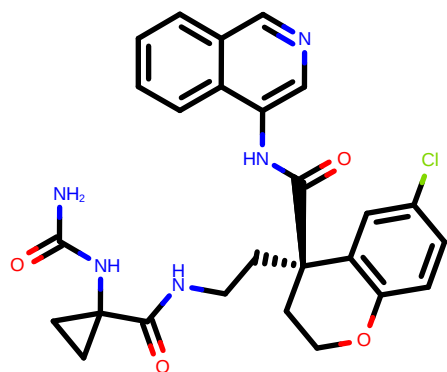
SMILES: C[C@]1(C)CCS(=O)(=O)C1NC(=O)CO[C@]2(C)C(=O)C3C2C(C3)C(=O)Nc4ccc5c4ccccc5

RUN: RUN341

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.35

EN300-123614_3_1



CID: EN300-123614_3_1

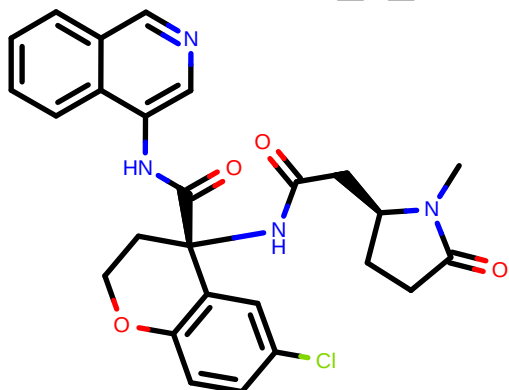
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@]3(C)C(=O)C4C3C(C4)C(=O)Nc5ccc6c5ccccc6

RUN: RUN606

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.32

EN300-207765_1_1



CID: EN300-207765_1_1

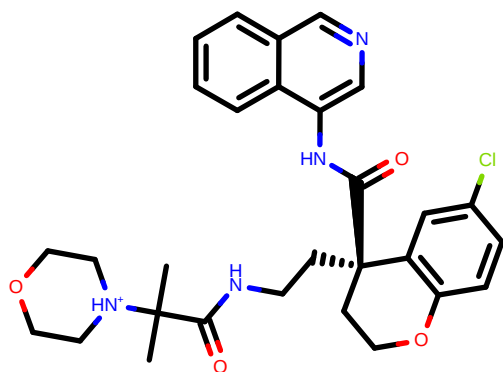
SMILES: CN1[C@@H](CCC1=O)CC(=O)N[C@]2(C)C(=O)C3C2C(C3)C(=O)Nc4ccc5c4ccccc5

RUN: RUN1197

DDG (kcal/mol): -1.25

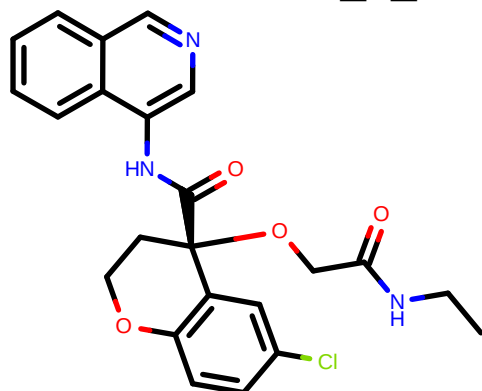
dDDG (kcal/mol): 0.26

EN300-64247_3_1



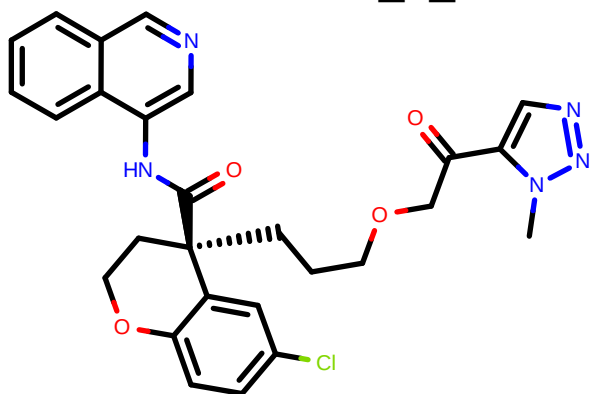
CID:	EN300-64247_3_1
SMILES:	<chem>CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)[NH+]5CCOCC5</chem>
RUN:	RUN630
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.44

EN300-7003350_1_1



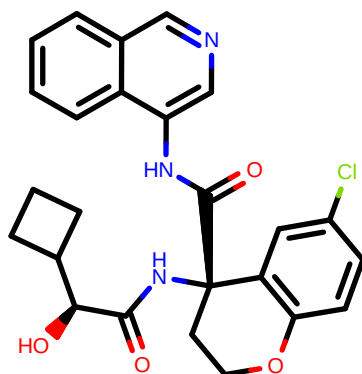
CID:	EN300-7003350_1_1
SMILES:	<chem>CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN731
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.20

EN300-204936_4_1



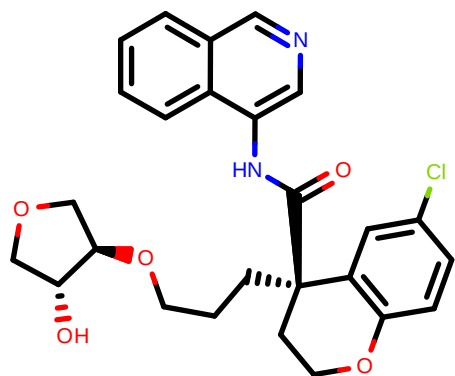
CID:	EN300-204936_4_1
SMILES:	<chem>Cn1c(cnn1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1726
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.31

EN300-249764_1_2



CID:	EN300-249764_1_2
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5CCCC5)O</chem>
RUN:	RUN949
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.26

EN300-331828_4_1



CID:

EN300-331828_4_1

SMILES:

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

RUN:

RUN1447

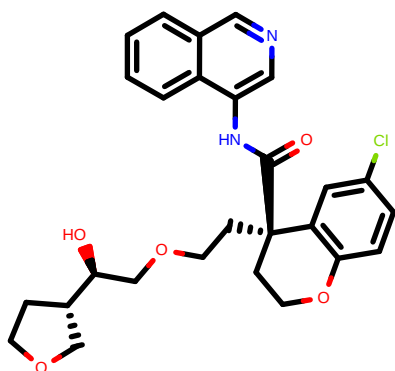
DDG (kcal/mol):

-1.24

dDDG (kcal/mol):

0.27

EN300-1911992_3_3



CID:

EN300-1911992_3_3

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](C)[C@@H]5CCOC5O

RUN:

RUN695

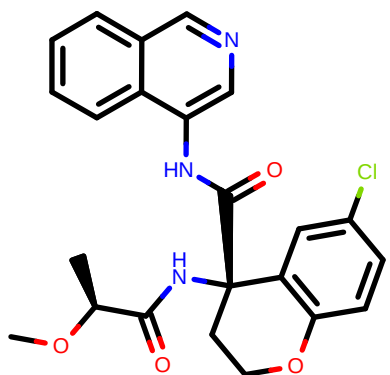
DDG (kcal/mol):

-1.23

dDDG (kcal/mol):

0.37

EN300-51257_1_1



CID:

EN300-51257_1_1

SMILES:

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

RUN:

RUN782

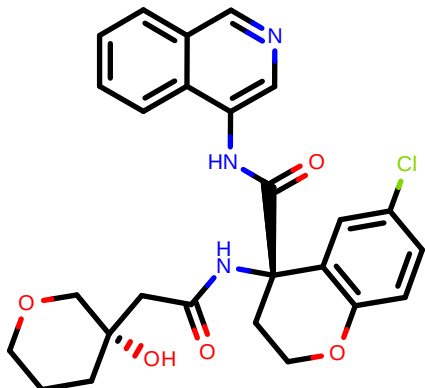
DDG (kcal/mol):

-1.23

dDDG (kcal/mol):

0.22

EN300-1071940_1_2



CID:

EN300-1071940_1_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5(CCCOC5)O

RUN:

RUN681

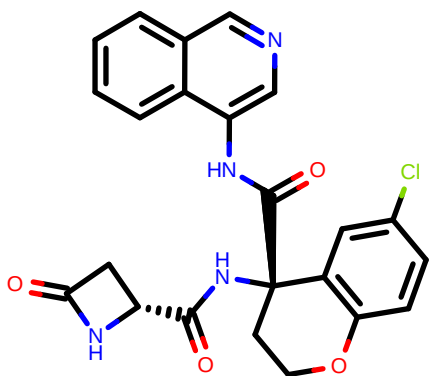
DDG (kcal/mol):

-1.23

dDDG (kcal/mol):

0.28

EN300-101505_1_2



CID: EN300-101505_1_2

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5

RUN:

RUN1277

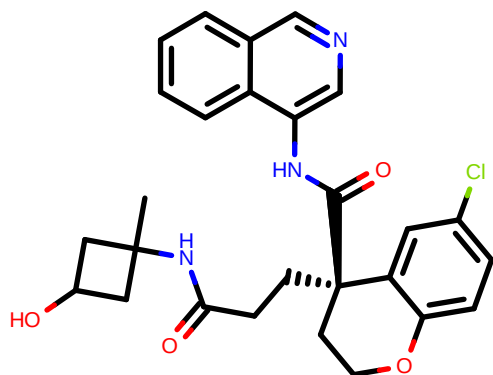
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.23

EN300-7396882_2_1



CID: EN300-7396882_2_1

SMILES:

CC1(CC(C1)O)NC(=O)CC[C@]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4ccc5ccccc5

RUN:

RUN939

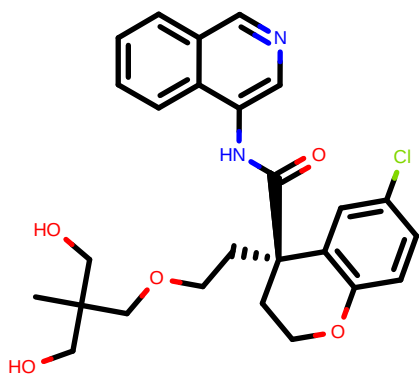
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.29

EN300-218116_3_1



CID: EN300-218116_3_1

SMILES:

CC(CO)(CO)COC[C@]1(CCOc2cc1cc(cc2)Cl)C(=O)Nc3ccc4cc3ccccc4

RUN:

RUN289

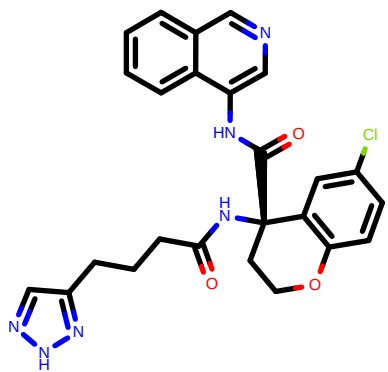
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

0.34

EN300-156995_1_1



CID: EN300-156995_1_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)NC(=O)CCC5cn[nH]5

RUN:

RUN1173

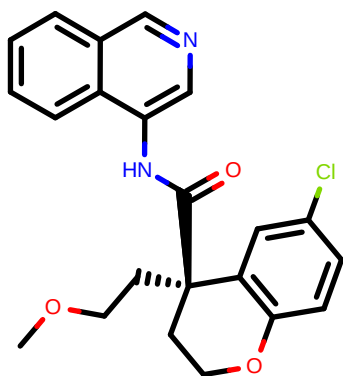
DDG (kcal/mol):

-1.22

dDDG (kcal/mol):

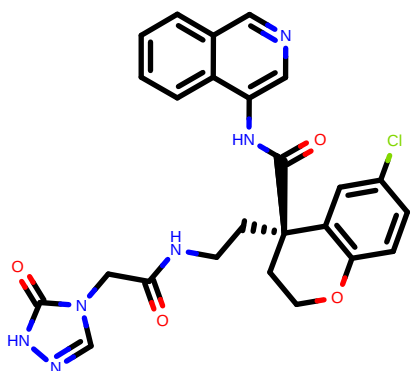
0.28

EDJ-MED-28ec730d-2_1



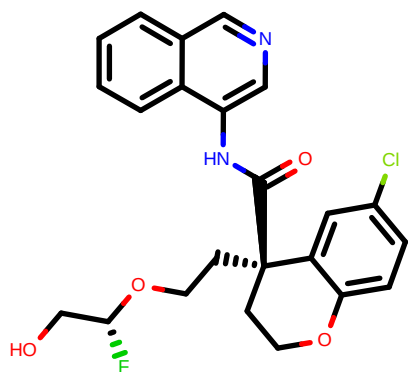
CID:	EDJ-MED-28ec730d-2_1
SMILES:	<chem>COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN77
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.20

EN300-120820_3_1



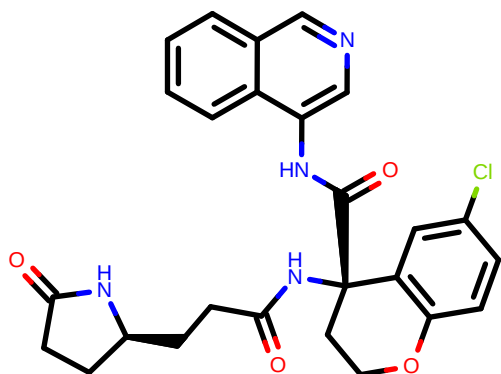
CID:	EN300-120820_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cn[nH]c5=O</chem>
RUN:	RUN914
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.31

EN300-861925_3_1



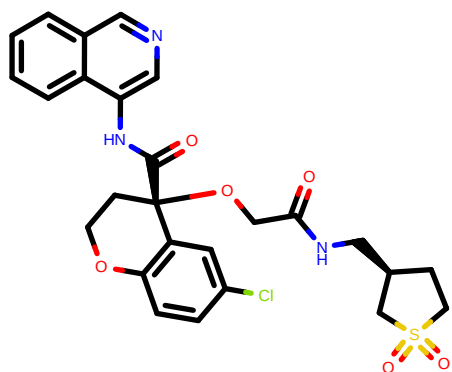
CID:	EN300-861925_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H](CO)F</chem>
RUN:	RUN1068
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.28

EN300-104592_1_2



CID:	EN300-104592_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H]5CCC(=O)N5</chem>
RUN:	RUN378
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.32

EN300-47606_1_2



CID: EN300-47606_1_2

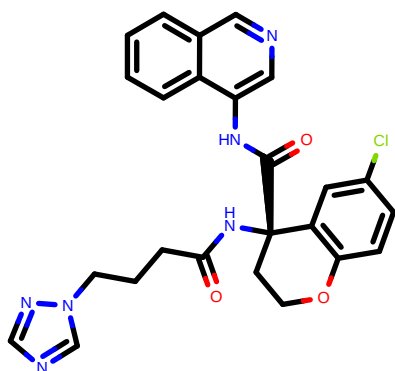
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5CCS(=O)(=O)C5

RUN: RUN1512

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.31

EN300-316216_1_1



CID: EN300-316216_1_1

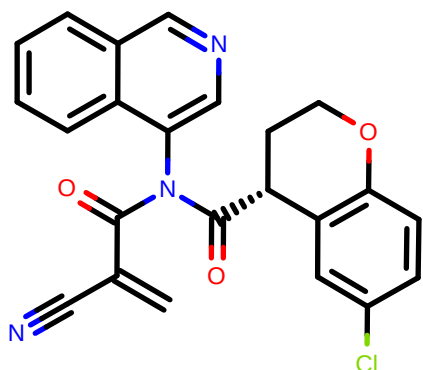
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5

RUN: RUN1740

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.43

VLA-UCB-34f3ed0c-1_1



CID: VLA-UCB-34f3ed0c-1_1

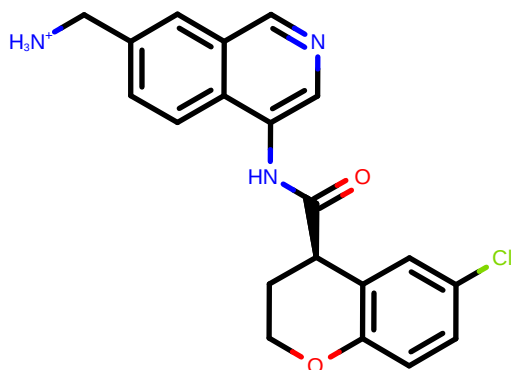
SMILES: C=C(C#N)C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN233

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.18

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

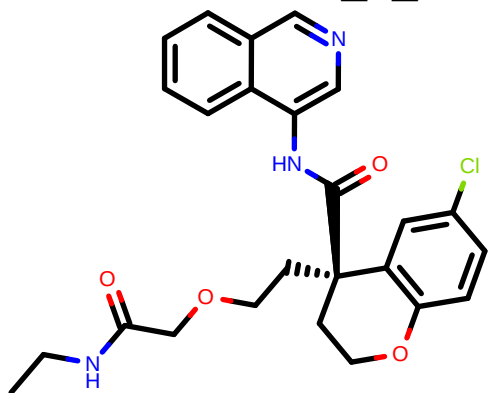
SMILES: c1cc2c(cc1C[NH3+])cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl

RUN: RUN19

DDG (kcal/mol): -1.21

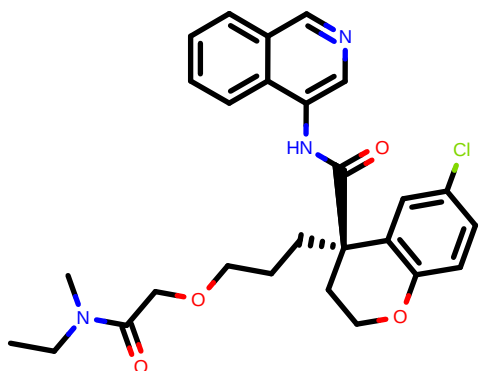
dDDG (kcal/mol): 0.14

EN300-7003350_3_1



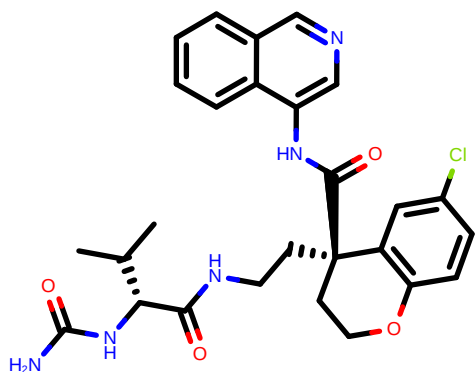
CID:	EN300-7003350_3_1
SMILES:	<chem>CCNC(=O)COC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1500
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.27

EN300-1253122_4_1



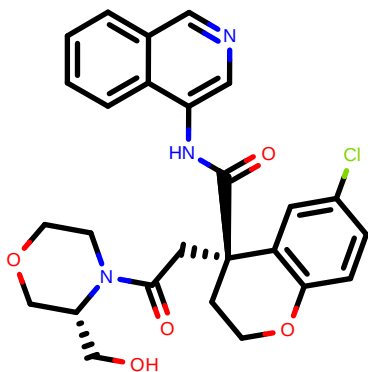
CID:	EN300-1253122_4_1
SMILES:	<chem>CCN(C)C(=O)COC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN698
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.34

EN300-2972220_3_1



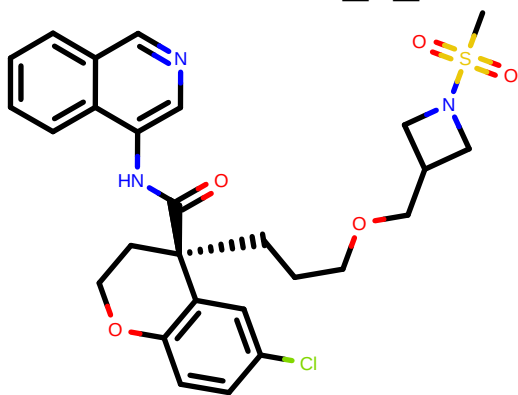
CID:	EN300-2972220_3_1
SMILES:	<chem>CC(C)[C@H](C(=O)NCC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N</chem>
RUN:	RUN1362
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.30

EN300-154201_1_2



CID:	EN300-154201_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(COC4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO</chem>
RUN:	RUN1202
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.38

EN300-302290_4_1



CID: EN300-302290_4_1

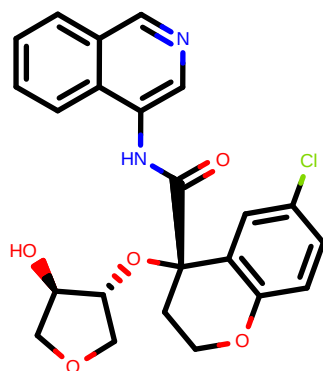
SMILES: CS(=O)(=O)N1CC(C1)COC[C@]2(C)C(=O)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1199

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.35

EN300-331828_1_1



CID: EN300-331828_1_1

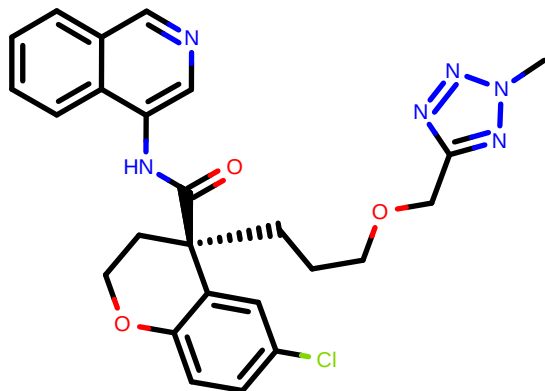
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)COCc4c3cc(cc4Cl)O[C@H]5COC[C@H]5O

RUN: RUN1591

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.19

EN300-90225_4_1



CID: EN300-90225_4_1

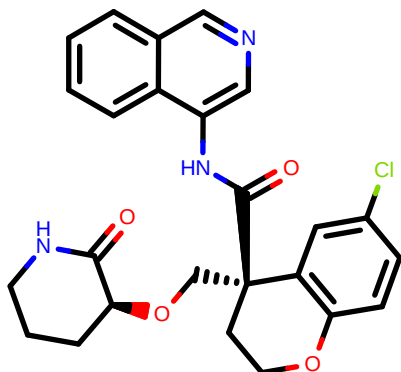
SMILES: Cn1nc(n1)COC[C@]2(C)C(=O)C(=O)Nc4cnc5c4ccccc5

RUN: RUN587

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.32

EN300-107267_2_2



CID: EN300-107267_2_2

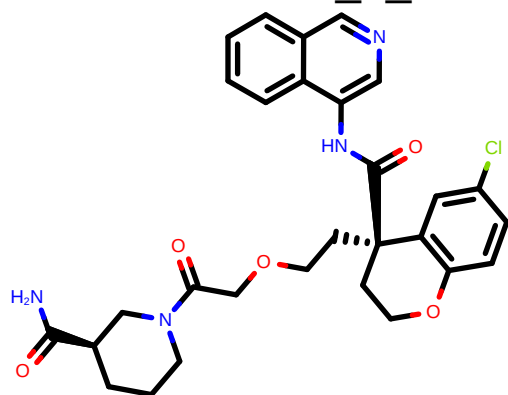
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)COCc4c3cc(cc4Cl)CO[C@H]5CCNC5=O

RUN: RUN966

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.25

EN300-22880_3_2



CID: EN300-22880_3_2

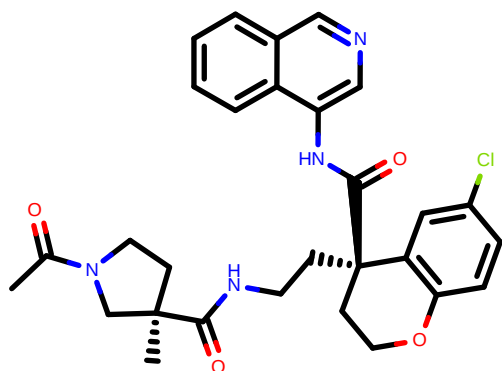
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N5CCC[C@H](C5)C(=O)N

RUN: RUN852

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.36

EN300-98018_3_1



CID: EN300-98018_3_1

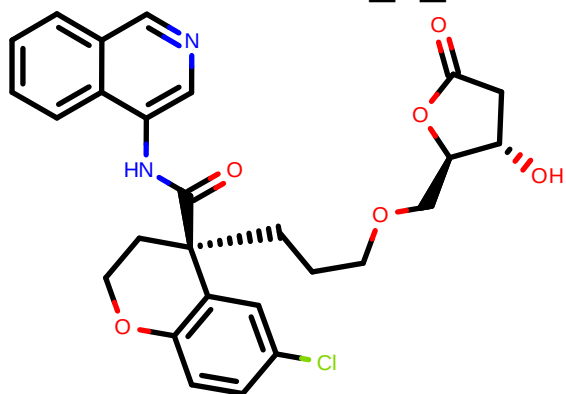
SMILES: CC(=O)N1CC[C@]([C1])(C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN319

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.40

EN300-6487407_4_1



CID: EN300-6487407_4_1

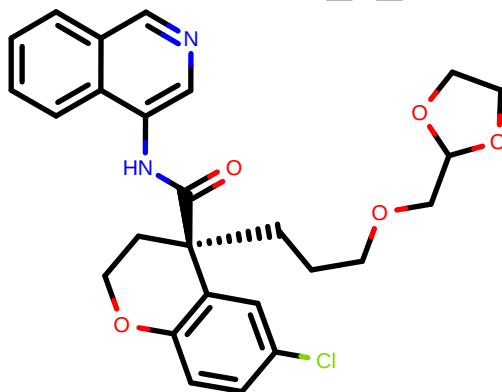
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5[C@H](CC(=O)O5)O

RUN: RUN1167

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.60

EN300-77092_4_1



CID: EN300-77092_4_1

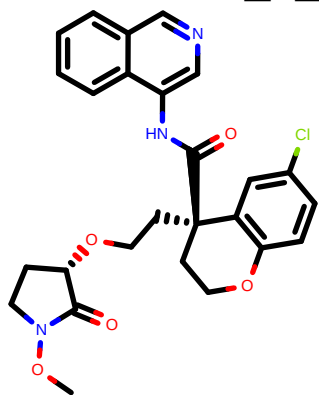
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5OCCO5

RUN: RUN651

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.32

EN300-302058_3_1



CID: EN300-302058_3_1

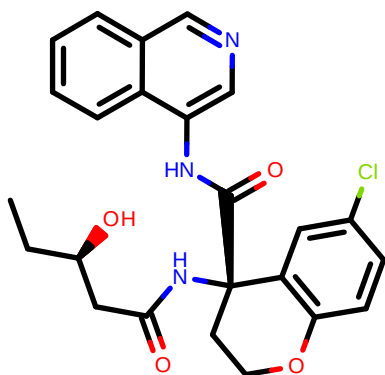
SMILES: CON1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN1707

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.27

EN300-224741_1_2



CID: EN300-224741_1_2

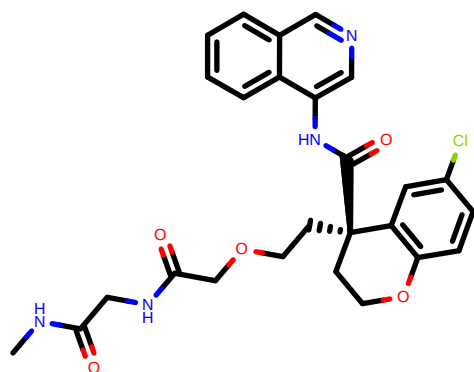
SMILES: CC[C@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4)O

RUN: RUN853

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.29

EN300-23223_3_1



CID: EN300-23223_3_1

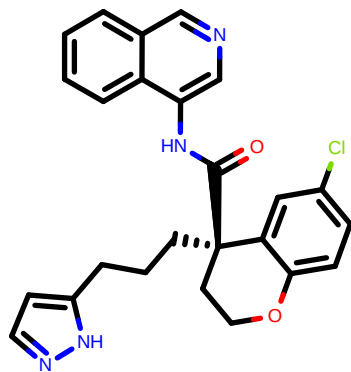
SMILES: CNC(=O)CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN: RUN1148

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.32

VLA-UCB-34f3ed0c-10_1



CID: VLA-UCB-34f3ed0c-10_1

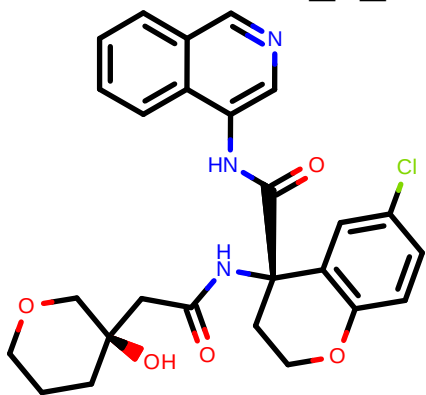
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5cc[nH]5

RUN: RUN125

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.30

EN300-1071940_1_1



CID:

EN300-1071940_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C[C@@]5(CCCOC5)O

RUN:

RUN1013

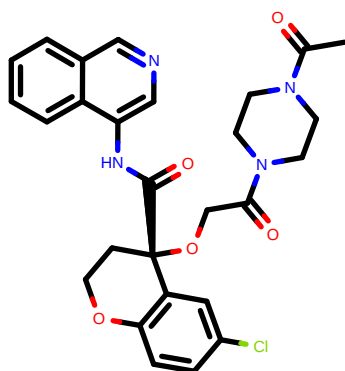
DDG (kcal/mol):

-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(cc3Cl)C(=O)Nc4cncc5c4ccccc5

RUN:

RUN936

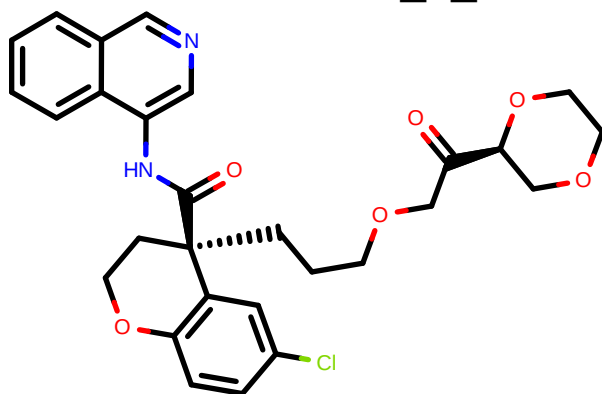
DDG (kcal/mol):

-1.18

dDDG (kcal/mol):

0.28

EN300-6238494_4_1



CID:

EN300-6238494_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCCOCC(=O)C[C@@]5(C)COC5

RUN:

RUN951

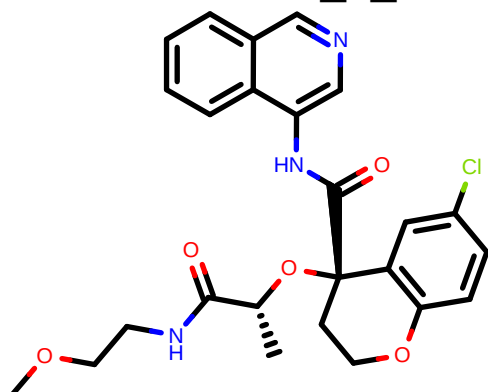
DDG (kcal/mol):

-1.17

dDDG (kcal/mol):

0.40

EN300-23317_1_2



CID:

EN300-23317_1_2

SMILES:

C[C@@H](C(=O)NCCOC)O[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1320

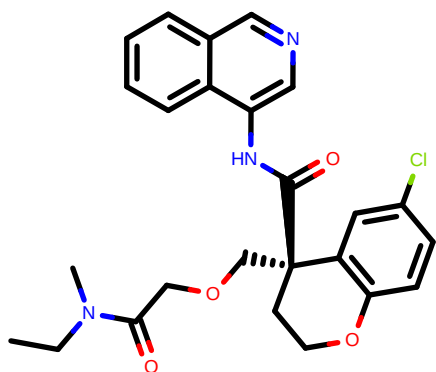
DDG (kcal/mol):

-1.17

dDDG (kcal/mol):

0.35

EN300-1253122_2_1



CID: EN300-1253122_2_1

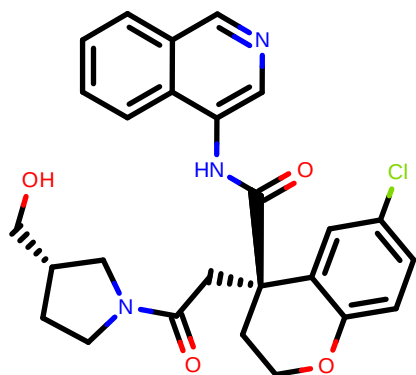
SMILES: CCN(C)C(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1454

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.24

EN300-256053_1_1



CID: EN300-256053_1_1

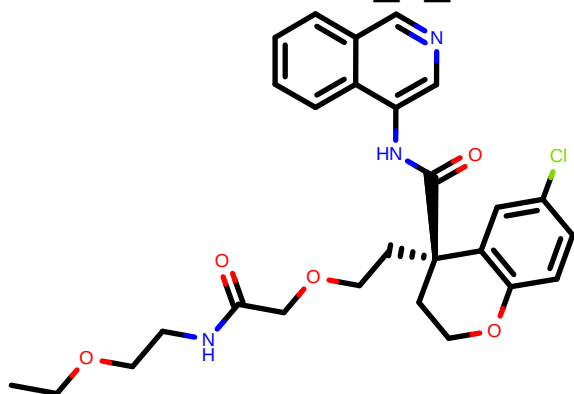
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN1458

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.25

EN300-103187_3_1



CID: EN300-103187_3_1

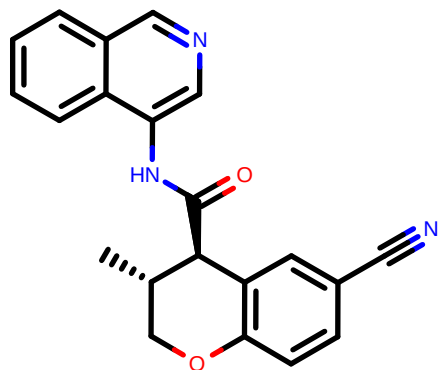
SMILES: CCOCCNC(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN632

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.46

DAR-DIA-0d514e7d-8_1



CID: DAR-DIA-0d514e7d-8_1

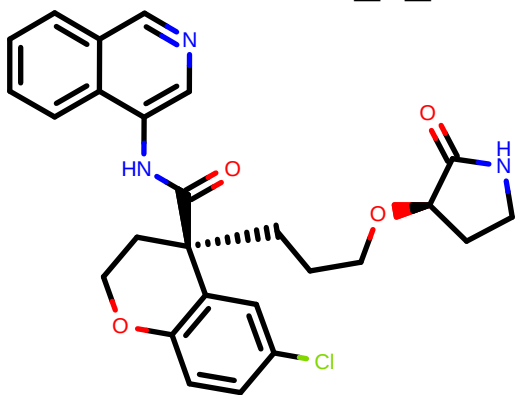
SMILES: C[C@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)C#N

RUN: RUN18

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.07

EN300-6736413_4_1



CID: EN300-6736413_4_1

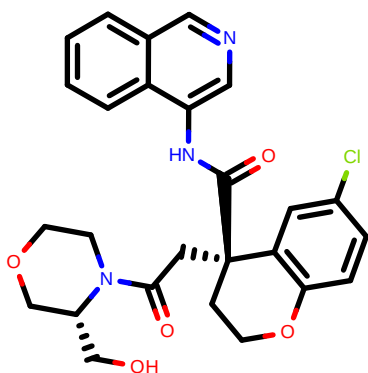
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN975

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.31

EN300-173903_1_1



CID: EN300-173903_1_1

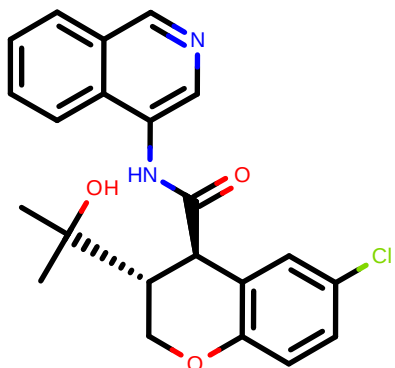
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN1210

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.32

BEN-BAS-5c03e89e-1_2



CID: BEN-BAS-5c03e89e-1_2

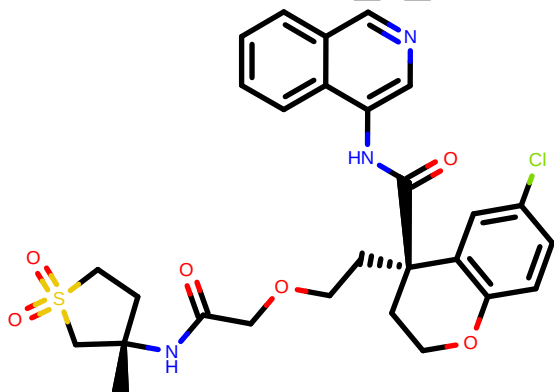
SMILES: CC(C)([C@@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O

RUN: RUN14

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.11

EN300-10414_3_1



CID: EN300-10414_3_1

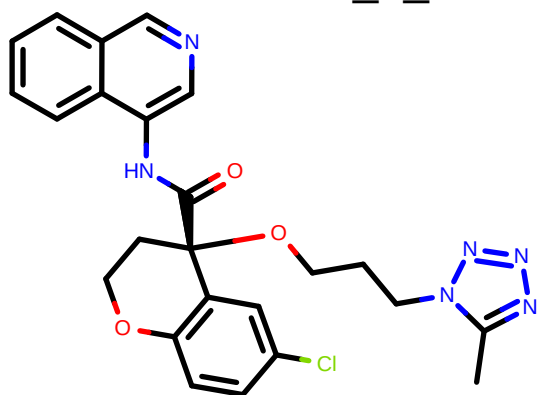
SMILES: C[C@@]1(CCS(=O)(=O)C1)NC(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN884

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.44

EN300-197715_1_1



CID: EN300-197715_1_1

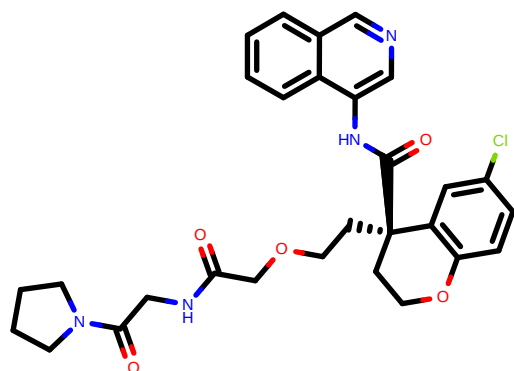
SMILES: Cc1nnnn1CCCO[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN888

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.32

EN300-28340_3_1



CID: EN300-28340_3_1

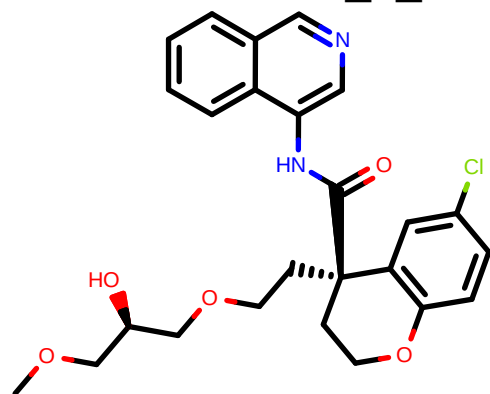
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)C(=O)NCC(=O)N5CCCC5

RUN: RUN1388

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.45

EN300-1915260_3_2



CID: EN300-1915260_3_2

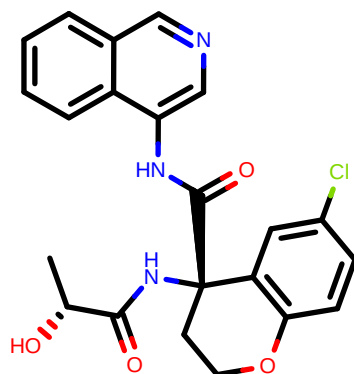
SMILES: COC[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN361

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.32

EN300-19542_1_2



CID: EN300-19542_1_2

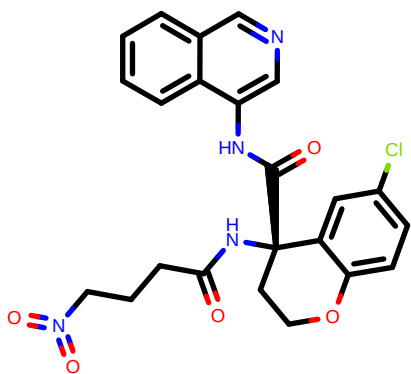
SMILES: C[C@H](C(=O)N[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN1389

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.20

EN300-143449_1_1



CID: EN300-143449_1_1

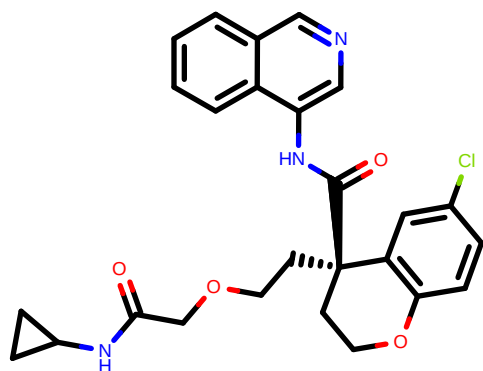
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCN(=O)=O

RUN: RUN736

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.30

EN300-1253178_3_1



CID: EN300-1253178_3_1

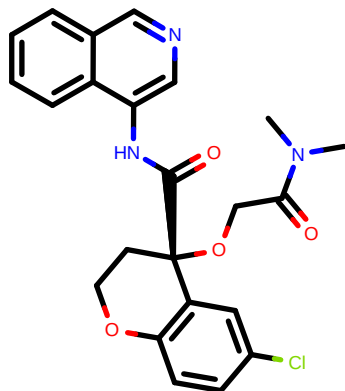
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)NC5CC5

RUN: RUN1683

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.29

EN300-216063_1_1



CID: EN300-216063_1_1

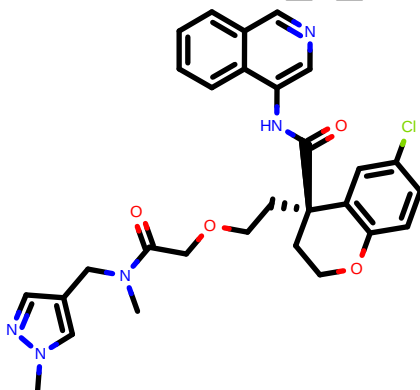
SMILES: CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN793

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.22

EN300-65978_3_1



CID: EN300-65978_3_1

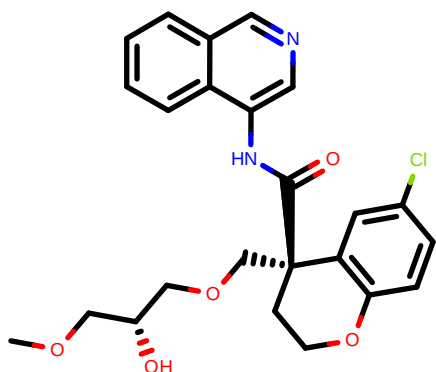
SMILES: Cn1cc(cn1)CN(C)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN1731

DDG (kcal/mol): -1.13

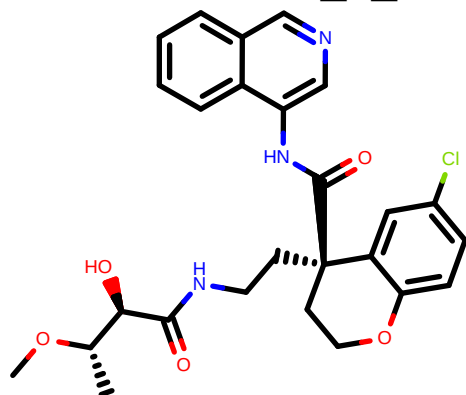
dDDG (kcal/mol): 0.55

EN300-1915260_2_2



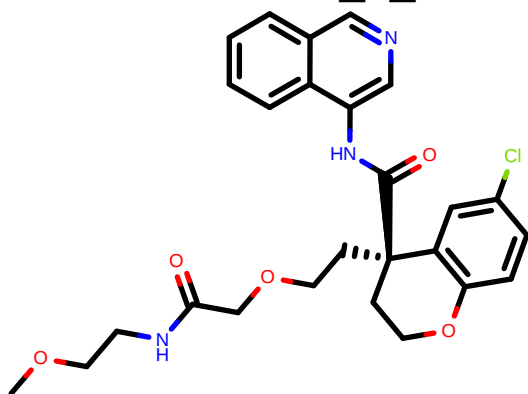
CID:	EN300-1915260_2_2
SMILES:	<chem>COC[C@H](COC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O</chem>
RUN:	RUN1030
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.38

EN300-220194_3_3



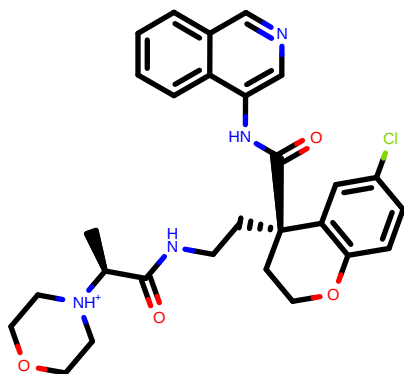
CID:	EN300-220194_3_3
SMILES:	<chem>ClC@@H](C@H)(C(=O)NCC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O)OC</chem>
RUN:	RUN1721
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.37

EN300-02015_3_1



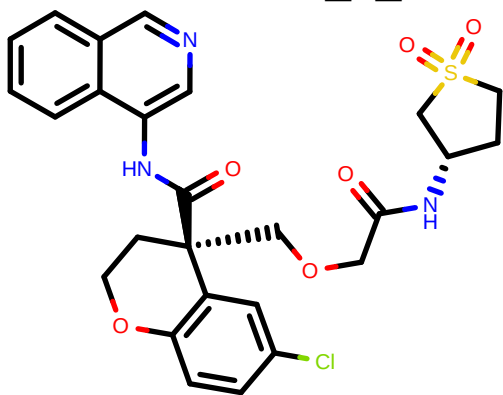
CID:	EN300-02015_3_1
SMILES:	<chem>COCCNC(=O)COCC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4</chem>
RUN:	RUN393
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.34

EN300-208191_3_1



CID:	EN300-208191_3_1
SMILES:	<chem>ClC@@H](C(=O)NCC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)[NH+]5COCOC5</chem>
RUN:	RUN709
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.32

EN300-05512_2_2



CID: EN300-05512_2_2

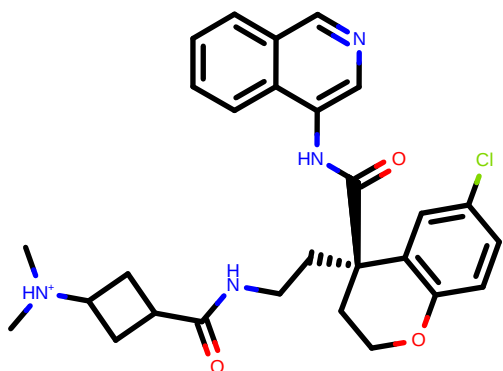
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4C3cc(cc4)Cl)COC(=O)N[C@H]5CCS(=O)(=O)C5

RUN: RUN467

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.46

EN300-6739235_3_1



CID: EN300-6739235_3_1

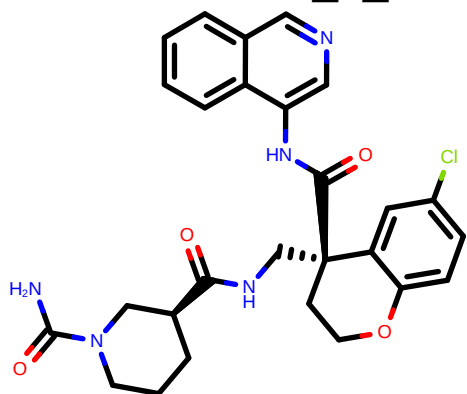
SMILES: C[NH+][C@H]1C[C@@H](C1)C(=O)NCC[C@@]2(C3C(CCC(C3)COC(=O)N[C@H]4C5C(CCC5)C

RUN: RUN1274

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.34

EN300-14767_2_2



CID: EN300-14767_2_2

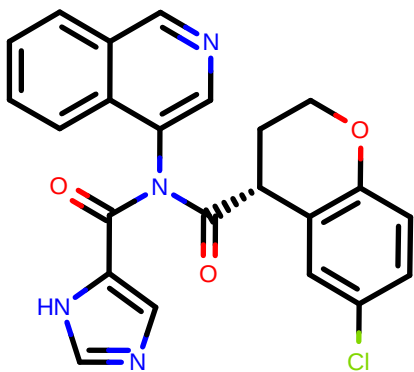
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4C3cc(cc4)Cl)CNC(=O)[C@H]5CCCCN(C5)C(=O)N

RUN: RUN1385

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.32

VLA-UCB-34f3ed0c-20_1



CID: VLA-UCB-34f3ed0c-20_1

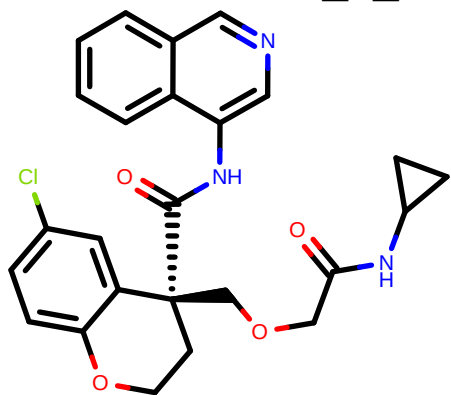
SMILES: c1ccc2c(c1)cncc2N(C(=O)c3cnc[nH]3)C(=O)[C@@H](C@H)4CCOC5C4C(C5)Cl

RUN: RUN242

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.28

EN300-1253178_2_1



CID: EN300-1253178_2_1

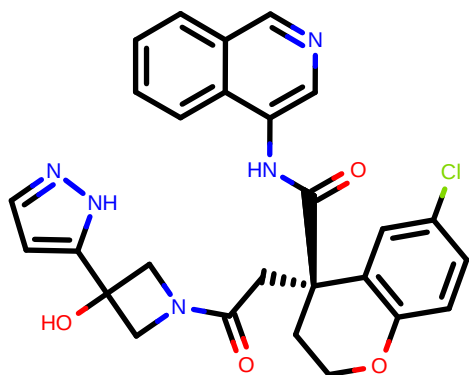
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CC5

RUN: RUN1086

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.25

EN300-1667046_1_1



CID: EN300-1667046_1_1

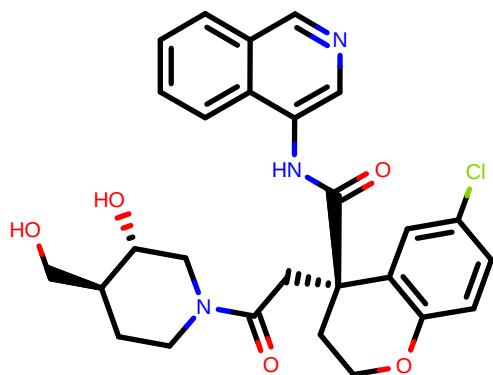
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6ccn[nH]6)O

RUN: RUN1673

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.29

EN300-95639_1_2



CID: EN300-95639_1_2

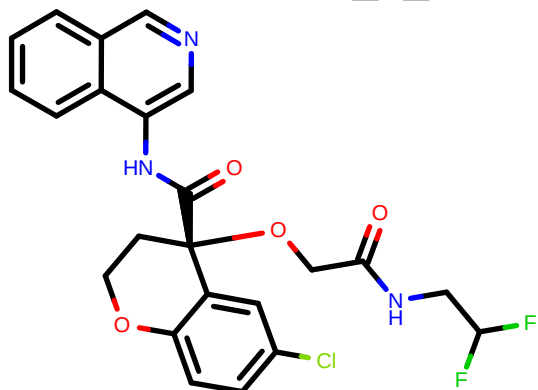
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)OCCO

RUN: RUN343

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.39

EN300-120586_1_1



CID: EN300-120586_1_1

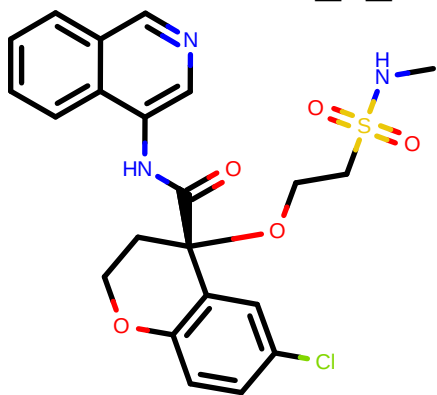
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCC(F)F

RUN: RUN429

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-6482967_1_1



CID:

EN300-6482967_1_1

SMILES:

CNS(=O)(=O)CCOC[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1599

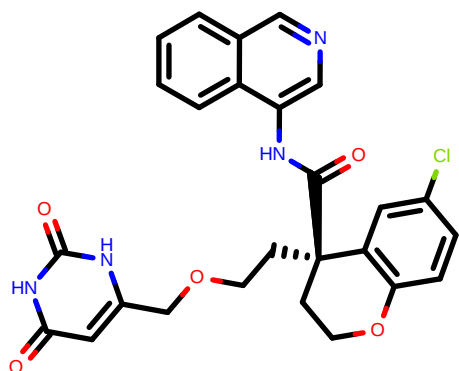
DDG (kcal/mol):

-1.11

dDDG (kcal/mol):

0.24

EN300-11300_3_1



CID:

EN300-11300_3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCOCc5cc(=O)[nH]c1=O)[nH]5

RUN:

RUN281

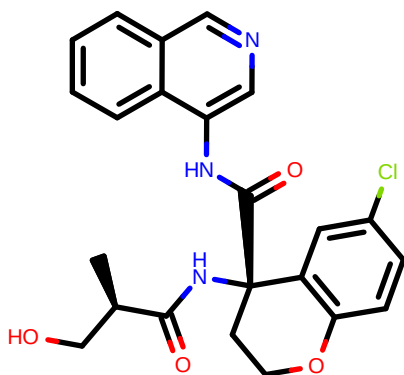
DDG (kcal/mol):

-1.10

dDDG (kcal/mol):

0.31

EN300-55072_1_2



CID:

EN300-55072_1_2

SMILES:

C[C@H](CO)C(=O)N[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN:

RUN1493

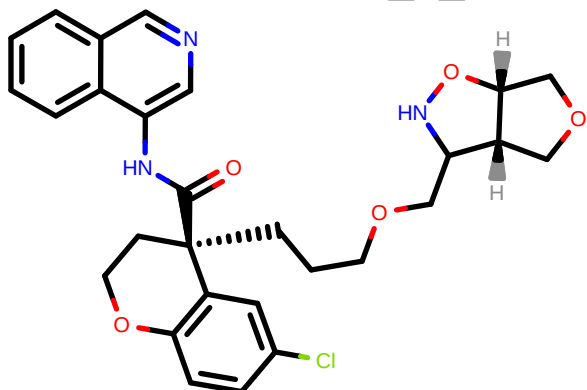
DDG (kcal/mol):

-1.10

dDDG (kcal/mol):

0.31

EN300-7436306_4_1



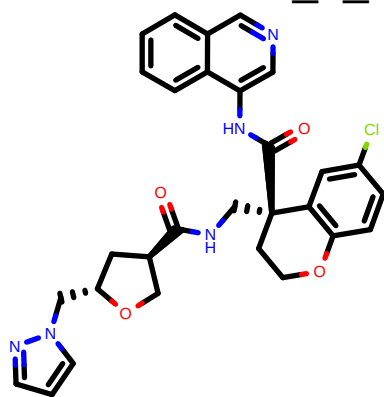
CID:

EN300-7436306_4_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCOCc5c6c7c8c5c6c7c8c9c10c7c8c9c10c11c12c13c11c12c13c14c15c16c14c15c16c17c18c19c17c18c19c20c21c22c20c21c22c23c24c25c23c24c25c26c27c28c26c27c28c29c30c31c29c30c31c32c33c34c32c33c34c35c36c37c35c36c37c38c39c40c38c39c40c41c42c43c41c42c43c44c45c46c44c45c46c47c48c49c47c48c49c50c51c52c50c51c52c53c54c55c53c54c55c56c57c58c56c57c58c59c60c61c59c60c61c62c63c64c62c63c64c65c66c67c65c66c67c68c69c70c68c69c70c71c72c73c71c72c73c74c75c76c74c75c76c77c78c79c77c78c79c80c81c82c80c81c82c83c84c85c83c84c85c86c87c88c86c87c88c89c90c91c89c90c91c92c93c94c92c93c94c95c96c97c95c96c97c98c99c100c98c99c100c101c102c103c101c102c103c104c105c106c104c105c106c107c108c109c107c108c109c110c111c112c110c111c112c113c114c115c113c114c115c116c117c118c116c117c118c119c120c121c119c120c121c122c123c124c122c123c124c125c126c127c125c126c127c128c129c130c128c129c130c131c132c133c131c132c133c134c135c136c134c135c136c137c138c139c137c138c139c140c141c142c140c141c142c143c144c145c143c144c145c146c147c148c146c147c148c149c150c151c149c150c151c152c153c154c152c153c154c155c156c157c155c156c157c158c159c160c158c159c160c161c162c163c161c162c163c164c165c166c164c165c166c167c168c169c167c168c169c170c171c172c170c171c172c173c174c175c173c174c175c176c177c178c176c177c178c179c180c181c179c180c181c182c183c184c182c183c184c185c186c187c185c186c187c188c189c190c188c189c190c191c192c193c191c192c193c194c195c196c194c195c196c197c198c199c197c198c199c200c201c202c200c201c202c203c204c205c203c204c205c206c207c208c206c207c208c209c210c211c209c210c211c212c213c214c212c213c214c215c216c217c215c216c217c218c219c220c218c219c220c221c222c223c221c222c223c224c225c226c224c225c226c227c228c229c227c228c229c230c231c232c230c231c232c233c234c235c233c234c235c236c237c238c236c237c238c239c240c241c239c240c241c242c243c244c242c243c244c245c246c247c245c246c247c248c249c250c248c249c250c251c252c253c251c252c253c254c255c256c254c255c256c257c258c259c257c258c259c260c261c262c260c261c262c263c264c265c263c264c265c266c267c268c266c267c268c269c270c271c269c270c271c272c273c274c272c273c274c275c276c277c275c276c277c278c279c280c278c279c280c281c282c283c281c282c283c284c285c286c284c285c286c287c288c289c287c288c289c290c291c292c290c291c292c293c294c295c293c294c295c296c297c298c296c297c298c299c300c301c299c300c301c302c303c304c302c303c304c305c306c307c305c306c307c308c309c310c308c309c310c311c312c313c311c312c313c314c315c316c314c315c316c317c318c319c317c318c319c320c321c322c320c321c322c323c324c325c323c324c325c326c327c328c326c327c328c329c330c331c329c330c331c332c333c334c332c333c334c335c336c337c335c336c337c338c339c340c338c339c340c341c342c343c341c342c343c344c345c346c344c345c346c347c348c349c347c348c349c350c351c352c350c351c352c353c354c355c353c354c355c356c357c358c356c357c358c359c360c361c359c360c361c362c363c364c362c363c364c365c366c367c365c366c367c368c369c370c368c369c370c371c372c373c371c372c373c374c375c376c374c375c376c377c378c379c377c378c379c380c381c382c380c381c382c383c384c385c383c384c385c386c387c388c386c387c388c389c390c391c389c390c391c392c393c394c392c393c394c395c396c397c395c396c397c398c399c400c398c399c400c401c402c403c401c402c403c404c405c406c404c405c406c407c408c409c407c408c409c410c411c412c410c411c412c413c414c415c413c414c415c416c417c418c416c417c418c419c420c421c419c420c421c422c423c424c422c423c424c425c426c427c425c426c427c428c429c430c428c429c430c431c432c433c431c432c433c434c435c436c434c435c436c437c438c439c437c438c439c440c441c442c440c441c442c443c444c445c443c444c445c446c447c448c446c447c448c449c450c451c449c450c451c452c453c454c452c453c454c455c456c457c455c456c457c458c459c460c458c459c460c461c462c463c461c462c463c464c465c466c464c465c466c467c468c469c467c468c469c470c471c472c470c471c472c473c474c475c473c474c475c476c477c478c476c477c478c479c480c481c479c480c481c482c483c484c482c483c484c485c486c487c485c486c487c488c489c490c488c489c490c491c492c493c491c492c493c494c495c496c494c495c496c497c498c499c497c498c499c500c501c502c500c501c502c503c504c505c503c504c505c506c507c508c506c507c508c509c510c511c509c510c511c512c513c514c512c513c514c515c516c517c515c516c517c518c519c520c518c519c520c521c522c523c521c522c523c524c525c526c524c525c526c527c528c529c527c528c529c530c531c532c530c531c532c533c534c535c533c534c535c536c537c538c536c537c538c539c540c541c539c540c541c542c543c544c542c543c544c545c546c547c545c546c547c548c549c550c548c549c550c551c552c553c551c552c553c554c555c556c554c555c556c557c558c559c557c558c559c560c561c562c560c561c562c563c564c565c563c564c565c566c567c568c566c567c568c569c570c571c569c570c571c572c573c574c572c573c574c575c576c577c575c576c577c578c579c580c578c579c580c581c582c583c581c582c583c584c585c586c584c585c586c587c588c589c587c588c589c590c591c592c590c591c592c593c594c595c593c594c595c596c597c598c596c597c598c599c600c601c599c600c601c602c603c604c602c603c604c605c606c607c605c606c607c608c609c610c608c609c610c611c612c613c611c612c613c614c615c616c614c615c616c617c618c619c617c618c619c620c621c622c620c621c622c623c624c625c623c624c625c626c627c628c626c627c628c629c630c631c629c630c631c632c633c634c632c633c634c635c636c637c635c636c637c638c639c640c638c639c640c641c642c643c641c642c643c644c645c646c644c645c646c647c648c649c647c648c649c650c651c652c650c651c652c653c654c655c653c654c655c656c657c658c656c657c658c659c660c661c659c660c661c662c663c664c662c663c664c665c666c667c665c666c667c668c669c670c668c669c670c671c672c673c671c672c673c674c675c676c674c675c676c677c678c679c677c678c679c680c681c682c680c681c682c683c684c685c683c684c685c686c687c688c686c687c688c689c690c691c689c690c691c692c693c694c692c693c694c695c696c697c695c696c697c698c699c700c698c699c700c701c702c703c701c702c703c704c705c706c704c705c706c707c708c709c707c708c709c710c711c712c710c711c712c713c714c715c713c714c715c716c717c718c716c717c718c719c720c721c719c720c721c722c723c724c722c723c724c725c726c727c725c726c727c728c729c730c728c729c730c731c732c733c731c732c733c734c735c736c734c735c736c737c738c739c737c738c739c740c741c742c740c741c742c743c744c745c743c744c745c746c747c748c746c747c748c749c750c751c749c750c751c752c753c754c752c753c754c755c756c757c755c756c757c758c759c760c758c759c760c761c762c763c761c762c763c764c765c766c764c765c766c767c768c769c767c768c769c770c771c772c770c771c772c773c774c775c773c774c775c776c777c778c776c777c778c779c780c781c779c780c781c782c783c784c782c783c784c785c786c787c785c786c787c788c789c790c788c789c790c791c792c793c791c792c793c794c795c796c794c795c796c797c798c799c797c798c799c800c801c802c800c801c802c803c804c805c803c804c805c806c807c808c806c807c808c809c810c811c809c810c811c812c813c814c812c813c814c815c816c817c815c816c817c818c819c820c818c819c820c821c822c823c821c822c823c824c825c826c824c825c826c827c828c829c827c828c829c830c831c832c830c831c832c833c834c835c833c834c835c836c837c838c836c837c838c839c840c841c839c840c841c842c843c844c842c843c844c845c846c847c845c846c847c848c849c850c848c849c850c851c852c853c851c852c853c854c855c856c854c855c856c857c858c859c857c858c859c860c861c862c860c861c862c863c864c865c863c864c865c866c867c868c866c867c868c869c870c871c869c870c871c872c873c874c872c873c874c875c876c877c875c876c877c878c879c880c878c879c880c881c882c883c881c882c883c884c885c886c884c885c886c887c888c889c887c888c889c890c891c892c890c891c892c893c894c895c893c894c895c896c897c898c896c897c898c899c900c901c899c900c901c902c903c904c902c903c904c905c906c907c905c906c907c908c909c910c908c909c910c911c912c913c911c912c913c914c915c916c914c915c916c917c918c919c917c918c919c920c921c922c920c921c922c923c924c925c923c924c925c926c927c928c926c927c928c929c930c931c929c930c931c932c933c934c932c933c934c935c936c937c935c936c937c938c939c940c938c939c940c941c942c943c941c942c943c944c945c946c944c945c946c947c948c949c947c948c949c950c951c952c950c951c952c953c954c955c953c954c955c956c957c958c956c957c958c959c960c961c959c960c961c962c963c964c962c963c964c965c966c967c965c966c967c968c969c970c968c969c970c971c972c973c971c972c973c974c975c976c974c975c976c977c978c979c977c978c979c980c981c982c980c981c982c983c984c985c983c984c985c986c987c988c986c987c988c989c990c991c989c990c991c992c993c994c992c993c994c995c996c997c995c996c997c998c999c1000c998c999c1000c1001c1002c1003c1001c1002c1003c1004c1005c1006c1004c1005c1006c1007c1008c1009c1007c1008c1009c1010c1011c1012c1010c1011c1012c1013c1014c1015c1013c1014c1015c1016c1017c1018c1016c1017c1018c1019c1020c1021c1019c1020c1021c1022c1023c1024c1022c1023c1024c1025c1026c1027c1025c1026c1027c1028c1029c1030c1028c1029c1030c1031c1032c1033c1031c1032c1033c1034c1035c1036c1034c1035c1036c1037c1038c1039c1037c1038c1039c1040c1041c1042c1040c1041c1042c1043c1044c1045c1043c1044c1045c1046c1047c1048c1046c1047c1048c1049c1050c1051c1049c1050c1051c1052c1053c1054c1052c1053c1054c1055c1056c1057c1055c1056c1057c1058c1059c1060c1058c1059c1060c1061c1062c1063c1061c1062c1063c1064c1065c1066c1064c1065c1066c1067c1068c1069c1067c1068c1069c1070c1071c1072c1070c1071c1072c1073c1074c1075c1073c1074c1075c1076c1077c1078c1076c1077c1078c1079c1080c1081c1079c1080c1081c1082c1083c1084c1082c1083c1084c1085c1086c1087c1085c1086c1087c1088c1089c1090c1088c1089c1090c1091c1092c1093c1091c1092c1093c1094c1095c1096c1094c1095c1096c1097c1098c1099c1097c1098c1099c1100c1101c1102c1100c1101c1102c1103c1104c1105c1103c1104c1105c1106c1107c1108c1106c1107c1108c1109c1110c1111c1109c1110c1111c1112c1113c1114c1112c1113c1114c1115c1116c1115c1116c1117c1118c1117c1118c1119c1120c1121c1119c1120c1121c1122c1123c1124c1122c1123c1124c1125c1126c1127c1125c1126c1127c1128c1129c1130c1128c1129c1130c1131c1132c1133c1131c1132c1133c1134c1135c1136c1134c1135c1136c1137c1138c1139c1137c1138c1139c1140c1141c1142c1140c1141c1142c1143c1144c1145c1143c1144c1145c1146c1147c1148c1146c1147c1148c1149c1150c1151c1149c1150c1151c1152c1153c1154c1152c1153c1154c1155c1156c1157c1155c1156c1157c1158c1159c1160c1158c1159c1160c1161c1162c1163c1161c1162c1163c1164c1165c1166c1164c1165c1166c1167c1168c1169c1167c1168c1169c1170c1171c1172c1170c1171c1172c1173c1174c1175c1173c1174c1175c1176c1177c1178c1176c1177c1178c1179c1180c1181c1179c1180c1181c1182c1183c1184c1182c1183c1184c1185c1186c1187c1185c1186c1187c1188c1189c1190c1188c1189c1190c1191c1192c1193c1191c1192c1193c1194c1195c1196c1194c1195c1196c1197c1198c1199c1197c1198c1199c1200c1201c1202c1200c1201c1202c1203c1204c1205c1203c1204c1205c1206c1207c1208c1206c1207c1208c1209c1210c1211c1209c1210c1211c1212c1213c1214c1212c1213c1214c1215c1216c1217c1215c1216c1217c1218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EN300-6494859_2_3



CID:

EN300-6494859_2_3

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@H3[C@@H](COC(=O)C4=CC=CC=C4)CNC(=O)C@H4[C@@H](C5=CC=CC=C5)C6=CC=CC=C6

RUN:

RUN1297

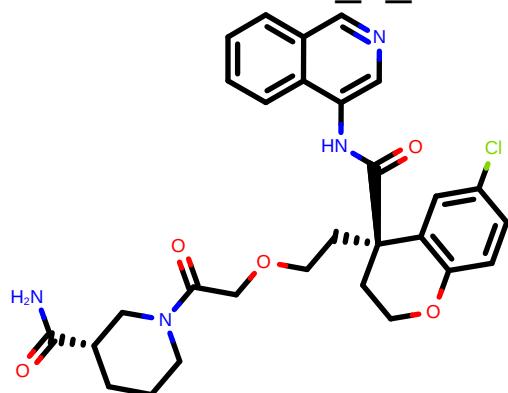
DDG (kcal/mol):

-1.08

dDDG (kcal/mol):

0.38

EN300-22880_3_1



CID:

EN300-22880_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)C@H3[C@@H](COC(=O)C4=CC=CC=C4)CNC(=O)C@H4[C@@H](C5=CC=CC=C5)C6=CC=CC=C6

RUN:

RUN1204

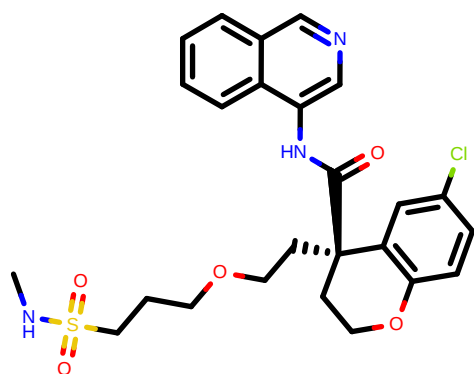
DDG (kcal/mol):

-1.08

dDDG (kcal/mol):

0.39

EN300-68875_3_1



CID:

EN300-68875_3_1

SMILES:

CNS(=O)(=O)CCCCC[C@H]1(COC(=O)C2=CC=CC=C2)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN1452

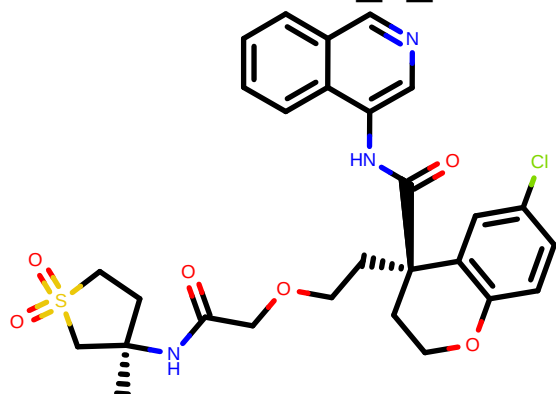
DDG (kcal/mol):

-1.08

dDDG (kcal/mol):

0.36

EN300-10414_3_2



CID:

EN300-10414_3_2

SMILES:

C[C@H]1(CCS(=O)(=O)C1)NC(=O)COC[C@H]2(COC(=O)C3=CC=CC=C3)C(=O)Nc4ncnc5c4ccccc5

RUN:

RUN988

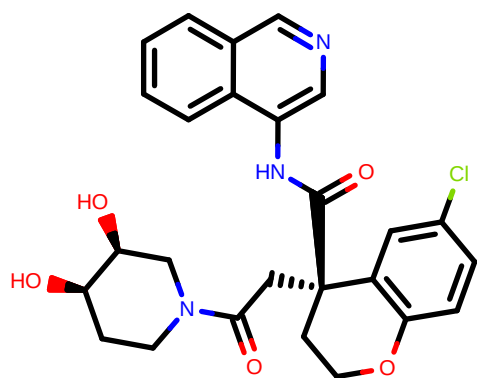
DDG (kcal/mol):

-1.08

dDDG (kcal/mol):

0.34

EN300-349304_1_1



CID: EN300-349304_1_1

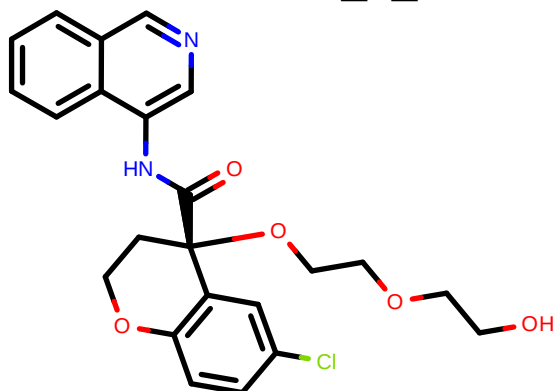
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC@H(C5)O)O

RUN: RUN1082

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.28

EN300-52467_1_1



CID: EN300-52467_1_1

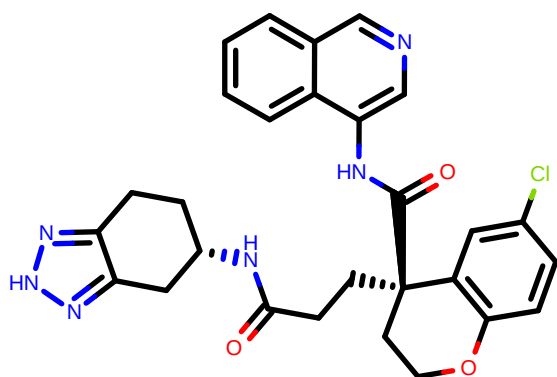
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN920

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-6491682_2_2



CID: EN300-6491682_2_2

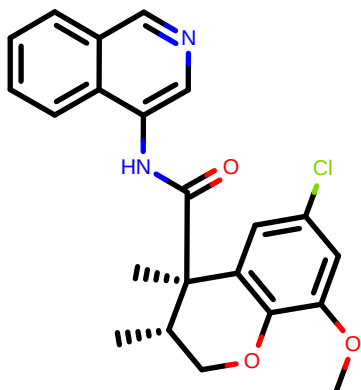
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCc6c(n[nH]n6)C5

RUN: RUN867

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-25_1



CID: DAR-DIA-0d514e7d-25_1

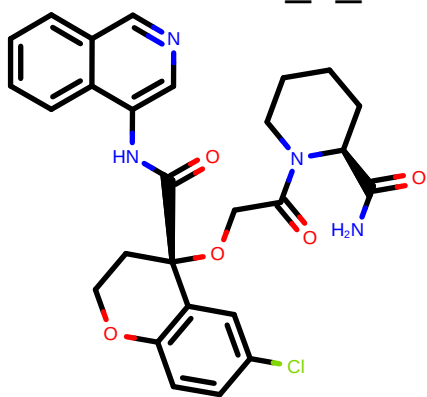
SMILES: C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4

RUN: RUN73

DDG (kcal/mol): -1.07

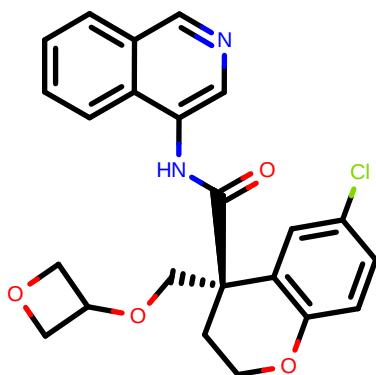
dDDG (kcal/mol): 0.13

EN300-22879_1_2



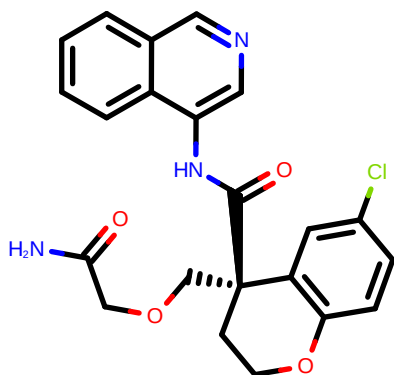
CID:	EN300-22879_1_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@H]5C(=O)N</chem>
RUN:	RUN325
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.28

EN300-317082_2_1



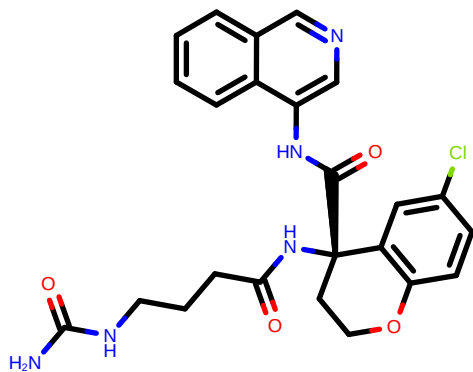
CID:	EN300-317082_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC5COC5</chem>
RUN:	RUN1462
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.22

EN300-18249_2_1



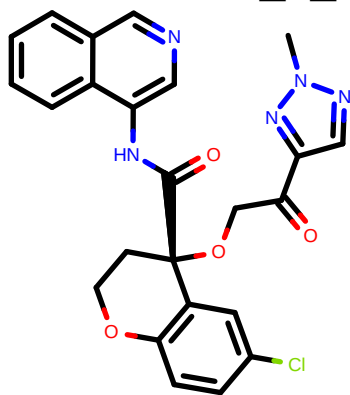
CID:	EN300-18249_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N</chem>
RUN:	RUN744
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.19

EN300-05620_1_1



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

EN300-204935_1_1



CID:

EN300-204935_1_1

SMILES:

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

RUN:

RUN1536

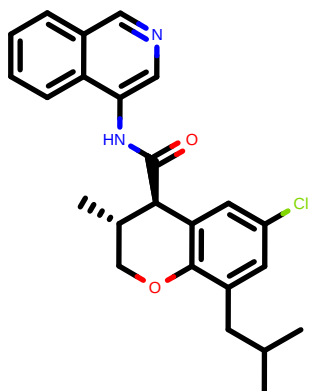
DDG (kcal/mol):

-1.04

dDDG (kcal/mol):

0.26

DAR-DIA-0d514e7d-24_1



CID:

DAR-DIA-0d514e7d-24_1

SMILES:

C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)CC(C)C

RUN:

RUN109

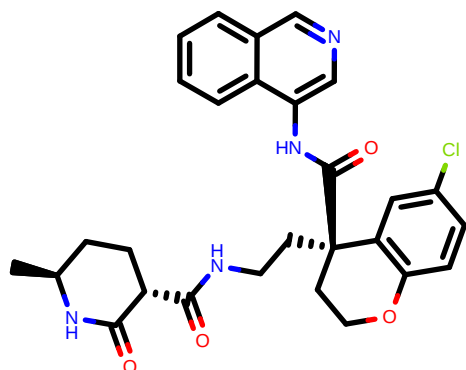
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.16

EN300-6505003_3_2



CID:

EN300-6505003_3_2

SMILES:

C[C@H]1CC[C@H](C(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

RUN1617

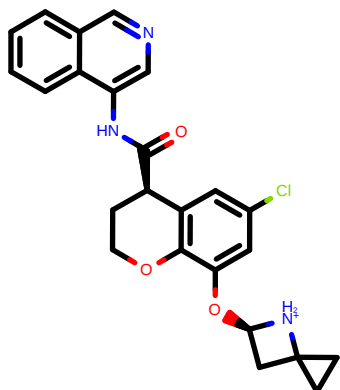
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.36

DAR-DIA-23e5a6a0-5_1



CID:

DAR-DIA-23e5a6a0-5_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)[C@@H]5CC6([NH2+][5]CC6)Cl

RUN:

RUN84

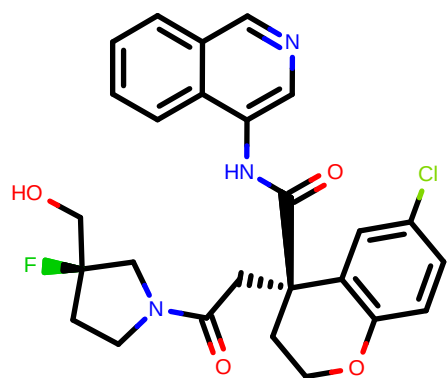
DDG (kcal/mol):

-1.03

dDDG (kcal/mol):

0.45

EN300-203118_1_1



CID: EN300-203118_1_1

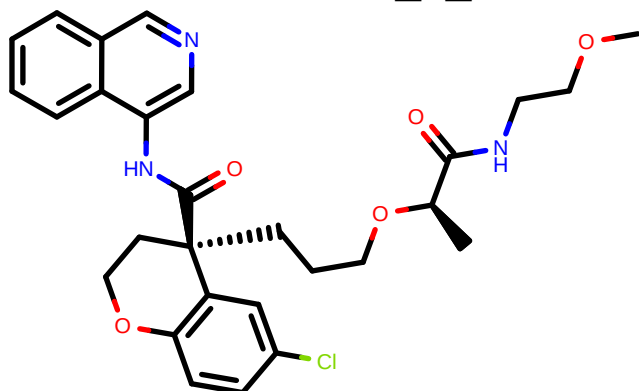
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(CO)F

RUN: RUN1737

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.46

EN300-23317_4_2



CID: EN300-23317_4_2

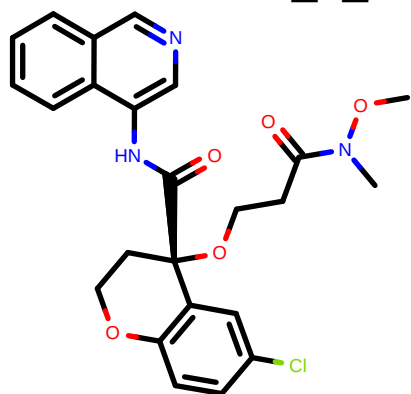
SMILES: C[C@H](C(=O)NCCOC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1551

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.37

EN300-174603_1_1



CID: EN300-174603_1_1

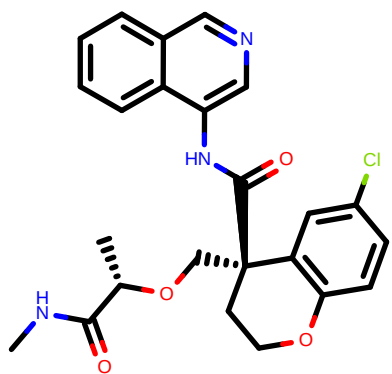
SMILES: CN(C(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4)OC

RUN: RUN1272

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.25

EN300-211482_2_1



CID: EN300-211482_2_1

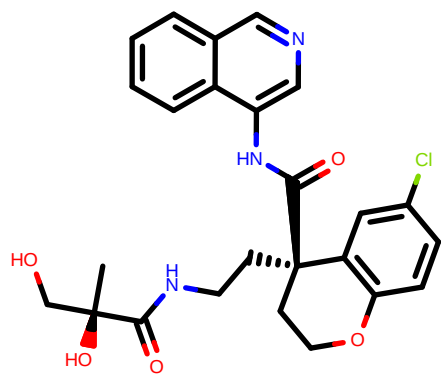
SMILES: C[C@@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1326

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.28

EN300-89418_3_1



CID: EN300-89418_3_1

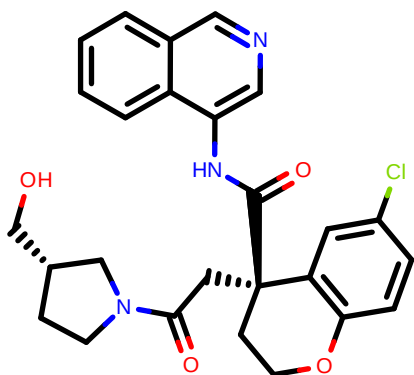
SMILES: C[C@@]([CO])(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN1577

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.44

EN300-256053_1_1



CID: EN300-256053_1_1

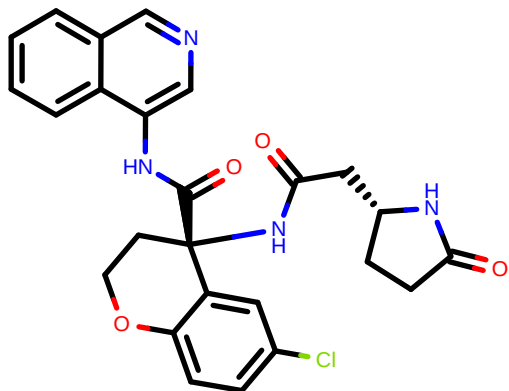
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO

RUN: RUN1450

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.29

EN300-68203_1_2



CID: EN300-68203_1_2

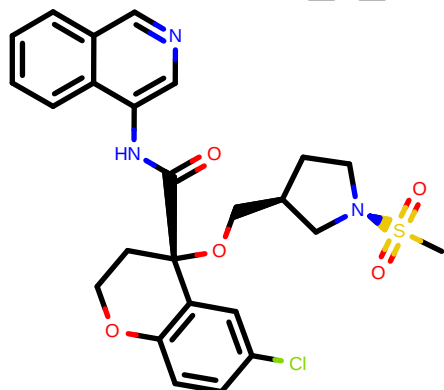
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCC(=O)N5

RUN: RUN1684

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.30

EN300-261986_1_1



CID: EN300-261986_1_1

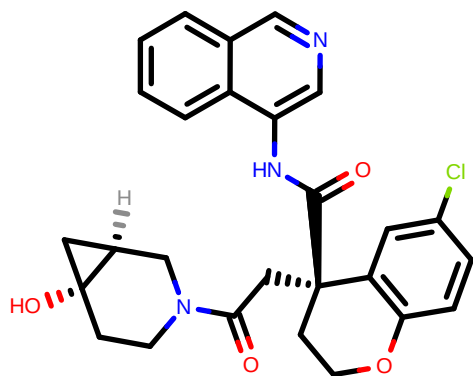
SMILES: CS(=O)(=O)[N@@]1CC[C@H](C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN516

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.32

EN300-303908_1_1



CID: EN300-303908_1_1

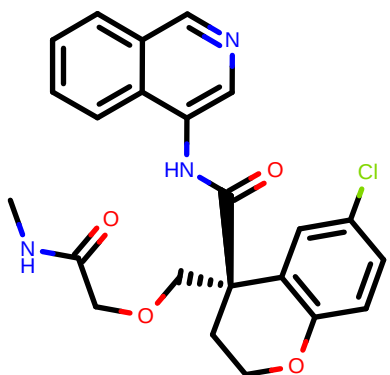
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]6(C[C@H]6C5)O

RUN: RUN827

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.35

EN300-2977549_2_1



CID: EN300-2977549_2_1

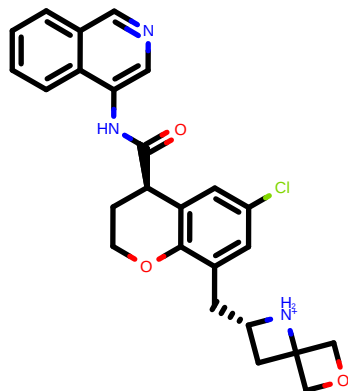
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1070

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.21

DAR-DIA-23e5a6a0-8_2



CID: DAR-DIA-23e5a6a0-8_2

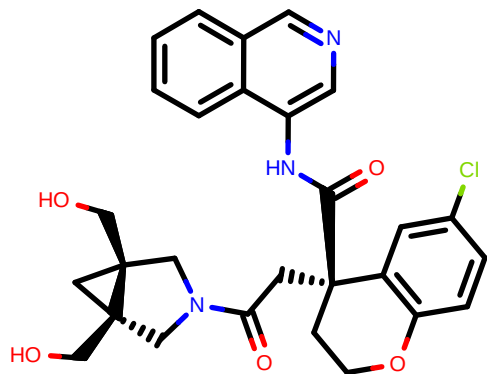
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[C@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN131

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.39

EN300-1270211_1_1



CID: EN300-1270211_1_1

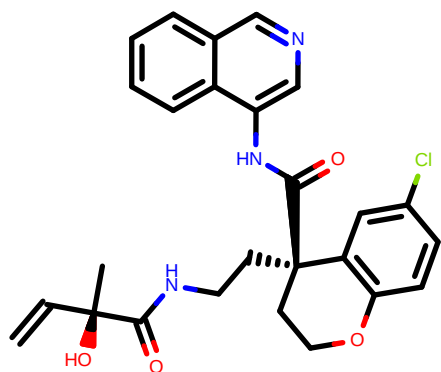
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]6(C[C@H]6(C5)CO)CO

RUN: RUN1522

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-248888_3_1



CID: EN300-248888_3_1

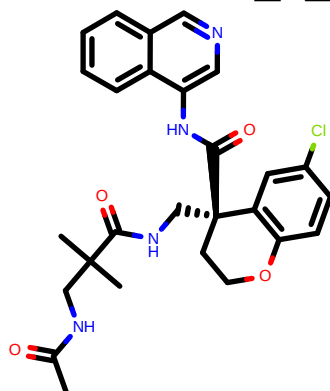
SMILES: C[C@@]([C=C])(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4)O

RUN: RUN763

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.40

EN300-189495_2_1



CID: EN300-189495_2_1

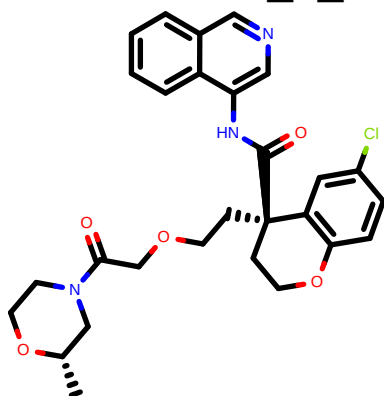
SMILES: CC(=O)NCC(C)(C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN: RUN613

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

EN300-25572_3_2



CID: EN300-25572_3_2

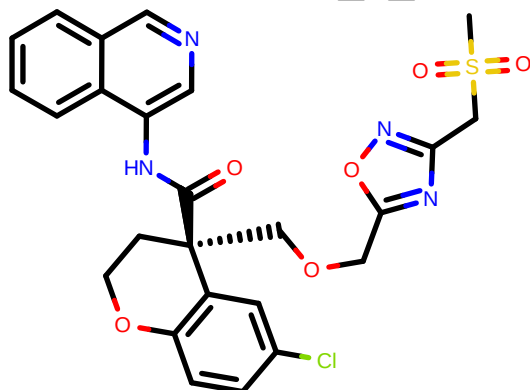
SMILES: C[C@H]1CN(CCO1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN592

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.31

EN300-94900_2_1



CID: EN300-94900_2_1

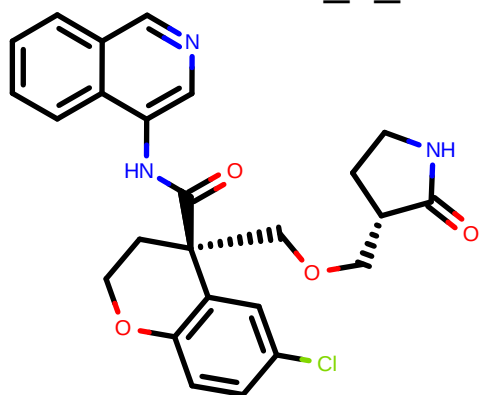
SMILES: CS(=O)(=O)Cc1nc(on1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN: RUN451

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.48

EN300-246248_2_1



CID: EN300-246248_2_1

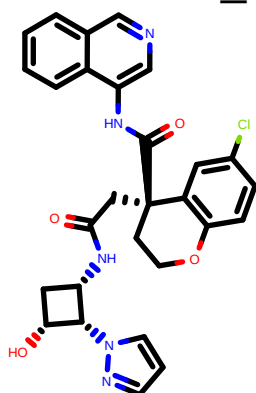
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O

RUN: RUN323

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.26

EN300-260696_1_8



CID: EN300-260696_1_8

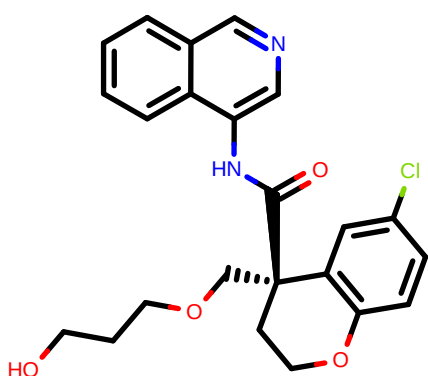
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H](C)[C@@H]5m6ccc6)O

RUN: RUN1785

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.62

EN300-221518_2_1



CID: EN300-221518_2_1

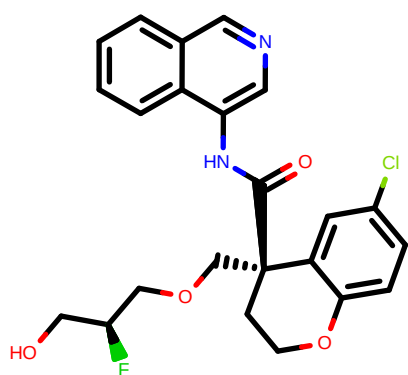
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(CO)C

RUN: RUN823

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.23

EN300-1600517_2_2



CID: EN300-1600517_2_2

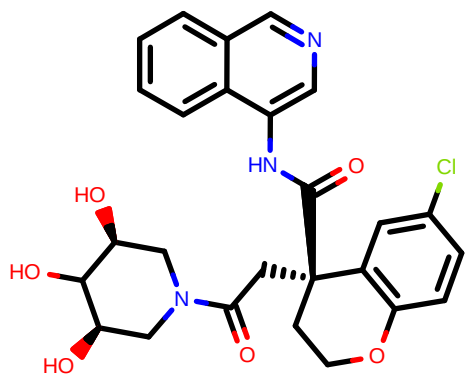
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CO)F

RUN: RUN1134

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.29

EN300-299920_1_1



CID: EN300-299920_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)CC(=O)N6C[C@H](C)[C@H](C5)OYO

RUN:

RUN1777

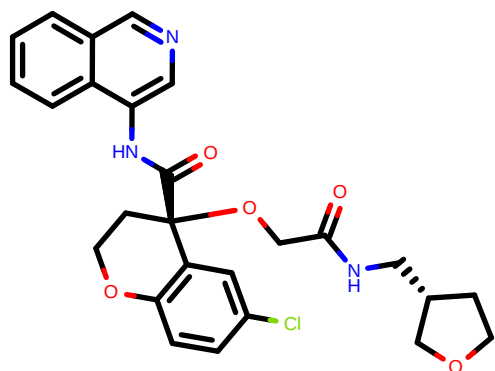
DDG (kcal/mol):

-0.98

dDDG (kcal/mol):

0.55

EN300-46832_1_1



CID: EN300-46832_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)OCC(=O)NC[C@H]5CCOC5

RUN:

RUN1472

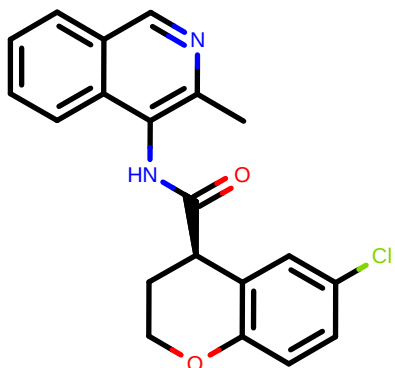
DDG (kcal/mol):

-0.98

dDDG (kcal/mol):

0.32

ADA-UCB-dc2b944c-10_1



CID: ADA-UCB-dc2b944c-10_1

SMILES:

Cc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN:

RUN51

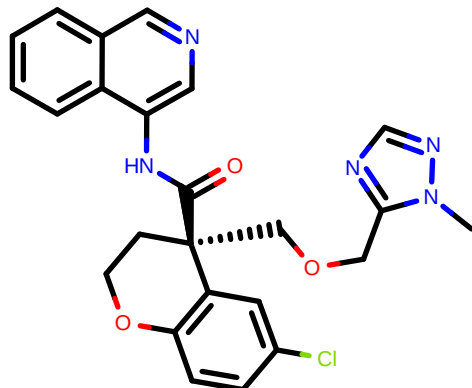
DDG (kcal/mol):

-0.97

dDDG (kcal/mol):

0.09

EN300-87334_2_1



CID: EN300-87334_2_1

SMILES:

Cn1c(ncn1)COC[C@@H]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN:

RUN1653

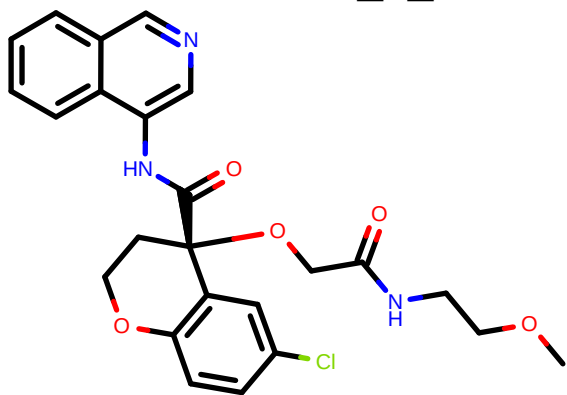
DDG (kcal/mol):

-0.97

dDDG (kcal/mol):

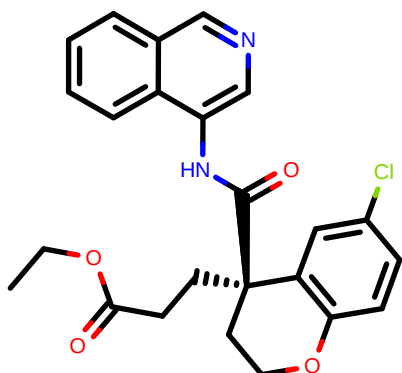
0.26

EN300-02015_1_1



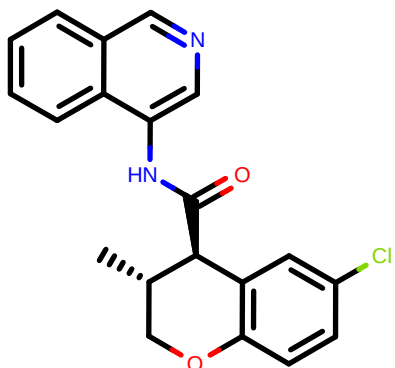
CID:	EN300-02015_1_1
SMILES:	<chem>COCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN413
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.34

JAG-UCB-706446eb-4_1



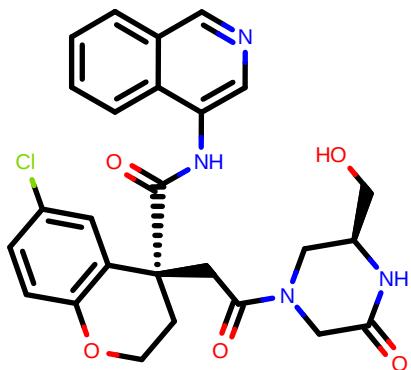
CID:	JAG-UCB-706446eb-4_1
SMILES:	<chem>CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-11_1



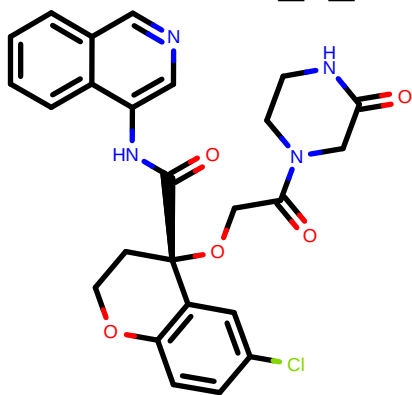
CID:	EDJ-MED-e4b030d8-11_1
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN12
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.05

EN300-100700_1_1



CID:	EN300-100700_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](NC(=O)C5)CO</chem>
RUN:	RUN1218
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.41

EN300-22884_1_1



CID: EN300-22884_1_1

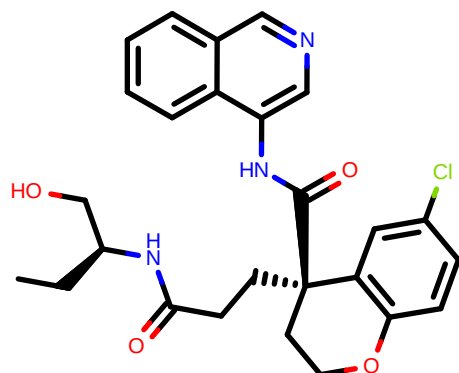
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCNC(=O)C5

RUN: RUN707

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EN300-157897_2_1



CID: EN300-157897_2_1

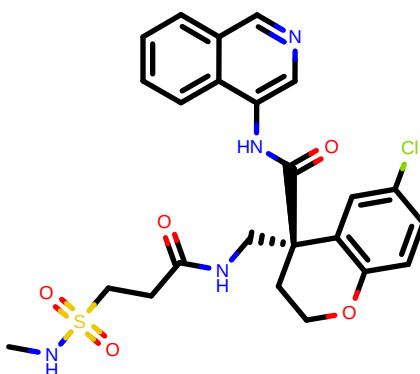
SMILES: CC[C@H](CO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN780

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.36

EN300-123205_2_1



CID: EN300-123205_2_1

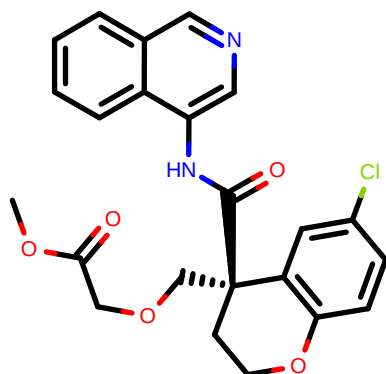
SMILES: CNS(=O)(=O)CCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN557

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.39

EN300-19700_2_1



CID: EN300-19700_2_1

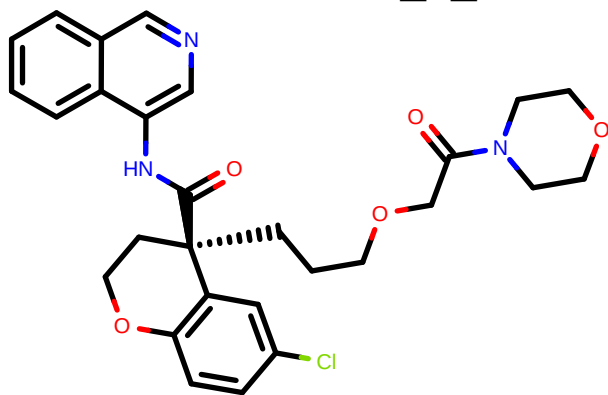
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1422

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.20

EN300-1241327_4_1



CID: EN300-1241327_4_1

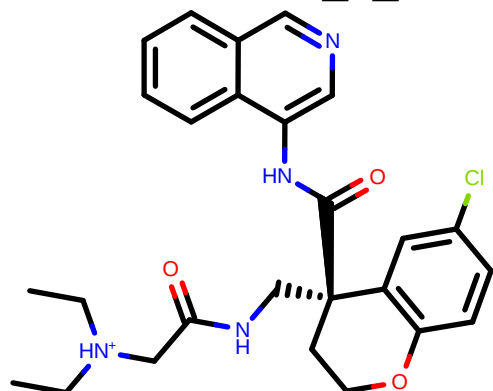
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOC5

RUN: RUN1183

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.33

EN300-82457_2_1



CID: EN300-82457_2_1

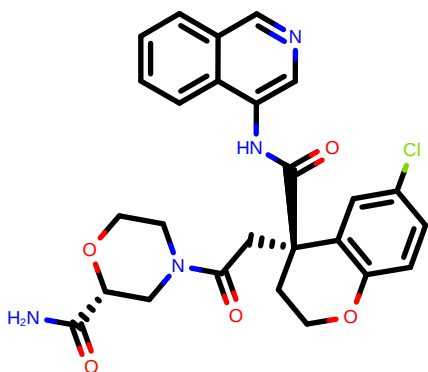
SMILES: CC[NH+](CC)CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4

RUN: RUN1249

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.42

EN300-60862_1_2



CID: EN300-60862_1_2

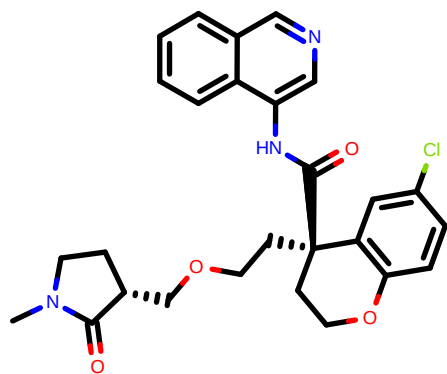
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)C(=O)N

RUN: RUN866

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.28

EN300-260816_3_1



CID: EN300-260816_3_1

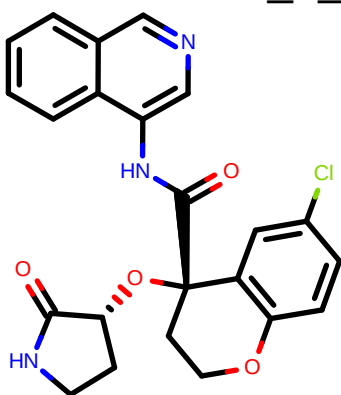
SMILES: CN1CC[C@@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN1763

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.52

EN300-6736413_1_1



CID: EN300-6736413_1_1

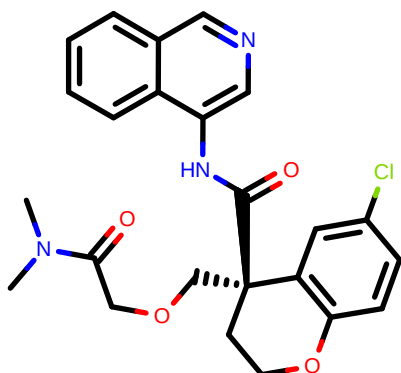
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@H]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCNC5=O

RUN: RUN1679

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.20

EN300-216063_2_1



CID: EN300-216063_2_1

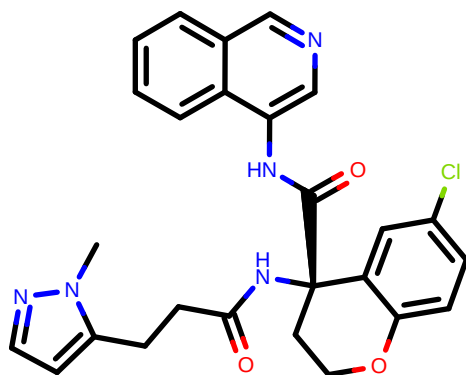
SMILES: CN(C)C(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN1198

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.22

EN300-92662_1_1



CID: EN300-92662_1_1

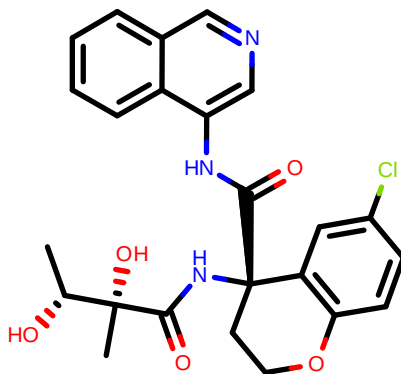
SMILES: Cn1c(ccn1)CCC(=O)N[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN537

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.26

EN300-202922_1_4



CID: EN300-202922_1_4

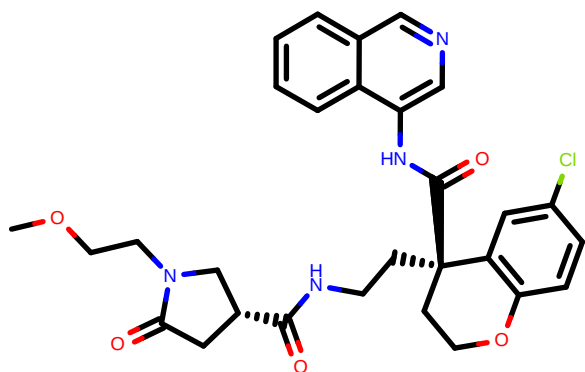
SMILES: C[C@H](C)(C)C(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4O)O

RUN: RUN1357

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.34

EN300-31845_3_1



CID: EN300-31845_3_1

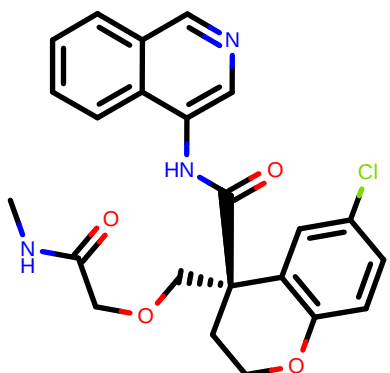
SMILES: COCN1C[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5

RUN: RUN1546

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.43

EN300-2977549_2_1



CID: EN300-2977549_2_1

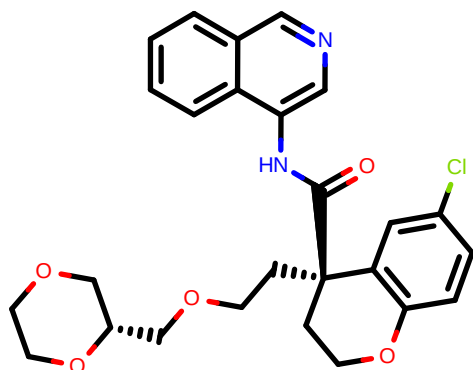
SMILES: CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3cccc4

RUN: RUN1078

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.22

EN300-139167_3_2



CID: EN300-139167_3_2

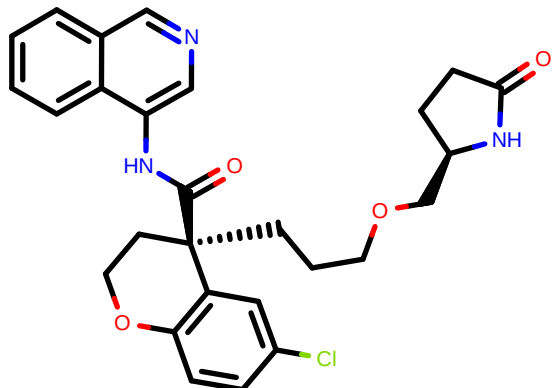
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCCCO5

RUN: RUN672

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.32

EN300-195756_4_2



CID: EN300-195756_4_2

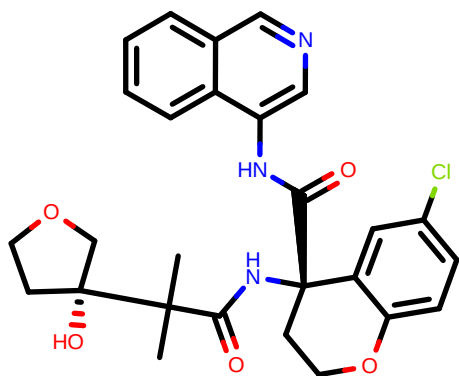
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCCC(=O)N5

RUN: RUN683

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-1630093_1_2



CID: EN300-1630093_1_2

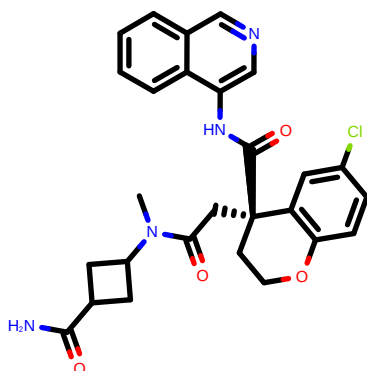
SMILES: CC(C)(C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)[C@]5(CCOCS)O

RUN: RUN1509

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.24

EN300-321459_1_1



CID: EN300-321459_1_1

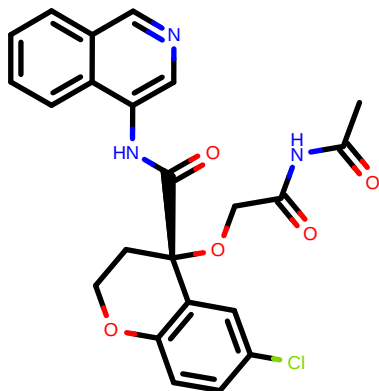
SMILES: CN(C(=O)C[C@@]1(Cc2cc(cc2)OCC1)C(=O)Nc3c4c(nc34)cccc4)[C@H]5C[C@H](C5)Cl=ON

RUN: RUN811

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-249475_1_1



CID: EN300-249475_1_1

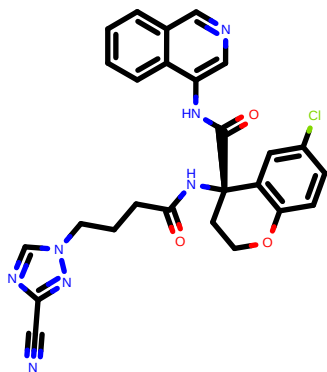
SMILES: CC(=O)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN896

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.23

EN300-245265_1_1



CID: EN300-245265_1_1

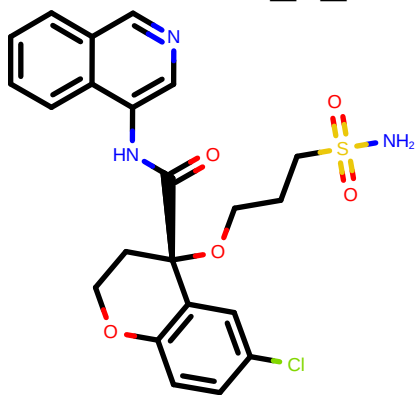
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5nc(n5)C#N

RUN: RUN1477

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.33

EN300-79588_1_1



CID: EN300-79588_1_1

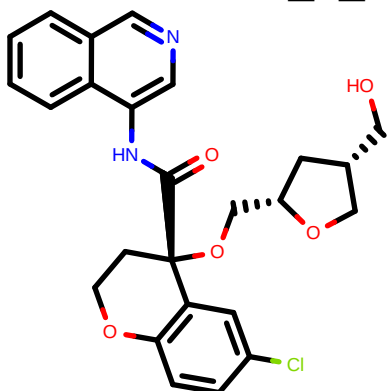
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCS(=O)(=O)N

RUN: RUN1120

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.29

EN300-6494158_1_1



CID: EN300-6494158_1_1

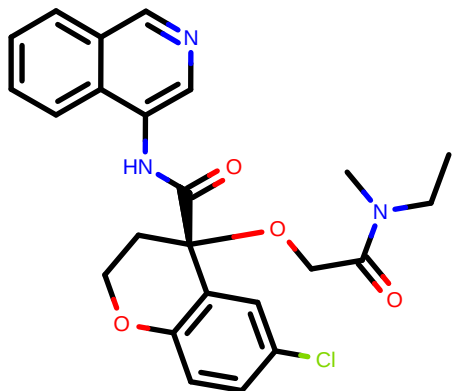
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@H](CO)CO

RUN: RUN1360

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.29

EN300-1253122_1_1



CID: EN300-1253122_1_1

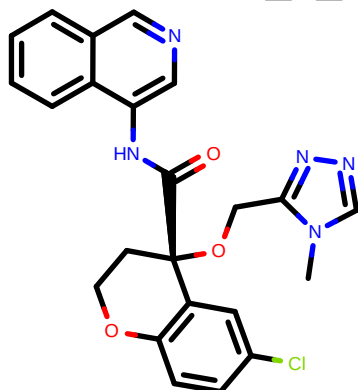
SMILES: CCN(C)C(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN548

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.25

EN300-113112_1_1



CID: EN300-113112_1_1

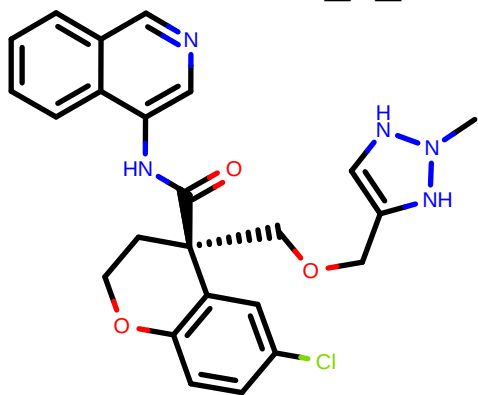
SMILES: Cn1cnnc1CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1200

DDG (kcal/mol): -0.92

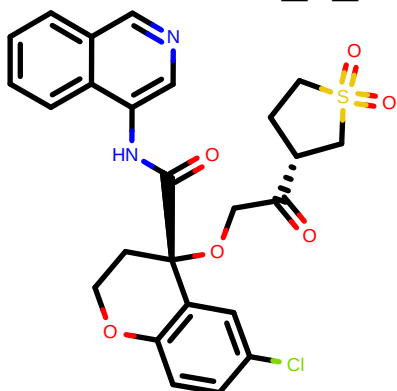
dDDG (kcal/mol): 0.23

EN300-219020_2_1



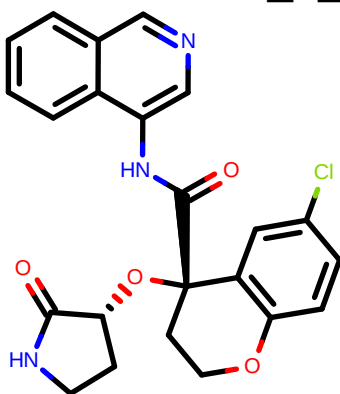
CID:	EN300-219020_2_1
SMILES:	<chem>Cn1ncc(n1)COC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5</chem>
RUN:	RUN1725
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.24

EN300-226314_1_1



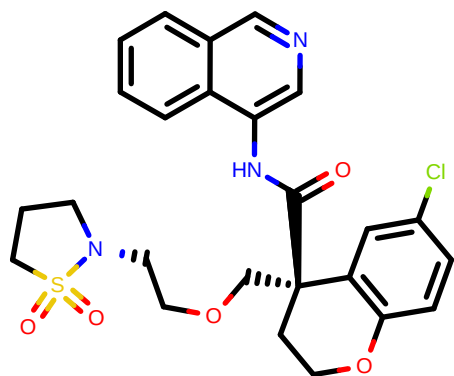
CID:	EN300-226314_1_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)OCC(=O)[C@@H]5SCCS(=O)(=O)C5</chem>
RUN:	RUN285
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.29

EN300-6736413_1_1



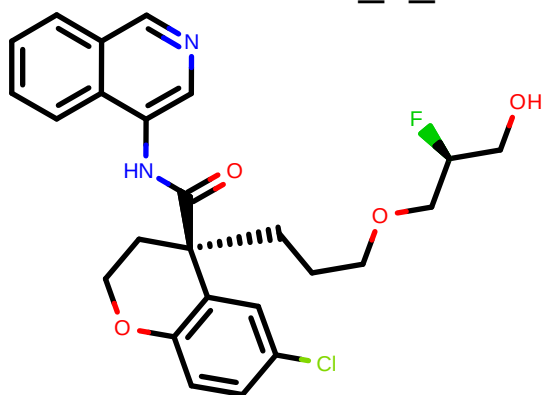
CID:	EN300-6736413_1_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)O[C@@H]5CCNC5=O</chem>
RUN:	RUN1671
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.20

EN300-114134_2_1



CID:	EN300-114134_2_1
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COC[C@H]5SCCS(=O)(=O)N5</chem>
RUN:	RUN347
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.35

EN300-1600517_4_2



CID:

EN300-1600517_4_2

SMILES:

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

RUN:

RUN492

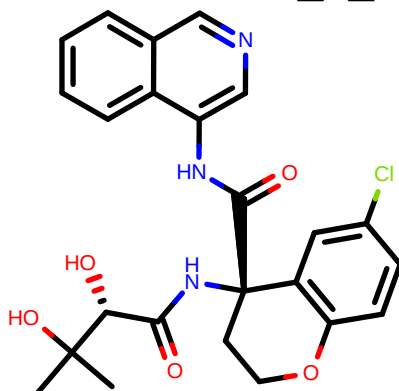
DDG (kcal/mol):

-0.91

dDDG (kcal/mol):

0.39

EN300-299532_1_1



CID:

EN300-299532_1_1

SMILES:

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

RUN:

RUN1141

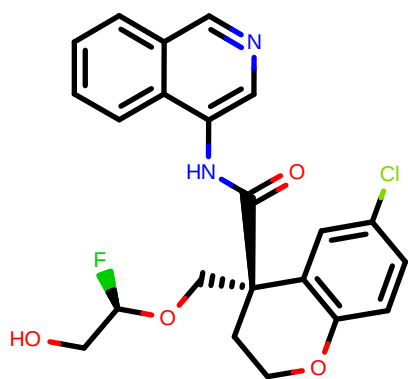
DDG (kcal/mol):

-0.91

dDDG (kcal/mol):

0.27

EN300-861925_2_1



CID:

EN300-861925_2_1

SMILES:

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

RUN:

RUN910

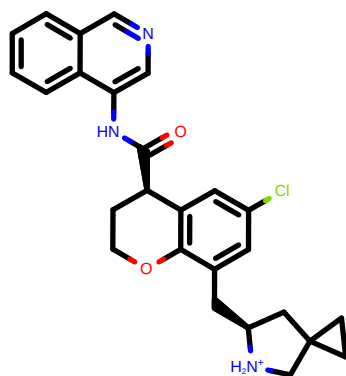
DDG (kcal/mol):

-0.91

dDDG (kcal/mol):

0.26

DAR-DIA-23e5a6a0-9_2



CID:

DAR-DIA-23e5a6a0-9_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)[C@H]5CC6(CC6)C[NH2+][5]Cl

RUN:

RUN157

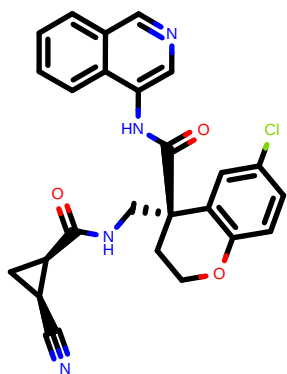
DDG (kcal/mol):

-0.91

dDDG (kcal/mol):

0.29

EN300-1588617_2_1



CID:

EN300-1588617_2_1

SMILES:

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

RUN:

RUN1481

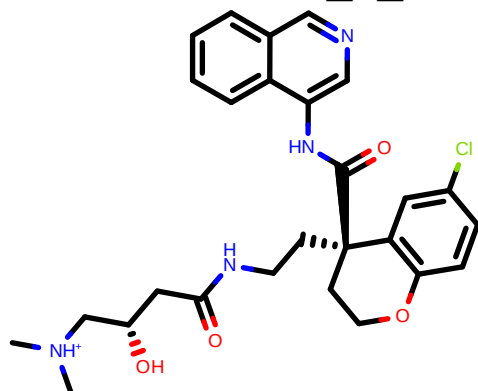
DDG (kcal/mol):

-0.90

dDDG (kcal/mol):

0.19

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)Nc3ncc4c3ccccc4)O

RUN:

RUN1370

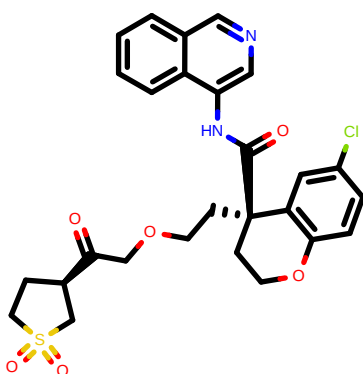
DDG (kcal/mol):

-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

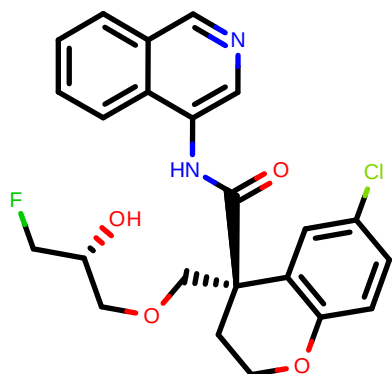
DDG (kcal/mol):

-0.89

dDDG (kcal/mol):

0.37

EN300-1968342_2_2



CID:

EN300-1968342_2_2

SMILES:

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

RUN:

RUN514

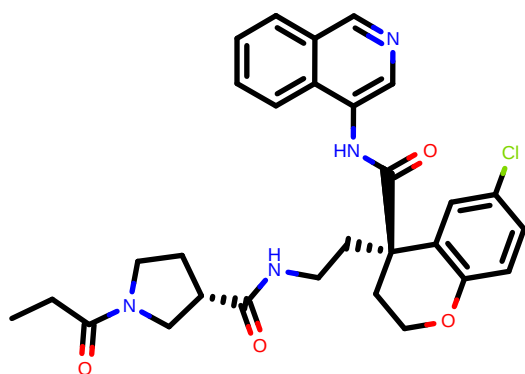
DDG (kcal/mol):

-0.89

dDDG (kcal/mol):

0.32

EN300-114133_3_1



CID: EN300-114133_3_1

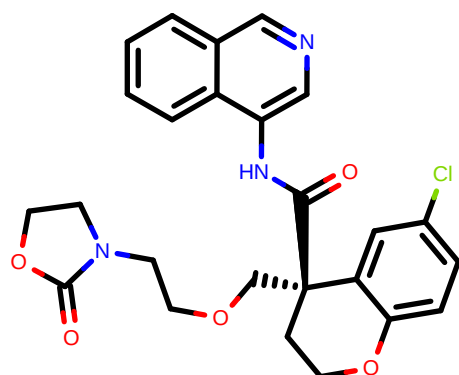
SMILES: CCC(=O)N1CC[C@@H](C1)C(=O)NCC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cccc5ccccc5

RUN: RUN1681

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.44

EN300-370967_2_1



CID: EN300-370967_2_1

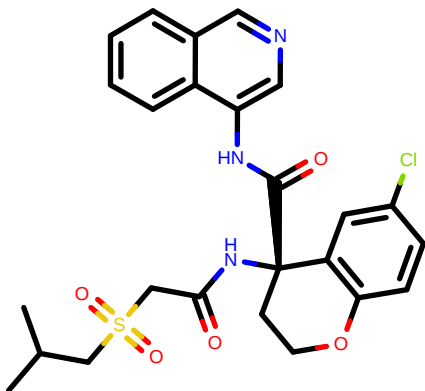
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5ccccc5=O

RUN: RUN807

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-42243_1_1



CID: EN300-42243_1_1

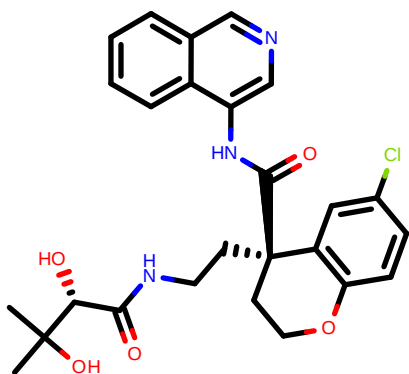
SMILES: CC(C)CS(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3ccccc4

RUN: RUN798

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.32

EN300-299532_3_1



CID: EN300-299532_3_1

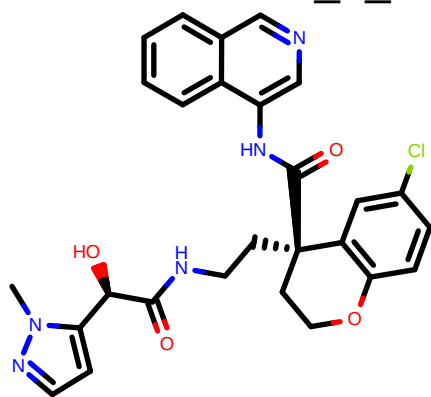
SMILES: CC(C)([C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3ccccc4)O)O

RUN: RUN1474

DDG (kcal/mol): -0.88

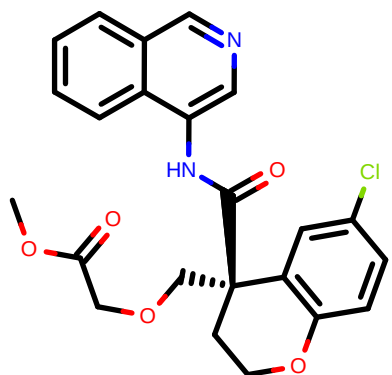
dDDG (kcal/mol): 0.38

EN300-6473273_3_2



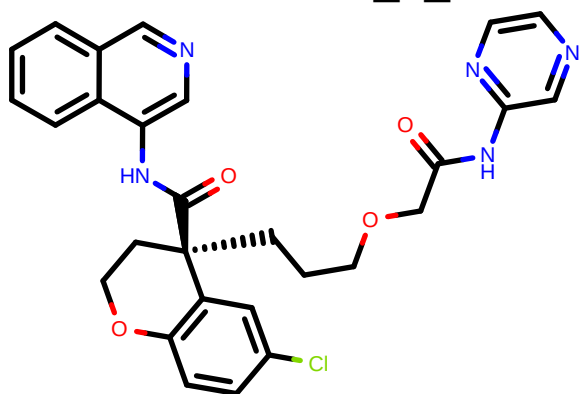
CID:	EN300-6473273_3_2
SMILES:	<chem>Cn1c(cn1)[C@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O</chem>
RUN:	RUN1106
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.37

EN300-19700_2_1



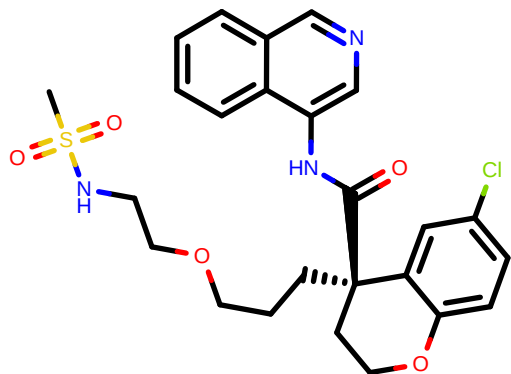
CID:	EN300-19700_2_1
SMILES:	<chem>COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1414
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.21

EN300-105267_4_1



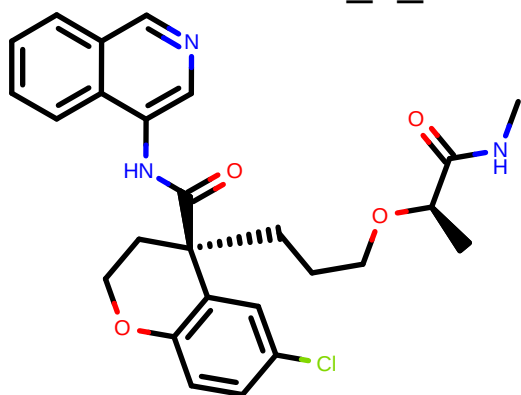
CID:	EN300-105267_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCOC(=O)Nc5cnccn5</chem>
RUN:	RUN1135
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.31

EN300-1238839_4_1



CID:	EN300-1238839_4_1
SMILES:	<chem>CS(=O)(=O)NCCOCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1231
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.40

EN300-211482_4_2



CID:

EN300-211482_4_2

SMILES:

C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN372

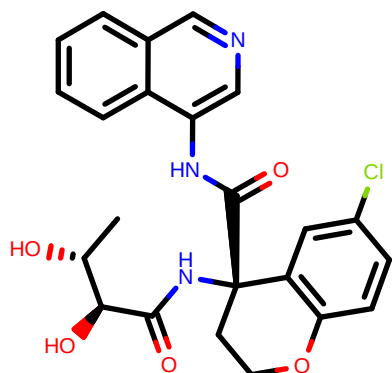
DDG (kcal/mol):

-0.87

dDDG (kcal/mol):

0.33

EN300-6974806_1_1



CID:

EN300-6974806_1_1

SMILES:

CC@H(C(=O)N)[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4O

RUN:

RUN997

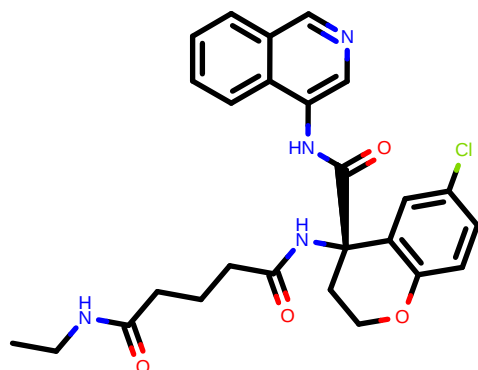
DDG (kcal/mol):

-0.87

dDDG (kcal/mol):

0.25

EN300-68635_1_1



CID:

EN300-68635_1_1

SMILES:

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

RUN:

RUN649

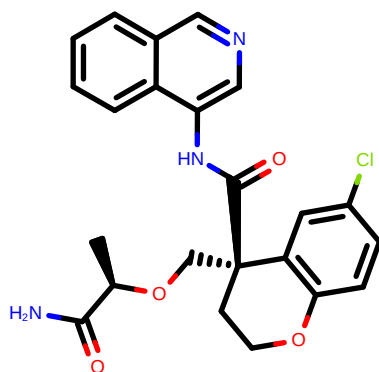
DDG (kcal/mol):

-0.87

dDDG (kcal/mol):

0.31

EN300-17381_2_2



CID:

EN300-17381_2_2

SMILES:

C[C@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1238

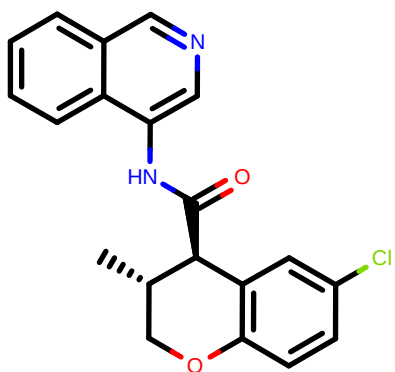
DDG (kcal/mol):

-0.87

dDDG (kcal/mol):

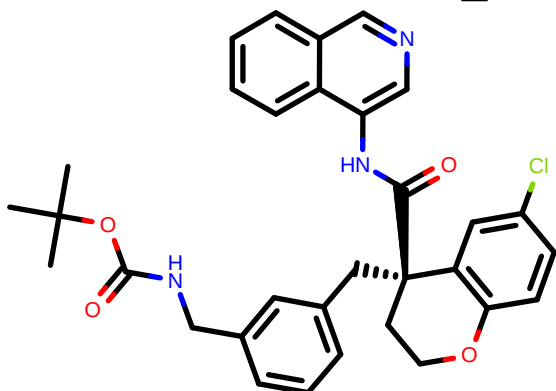
0.24

MAT-POS-8a69d52e-4_2



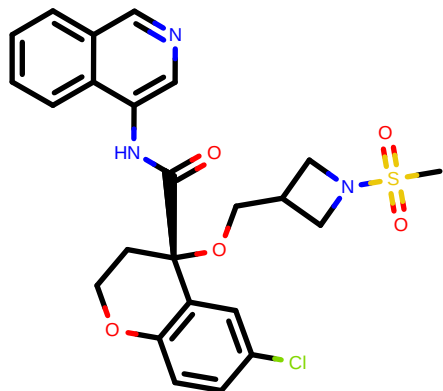
CID:	MAT-POS-8a69d52e-4_2
SMILES:	<chem>C[C@H]1COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN13
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.06

JAG-UCB-7b680c2b-1_1



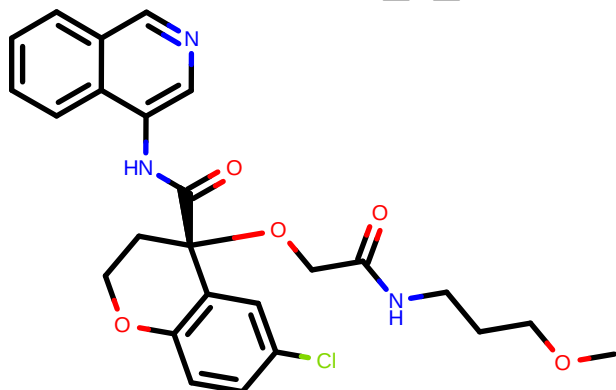
CID:	JAG-UCB-7b680c2b-1_1
SMILES:	<chem>CC(C)(C)OC(=O)Nc1cccc(c1)[C@H]2(COC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN255
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.36

EN300-302290_1_1



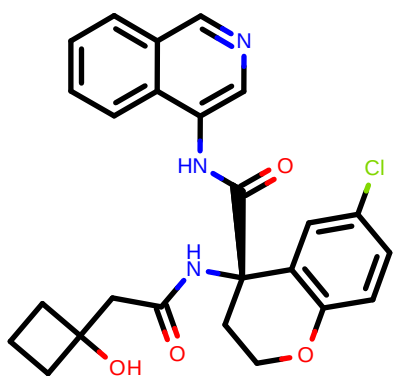
CID:	EN300-302290_1_1
SMILES:	<chem>CS(=O)(=O)N1CC(C1)CO[C@H]2(COC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN493
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.26

EN300-04492_1_1



CID:	EN300-04492_1_1
SMILES:	<chem>COCCCN(C(=O)CO[C@H]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1663
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.22

EN300-246423_1_1



CID: EN300-246423_1_1

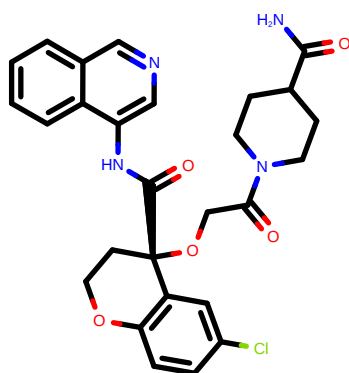
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)NC(=O)CC5(CCC5)O

RUN: RUN545

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.25

EN300-08063_1_1



CID: EN300-08063_1_1

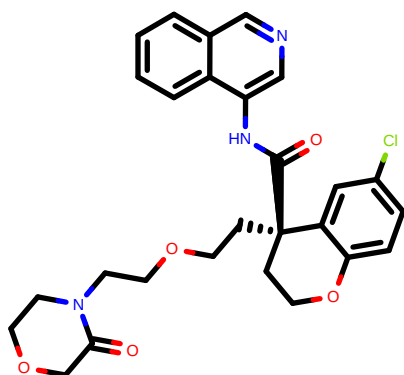
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)OCC(=O)N5CCCC(C5)C(=O)N

RUN: RUN1392

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.24

EN300-219330_3_1



CID: EN300-219330_3_1

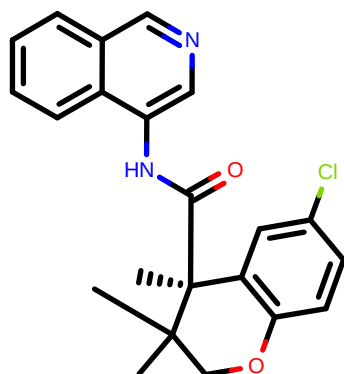
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)CCOCC5NCCOCC5=O

RUN: RUN536

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.34

DAR-DIA-0d514e7d-30_1



CID: DAR-DIA-0d514e7d-30_1

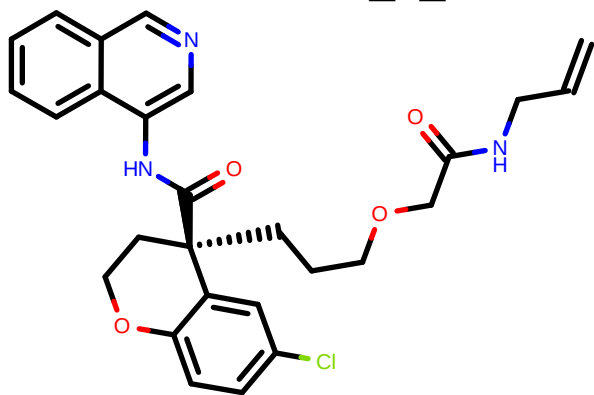
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN112

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.15

EN300-17184_4_1



CID: EN300-17184_4_1

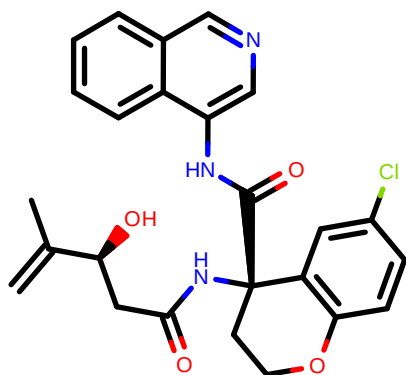
SMILES: C=CCNC(=O)COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1567

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.38

EN300-155498_1_1



CID: EN300-155498_1_1

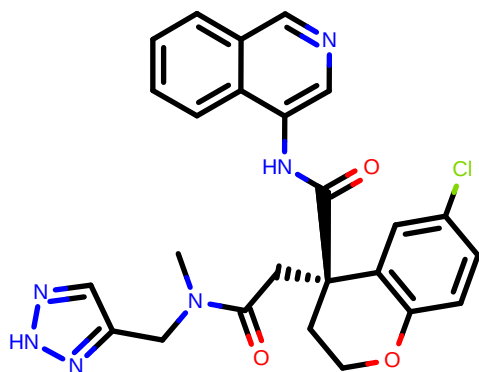
SMILES: CC(=C)[C@H](CC(=O)N[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN442

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.26

EN300-1265071_1_1



CID: EN300-1265071_1_1

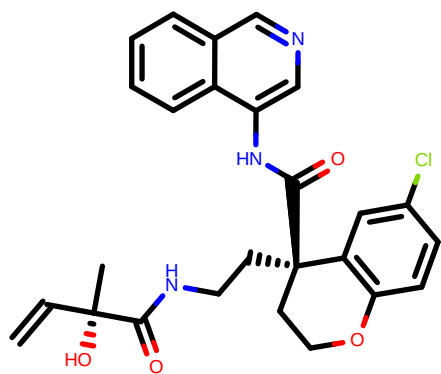
SMILES: CN(Cc1cn[nH]n1)C(=O)[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1322

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.29

EN300-248888_3_2



CID: EN300-248888_3_2

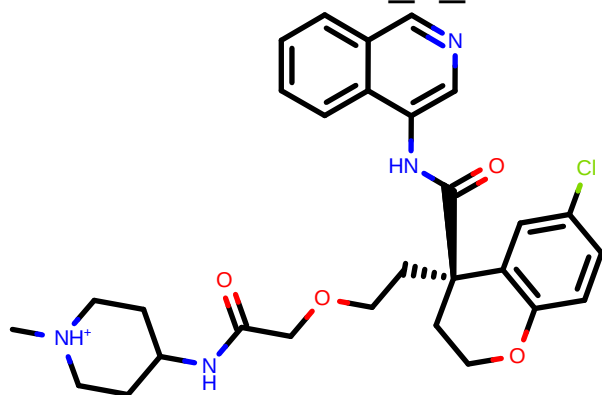
SMILES: C[C@](C=C)(C(=O)NCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN678

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.37

EN300-342462_3_1



CID:

EN300-342462_3_1

SMILES:

C[NH+]1CCC(CC1)NC(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN:

RUN1132

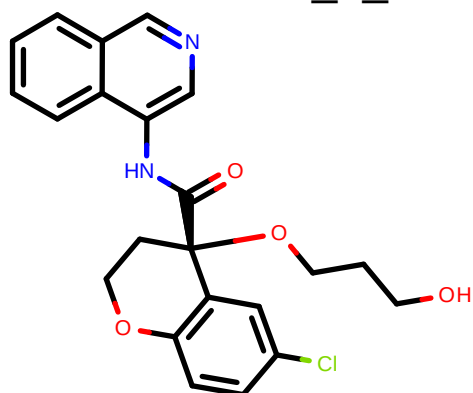
DDG (kcal/mol):

-0.85

dDDG (kcal/mol):

0.45

EN300-221518_1_1



CID:

EN300-221518_1_1

SMILES:

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

RUN:

RUN992

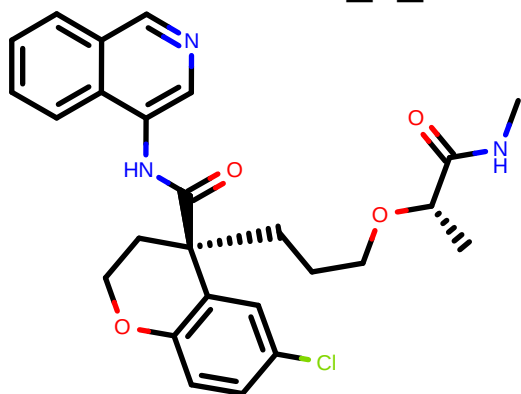
DDG (kcal/mol):

-0.84

dDDG (kcal/mol):

0.20

EN300-211482_4_1



CID:

EN300-211482_4_1

SMILES:

C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN:

RUN1015

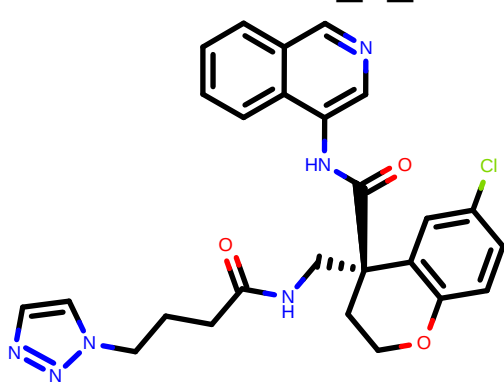
DDG (kcal/mol):

-0.84

dDDG (kcal/mol):

0.35

EN300-124301_2_1



CID:

EN300-124301_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCn5ccnn5

RUN:

RUN754

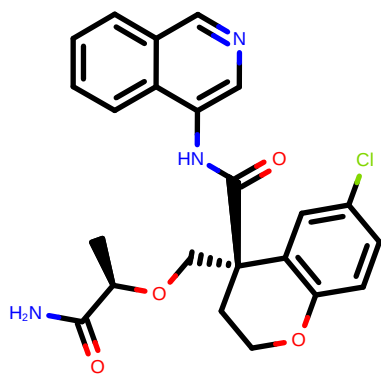
DDG (kcal/mol):

-0.84

dDDG (kcal/mol):

0.32

EN300-17381_2_2



CID: EN300-17381_2_2

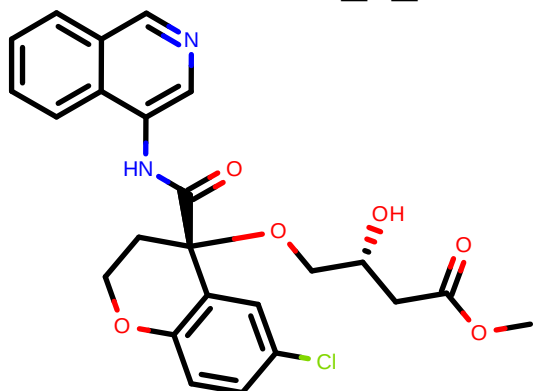
SMILES: C[C@H](C(=O)N)OC[C@]1(COC(=O)Cc2cc(C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1230

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.26

EN300-73662_1_1



CID: EN300-73662_1_1

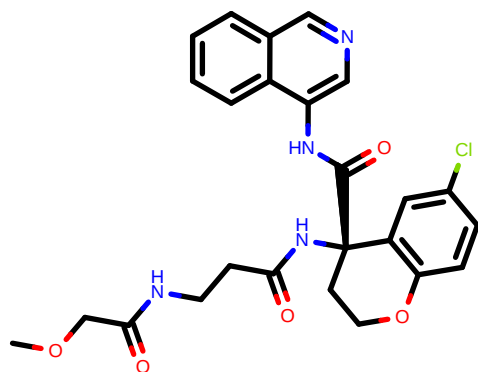
SMILES: COC(=O)C[C@H](CO[C@]1(COC(=O)Cc2cc(C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1288

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.32

EN300-31242_1_1



CID: EN300-31242_1_1

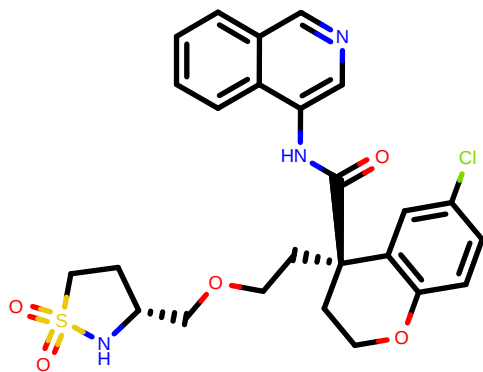
SMILES: COCC(=O)NCCC(=O)N[C@]1(COC(=O)Cc2cc(C)C(=O)Nc3cncc4c3ccccc4

RUN: RUN553

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.28

EN300-1699871_3_2



CID: EN300-1699871_3_2

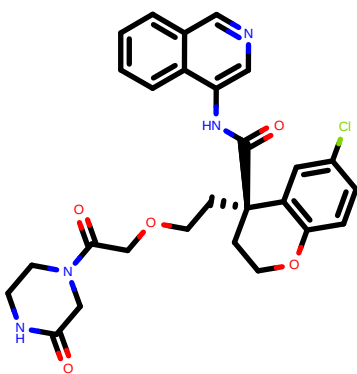
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(C)C)CCOC[C@H]5CCS(=O)(=O)N5

RUN: RUN1611

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-22884_3_1



CID: EN300-22884_3_1

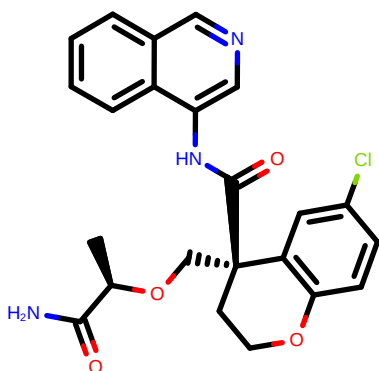
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCNC(=O)C5

RUN: RUN544

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.32

EN300-17381_2_2



CID: EN300-17381_2_2

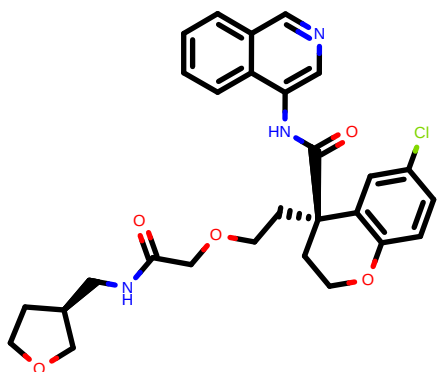
SMILES: C[C@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN1246

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.24

EN300-46832_3_1



CID: EN300-46832_3_1

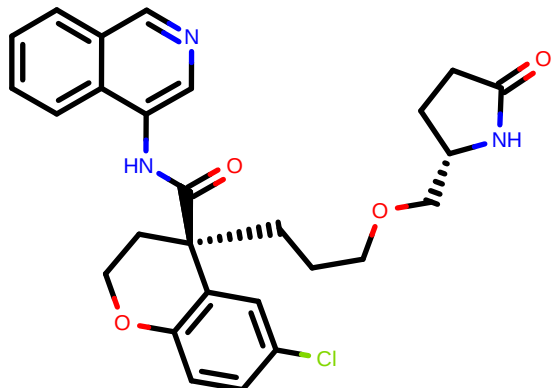
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@@H]5CCOC5

RUN: RUN1667

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.38

EN300-195756_4_1



CID: EN300-195756_4_1

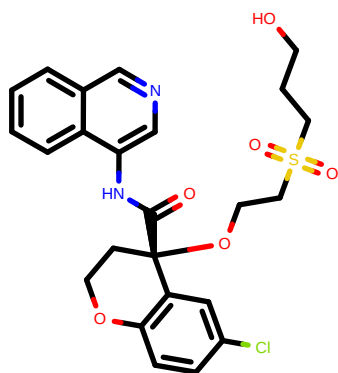
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC[C@@H]5CCC(=O)N5

RUN: RUN1455

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.37

EN300-7456499_1_1



CID: EN300-7456499_1_1

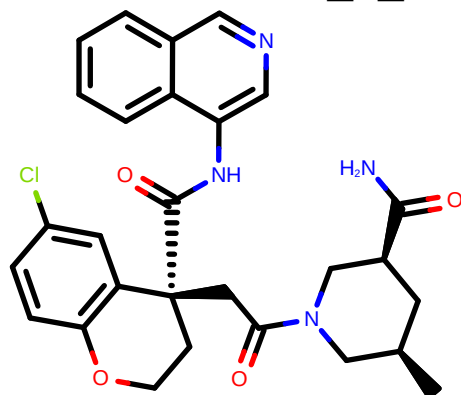
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCCO

RUN: RUN501

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.35

EN300-1724086_1_1



CID: EN300-1724086_1_1

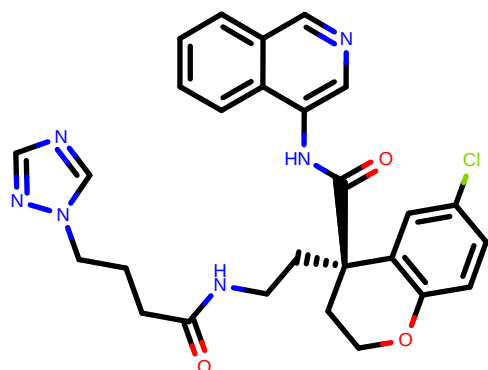
SMILES: ClC@@H1C[C@@H]2CN(C1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)N4Cncc5c4cccc5)Cl=O)N

RUN: RUN670

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.25

EN300-316216_3_1



CID: EN300-316216_3_1

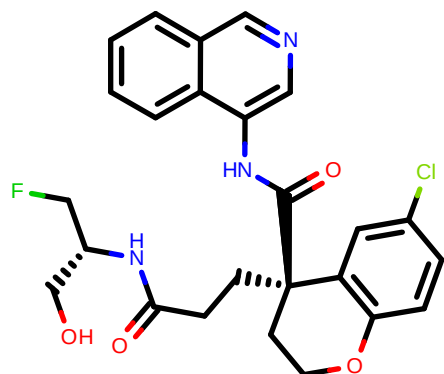
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCn5cnnc5

RUN: RUN755

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.33

EN300-6498726_2_1



CID: EN300-6498726_2_1

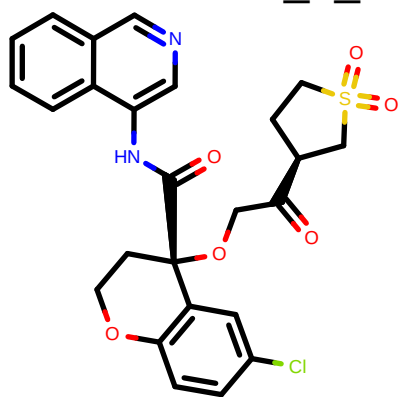
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CO)CF

RUN: RUN1539

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.36

EN300-226314_1_2



CID: EN300-226314_1_2

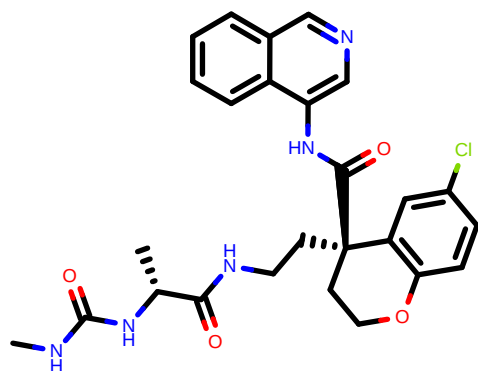
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5SCCS(=O)(=O)C5

RUN: RUN277

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.29

EN300-1258964_3_2



CID: EN300-1258964_3_2

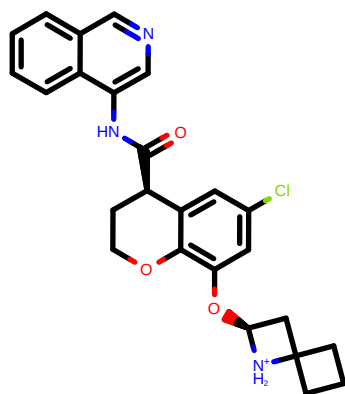
SMILES: C[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)NC(=O)NC

RUN: RUN1026

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.50

DAR-DIA-23e5a6a0-2_2



CID: DAR-DIA-23e5a6a0-2_2

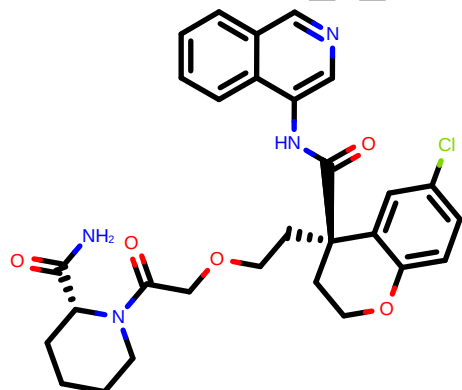
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)[C@H]5CC6([NH2+][5])CC6)Cl

RUN: RUN88

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.27

EN300-22879_3_1



CID: EN300-22879_3_1

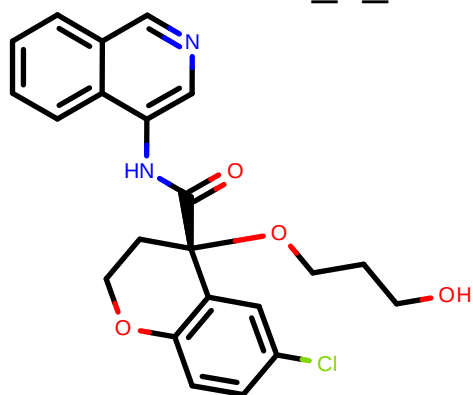
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)C(=O)N5CCCC[C@H]5[C@@H](C1=CN)C1=O

RUN: RUN765

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.42

EN300-221518_1_1



CID: EN300-221518_1_1

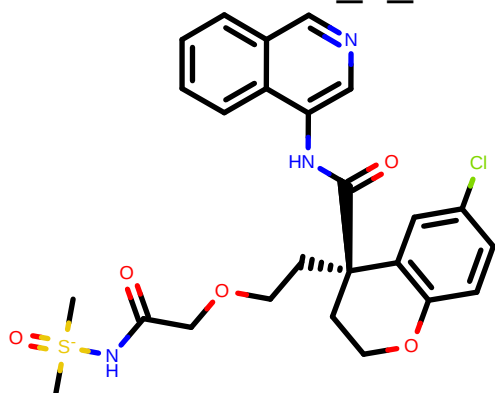
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO

RUN: RUN984

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.19

EN300-267469_3_1



CID: EN300-267469_3_1

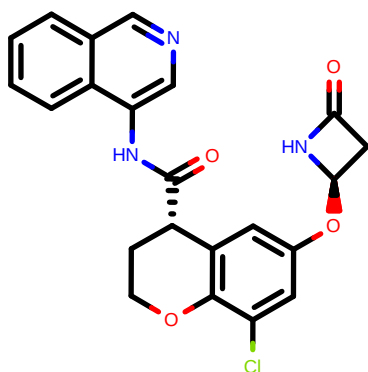
SMILES: CS(=NC(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4(=O)C

RUN: RUN377

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.41

FRA-DIA-b66f7109-3_1



CID: FRA-DIA-b66f7109-3_1

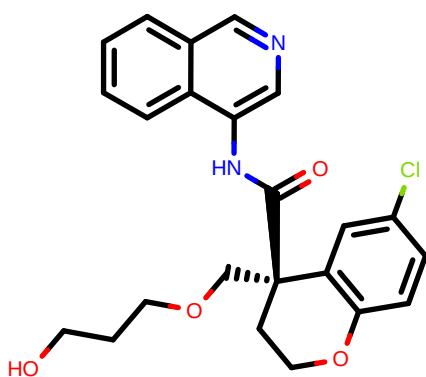
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)O[C@@H]5CC(=O)N5

RUN: RUN187

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.23

EN300-221518_2_1



CID: EN300-221518_2_1

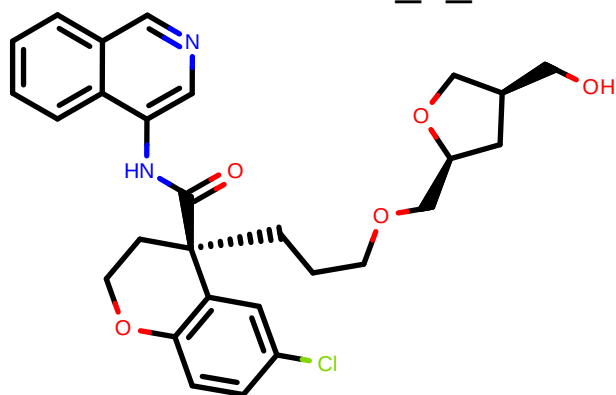
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCO

RUN: RUN838

DDG (kcal/mol): -0.80

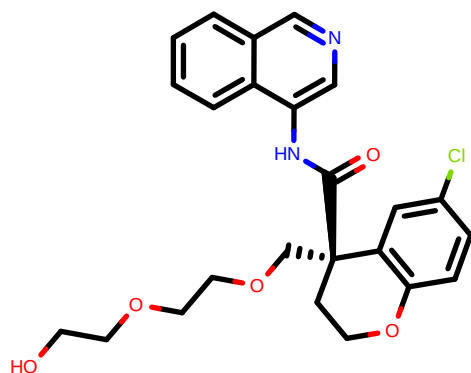
dDDG (kcal/mol): 0.27

EN300-6494158_4_1



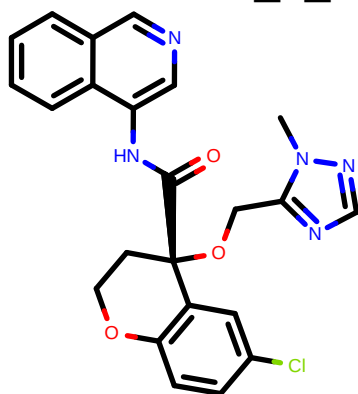
CID:	EN300-6494158_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5C[C@@H](CO)CO</chem>
RUN:	RUN1007
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.49

EN300-52467_2_1



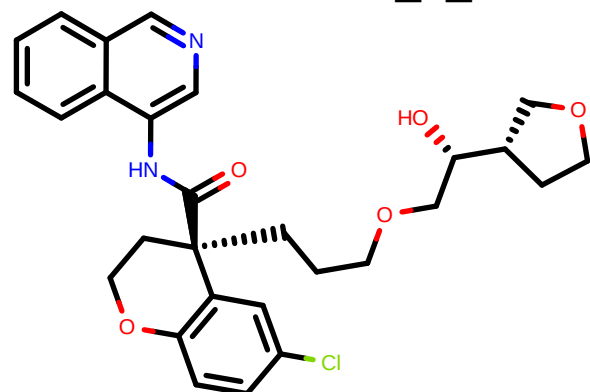
CID:	EN300-52467_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCOCO</chem>
RUN:	RUN1581
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.27

EN300-87334_1_1



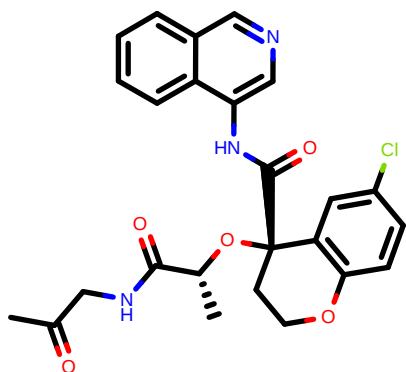
CID:	EN300-87334_1_1
SMILES:	<chem>Cn1c(ncn1)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN580
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.23

EN300-1911992_4_3



CID:	EN300-1911992_4_3
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H](C)[C@@H]5CCOC5O</chem>
RUN:	RUN675
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.35

EN300-131093_1_2



CID: EN300-131093_1_2

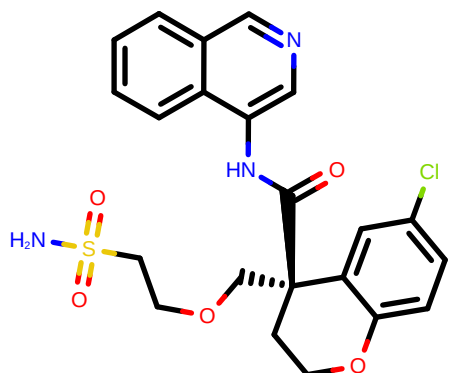
SMILES: C[C@H](C(=O)NCC(=O)C)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4

RUN: RUN1352

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.27

EN300-270710_2_1



CID: EN300-270710_2_1

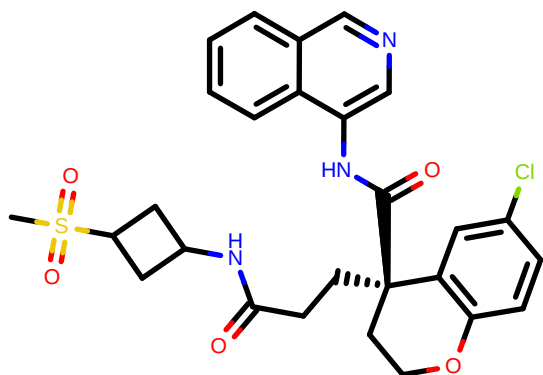
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)C(=O)N

RUN: RUN1286

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.26

EN300-378760_2_1



CID: EN300-378760_2_1

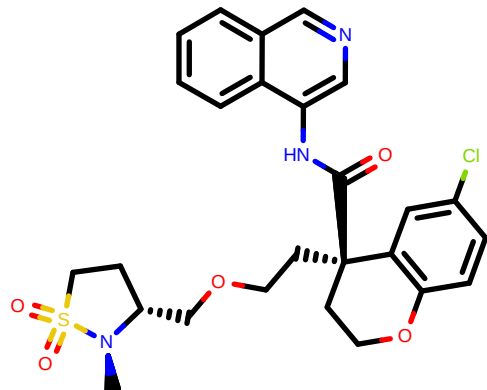
SMILES: CS(=O)(=O)[C@H]1C[C@H](C1)NC(=O)C[C@]2(C3c4cc(cc4)OCC2)C(=O)Nc4c5c(cnc4)ccc5

RUN: RUN1187

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.30

EN300-393148_3_2



CID: EN300-393148_3_2

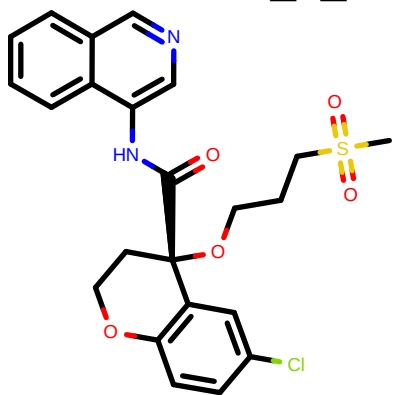
SMILES: C[N@@]1[C@H](CCS1(=O)=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5

RUN: RUN520

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.31

EN300-68794_1_1



CID: EN300-68794_1_1

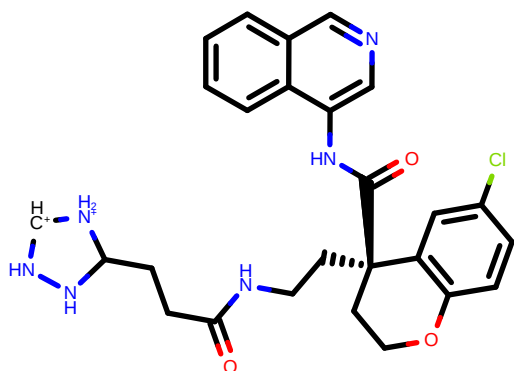
SMILES: CS(=O)(=O)CCCO[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4

RUN: RUN652

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.28

EN300-101197_3_1



CID: EN300-101197_3_1

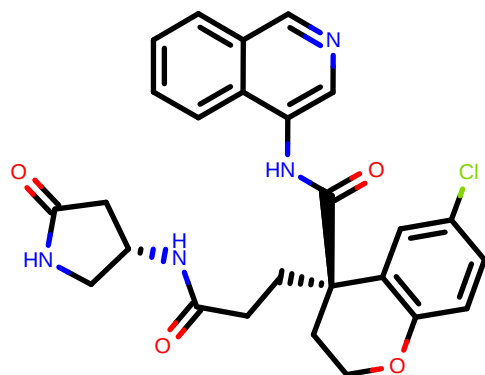
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCNC(=O)CCc5[nH]ncn5

RUN: RUN1178

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.32

EN300-127487_2_2



CID: EN300-127487_2_2

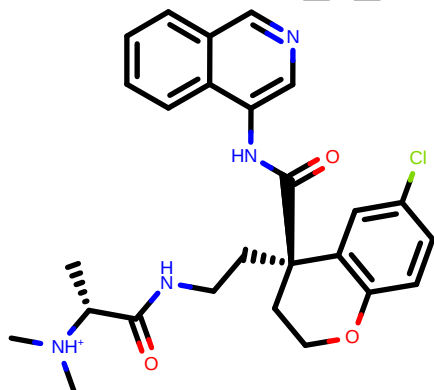
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(C(COC4c3cc(cc4)Cl)CCC(=O)N[C@H]5CC(=O)NCS

RUN: RUN615

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.31

EN300-312850_3_1



CID: EN300-312850_3_1

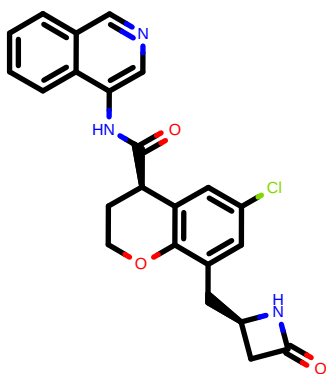
SMILES: C[C@H](C(=O)NCC[C@]1(C(COC2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4)[NH+](C)C

RUN: RUN407

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.41

DAR-DIA-6a508060-5_1



CID:

DAR-DIA-6a508060-5_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC(=O)N5)Cl

RUN:

RUN189

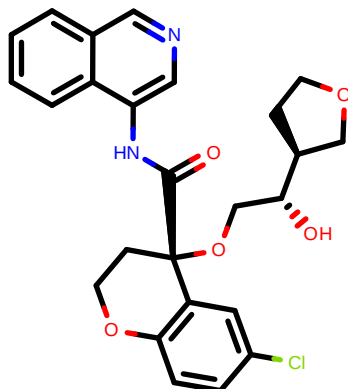
DDG (kcal/mol):

-0.78

dDDG (kcal/mol):

0.20

EN300-1911992_1_4



CID:

EN300-1911992_1_4

SMILES:

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

RUN:

RUN1703

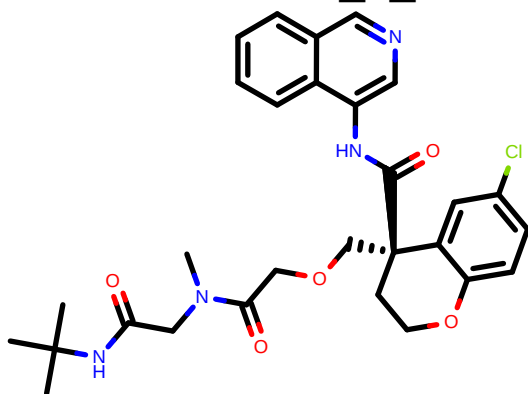
DDG (kcal/mol):

-0.78

dDDG (kcal/mol):

0.28

EN300-23019_2_1



CID:

EN300-23019_2_1

SMILES:

CC(C)(C)NC(=O)CN(C)C(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN:

RUN1118

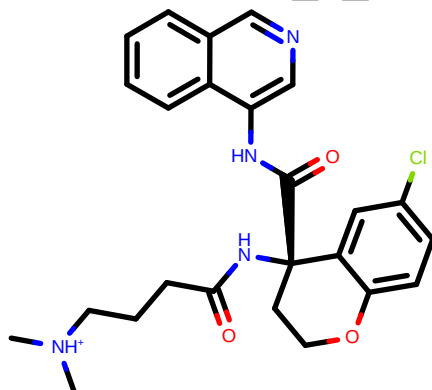
DDG (kcal/mol):

-0.77

dDDG (kcal/mol):

0.41

EN300-42520_1_1



CID:

EN300-42520_1_1

SMILES:

C[NH+](C)CCCC(=O)N[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN:

RUN925

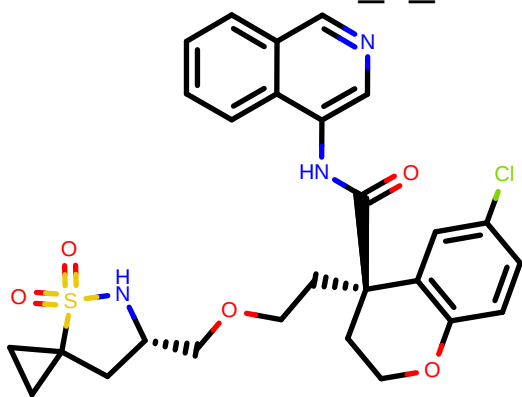
DDG (kcal/mol):

-0.77

dDDG (kcal/mol):

0.33

EN300-6504697_3_1



CID:

EN300-6504697_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4ccc(cc4)C)CCOC[C@@H]3C6(CO)S(=O)(=O)N6

RUN:

RUN892

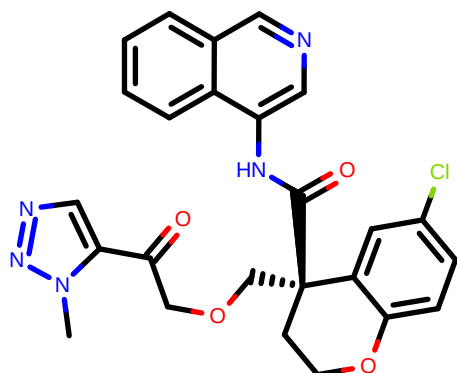
DDG (kcal/mol):

-0.77

dDDG (kcal/mol):

0.34

EN300-204936_2_1



CID:

EN300-204936_2_1

SMILES:

Cn1c(cnn1)C(=O)COC[C@H]2(CCOc3ccc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5

RUN:

RUN1773

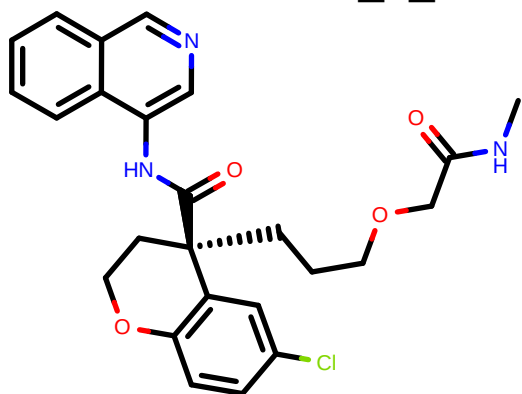
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.34

EN300-2977549_4_1



CID:

EN300-2977549_4_1

SMILES:

CNC(=O)COCCC[C@H]1(CCOc2ccc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN:

RUN603

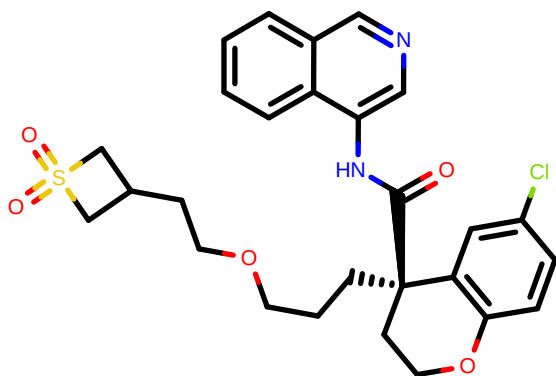
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.27

EN300-189563_4_1



CID:

EN300-189563_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4ccc(cc4)Cl)CCOCCSCS(=O)(=O)C5

RUN:

RUN847

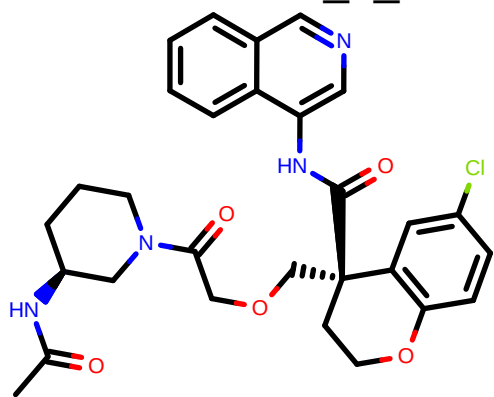
DDG (kcal/mol):

-0.76

dDDG (kcal/mol):

0.32

EN300-48886_2_2



CID: EN300-48886_2_2

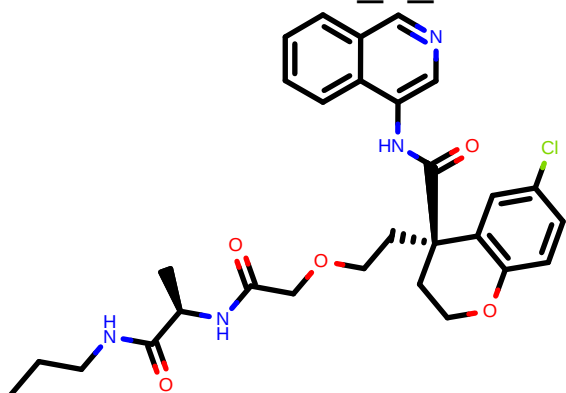
SMILES: CC(=O)N[C@H]1CCCN(C1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN1741

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.42

EN300-23214_3_1



CID: EN300-23214_3_1

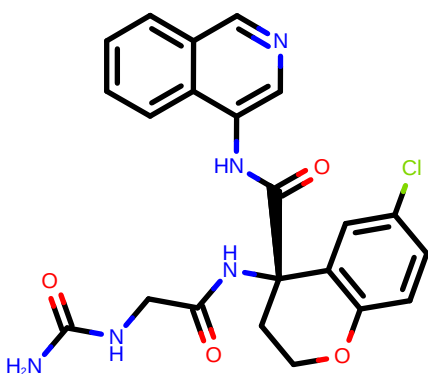
SMILES: CCCCNC(=O)[C@H](C)NC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1508

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.37

EN300-10397_1_1



CID: EN300-10397_1_1

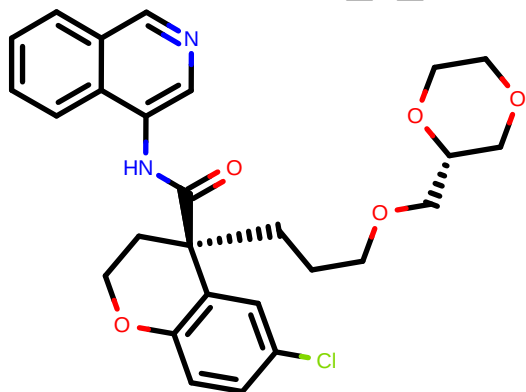
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N

RUN: RUN1525

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.22

EN300-139167_4_2



CID: EN300-139167_4_2

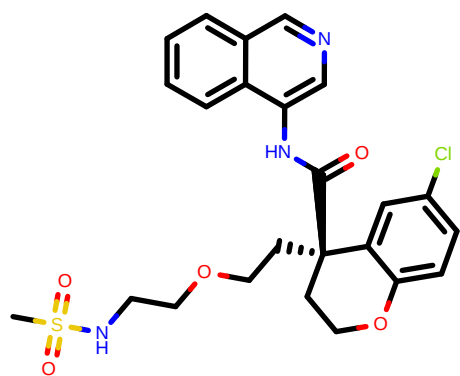
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5COCOC5

RUN: RUN1159

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.35

EN300-1238839_3_1



CID: EN300-1238839_3_1

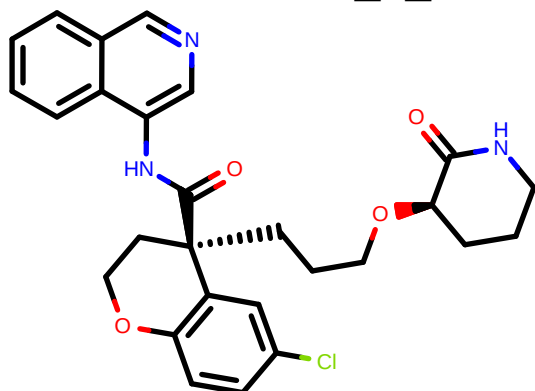
SMILES: CS(=O)(=O)NCCOC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1100

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.33

EN300-107267_4_1



CID: EN300-107267_4_1

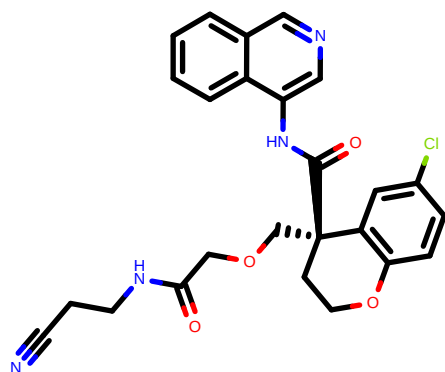
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCNCC5=O

RUN: RUN1670

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.32

EN300-10895_2_1



CID: EN300-10895_2_1

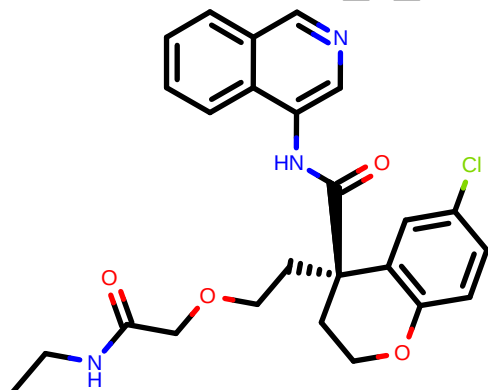
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCCC#N

RUN: RUN690

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.31

EN300-7003350_3_1



CID: EN300-7003350_3_1

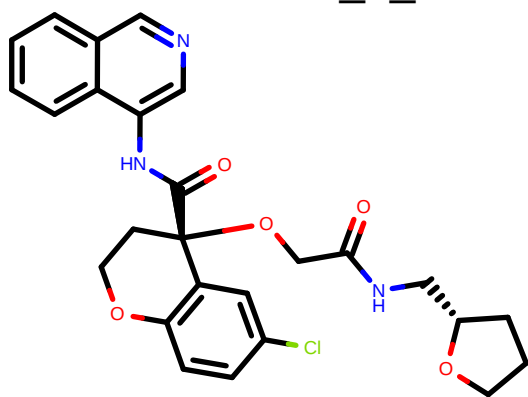
SMILES: CCNC(=O)COCC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1492

DDG (kcal/mol): -0.76

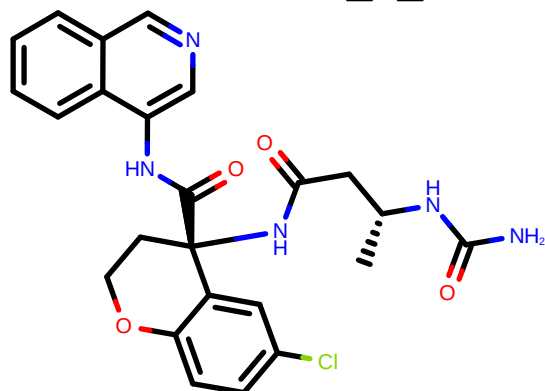
dDDG (kcal/mol): 0.27

EN300-01527_1_1



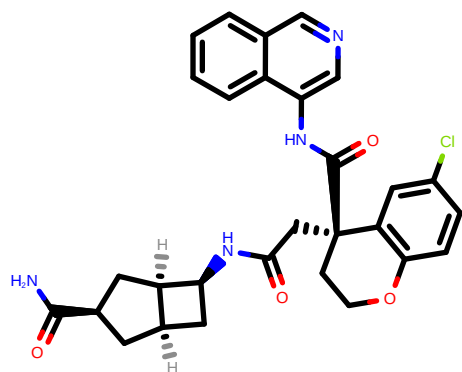
CID:	EN300-01527_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)OCC(=O)NC[C@@H]5CCCCO5</chem>
RUN:	RUN1623
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.27

EN300-268198_1_2



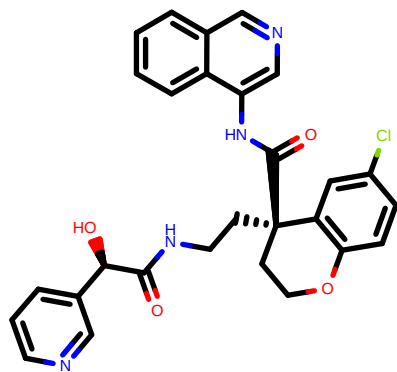
CID:	EN300-268198_1_2
SMILES:	<chem>C[C@H](CC(=O)N[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3ccoc4)NC(=O)N</chem>
RUN:	RUN1053
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.29

EN300-1268016_1_6



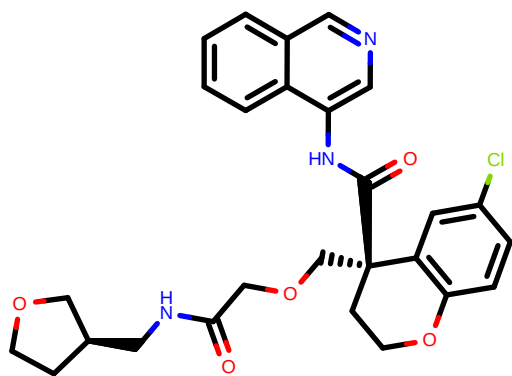
CID:	EN300-1268016_1_6
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)OCC(=O)N[C@@H]5C[C@@H]6[C@@H]5C[C@@H]6Cl=O)N</chem>
RUN:	RUN994
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.34

EN300-134855_3_1



CID:	EN300-134855_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@H](c5ccncc5)O</chem>
RUN:	RUN1258
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.47

EN300-46832_2_2



CID:

EN300-46832_2_2

SMILES:

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

RUN:

RUN618

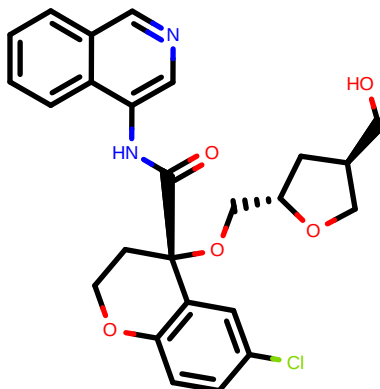
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.33

EN300-6494158_1_3



CID:

EN300-6494158_1_3

SMILES:

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

RUN:

RUN1104

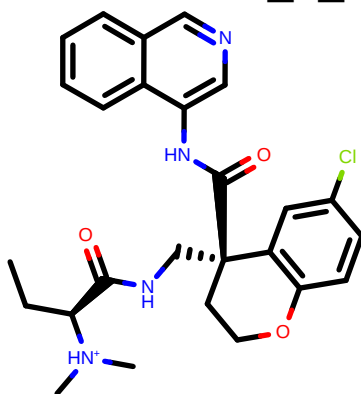
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.27

EN300-110012_2_1



CID:

EN300-110012_2_1

SMILES:

CC[C@H](C(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccccc4)[NH+](C)C

RUN:

RUN1760

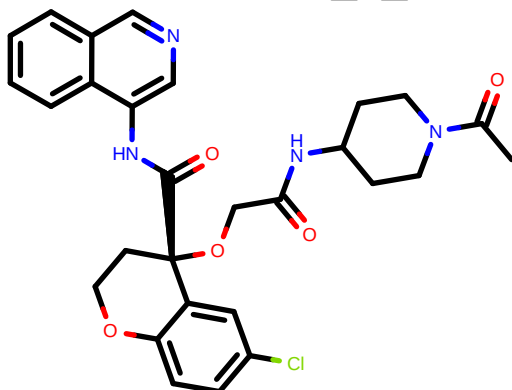
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.67

EN300-23226_1_1



CID:

EN300-23226_1_1

SMILES:

CC(=O)N1CCC(CC1)NC(=O)CO[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccccc5

RUN:

RUN1695

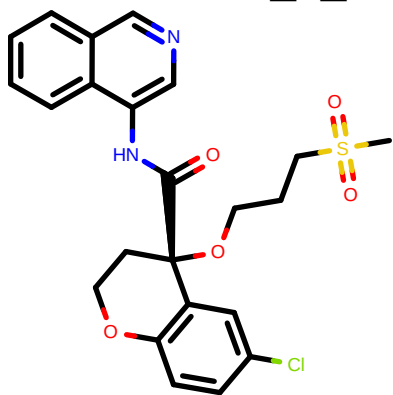
DDG (kcal/mol):

-0.75

dDDG (kcal/mol):

0.35

EN300-68794_1_1



CID:

EN300-68794_1_1

SMILES:

CS(=O)(=O)CCCO[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN660

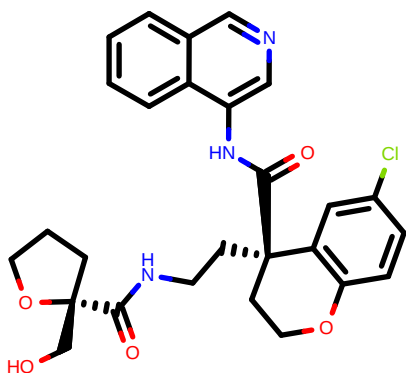
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.30

EN300-1425677_3_2



CID:

EN300-1425677_3_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(COC4c3cc(cc4)Cl)CCNC(=O)[C@]5(C)C(CCO5)CO

RUN:

RUN1665

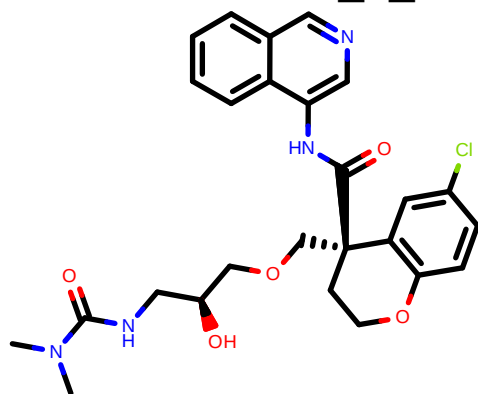
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.39

EN300-6501360_2_1



CID:

EN300-6501360_2_1

SMILES:

CN(C)C(=O)NC[C@@H](COC[C@]1(C)C(COC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN:

RUN1046

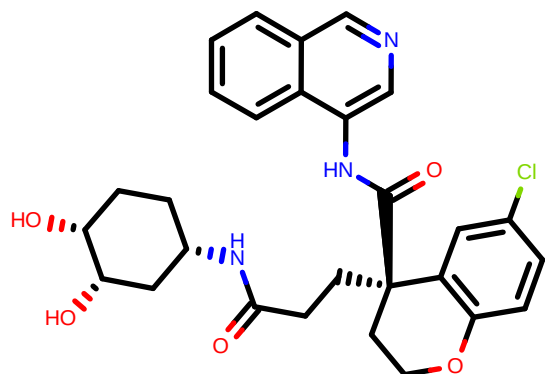
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.48

EN300-741822_2_2



CID:

EN300-741822_2_2

SMILES:

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

RUN:

RUN1267

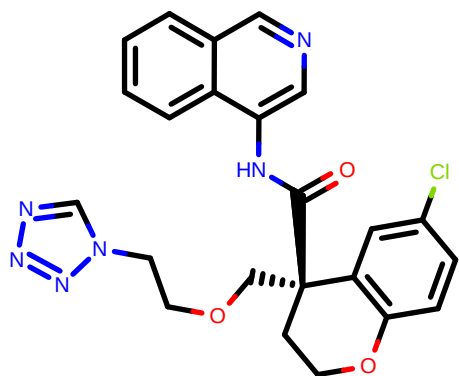
DDG (kcal/mol):

-0.74

dDDG (kcal/mol):

0.36

EN300-364679_2_1



CID: EN300-364679_2_1

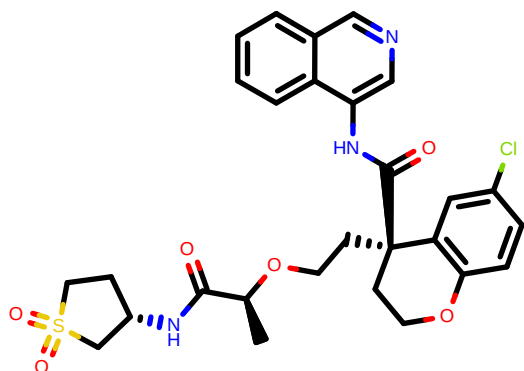
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cnnn5

RUN: RUN1526

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.25

EN300-23318_3_3



CID: EN300-23318_3_3

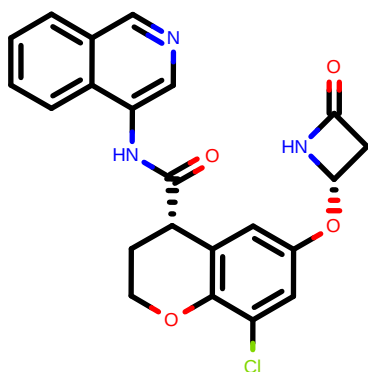
SMILES: C[C@@H](Cl)(=O)N[C@@H](CCS(=O)(=O)Cl)OCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1348

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.46

FRA-DIA-b66f7109-3_2



CID: FRA-DIA-b66f7109-3_2

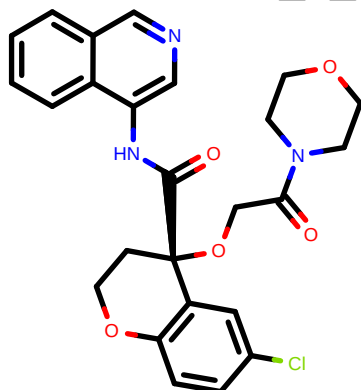
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4)ClO[C@@H]5CC(=O)N5

RUN: RUN210

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.23

EN300-1241327_1_1



CID: EN300-1241327_1_1

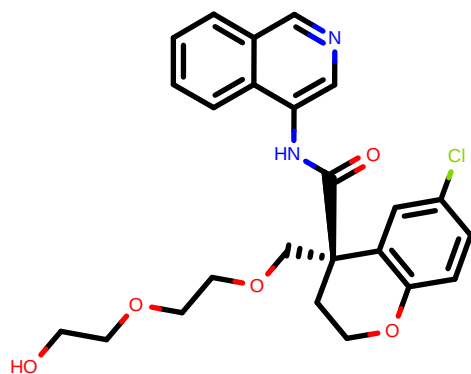
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCOCC5

RUN: RUN540

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.24

EN300-52467_2_1



CID:

EN300-52467_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCOCO

RUN:

RUN1573

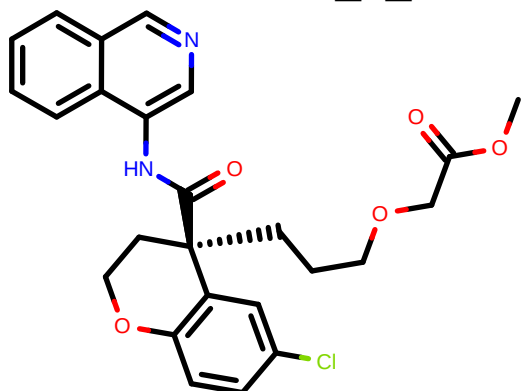
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.27

EN300-19700_4_1



CID:

EN300-19700_4_1

SMILES:

COC(=O)COCOC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4

RUN:

RUN436

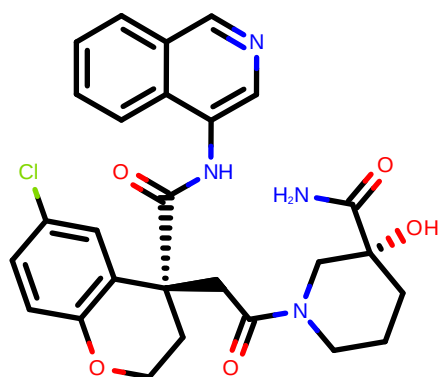
DDG (kcal/mol):

-0.73

dDDG (kcal/mol):

0.30

EN300-210553_1_1



CID:

EN300-210553_1_1

SMILES:

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

RUN:

RUN1490

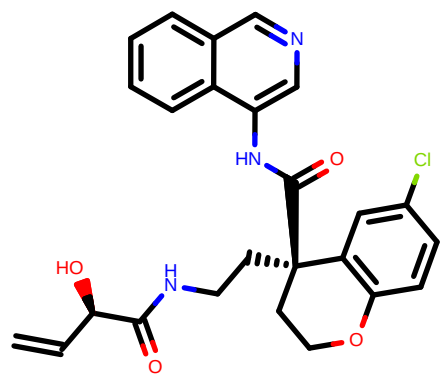
DDG (kcal/mol):

-0.72

dDDG (kcal/mol):

0.46

EN300-181492_3_2



CID:

EN300-181492_3_2

SMILES:

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

RUN:

RUN1713

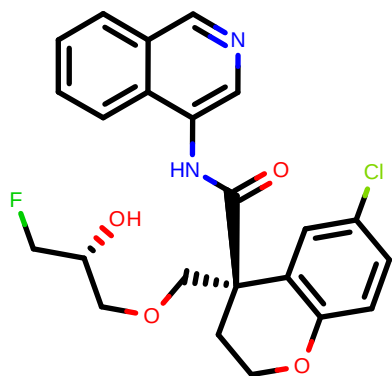
DDG (kcal/mol):

-0.72

dDDG (kcal/mol):

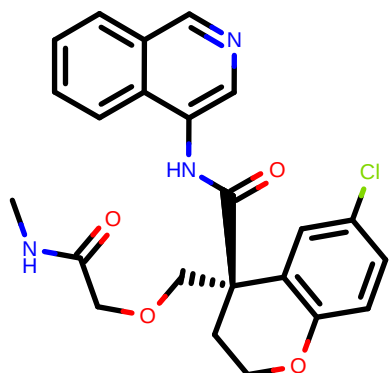
0.32

EN300-1968342_2_2



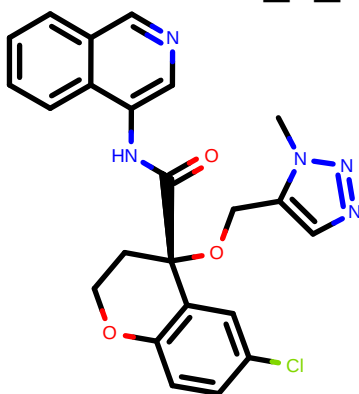
CID:	EN300-1968342_2_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O</chem>
RUN:	RUN507
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.35

EN300-2977549_2_1



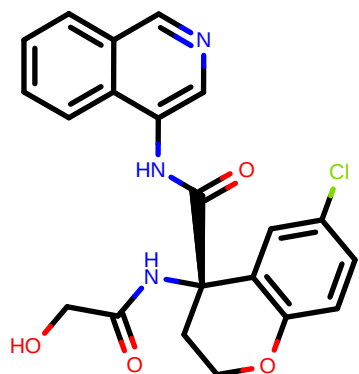
CID:	EN300-2977549_2_1
SMILES:	<chem>CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN1062
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.25

EN300-216673_1_1



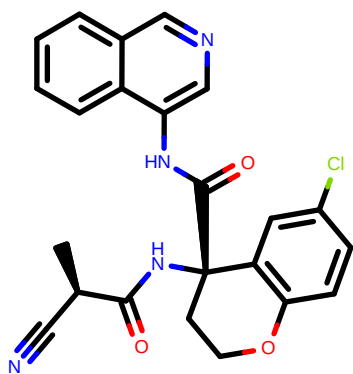
CID:	EN300-216673_1_1
SMILES:	<chem>Cn1c(cnn1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN564
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.25

EN300-19242_1_1



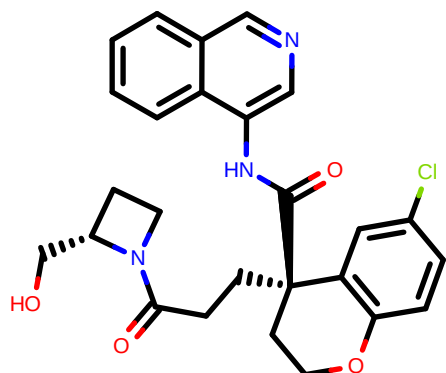
CID:	EN300-19242_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO</chem>
RUN:	RUN1780
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.26

EN300-72730_1_2



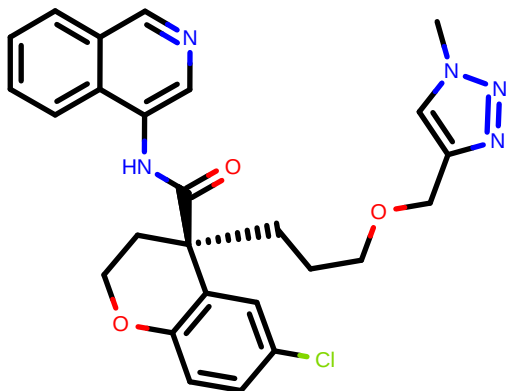
CID:	EN300-72730_1_2
SMILES:	<chem>C[C@H](C#N)C(=O)N[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4</chem>
RUN:	RUN1261
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.22

EN300-154332_2_2



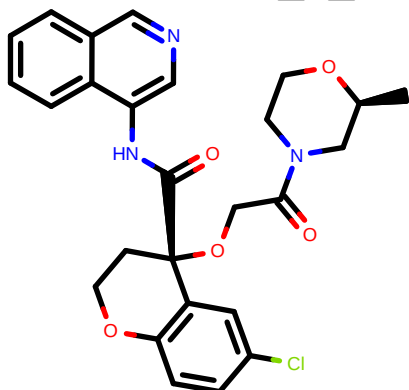
CID:	EN300-154332_2_2
SMILES:	<chem>c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@H]5CO</chem>
RUN:	RUN559
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.28

EN300-120282_4_1



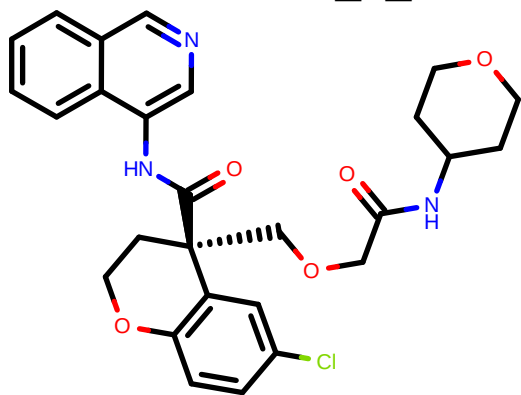
CID:	EN300-120282_4_1
SMILES:	<chem>Cn1cc(nn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN356
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.28

EN300-25572_1_2



CID:	EN300-25572_1_2
SMILES:	<chem>C[C@H]1CN(CCO1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN604
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.24

EN300-67573_2_1



CID: EN300-67573_2_1

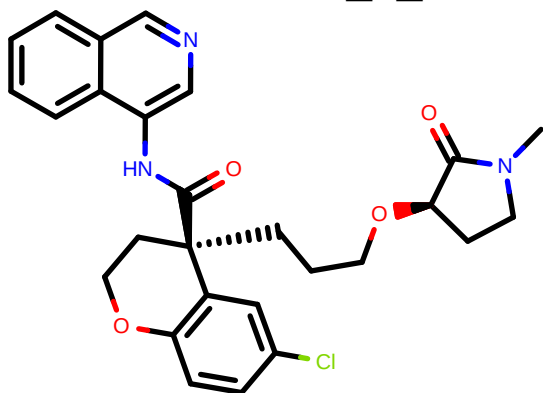
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)NC5CCOC5

RUN: RUN626

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.28

EN300-98648_4_2



CID: EN300-98648_4_2

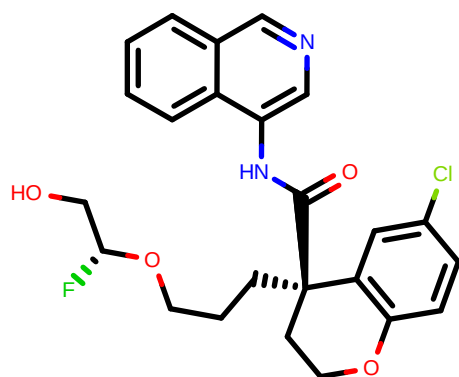
SMILES: CN1CC[C@H](C1=O)OCCC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ncc5c4cccs5

RUN: RUN1686

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

EN300-861925_4_1



CID: EN300-861925_4_1

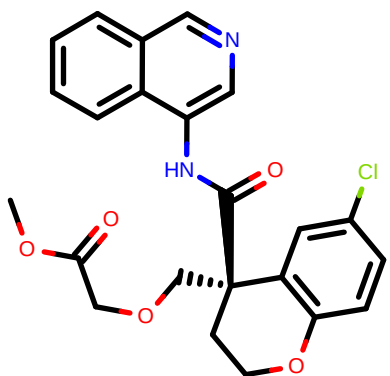
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCO[C@H](CO)F

RUN: RUN753

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.48

EN300-19700_2_1



CID: EN300-19700_2_1

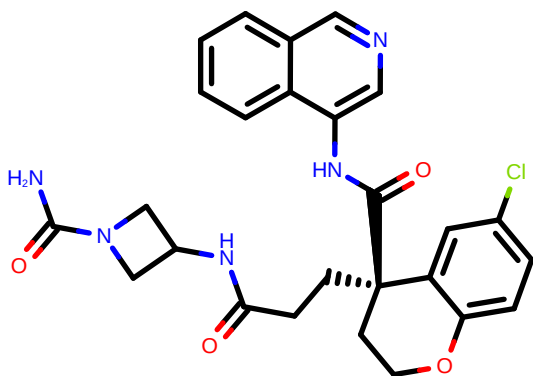
SMILES: COC(=O)COC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN1406

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.21

EN300-6472847_2_1



CID: EN300-6472847_2_1

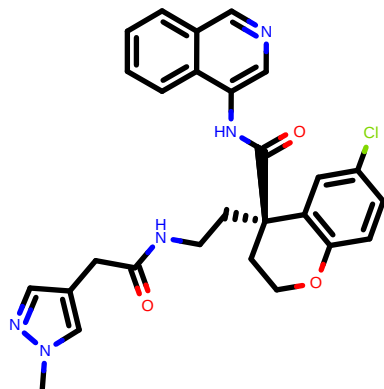
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5CN(C5)C(=O)N

RUN: RUN663

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.32

EN300-63872_3_1



CID: EN300-63872_3_1

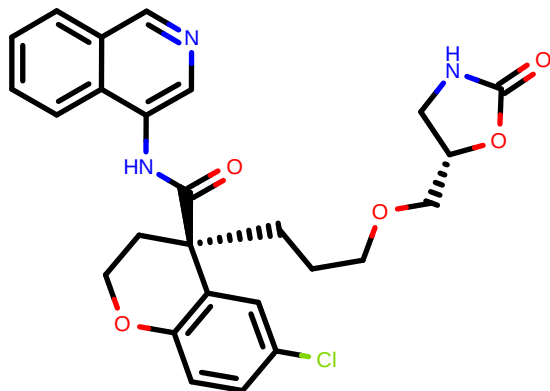
SMILES: Cn1cc(en1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1562

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.34

EN300-203293_4_1



CID: EN300-203293_4_1

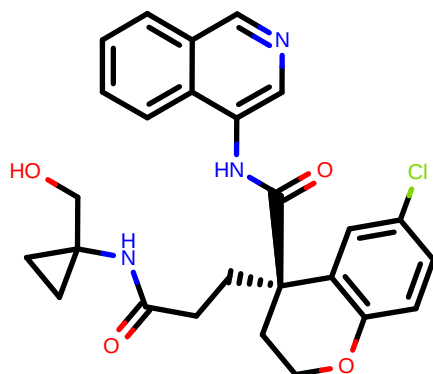
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5CNC(=O)O5

RUN: RUN476

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.47

EN300-117059_2_1



CID: EN300-117059_2_1

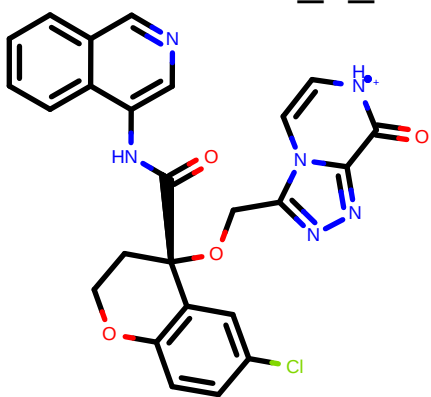
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CC5)CO

RUN: RUN1379

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.29

EN300-378316_1_1



CID: EN300-378316_1_1

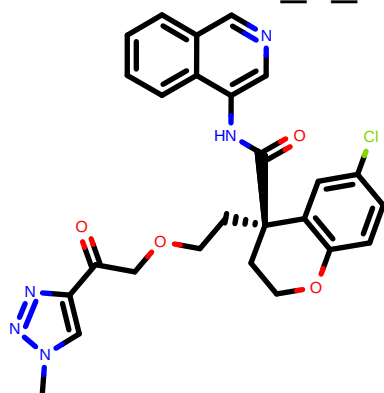
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCc5nnc6n5cc[nH]c6=O

RUN: RUN1160

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.25

EN300-263153_3_1



CID: EN300-263153_3_1

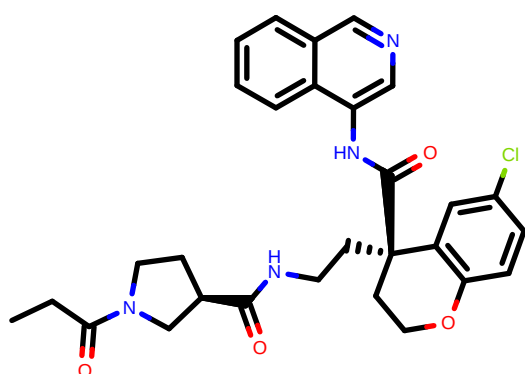
SMILES: Cn1cc(nn1)C(=O)COC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN719

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.31

EN300-114133_3_2



CID: EN300-114133_3_2

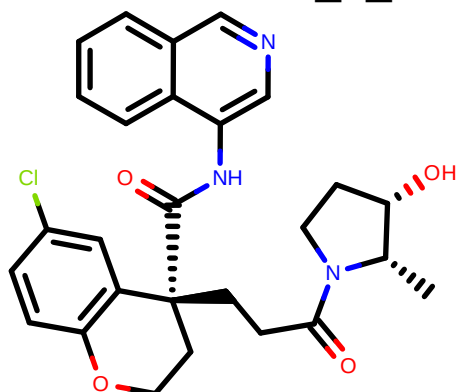
SMILES: CCC(=O)N1CC[C@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN646

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.48

EN300-2008120_2_1



CID: EN300-2008120_2_1

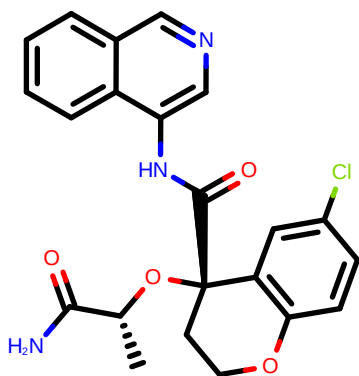
SMILES: C[C@H]1[C@H](CCN1C(=O)CC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4cccc5)O

RUN: RUN1107

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.29

EN300-17381_1_2



CID: EN300-17381_1_2

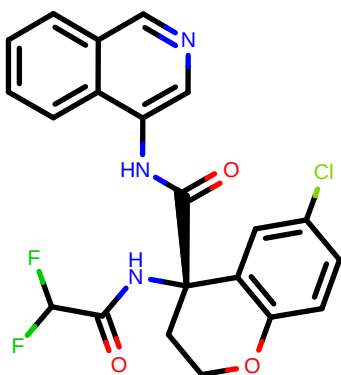
SMILES: C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN817

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.21

EN300-19507_1_1



CID: EN300-19507_1_1

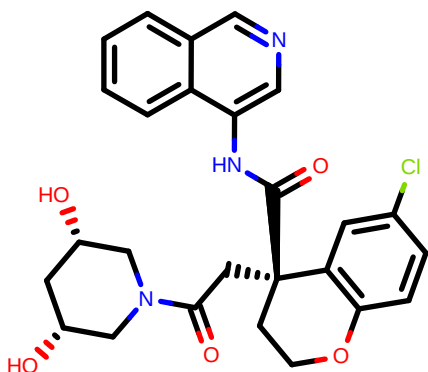
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(F)F

RUN: RUN1237

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.18

EN300-96886_1_1



CID: EN300-96886_1_1

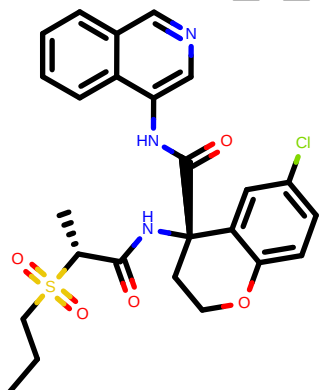
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C)[C@H](C5)O

RUN: RUN1410

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.33

EN300-52768_1_2



CID: EN300-52768_1_2

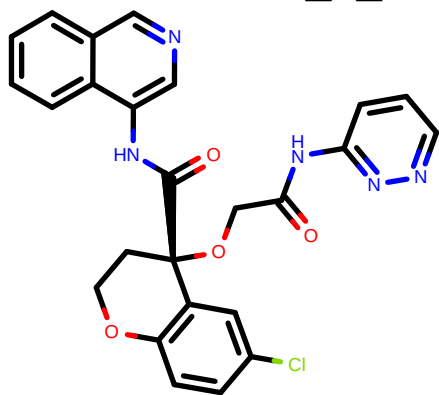
SMILES: CCCS(=O)(=O)[C@H](C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1772

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.54

EN300-761618_1_1



CID: EN300-761618_1_1

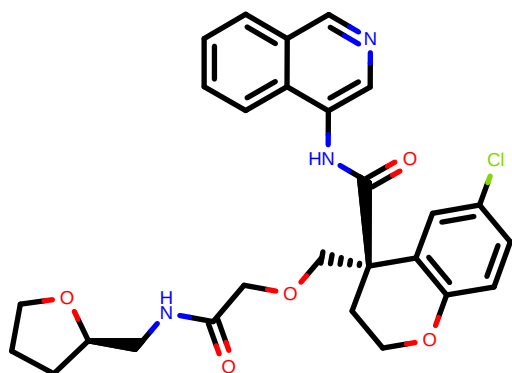
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5cccn5

RUN: RUN1607

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.19

EN300-01527_2_2



CID: EN300-01527_2_2

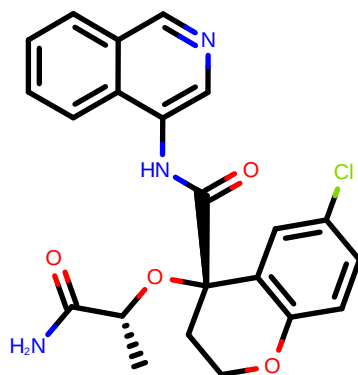
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC[C@H]5CCCCO5

RUN: RUN594

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.35

EN300-17381_1_2



CID: EN300-17381_1_2

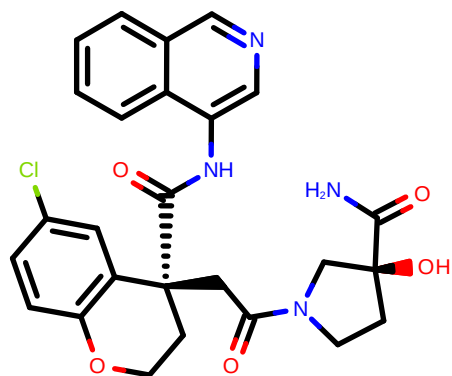
SMILES: C[C@H](C(=O)N)O[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN825

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.23

EN300-172481_1_2



CID: EN300-172481_1_2

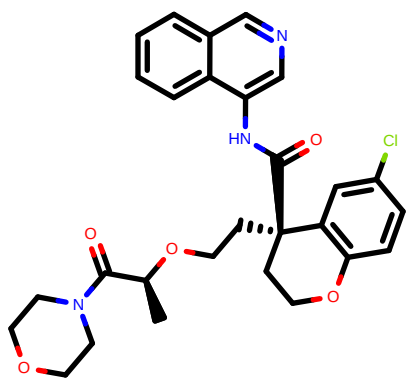
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]5(C5)(C(=O)N)O

RUN: RUN367

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.43

EN300-05754_3_1



CID:

EN300-05754_3_1

SMILES:

C[C@@H](C(=O)N1CCOCC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5

RUN:

RUN956

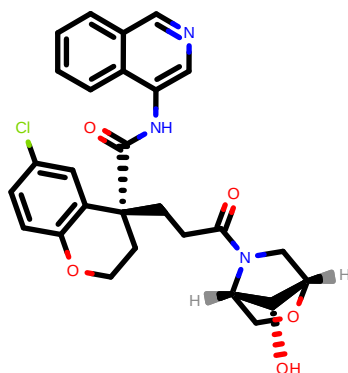
DDG (kcal/mol):

-0.66

dDDG (kcal/mol):

0.41

EN300-6493060_2_1



CID:

EN300-6493060_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C@@H5CO6O

RUN:

RUN1139

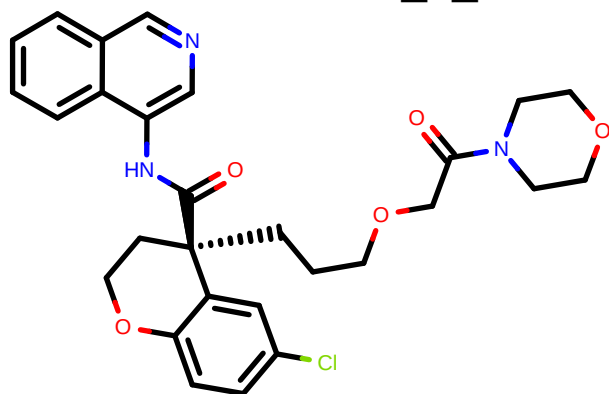
DDG (kcal/mol):

-0.66

dDDG (kcal/mol):

0.23

EN300-1241327_4_1



CID:

EN300-1241327_4_1

SMILES:

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

RUN:

RUN1191

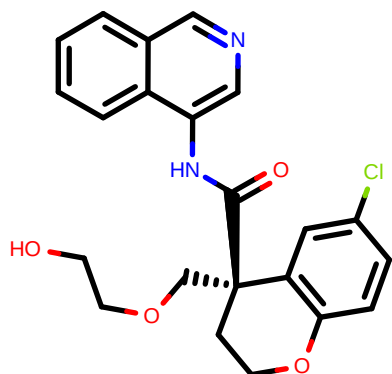
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.31

EN300-21258_2_1



CID:

EN300-21258_2_1

SMILES:

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

RUN:

RUN783

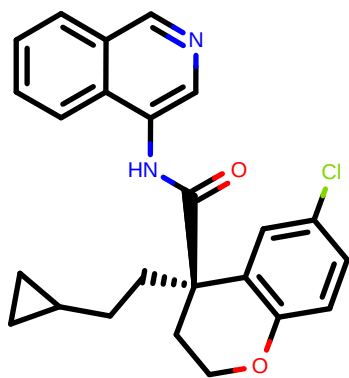
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.22

ALP-POS-477dc5b7-3_1



CID:

ALP-POS-477dc5b7-3_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCC5

RUN:

RUN96

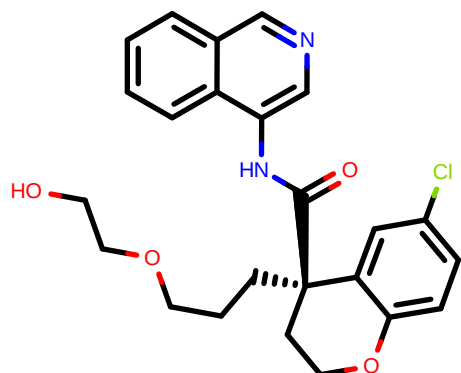
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.23

EN300-21258_4_1



CID:

EN300-21258_4_1

SMILES:

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

RUN:

RUN563

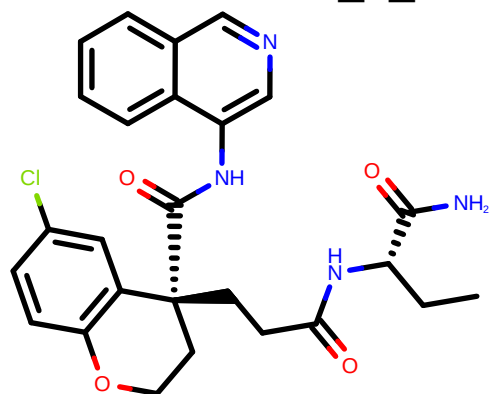
DDG (kcal/mol):

-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)Nc3ncc4c3ccccc4

RUN:

RUN1083

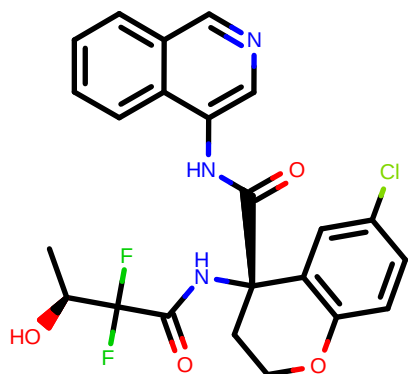
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.29

EN300-185398_1_1



CID:

EN300-185398_1_1

SMILES:

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

RUN:

RUN1437

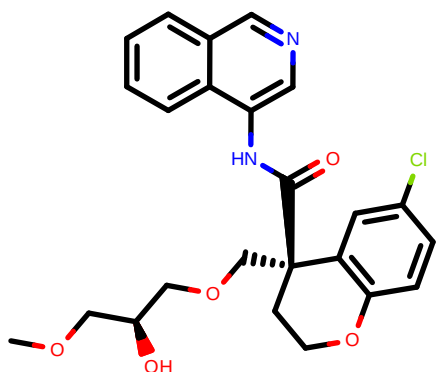
DDG (kcal/mol):

-0.65

dDDG (kcal/mol):

0.23

EN300-1915260_2_1



CID: EN300-1915260_2_1

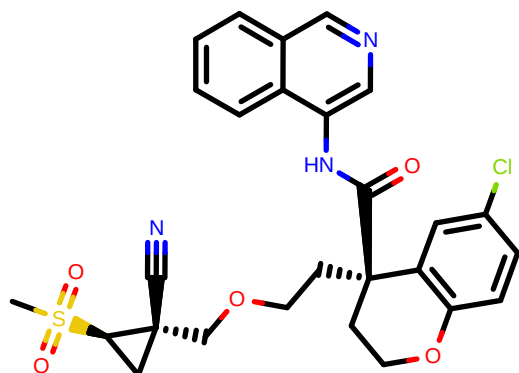
SMILES: COC[C@@H](COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)O

RUN: RUN934

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.40

EN300-633533_3_1



CID: EN300-633533_3_1

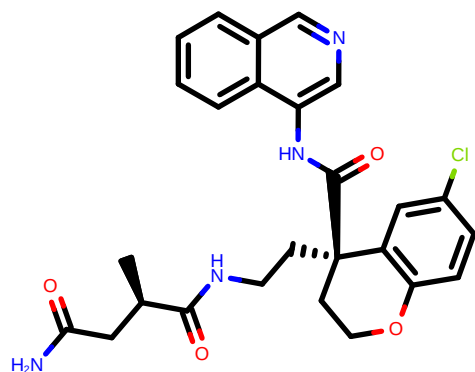
SMILES: CS(=O)(=O)[C@@H](C)[C@]1(C(COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5)C#N

RUN: RUN781

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.47

EN300-202757_3_2



CID: EN300-202757_3_2

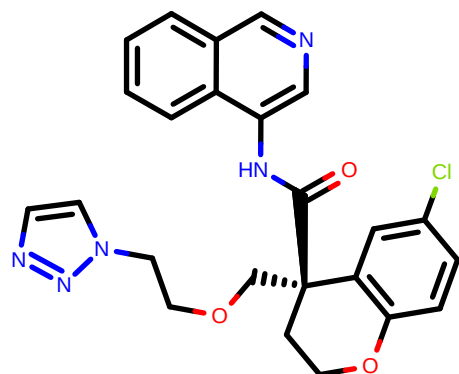
SMILES: C[C@H](CC(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1761

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.49

EN300-1715993_2_1



CID: EN300-1715993_2_1

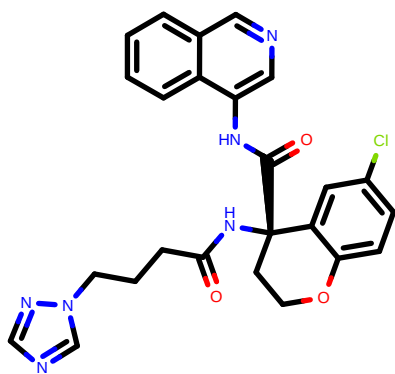
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cnnn5

RUN: RUN1550

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.32

EN300-316216_1_1



CID: EN300-316216_1_1

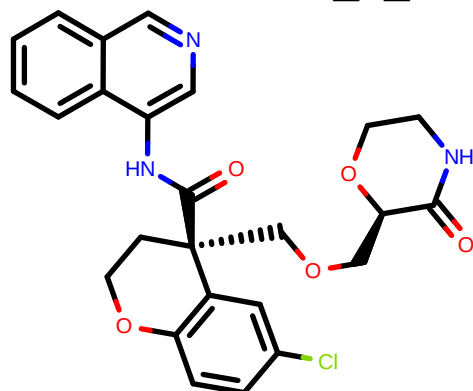
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5

RUN: RUN1748

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.38

EN300-1706036_2_1



CID: EN300-1706036_2_1

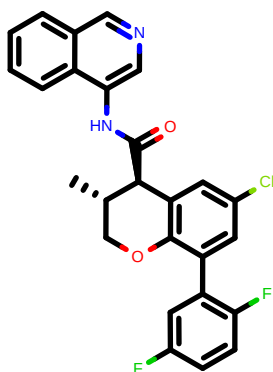
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C(=O)NCCO5

RUN: RUN1022

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.37

DAR-DIA-0d514e7d-15_1



CID: DAR-DIA-0d514e7d-15_1

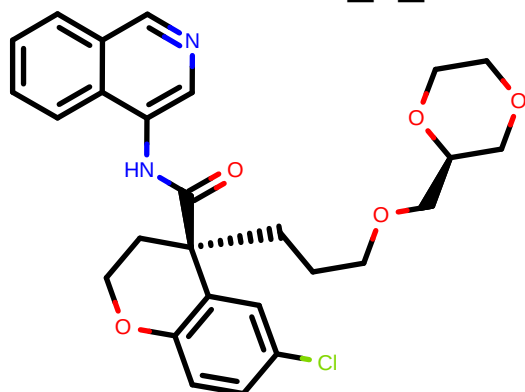
SMILES: C[C@@H]1COC2c(cc(cc2[C@@H]1C(=O)Nc3ncoc4c3ccc4)Cl)c5cc(ccc5)F

RUN: RUN263

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.24

EN300-139167_4_1



CID: EN300-139167_4_1

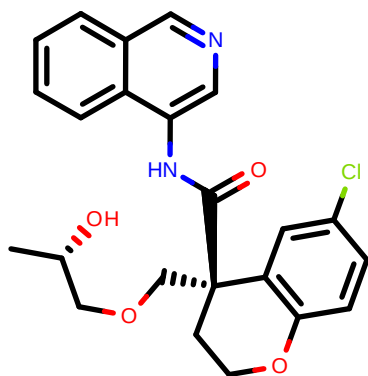
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN523

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.33

EN300-185378_2_1



CID: EN300-185378_2_1

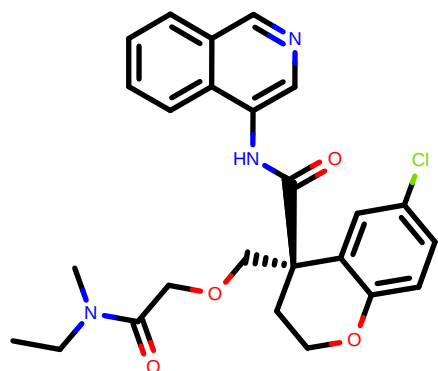
SMILES: C[C@@H](COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN1054

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.25

EN300-1253122_2_1



CID: EN300-1253122_2_1

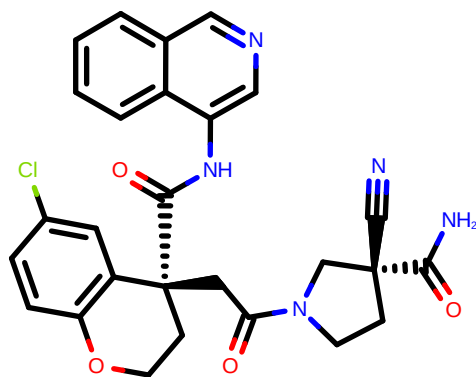
SMILES: CCN(C)C(=O)COC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1446

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

EN300-1608992_1_1



CID: EN300-1608992_1_1

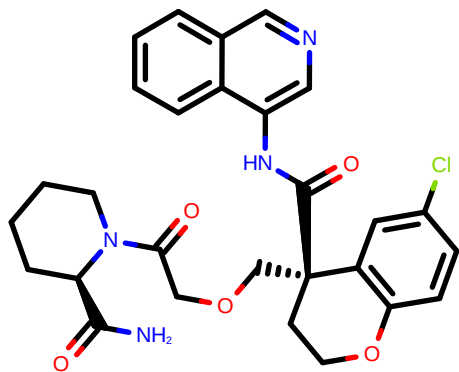
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(C#N)C(=O)N

RUN: RUN463

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.22

EN300-22879_2_1



CID: EN300-22879_2_1

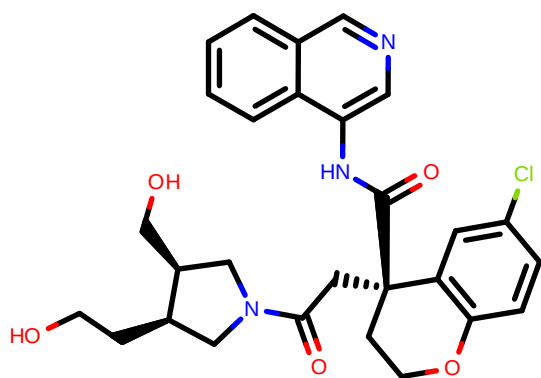
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN752

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.30

EN300-1425608_1_4



CID: EN300-1425608_1_4

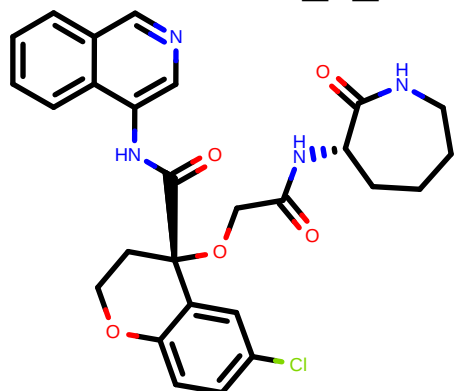
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N[C@@H]3C[C@H](O)C5COCCO

RUN: RUN351

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.42

EN300-37195_1_2



CID: EN300-37195_1_2

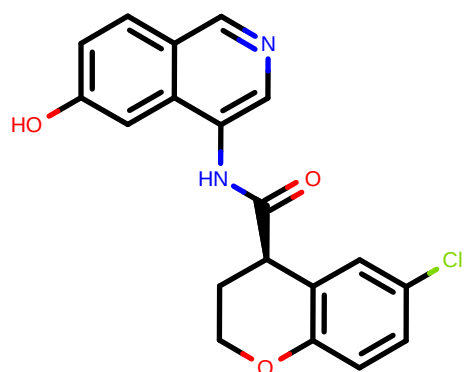
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N[C@@H]3C[C@H](O)C5COCCO

RUN: RUN1232

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

BEN-DND-c852c98b-4_1



CID: BEN-DND-c852c98b-4_1

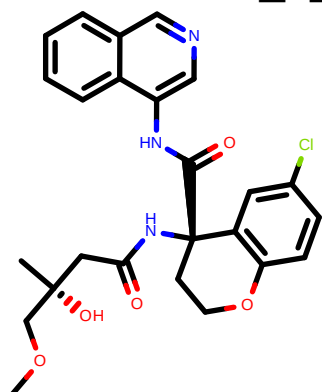
SMILES: c1cc2cncnc(c2cc1O)NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N[C@@H]3C[C@H](O)C5COCCO

RUN: RUN33

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.05

EN300-1296824_1_1



CID: EN300-1296824_1_1

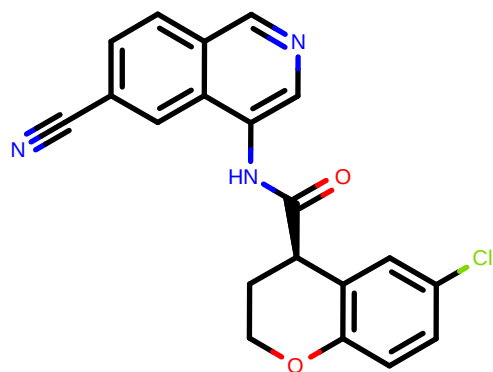
SMILES: C[C@@H](COC(=O)N[C@@H]1[C@@H](COCc2cc1cc2)C(=O)Nc3cnc4c3cc4)(COC)O

RUN: RUN957

DDG (kcal/mol): -0.61

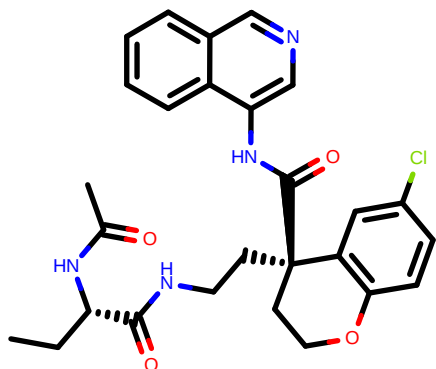
dDDG (kcal/mol): 0.39

BEN-DND-c852c98b-1_1



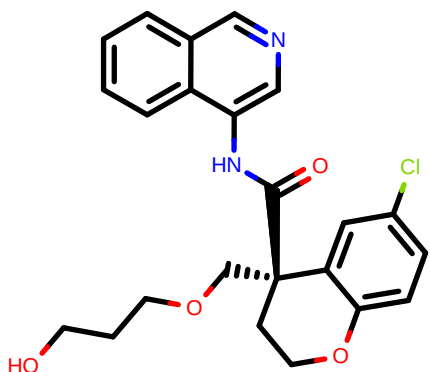
CID:	BEN-DND-c852c98b-1_1
SMILES:	<chem>c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN25
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.04

EN300-332601_3_1



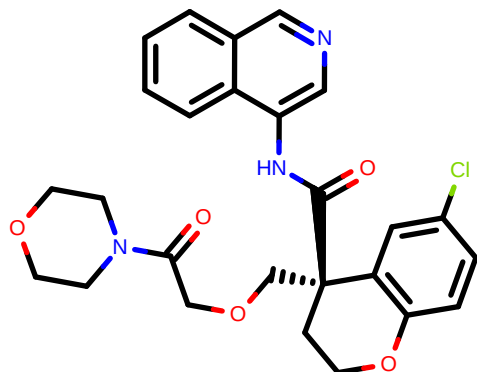
CID:	EN300-332601_3_1
SMILES:	<chem>CC[C@@H](C(=O)NCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc4)NC(=O)C</chem>
RUN:	RUN858
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.33

EN300-221518_2_1



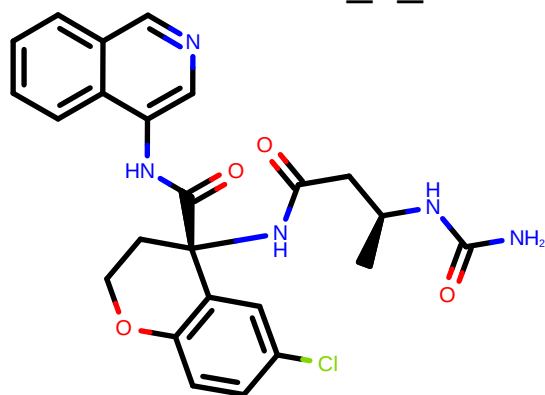
CID:	EN300-221518_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COC(CO)CO</chem>
RUN:	RUN831
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.23

EN300-1241327_2_1



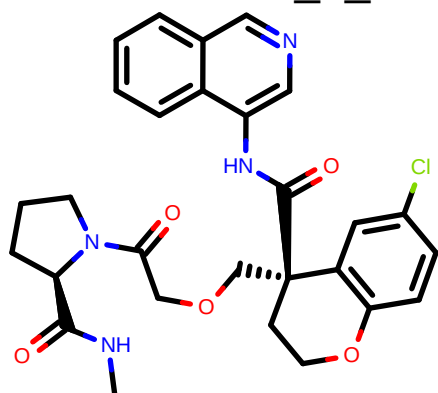
CID:	EN300-1241327_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCOCC5</chem>
RUN:	RUN411
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.42

EN300-268198_1_1



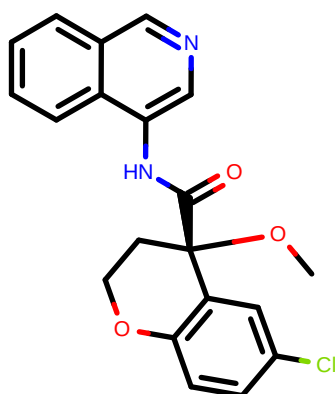
CID:	EN300-268198_1_1
SMILES:	<chem>C[C@@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)NC(=O)N</chem>
RUN:	RUN989
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.22

EN300-48902_2_2



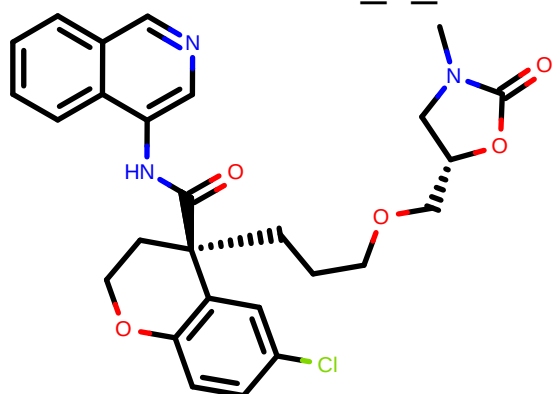
CID:	EN300-48902_2_2
SMILES:	<chem>CNC(=O)[C@H]1CCCN1C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN729
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.43

PET-UNK-29afea89-2_1

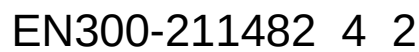
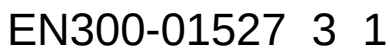
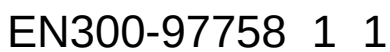


CID:	PET-UNK-29afea89-2_1
SMILES:	<chem>CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4</chem>
RUN:	RUN55
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.13

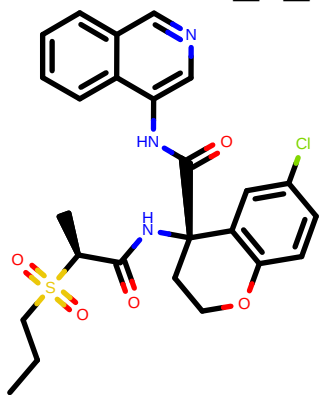
EN300-222969_4_2



CID:	EN300-222969_4_2
SMILES:	<chem>CN1C[C@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN1606
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.48



EN300-52768_1_1



CID:

EN300-52768_1_1

SMILES:

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

RUN:

RUN1612

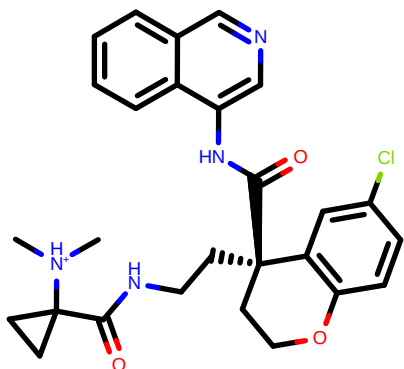
DDG (kcal/mol):

-0.56

dDDG (kcal/mol):

0.46

EN300-248786_3_1



CID:

EN300-248786_3_1

SMILES:

C[NH+](C)C1(CC1)C(=O)NCC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5

RUN:

RUN1641

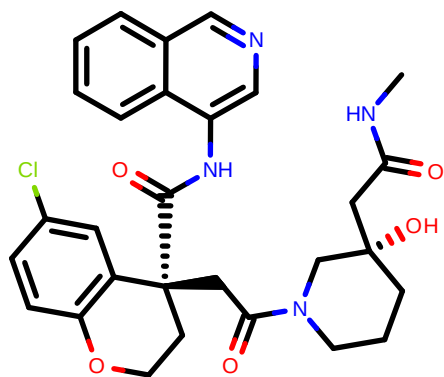
DDG (kcal/mol):

-0.56

dDDG (kcal/mol):

0.40

EN300-259062_1_2



CID:

EN300-259062_1_2

SMILES:

CNC(=O)C[C@H]1(CCCN(C1)C(=O)C[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncoc5c4ccoc5)O

RUN:

RUN1058

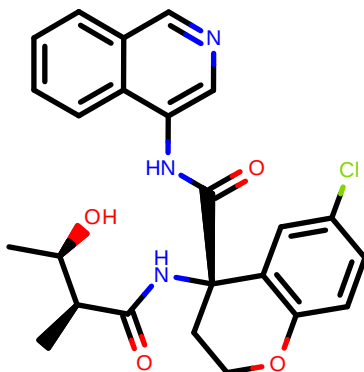
DDG (kcal/mol):

-0.56

dDDG (kcal/mol):

0.34

EN300-7089802_1_1



CID:

EN300-7089802_1_1

SMILES:

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

RUN:

RUN1668

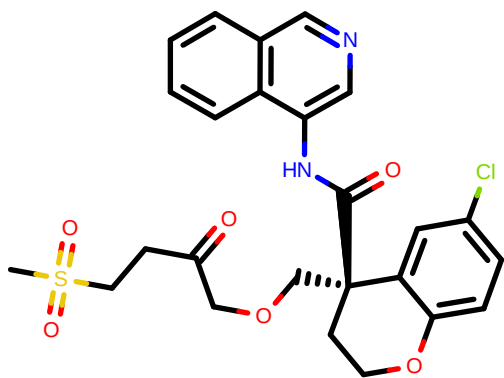
DDG (kcal/mol):

-0.56

dDDG (kcal/mol):

0.30

EN300-1988306_2_1



CID: EN300-1988306_2_1

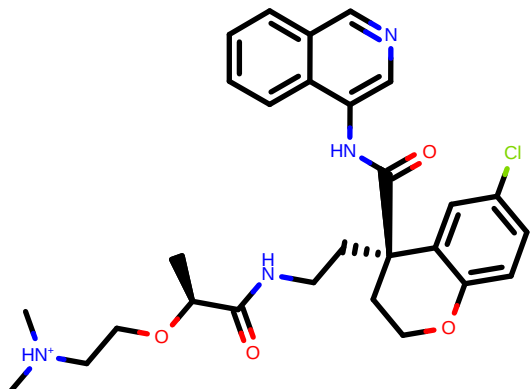
SMILES: CS(=O)(=O)CCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN1605

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.33

EN300-6497863_3_1



CID: EN300-6497863_3_1

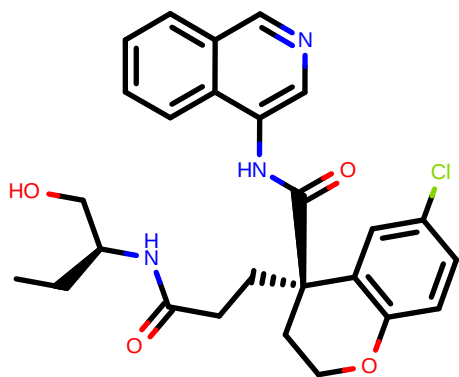
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4)OCC[NH+](C)C

RUN: RUN495

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.70

EN300-19709_2_1



CID: EN300-19709_2_1

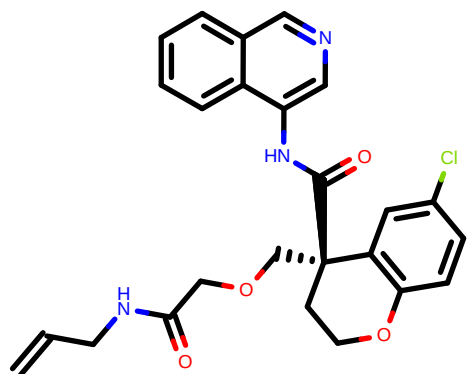
SMILES: CC[C@H](CO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN772

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.32

EN300-17184_2_1



CID: EN300-17184_2_1

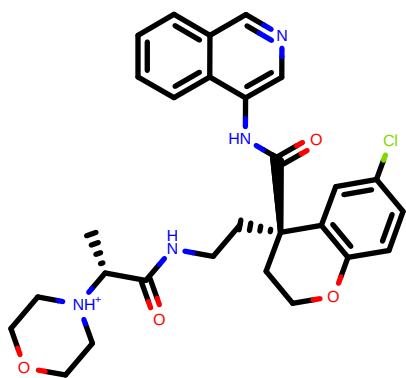
SMILES: C=CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN: RUN315

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.22

EN300-41473_3_2



CID:

EN300-41473_3_2

SMILES:

C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4)[NH+]5CCOCC5

RUN:

RUN962

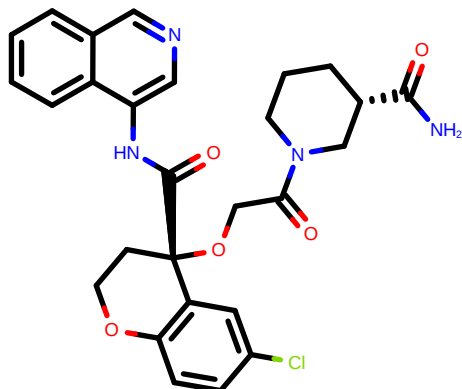
DDG (kcal/mol):

-0.55

dDDG (kcal/mol):

0.38

EN300-22880_1_1



CID:

EN300-22880_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCC[C@H](H)C5C(=O)N

RUN:

RUN1759

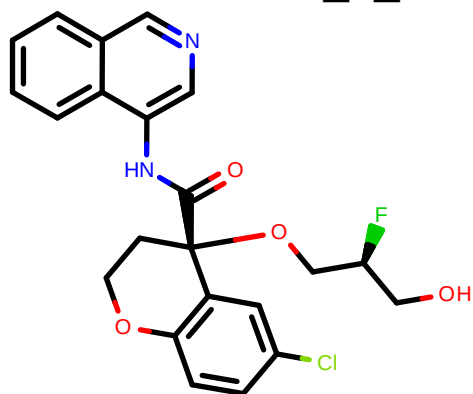
DDG (kcal/mol):

-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)C)OC[C@H](CO)F

RUN:

RUN1208

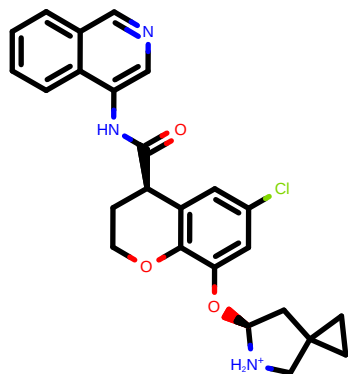
DDG (kcal/mol):

-0.54

dDDG (kcal/mol):

0.26

DAR-DIA-23e5a6a0-4_2



CID:

DAR-DIA-23e5a6a0-4_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4O)[C@H]5CC6(CC6)C[NH2+][5]Cl

RUN:

RUN111

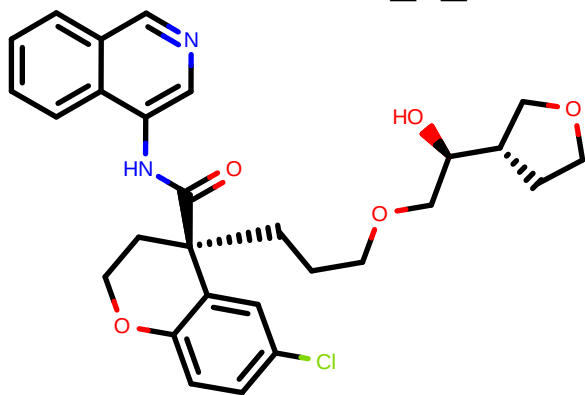
DDG (kcal/mol):

-0.53

dDDG (kcal/mol):

0.36

EN300-1911992_4_4



CID: EN300-1911992_4_4

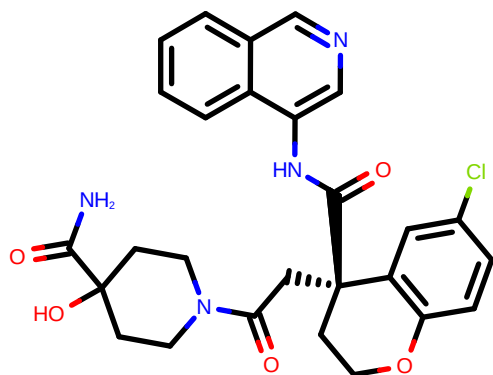
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC@H5CCOC5O

RUN: RUN903

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.39

EN300-203306_1_1



CID: EN300-203306_1_1

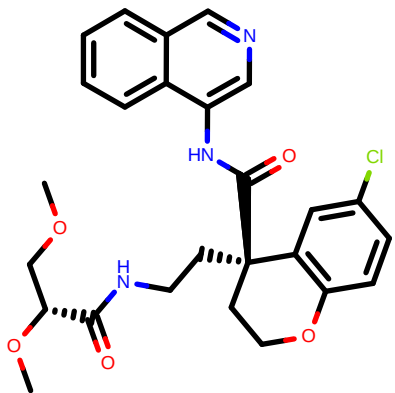
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)(C(=O)N)O

RUN: RUN1290

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.35

EN300-305282_3_2



CID: EN300-305282_3_2

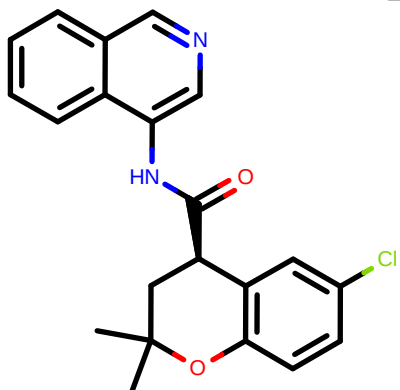
SMILES: COC[C@H](C(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)OC

RUN: RUN1506

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.40

ADA-UCB-dc2b944c-16_1



CID: ADA-UCB-dc2b944c-16_1

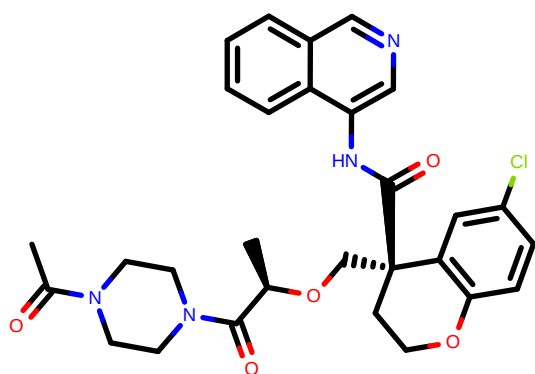
SMILES: CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3cccc4)C

RUN: RUN43

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.10

EN300-28106_2_2



CID: EN300-28106_2_2

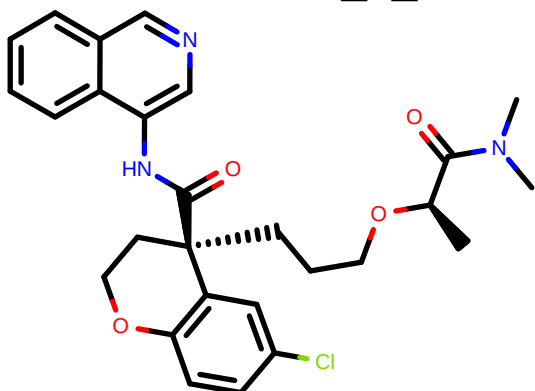
SMILES: C[C@H](C(=O)N1CCN(CC1)C(=O)C)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN1621

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.40

EN300-14458_4_2



CID: EN300-14458_4_2

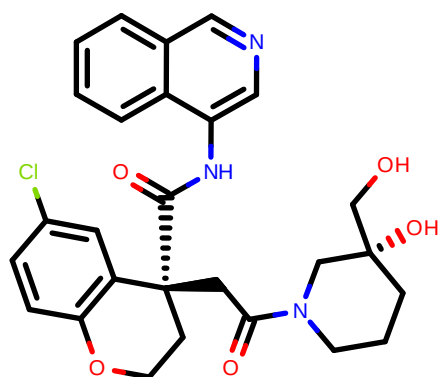
SMILES: C[C@H](C(=O)N(C)C)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cccc4c3cccc4

RUN: RUN316

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

EN300-251396_1_1



CID: EN300-251396_1_1

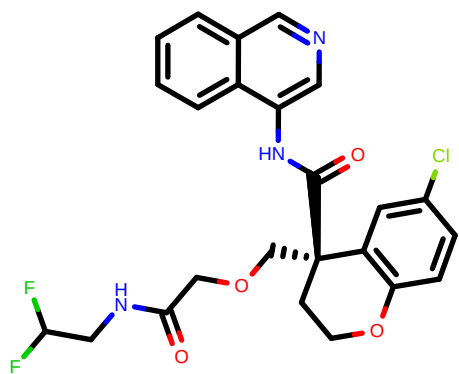
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@]3(C5)(CO)O

RUN: RUN431

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.39

EN300-120586_2_1



CID: EN300-120586_2_1

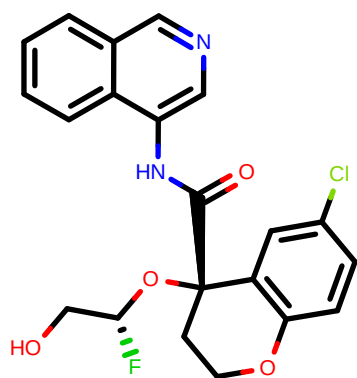
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCC(F)F

RUN: RUN371

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.31

EN300-861925_1_1



CID: EN300-861925_1_1

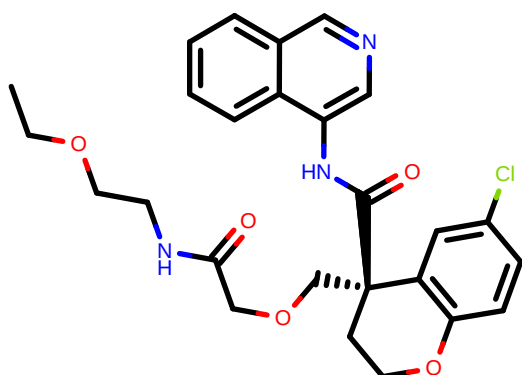
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H](CO)F

RUN: RUN1711

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.28

EN300-103187_2_1



CID: EN300-103187_2_1

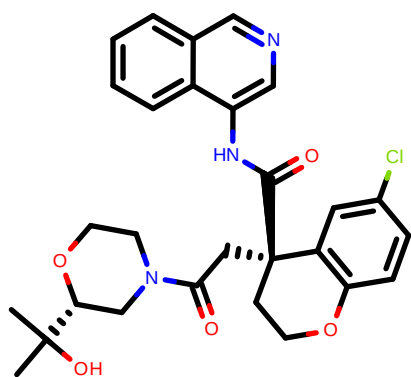
SMILES: CCOCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN586

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.34

EN300-7435544_1_2



CID: EN300-7435544_1_2

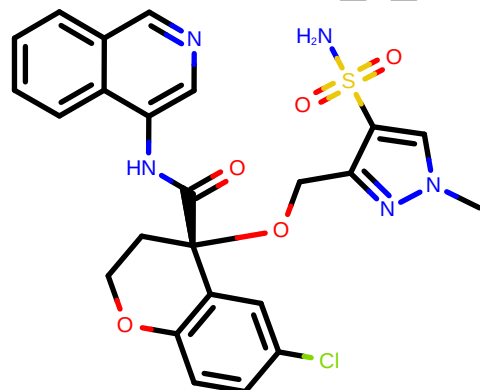
SMILES: CC(C)([C@@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN598

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.26

EN300-7355737_1_1



CID: EN300-7355737_1_1

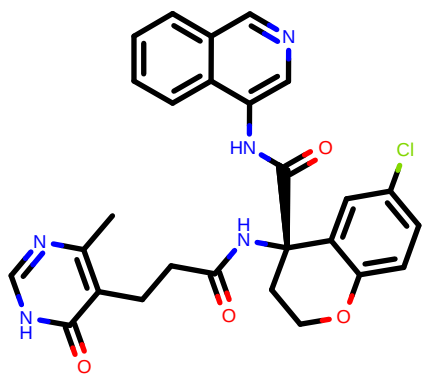
SMILES: Cn1cc(c(n1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)N

RUN: RUN1400

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.29

EN300-33553_1_1



CID: EN300-33553_1_1

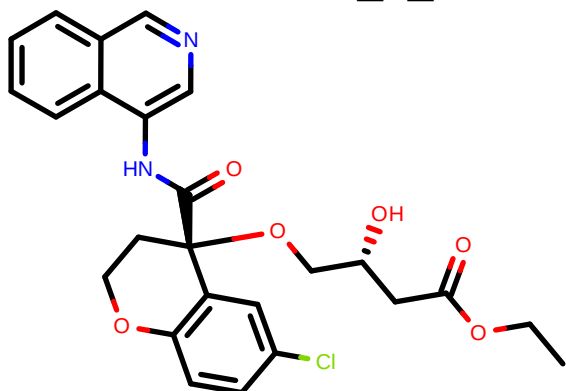
SMILES: Cc1c(c(=O)[nH]cn1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN362

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.28

EN300-82539_1_2



CID: EN300-82539_1_2

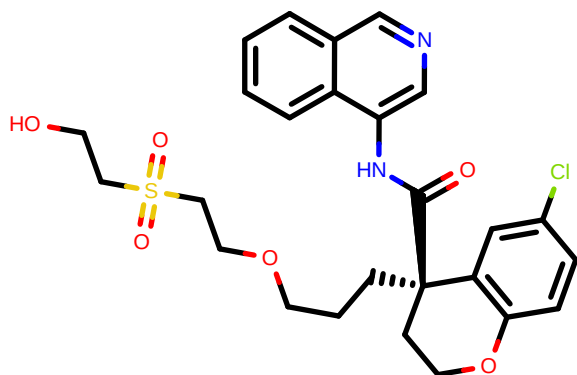
SMILES: CCOC(=O)C[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN960

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.27

EN300-7463171_4_1



CID: EN300-7463171_4_1

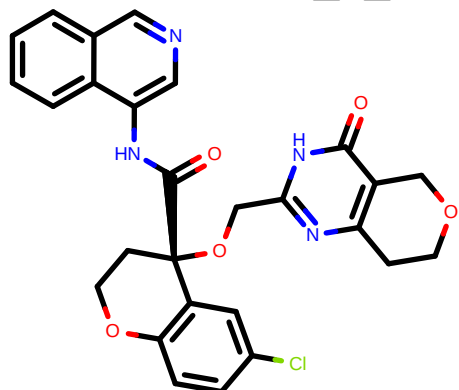
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCS(=O)(=O)CCO

RUN: RUN1535

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.71

EN300-343103_1_1



CID: EN300-343103_1_1

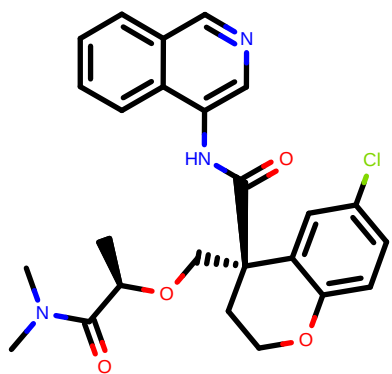
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5[nH]c(=O)c6c(n5)CCOC6

RUN: RUN1376

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.23

EN300-14458_2_2



CID: EN300-14458_2_2

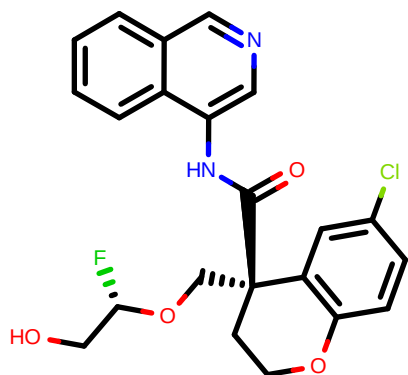
SMILES: C[C@H](C(=O)N(C)C)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN1510

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.30

EN300-861925_2_2



CID: EN300-861925_2_2

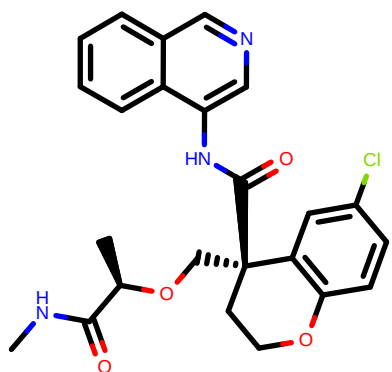
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H](CO)F

RUN: RUN737

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.25

EN300-211482_2_2



CID: EN300-211482_2_2

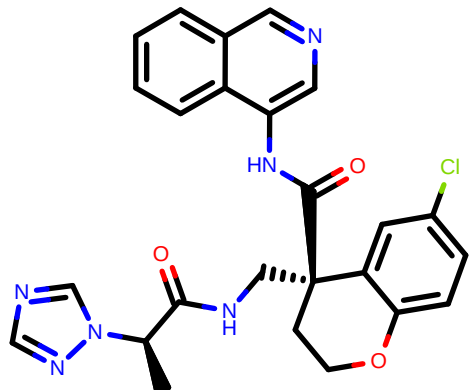
SMILES: C[C@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4

RUN: RUN1542

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.43

EN300-30397_2_2



CID: EN300-30397_2_2

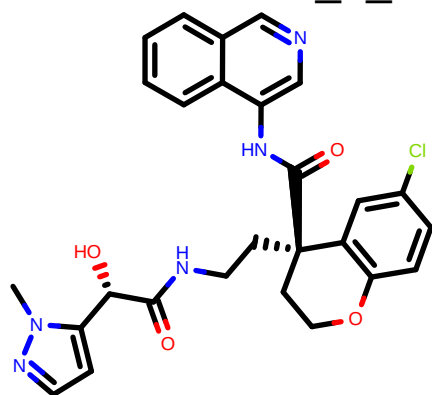
SMILES: C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccc4)n5cnfn5

RUN: RUN1553

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.24

EN300-6473273_3_1



CID: EN300-6473273_3_1

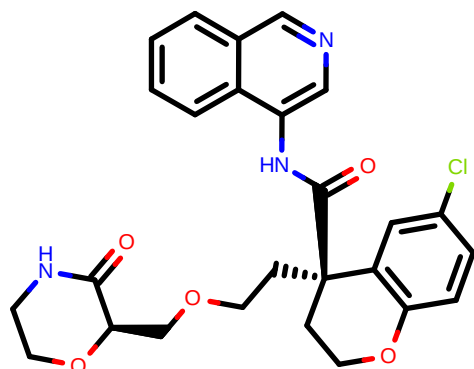
SMILES: Cn1c(ccn1)[C@@H](C(=O)NCC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccoc5)O

RUN: RUN1697

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.41

EN300-1706036_3_1



CID: EN300-1706036_3_1

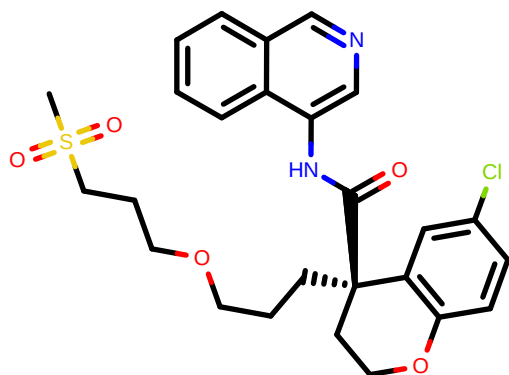
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C(=O)NCCO5

RUN: RUN1028

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.32

EN300-68794_4_1



CID: EN300-68794_4_1

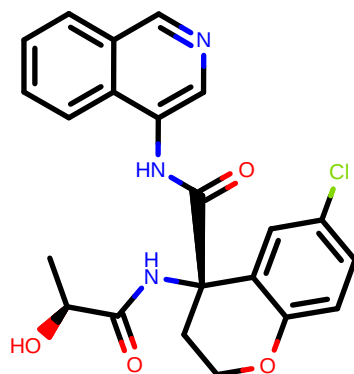
SMILES: CS(=O)(=O)CCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1503

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.36

EN300-91905_1_1



CID: EN300-91905_1_1

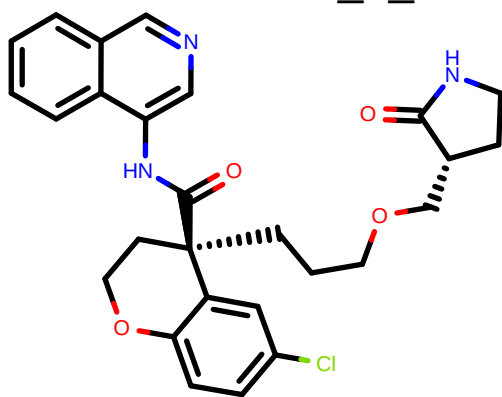
SMILES: C[C@@H](C(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)O

RUN: RUN1221

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.23

EN300-246248_4_2



CID: EN300-246248_4_2

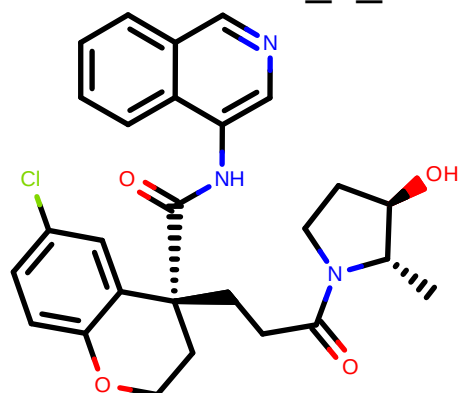
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CCCOC[C@H]5CCNCS=O

RUN: RUN800

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.46

EN300-245036_2_1



CID: EN300-245036_2_1

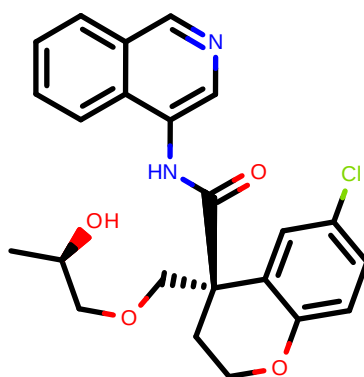
SMILES: C[C@H]1[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN955

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-185378_2_2



CID: EN300-185378_2_2

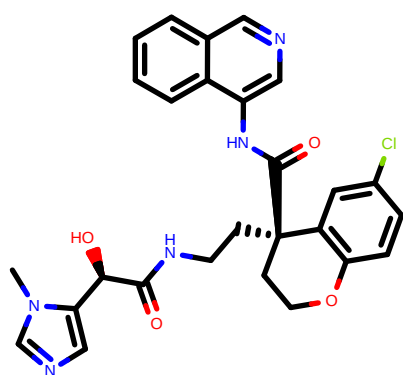
SMILES: C[C@H](COC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)O

RUN: RUN846

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-190283_3_2



CID: EN300-190283_3_2

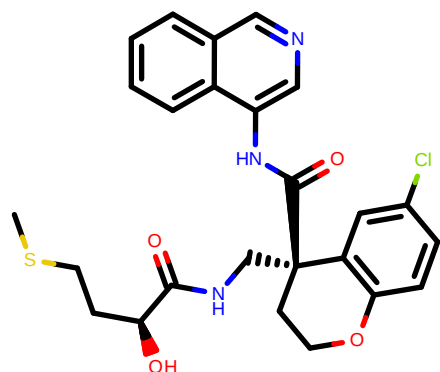
SMILES: Cn1cncc1[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5)O

RUN: RUN771

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.52

EN300-103144_2_1



CID: EN300-103144_2_1

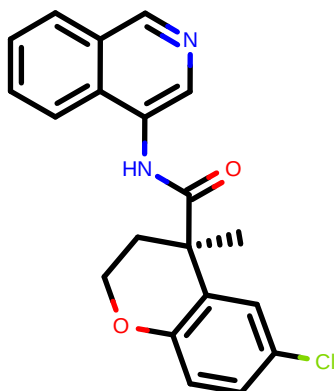
SMILES: CSCC[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4)O

RUN: RUN770

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.35

EDJ-MED-e4b030d8-13_1



CID: EDJ-MED-e4b030d8-13_1

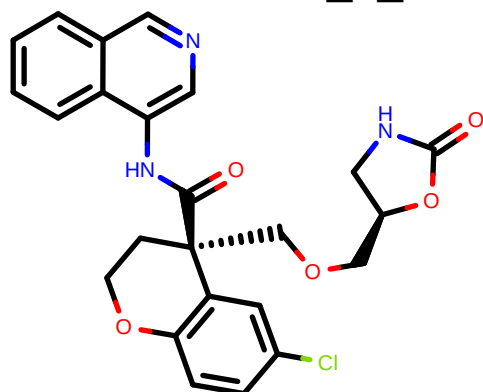
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN8

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.11

EN300-203293_2_2



CID: EN300-203293_2_2

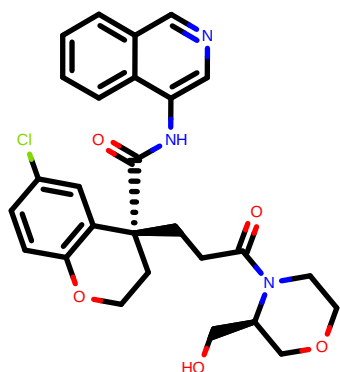
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CNC(=O)O5

RUN: RUN1637

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-154201_2_2



CID: EN300-154201_2_2

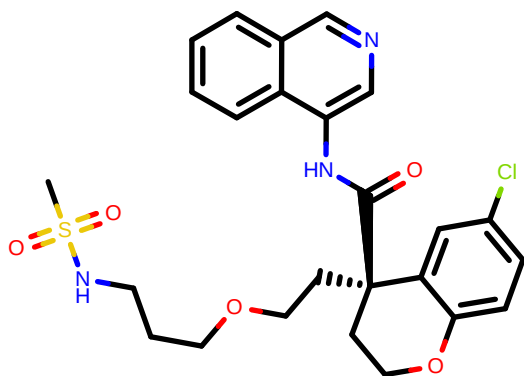
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@H]5CO

RUN: RUN1235

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-45485_3_1



CID: EN300-45485_3_1

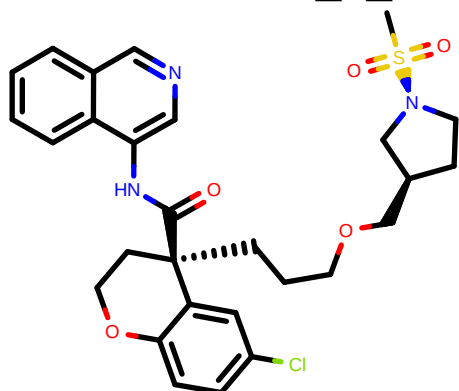
SMILES: CS(=O)(=O)NCCCOC[C@]1(C)C(=O)C2C1CC(C(=O)Nc3nccc4c3ccccc4

RUN: RUN353

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.41

EN300-261986_4_2



CID: EN300-261986_4_2

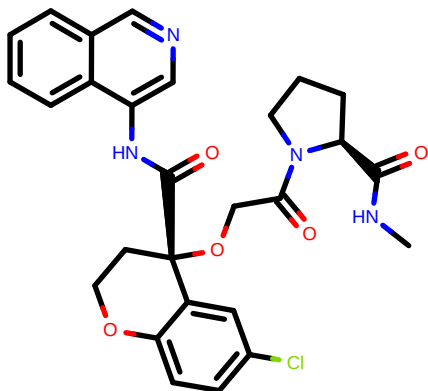
SMILES: CS(=O)(=O)N[C@]1(C)C[C@H](C1)C(=O)C[C@]2(C)C(=O)C3C2CC(C(=O)Nc4nccc5c4ccccc5

RUN: RUN1287

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.46

EN300-48902_1_1



CID: EN300-48902_1_1

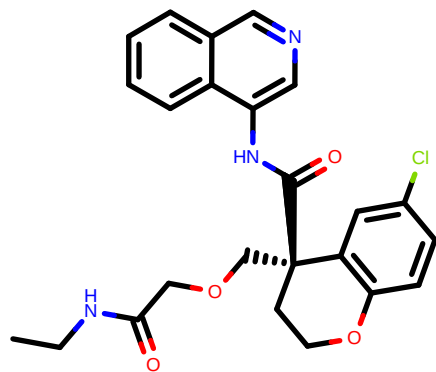
SMILES: CNC(=O)[C@]1(C)C[C@H](C1)C(=O)C[C@]2(C)C(=O)C3C2CC(C(=O)Nc4nccc5c4ccccc5

RUN: RUN365

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.27

EN300-7003350_2_1



CID: EN300-7003350_2_1

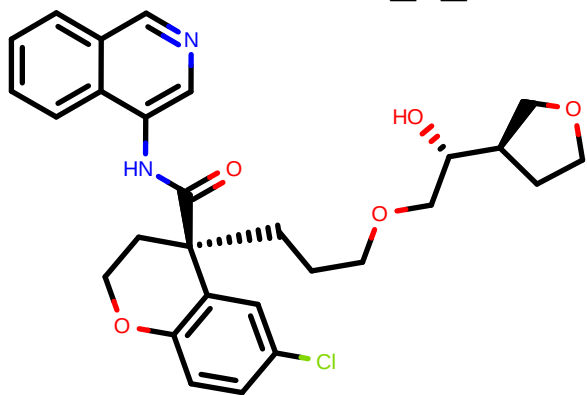
SMILES: CCNC(=O)COC[C@]1(C)C(=O)C2C1CC(C(=O)Nc3nccc4c3ccccc4

RUN: RUN958

DDG (kcal/mol): -0.46

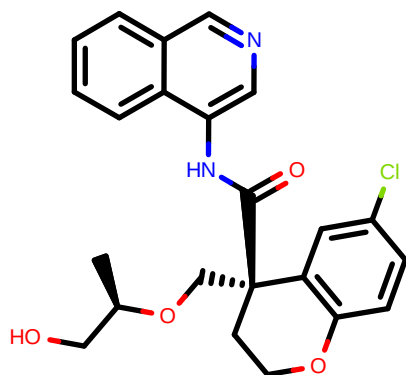
dDDG (kcal/mol): 0.26

EN300-1911992_4_1



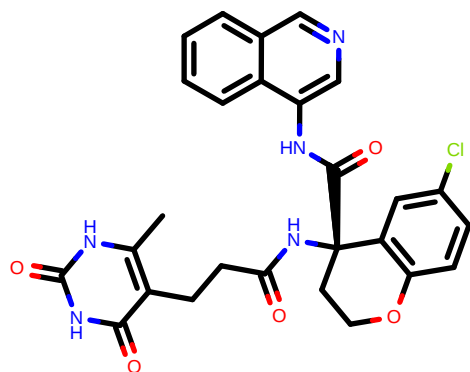
CID:	EN300-1911992_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]([C@@H]5CCOC5)O</chem>
RUN:	RUN832
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.32

EN300-175186_2_2



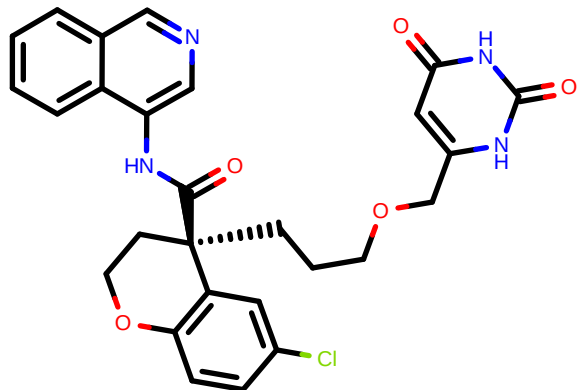
CID:	EN300-175186_2_2
SMILES:	<chem>C[C@H]([CO])OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN1390
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.27

EN300-25735_1_1



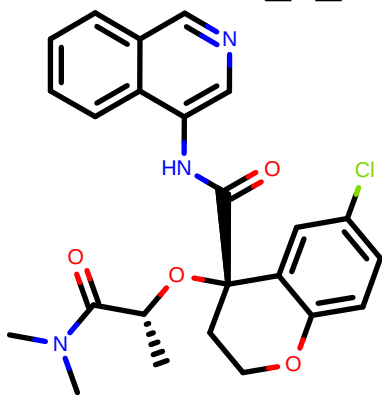
CID:	EN300-25735_1_1
SMILES:	<chem>Cc1c(c(=O)[nH]c(=O)[nH]1)CCC(=O)N[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN290
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.27

EN300-11300_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

EN300-14458_1_2



CID: EN300-14458_1_2

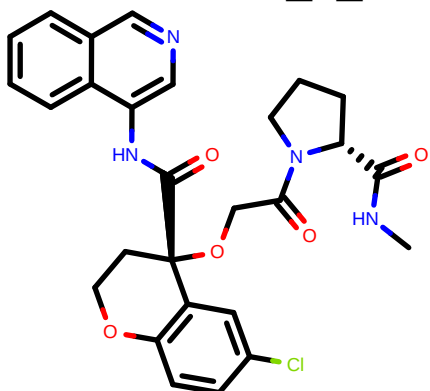
SMILES: C[C@H](C(=O)N(C)C)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1384

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.19

EN300-48902_1_2



CID: EN300-48902_1_2

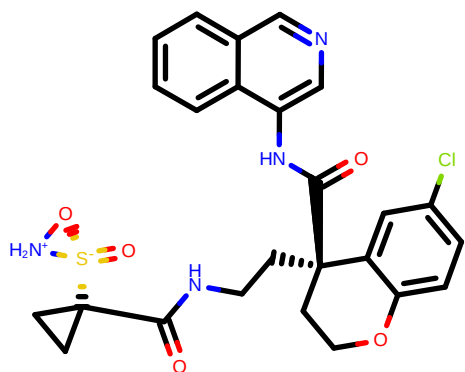
SMILES: CNC(=O)[C@H]1CCCN1C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1544

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.30

EN300-223741_3_1



CID: EN300-223741_3_1

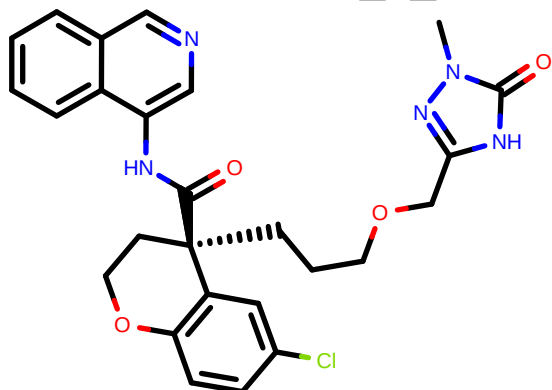
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(S(=O)(=O)N

RUN: RUN1346

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.38

EN300-124918_4_1



CID: EN300-124918_4_1

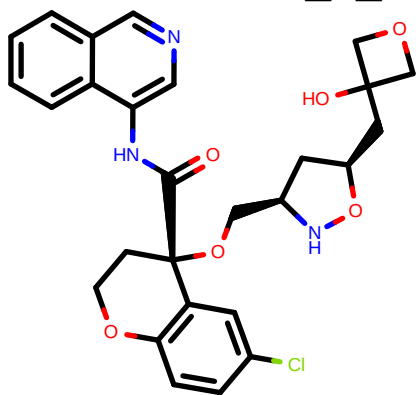
SMILES: Cn1c(=O)[nH]c(n1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN959

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.42

EN300-7457160_1_1



CID:

EN300-7457160_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NO[C@H](C5)CC6(COC6)O

RUN:

RUN1496

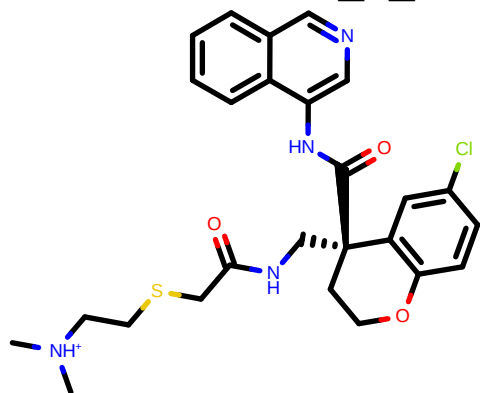
DDG (kcal/mol):

-0.44

dDDG (kcal/mol):

0.30

EN300-1708620_2_1



CID:

EN300-1708620_2_1

SMILES:

C[NH+](C)CCSCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN:

RUN1153

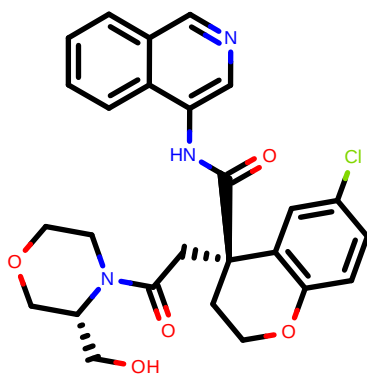
DDG (kcal/mol):

-0.44

dDDG (kcal/mol):

0.35

EN300-154201_1_2



CID:

EN300-154201_1_2

SMILES:

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

RUN:

RUN1194

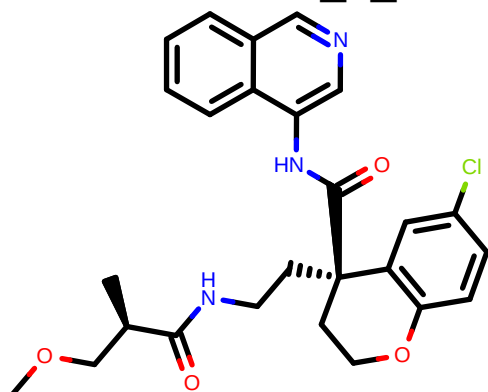
DDG (kcal/mol):

-0.44

dDDG (kcal/mol):

0.32

EN300-69162_3_2



CID:

EN300-69162_3_2

SMILES:

C[C@H](COC)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN:

RUN1585

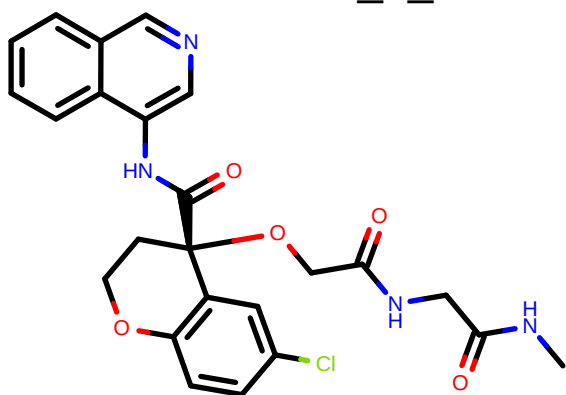
DDG (kcal/mol):

-0.44

dDDG (kcal/mol):

0.39

EN300-23223_1_1



CID: EN300-23223_1_1

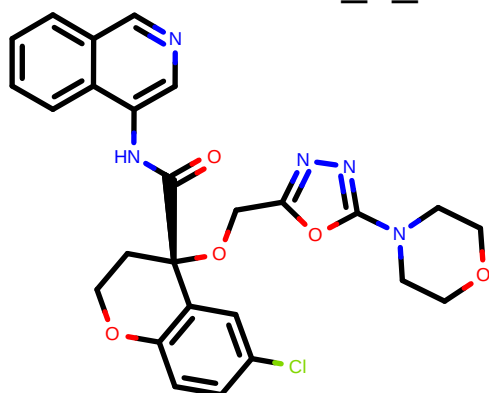
SMILES: CNC(=O)CNC(=O)CO[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN1152

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-6486576_1_1



CID: EN300-6486576_1_1

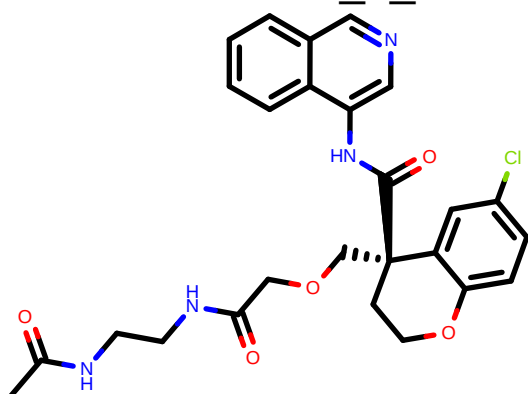
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@]3(COC4c3cc(cc4)Cl)OC5nnc(o5)N6CCOCC6

RUN: RUN1488

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.30

EN300-23129_2_1



CID: EN300-23129_2_1

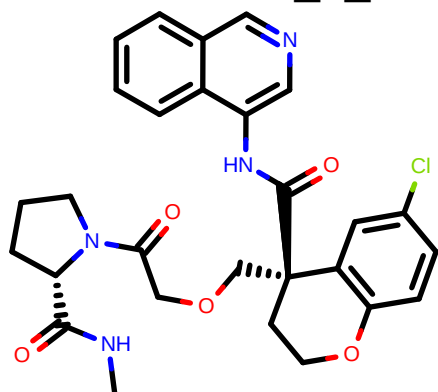
SMILES: CC(=O)NCCNC(=O)COC[C@]1(COC2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN363

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.38

EN300-48902_2_1



CID: EN300-48902_2_1

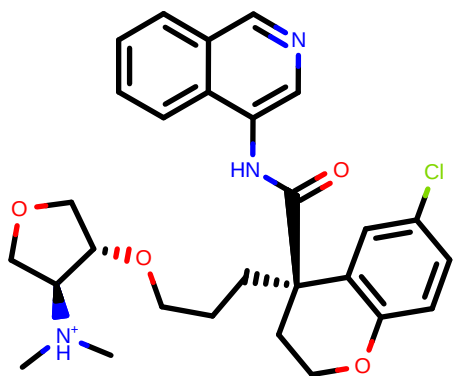
SMILES: CNC(=O)[C@]3(C)[C@@H]1CCCN1C(=O)COC[C@]2(COC3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN697

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.37

EN300-2723070_4_2



CID: EN300-2723070_4_2

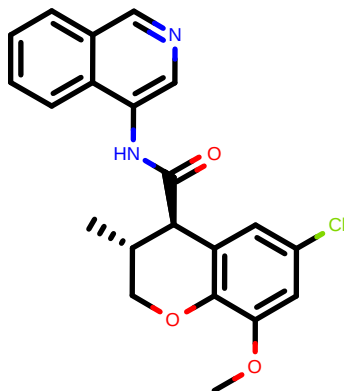
SMILES: C[NH+](C)[C@H]1COC[C@H]1OCCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1654

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.55

DAR-DIA-0d514e7d-1_1



CID: DAR-DIA-0d514e7d-1_1

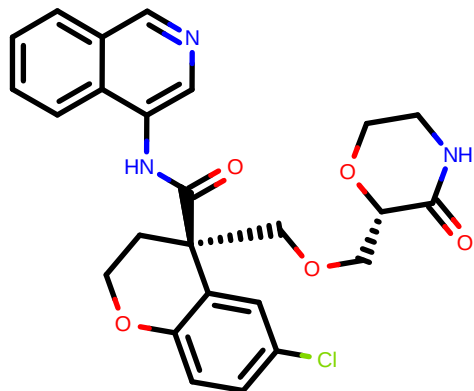
SMILES: C[C@H]1COC2c(cc(cc2OC)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4

RUN: RUN79

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.13

EN300-1706036_2_2



CID: EN300-1706036_2_2

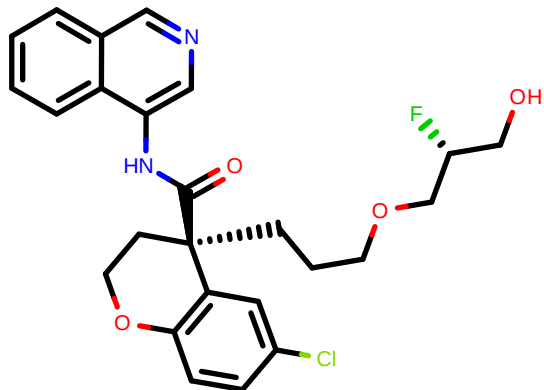
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C(=O)NCCO5

RUN: RUN1645

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.38

EN300-1600517_4_1



CID: EN300-1600517_4_1

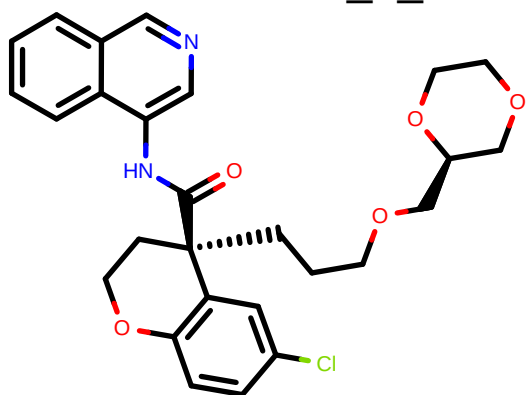
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H](CO)F

RUN: RUN706

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.46

EN300-139167_4_1



CID:

EN300-139167_4_1

SMILES:

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

RUN:

RUN508

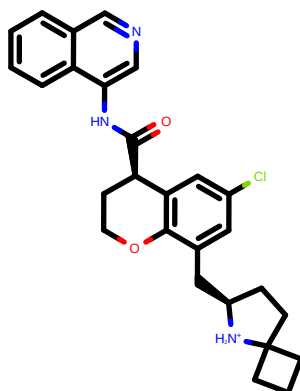
DDG (kcal/mol):

-0.43

dDDG (kcal/mol):

0.45

DAR-DIA-23e5a6a0-6_2



CID:

DAR-DIA-23e5a6a0-6_2

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)C[C@H]5CCCC6([NH2+][5])COC6)Cl

RUN:

RUN133

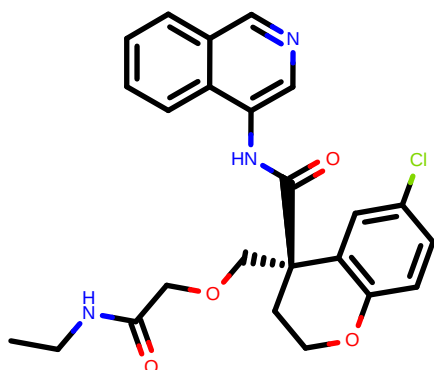
DDG (kcal/mol):

-0.42

dDDG (kcal/mol):

0.40

EN300-7003350_2_1



CID:

EN300-7003350_2_1

SMILES:

CCNC(=O)COC[C@@H]1(CCOc2c1cc(cc2Cl)C(=O)Nc3ncc4c3ccccc4

RUN:

RUN942

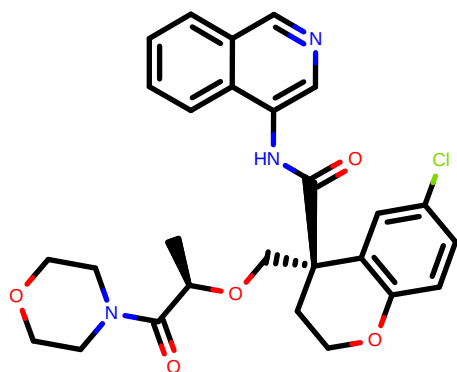
DDG (kcal/mol):

-0.42

dDDG (kcal/mol):

0.22

EN300-05754_2_2



CID:

EN300-05754_2_2

SMILES:

C[C@H](C(=O)N1CCOCC1)OC[C@@H]2(CCOc3c2cc(cc3Cl)C(=O)Nc4ncc5c4ccccc5

RUN:

RUN1757

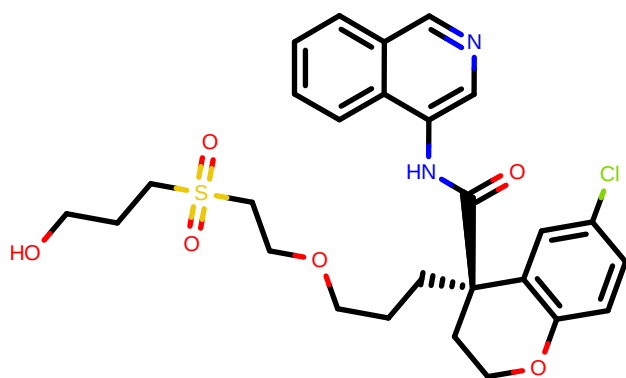
DDG (kcal/mol):

-0.42

dDDG (kcal/mol):

0.37

EN300-7456499_4_1



CID:

EN300-7456499_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COC(=O)C3)CCCC(=O)C(=O)CCO

RUN:

RUN1519

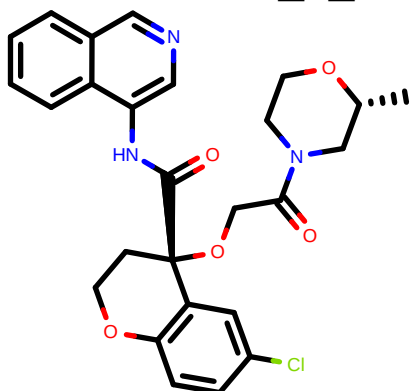
DDG (kcal/mol):

-0.42

dDDG (kcal/mol):

0.44

EN300-25572_1_1



CID:

EN300-25572_1_1

SMILES:

C[C@@H]1CN(CCO1)C(=O)CO[C@@H]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN:

RUN572

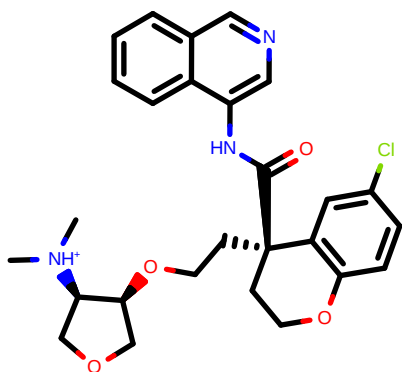
DDG (kcal/mol):

-0.41

dDDG (kcal/mol):

0.31

EN300-2723070_3_1



CID:

EN300-2723070_3_1

SMILES:

C[NH+](C)[C@@H]1COC[C@@H]1OCC[C@@H]2(CCOc3cc2cc(cc3)Cl)C(=O)Nc4ncnc5c4ccccc5

RUN:

RUN616

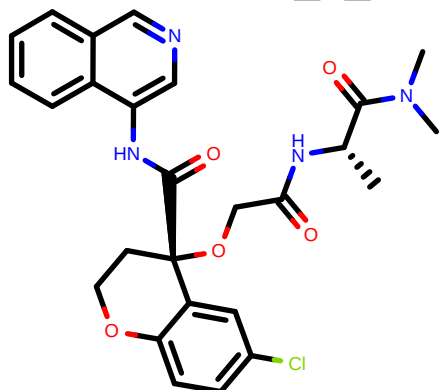
DDG (kcal/mol):

-0.41

dDDG (kcal/mol):

0.42

EN300-47657_1_1



CID:

EN300-47657_1_1

SMILES:

C[C@@H](C(=O)N(C)C)NC(=O)CO[C@@H]1(CCOc2cc1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN848

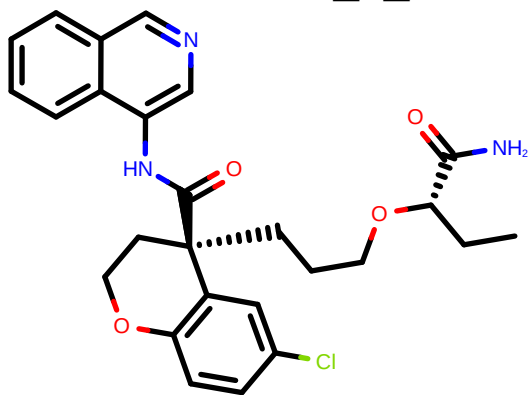
DDG (kcal/mol):

-0.41

dDDG (kcal/mol):

0.28

EN300-65839_4_1



CID:

EN300-65839_4_1

SMILES:

CC[C@@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccoc4

RUN:

RUN808

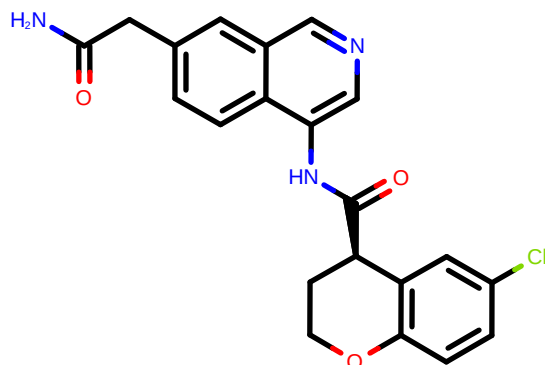
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.42

MAK-UNK-8be7dca9-2_1



CID:

MAK-UNK-8be7dca9-2_1

SMILES:

c1cc2c(cc1CC(=O)N)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN:

RUN59

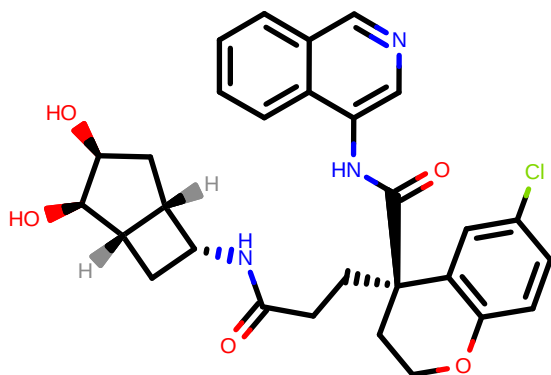
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.07

EN300-6736851_2_1



CID:

EN300-6736851_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCOC(=O)N[C@@H]5C[C@@H]6[C@@H]5C[C@@H]6[C@@H]5C[C@@H]5O

RUN:

RUN1099

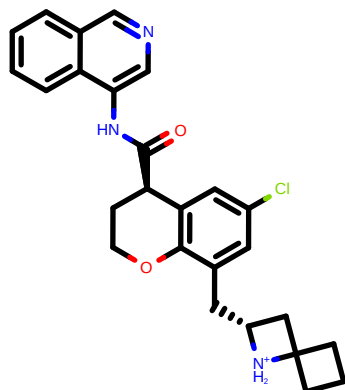
DDG (kcal/mol):

-0.40

dDDG (kcal/mol):

0.35

DAR-DIA-23e5a6a0-7_1



CID:

DAR-DIA-23e5a6a0-7_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C[C@@H]5CC6([NH2+][5])CCC6)Cl

RUN:

RUN223

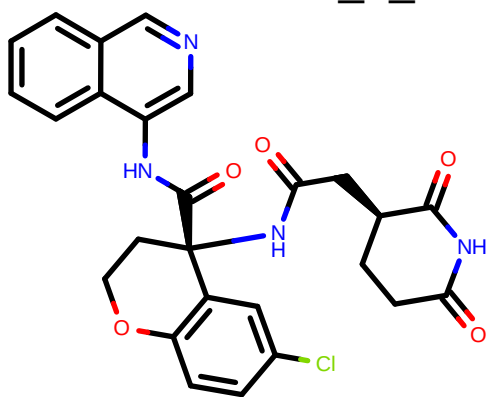
DDG (kcal/mol):

-0.39

dDDG (kcal/mol):

0.26

EN300-3451857_1_1



CID: EN300-3451857_1_1

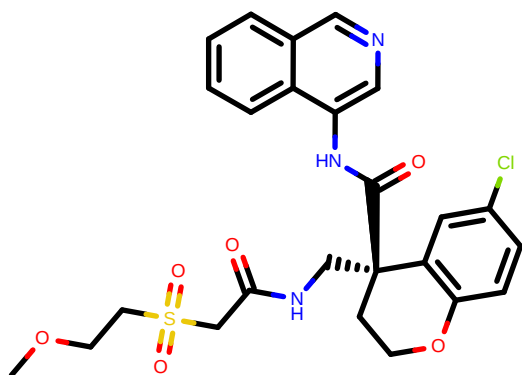
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(COCc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)NC5=O

RUN: RUN1085

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.26

EN300-39501_2_1



CID: EN300-39501_2_1

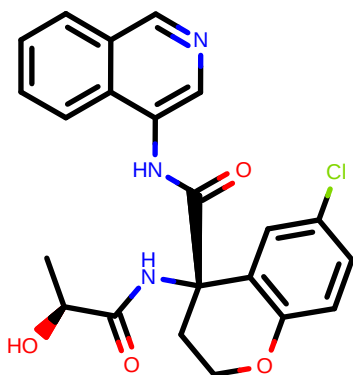
SMILES: COCCS(=O)(=O)CC(=O)NC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4

RUN: RUN873

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.35

EN300-19542_1_1



CID: EN300-19542_1_1

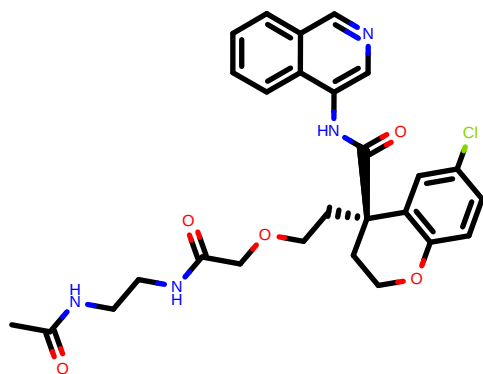
SMILES: C[C@@H](C(=O)N[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4)O

RUN: RUN1213

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.23

EN300-23129_3_1



CID: EN300-23129_3_1

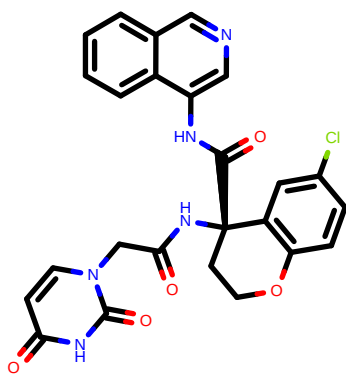
SMILES: CC(=O)NCCNC(=O)COCC[C@@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccccc4

RUN: RUN1316

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

EN300-13287_1_1



CID: EN300-13287_1_1

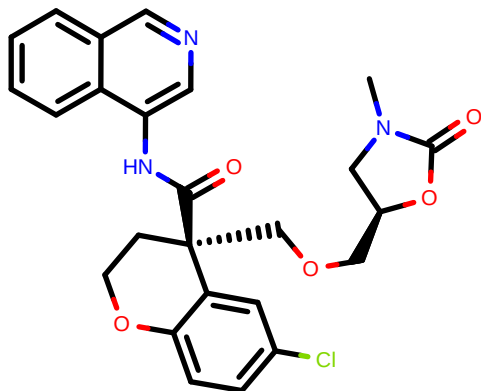
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccc(=O)[nH]c5=O

RUN: RUN601

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.30

EN300-222969_2_1



CID: EN300-222969_2_1

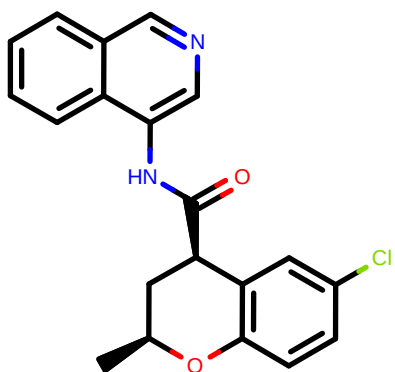
SMILES: CN1C[C@@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4ccc5

RUN: RUN1701

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.31

EDJ-MED-e4b030d8-3_1



CID: EDJ-MED-e4b030d8-3_1

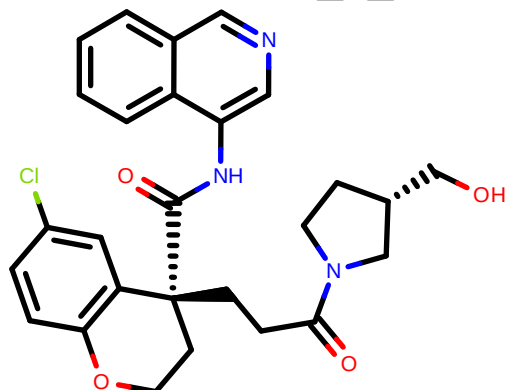
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3ccccc4

RUN: RUN22

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.10

EN300-88131_2_1



CID: EN300-88131_2_1

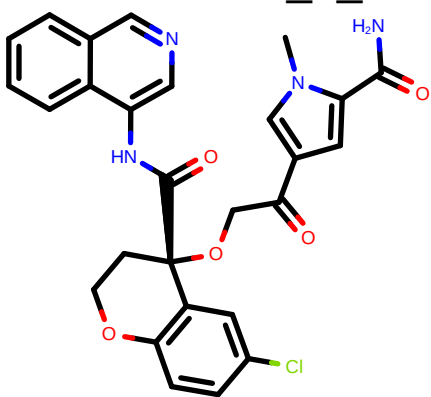
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](C5)CO

RUN: RUN1443

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.27

EN300-35592_1_1



CID: EN300-35592_1_1

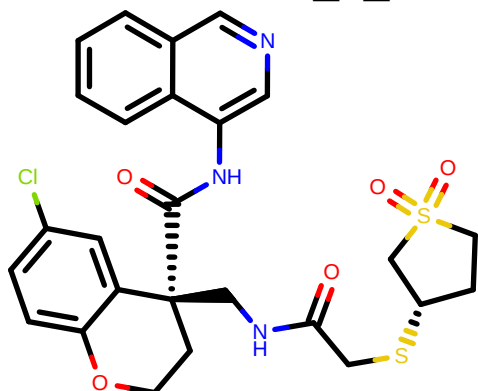
SMILES: Cn1cc(cc1C(=O)N)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5

RUN: RUN1016

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.33

EN300-13890_2_2



CID: EN300-13890_2_2

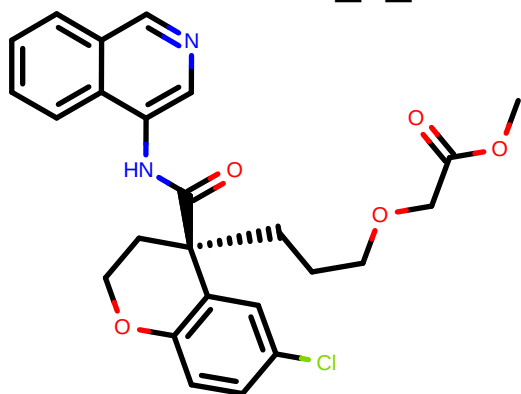
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS[C@H]5CCS(=O)(=O)C5

RUN: RUN1313

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.36

EN300-19700_4_1



CID: EN300-19700_4_1

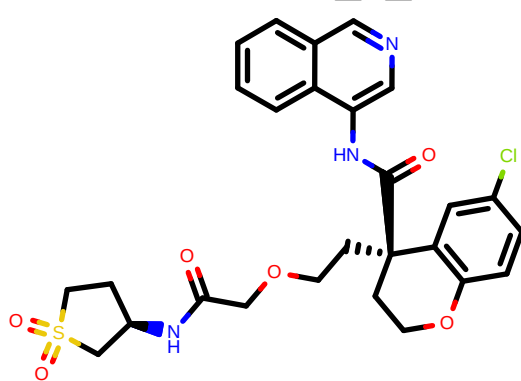
SMILES: COC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3cccc4

RUN: RUN420

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.32

EN300-05512_3_1



CID: EN300-05512_3_1

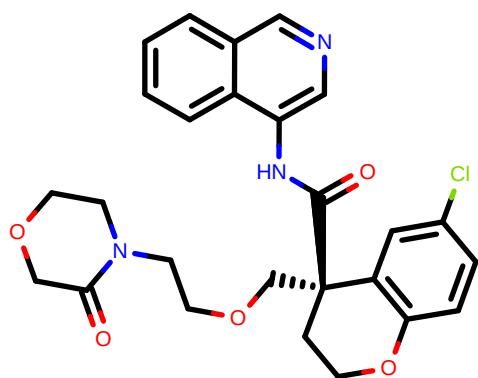
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@H]5CCS(=O)(=O)C5

RUN: RUN1196

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.36

EN300-219330_2_1



CID: EN300-219330_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5c5ccccc5=O

RUN:

RUN499

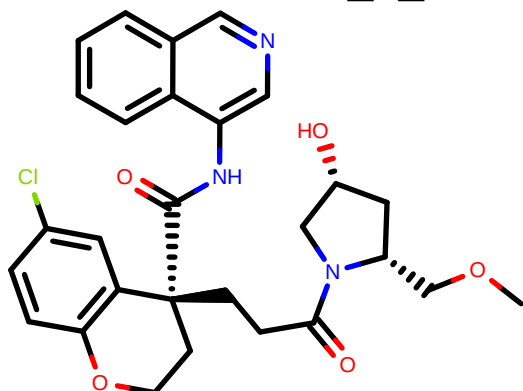
DDG (kcal/mol):

-0.36

dDDG (kcal/mol):

0.27

EN300-263601_2_1



CID: EN300-263601_2_1

SMILES:

COC[C@H]1C[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5)O

RUN:

RUN1698

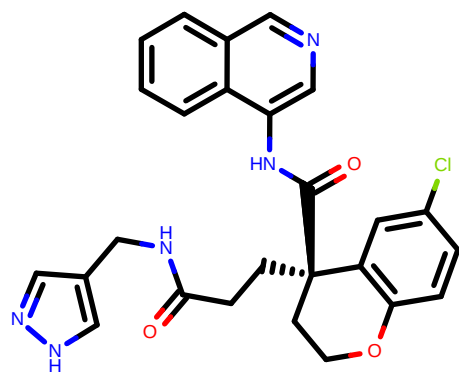
DDG (kcal/mol):

-0.35

dDDG (kcal/mol):

0.36

EN300-31562_2_1



CID: EN300-31562_2_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5c[nH]nc5

RUN:

RUN1051

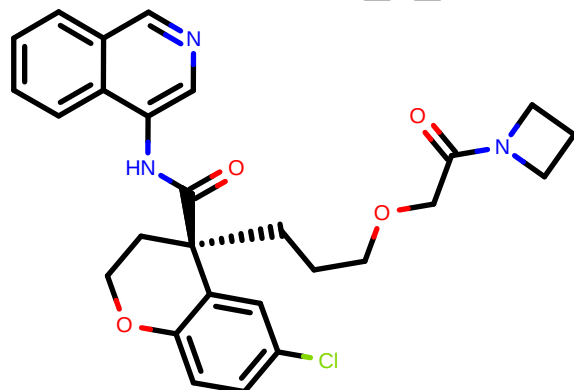
DDG (kcal/mol):

-0.35

dDDG (kcal/mol):

0.32

EN300-11195_4_1



CID: EN300-11195_4_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC(=O)N5CCCS5

RUN:

RUN1255

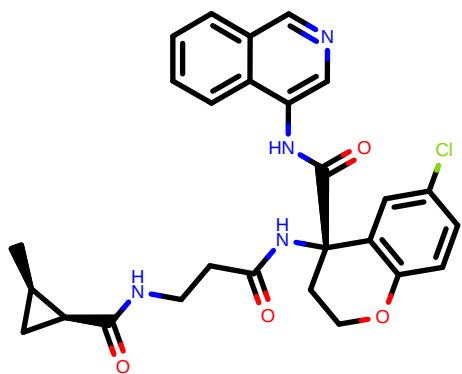
DDG (kcal/mol):

-0.35

dDDG (kcal/mol):

0.30

EN300-36851_1_1



CID: EN300-36851_1_1

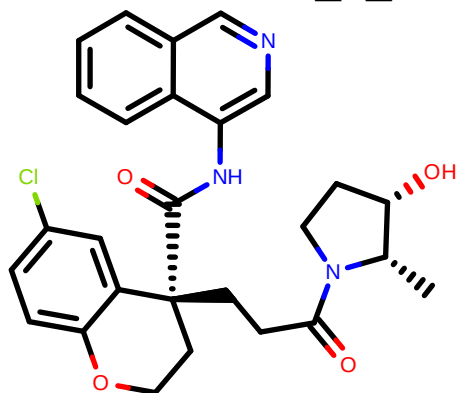
SMILES: C[C@@H]1C[C@@H]1C(=O)NCCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5

RUN: RUN1181

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.25

EN300-2008120_2_1



CID: EN300-2008120_2_1

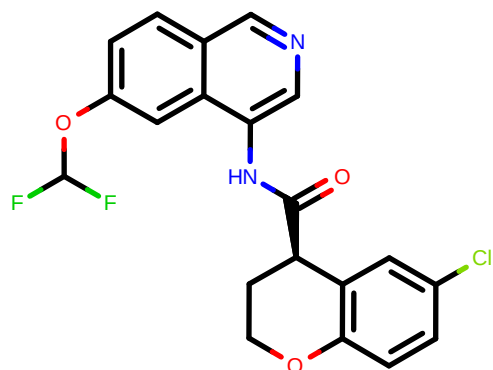
SMILES: C[C@H]1[C@H](CCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4ccc5)O

RUN: RUN1115

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.28

BEN-DND-c852c98b-6_1



CID: BEN-DND-c852c98b-6_1

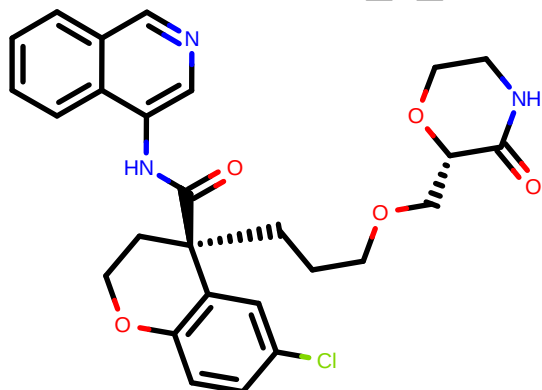
SMILES: c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN53

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.07

EN300-1706036_4_2



CID: EN300-1706036_4_2

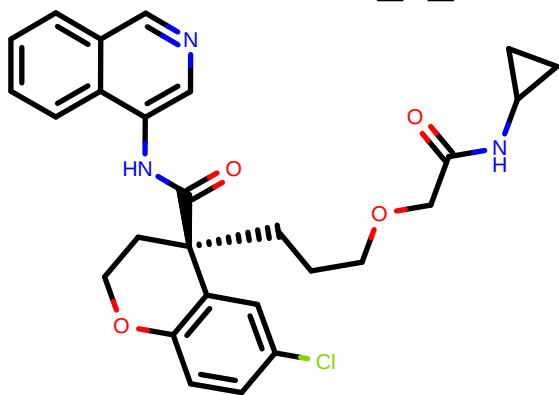
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5C(=O)NCCO5

RUN: RUN1407

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.33

EN300-1253178_4_1



CID: EN300-1253178_4_1

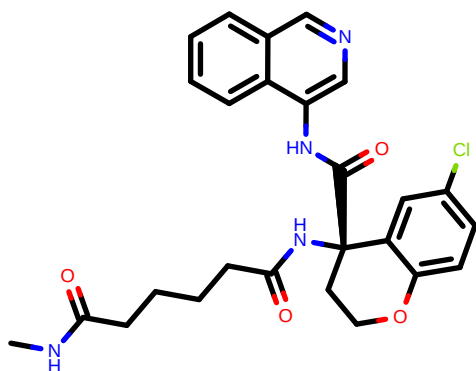
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC5CC5

RUN: RUN1431

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.44

EN300-154693_1_1



CID: EN300-154693_1_1

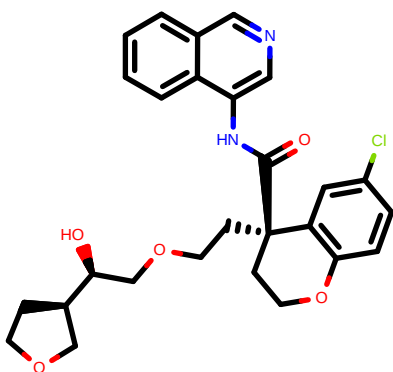
SMILES: CNC(=O)CCCCC(=O)N[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1021

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.33

EN300-1911992_3_1



CID: EN300-1911992_3_1

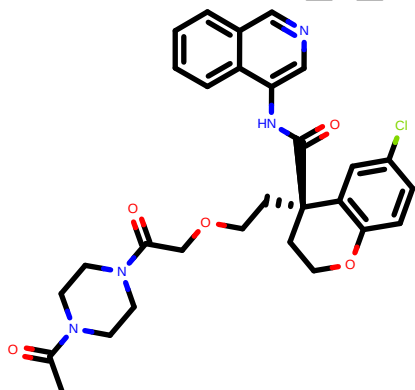
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]([C@@H]5CCOC5)O

RUN: RUN481

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.32

EN300-1724771_3_1



CID: EN300-1724771_3_1

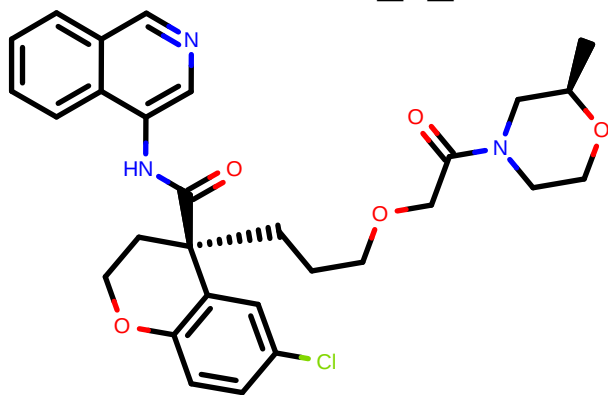
SMILES: CC(=O)N1CCN(CC1)C(=O)COC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1603

DDG (kcal/mol): -0.33

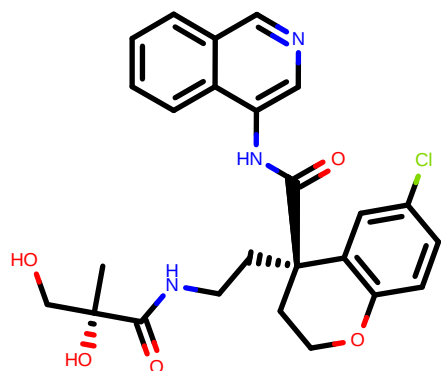
dDDG (kcal/mol): 0.47

EN300-25572_4_1



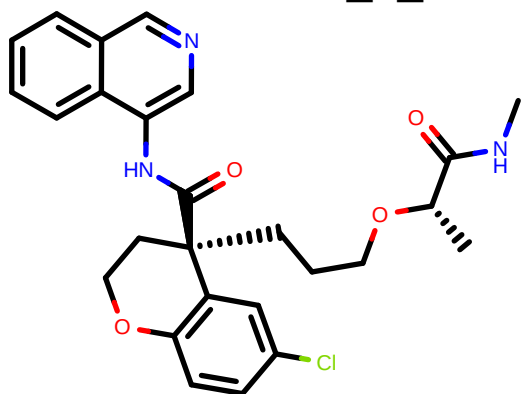
CID:	EN300-25572_4_1
SMILES:	<chem>C[C@@H]1CN(CCO1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5</chem>
RUN:	RUN999
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.38

EN300-89418_3_2



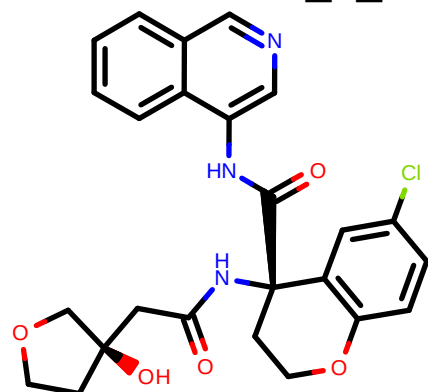
CID:	EN300-89418_3_2
SMILES:	<chem>C[C@](CO)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O</chem>
RUN:	RUN779
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.54

EN300-211482_4_1



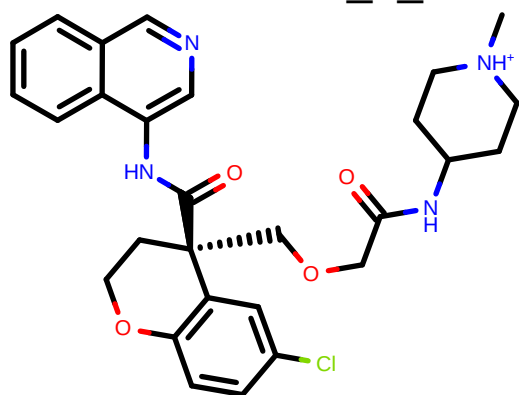
CID:	EN300-211482_4_1
SMILES:	<chem>C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4</chem>
RUN:	RUN1023
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.34

EN300-360157_1_1



CID:	EN300-360157_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCOCS5)O</chem>
RUN:	RUN766
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.34

EN300-342462_2_1



CID: EN300-342462_2_1

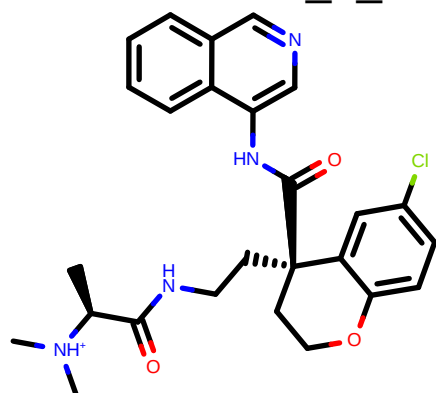
SMILES: C[NH+]1CCC(CC1)NC(=O)COC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4cncc5c4cccc5

RUN: RUN578

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.35

EN300-306495_3_1



CID: EN300-306495_3_1

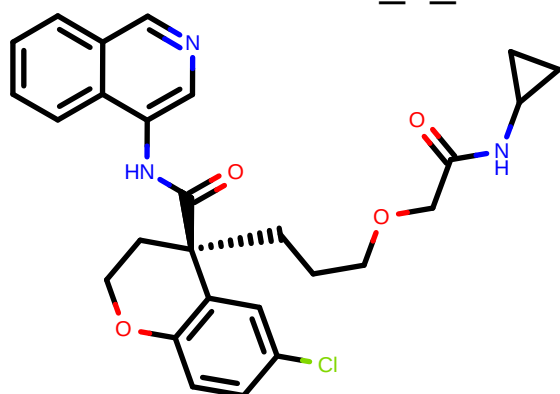
SMILES: C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)[NH+](C)C

RUN: RUN287

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.36

EN300-1253178_4_1



CID: EN300-1253178_4_1

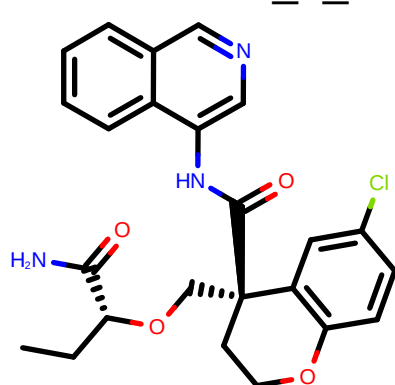
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCOC(=O)NC5CC5

RUN: RUN1423

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.34

EN300-65839_2_2



CID: EN300-65839_2_2

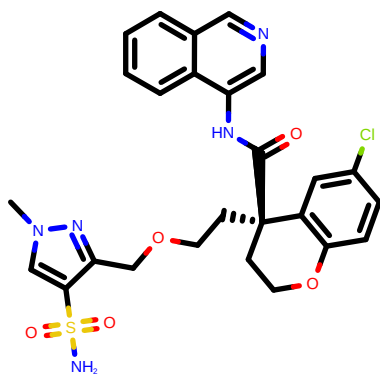
SMILES: CC[C@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4

RUN: RUN926

DDG (kcal/mol): -0.32

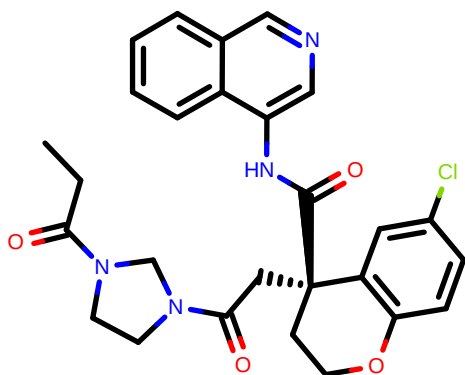
dDDG (kcal/mol): 0.31

EN300-7355737_3_1



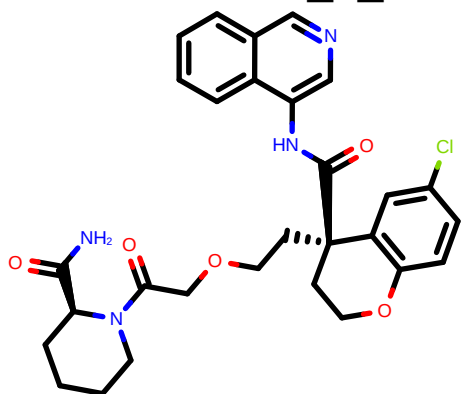
CID:	EN300-7355737_3_1
SMILES:	<chem>Cn1cc(c(n1)COC[C@]2(C(=O)C3C2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)N</chem>
RUN:	RUN1092
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.39

EN300-257790_1_1



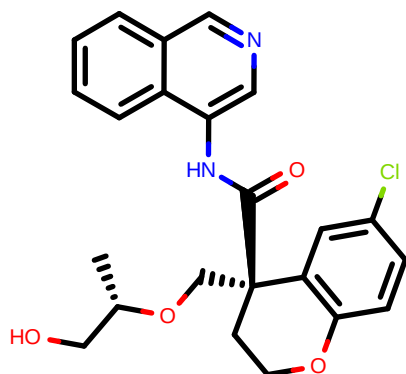
CID:	EN300-257790_1_1
SMILES:	<chem>CCC(=O)N1CCN(C1)C(=O)C[C@]2(C(=O)C3C2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1625
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.27

EN300-22879_3_2



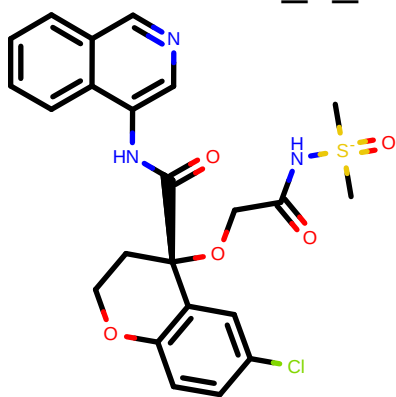
CID:	EN300-22879_3_2
SMILES:	<chem>c1cccc2c(c1)cncc2NC(=O)[C@@]3(C(=O)C4C3cc(cc4)Cl)CCOC(=O)N5CCCC[C@H]5C(=O)N</chem>
RUN:	RUN512
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.47

EN300-175186_2_1



CID:	EN300-175186_2_1
SMILES:	<chem>C[C@@H](CO)OC[C@]1(C(=O)C2C1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1374
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.25

EN300-267469_1_1



CID: EN300-267469_1_1

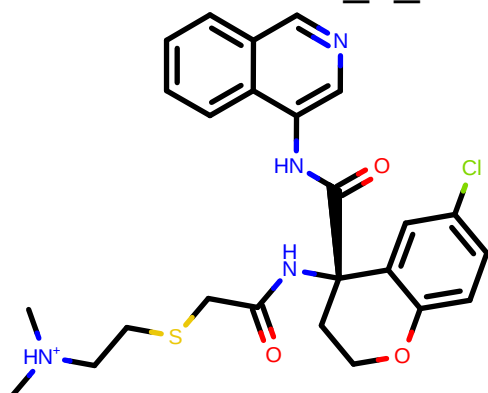
SMILES: CS(=NC(=O)CQ[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4)(=O)C

RUN: RUN715

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.27

EN300-1708620_1_1



CID: EN300-1708620_1_1

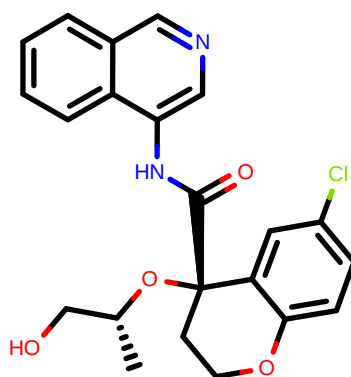
SMILES: C[NH+](C)CCSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN1101

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.34

EN300-175186_1_2



CID: EN300-175186_1_2

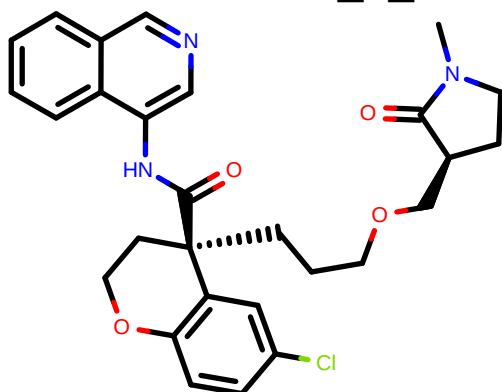
SMILES: C[C@H](CO)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN596

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

EN300-260816_4_2



CID: EN300-260816_4_2

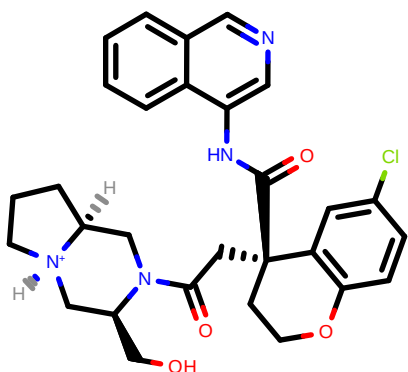
SMILES: CN1CC[C@H](C1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5

RUN: RUN855

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.36

EN300-365281_1_1



CID: EN300-365281_1_1

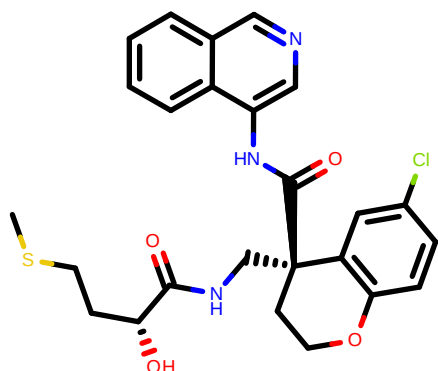
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4c3cc(cc4)C)CC(=O)N5C[C@@H]6CC[C@H]6[C@@H]3C[C@@H]5CO

RUN: RUN311

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.34

EN300-103144_2_2



CID: EN300-103144_2_2

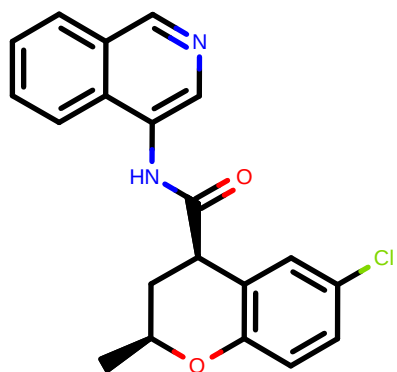
SMILES: CSCC[C@H](C(=O)NC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O

RUN: RUN669

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.31

ALP-POS-d3acb8cc-1_1



CID: ALP-POS-d3acb8cc-1_1

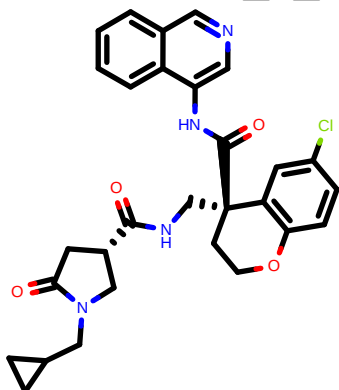
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN23

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.10

EN300-31969_2_2



CID: EN300-31969_2_2

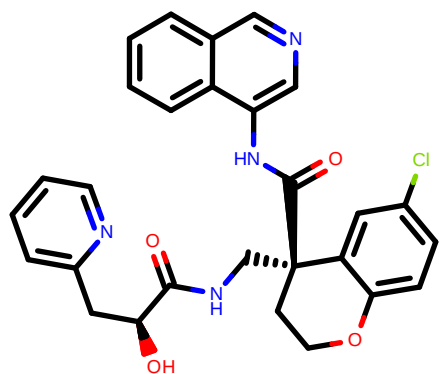
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4c3cc(cc4)C)CNC(=O)[C@H]5C[C@@H](C5)COC6C6

RUN: RUN708

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.31

EN300-6762327_2_2



CID: EN300-6762327_2_2

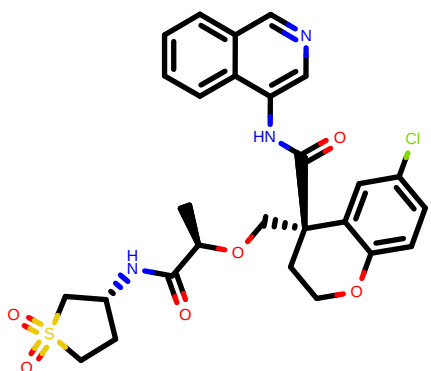
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](Cc5ccccc5)O

RUN: RUN1137

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.33

EN300-23318_2_2



CID: EN300-23318_2_2

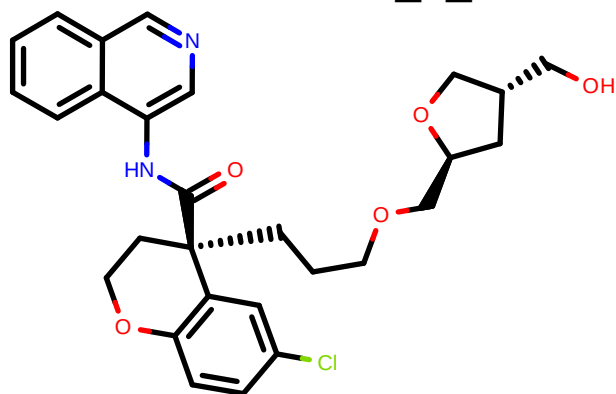
SMILES: ClC@H](C(=O)NC@H)1CCS(=O)(=O)C1OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cccc5c4cccc5

RUN: RUN658

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.40

EN300-6494158_4_3



CID: EN300-6494158_4_3

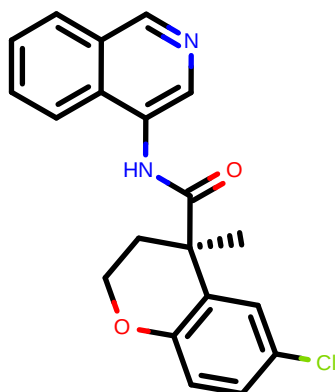
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCC[C@]4(C)[C@H](CO)C5C(=O)CO

RUN: RUN792

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.40

DAR-DIA-6a508060-10_2



CID: DAR-DIA-6a508060-10_2

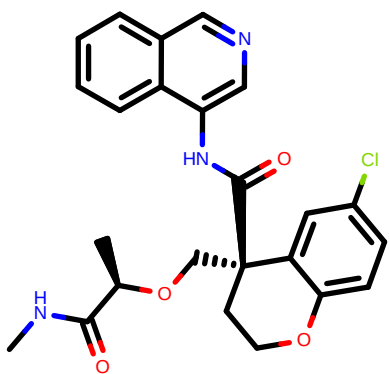
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN9

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.12

EN300-211482_2_2



CID: EN300-211482_2_2

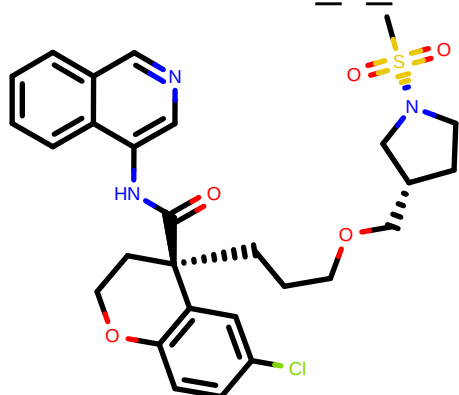
SMILES: C[C@H](C(=O)NC)OC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1534

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.33

EN300-261986_4_1



CID: EN300-261986_4_1

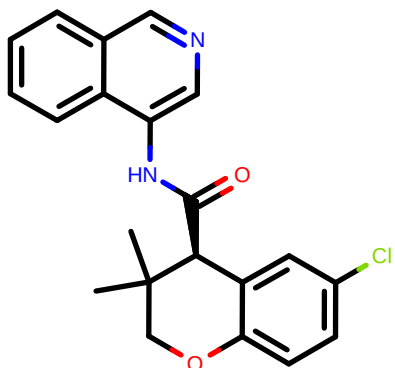
SMILES: CS(=O)(=O)N[C@@]1(C[C@H]2C(=O)OCC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN: RUN1335

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.36

ADA-UCB-dc2b944c-15_1



CID: ADA-UCB-dc2b944c-15_1

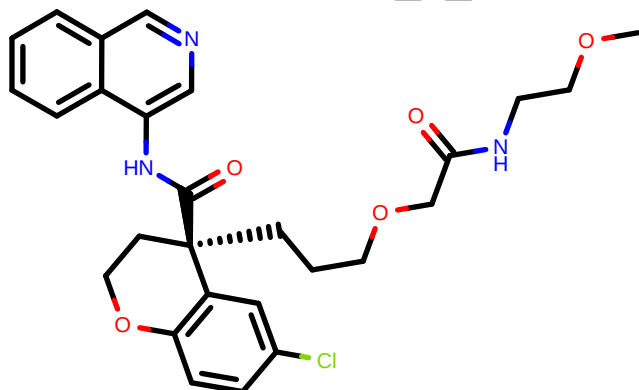
SMILES: CC1(COCc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C

RUN: RUN155

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.13

EN300-02015_4_1



CID: EN300-02015_4_1

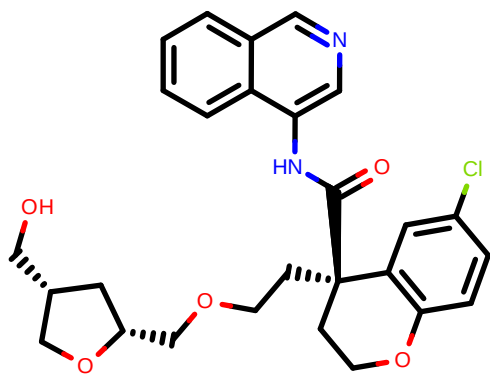
SMILES: COCCNC(=O)COCC[C@]1(COCc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN1646

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.39

EN300-6494158_3_4



CID: EN300-6494158_3_4

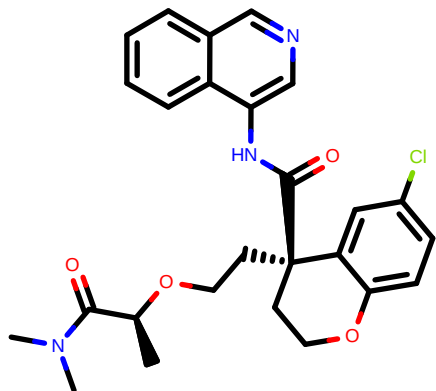
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C[C@H](CO5)CO

RUN: RUN932

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.33

EN300-14458_3_1



CID: EN300-14458_3_1

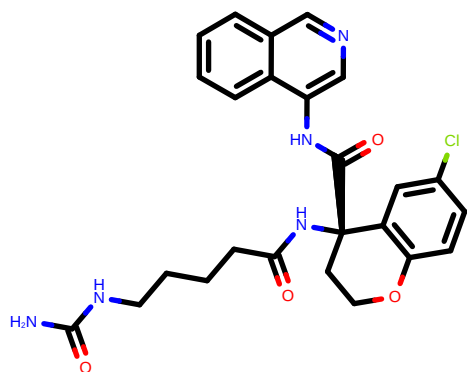
SMILES: C[C@@H](C(=O)N(C)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3ccoc4

RUN: RUN1524

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.32

EN300-13499_1_1



CID: EN300-13499_1_1

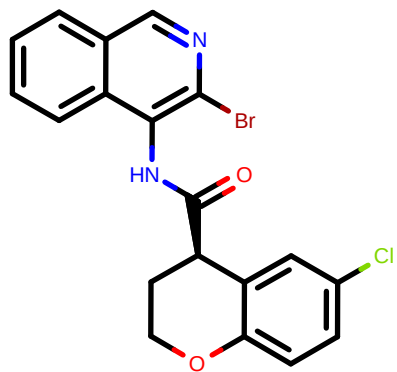
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCCNC(=O)N

RUN: RUN720

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.30

ADA-UCB-dc2b944c-9_1



CID: ADA-UCB-dc2b944c-9_1

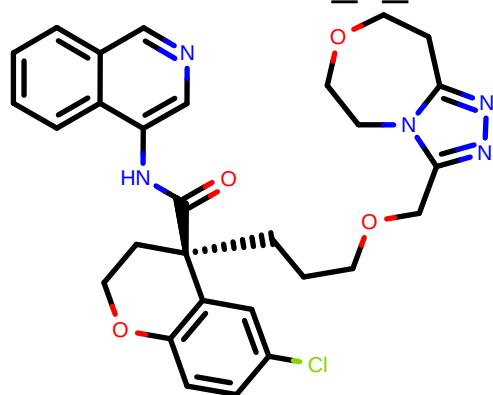
SMILES: c1ccc2c(c1)cnc(c2NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl)Br

RUN: RUN58

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.13

EN300-310888_4_1



CID: EN300-310888_4_1

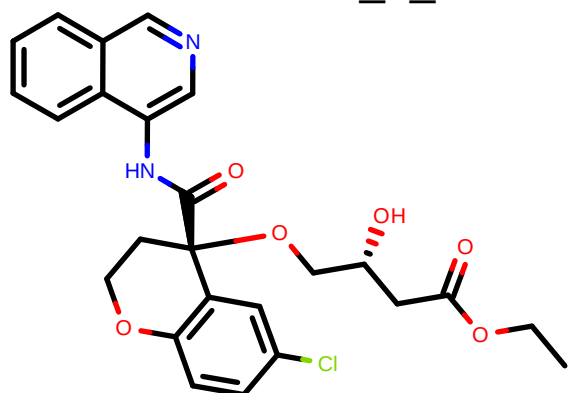
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nnc6n5CCOCC6

RUN: RUN1479

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.35

EN300-82539_1_2



CID: EN300-82539_1_2

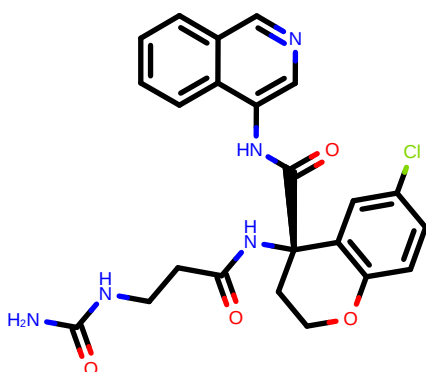
SMILES: CCOC(=O)C[C@H](CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4)O

RUN: RUN952

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.32

EN300-10729_1_1



CID: EN300-10729_1_1

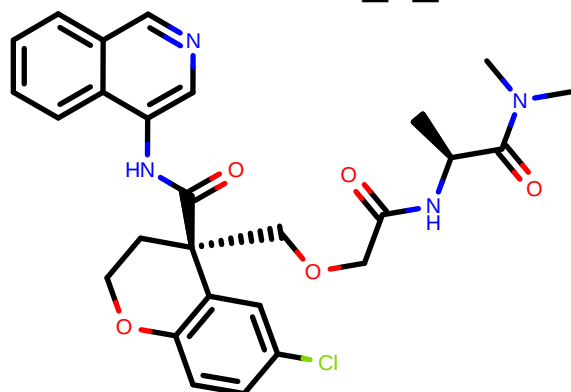
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)N

RUN: RUN1565

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.26

EN300-47657_2_1



CID: EN300-47657_2_1

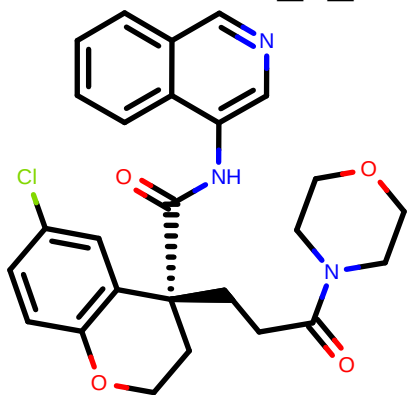
SMILES: C[C@@H](C(=O)N(C)C)NC(=O)COC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN530

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.29

EN300-18064_2_1



CID: EN300-18064_2_1

SMILES:

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

RUN:

RUN756

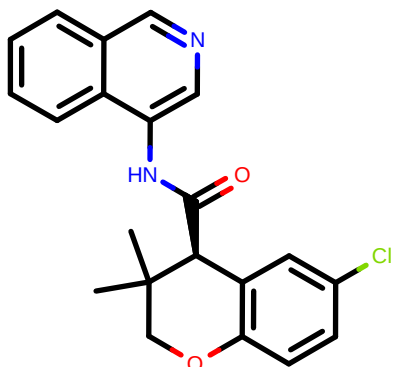
DDG (kcal/mol):

-0.26

dDDG (kcal/mol):

0.25

DAR-DIA-0d514e7d-3_1



CID: DAR-DIA-0d514e7d-3_1

SMILES:

CC1(COC2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C

RUN:

RUN156

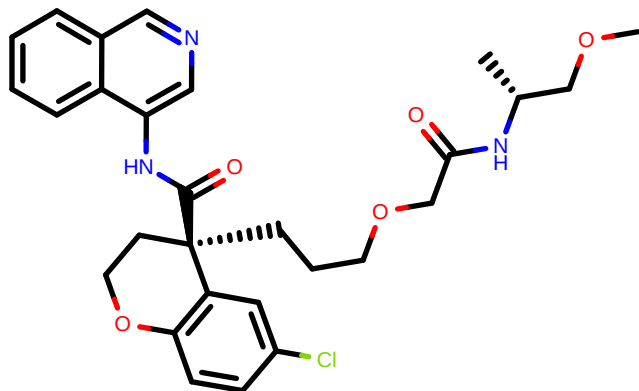
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.13

EN300-02067_4_2



CID: EN300-02067_4_2

SMILES:

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

RUN:

RUN1662

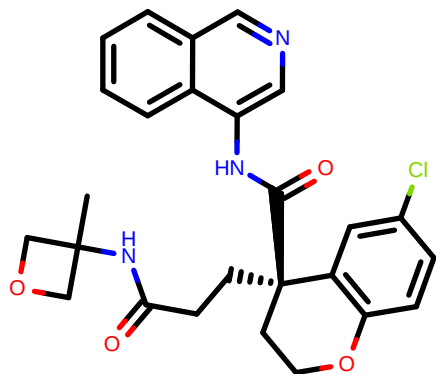
DDG (kcal/mol):

-0.25

dDDG (kcal/mol):

0.33

EN300-216032_2_1



CID: EN300-216032_2_1

SMILES:

CC1(COC1)NC(=O)CC[C@H]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5

RUN:

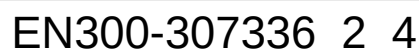
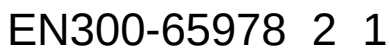
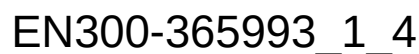
RUN575

DDG (kcal/mol):

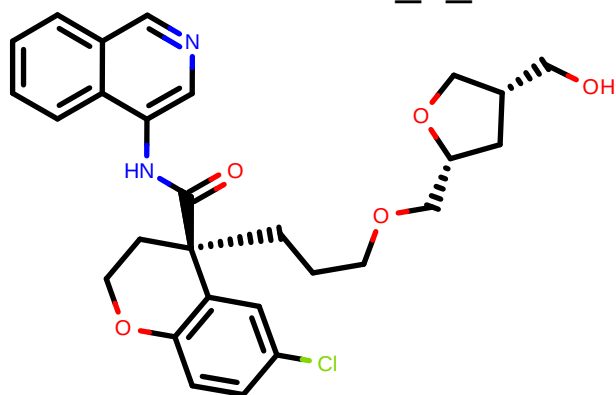
-0.25

dDDG (kcal/mol):

0.26

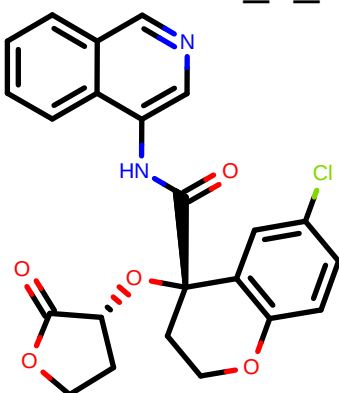


EN300-6494158_4_4



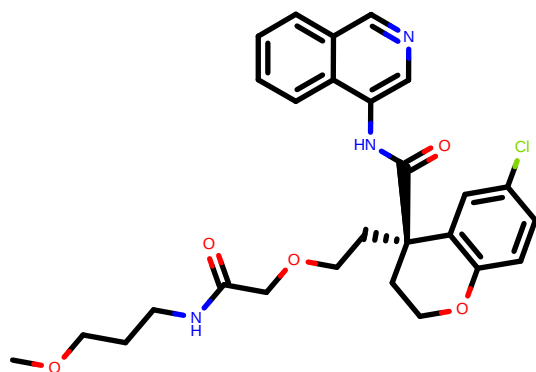
CID:	EN300-6494158_4_4
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C[C@H](CO5)CO</chem>
RUN:	RUN879
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.40

EN300-20496_1_1



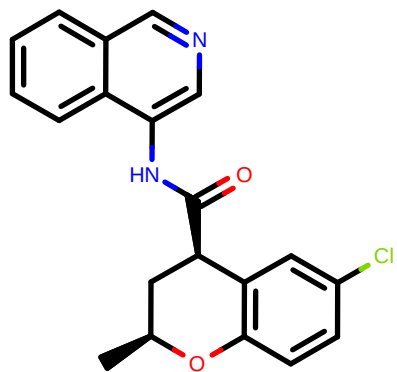
CID:	EN300-20496_1_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)O[C@H]5CCOC5=O</chem>
RUN:	RUN1344
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.22

EN300-04492_3_1



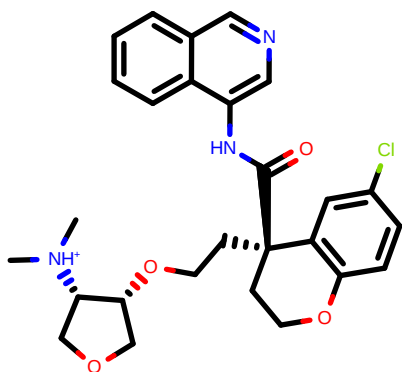
CID:	EN300-04492_3_1
SMILES:	<chem>COCCCN(C(=O)COCC[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN1651
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.32

MAT-POS-8a69d52e-1_4



CID:	MAT-POS-8a69d52e-1_4
SMILES:	<chem>C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN21
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.09

EN300-2723070_3_4



CID: EN300-2723070_3_4

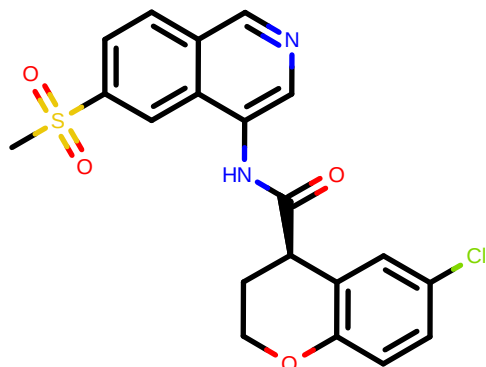
SMILES: C[NH+](C)[C@H]1COC[C@H]1OCC[C@]2(CCOc3c2cc(cc3C)C)C(=O)Nc4nc5c4ccccc5

RUN: RUN1052

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.38

BEN-DND-c852c98b-5_1



CID: BEN-DND-c852c98b-5_1

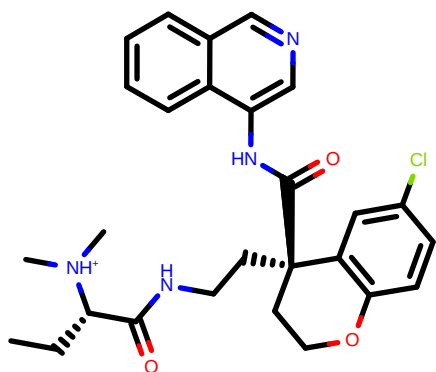
SMILES: CS(=O)(=O)c1ccc2nc(cc(c2c1)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN54

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.08

EN300-223964_3_1



CID: EN300-223964_3_1

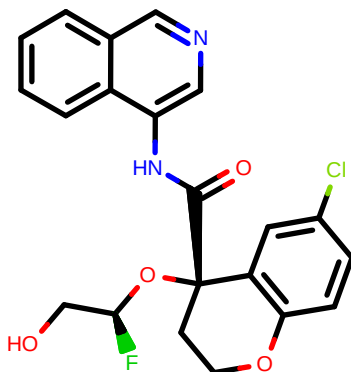
SMILES: CC[C@@H](C)(C=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccccc4)[NH+](C)C

RUN: RUN590

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.46

EN300-861925_1_2



CID: EN300-861925_1_2

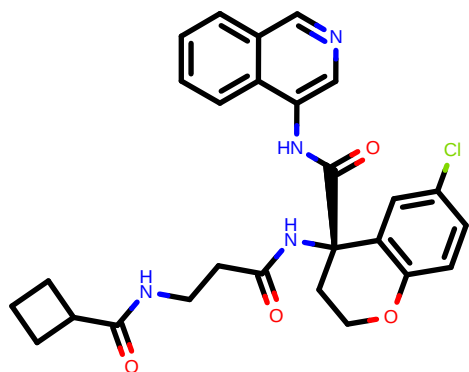
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@H](CO)F

RUN: RUN317

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-62449_1_1



CID: EN300-62449_1_1

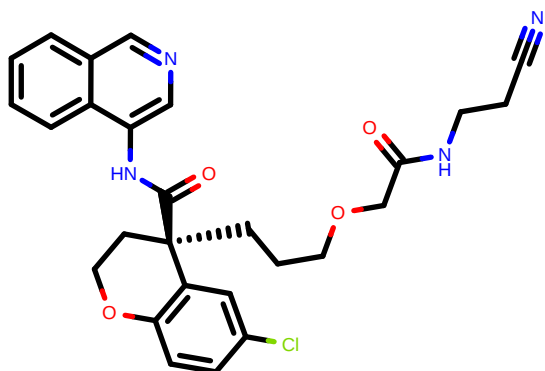
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5CCCS

RUN: RUN314

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.29

EN300-10895_4_1



CID: EN300-10895_4_1

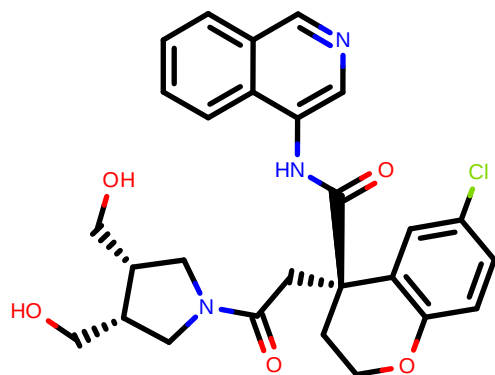
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCCC#N

RUN: RUN1766

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.47

EN300-333677_1_1



CID: EN300-333677_1_1

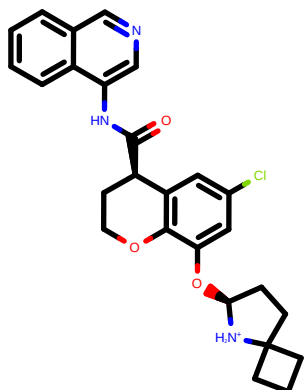
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C)[C@@H](C5)COCO

RUN: RUN550

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

DAR-DIA-23e5a6a0-1_2



CID: DAR-DIA-23e5a6a0-1_2

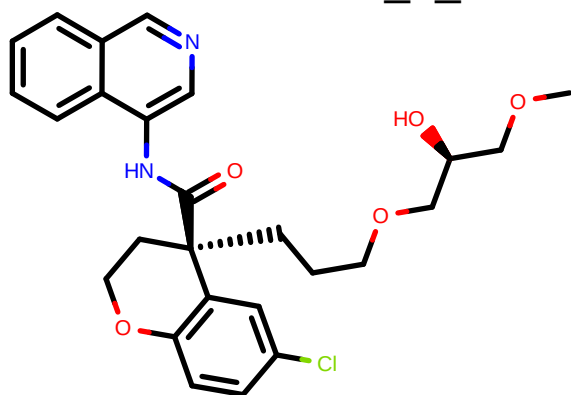
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOo4c3cc(cc4O)[C@H]5CCCC6([NH2+][5])CCC6)Cl

RUN: RUN108

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.34

EN300-1915260_4_1



CID: EN300-1915260_4_1

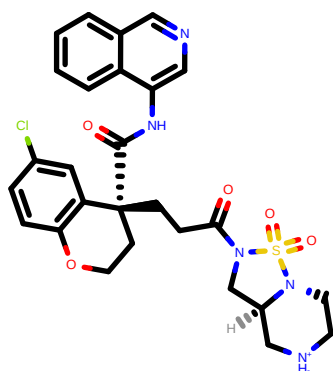
SMILES: COC[C@@H](COCCC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3ccc4c3cccc4)O

RUN: RUN714

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.41

EN300-717233_2_1



CID: EN300-717233_2_1

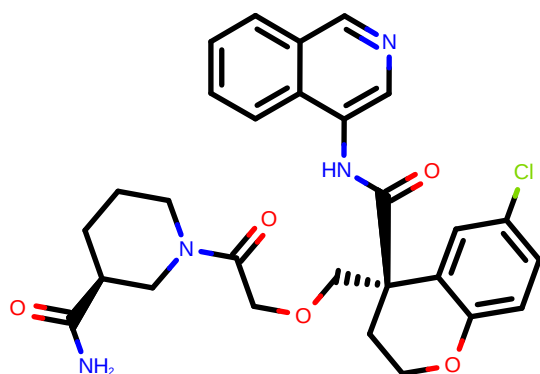
SMILES: c1ccc2c(c1)ncnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5C[C@@H]6C[NH2+]C[C@]7(N5)C(=O)O

RUN: RUN1754

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.47

EN300-22880_2_1



CID: EN300-22880_2_1

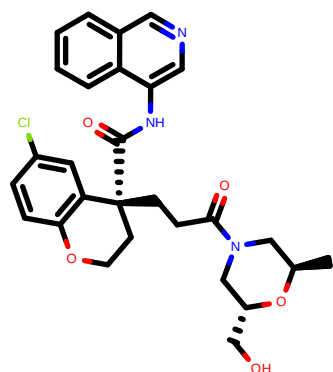
SMILES: c1ccc2c(c1)ncnc2N(C(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(C(=O)N5CCC[C@@H]6C5)C(=O)N

RUN: RUN1270

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.41

EN300-6759637_2_1



CID: EN300-6759637_2_1

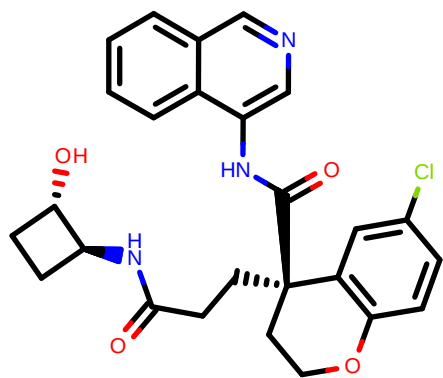
SMILES: C[C@@H]1CN(C[C@H](O1)CO)C(=O)CC[C@]2(CCOc3c2cc(cc3)C)C(=O)Nc4ccc5c4cccc5

RUN: RUN1650

DDG (kcal/mol): -0.19

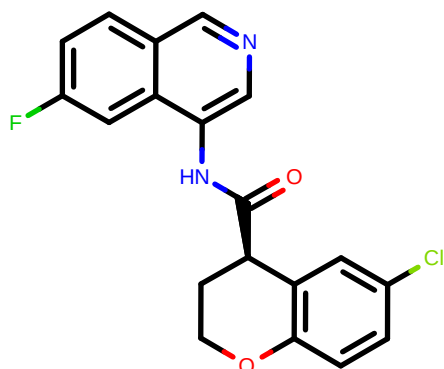
dDDG (kcal/mol): 0.32

EN300-129424_2_2



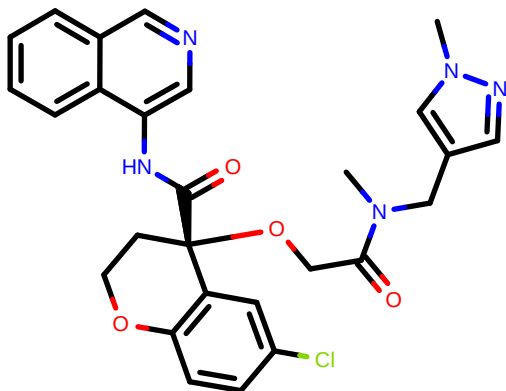
CID:	EN300-129424_2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOC4C3cc(cc4Cl)CCC(=O)N[C@@H]5CC[C@@H]5O</chem>
RUN:	RUN1459
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.31

ALP-POS-696356e4-1_1



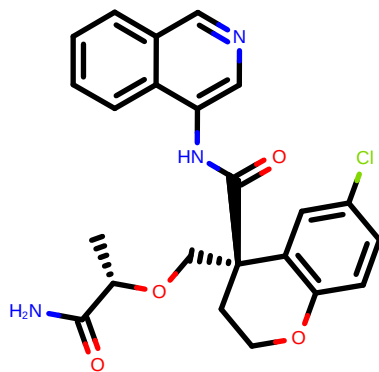
CID:	ALP-POS-696356e4-1_1
SMILES:	<chem>c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOC4C3cc(cc4Cl</chem>
RUN:	RUN20
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.04

EN300-65978_1_1



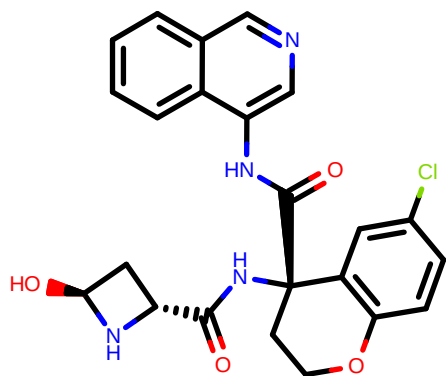
CID:	EN300-65978_1_1
SMILES:	<chem>Cn1cc(n1)CN(C)C(=O)CO[C@@H]2(CCOC3C2cc(cc3Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1312
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.34

EN300-17381_2_1



CID:	EN300-17381_2_1
SMILES:	<chem>C[C@@H](C(=O)N)OC[C@H]1(CCOC2C1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN878
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.27

EN300-184266_1_1



CID: EN300-184266_1_1

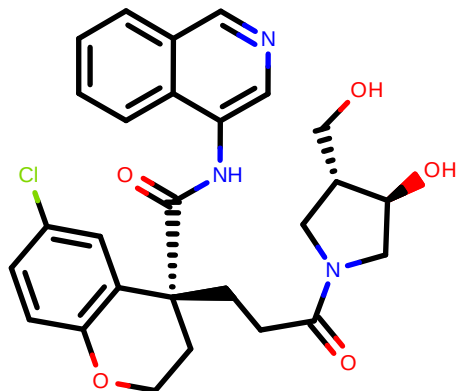
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5

RUN: RUN1269

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.22

EN300-248521_2_3



CID: EN300-248521_2_3

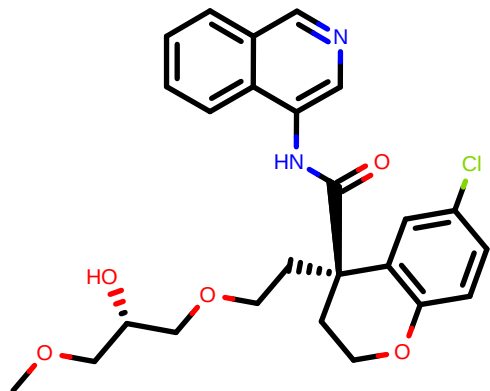
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C[C@H]6[C@H](C5)O[CO

RUN: RUN296

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.26

EN300-1915260_3_1



CID: EN300-1915260_3_1

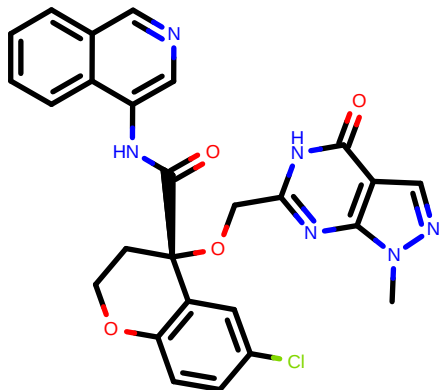
SMILES: COC[C@@H](COCC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nnc4c3cccc4)O

RUN: RUN1540

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.34

EN300-44149_1_1



CID: EN300-44149_1_1

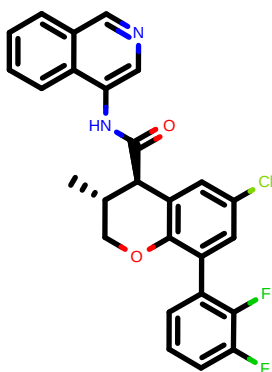
SMILES: Cn1c2c(cn1)c(=O)[nH]c(n2)CO[C@H]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5ncc6c5cccc6

RUN: RUN1528

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.25

DAR-DIA-0d514e7d-14_1



CID:

DAR-DIA-0d514e7d-14_1

SMILES:

C[C@H]1COC2c(cc2[C@@H]1C(=O)Nc3ncoc4c3ccoc4)Cl)c5ccoc(c5)F

RUN:

RUN206

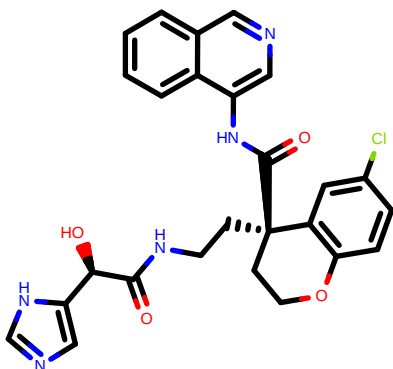
DDG (kcal/mol):

-0.18

dDDG (kcal/mol):

0.27

EN300-254121_3_1



CID:

EN300-254121_3_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CCNC(=O)[C@@H](c5nc[nH]5)O

RUN:

RUN383

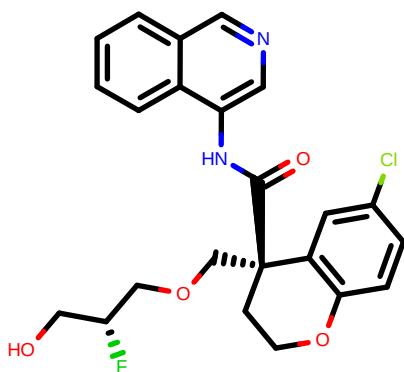
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.56

EN300-1600517_2_1



CID:

EN300-1600517_2_1

SMILES:

c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)COC[C@@H](CO)F

RUN:

RUN1262

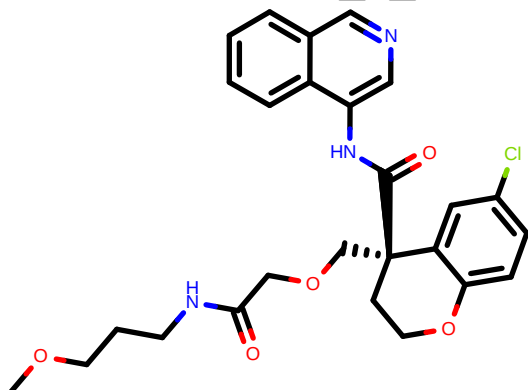
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.29

EN300-04492_2_1



CID:

EN300-04492_2_1

SMILES:

COCCCNc(=O)COC[C@@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3ncoc4c3ccoc4

RUN:

RUN1398

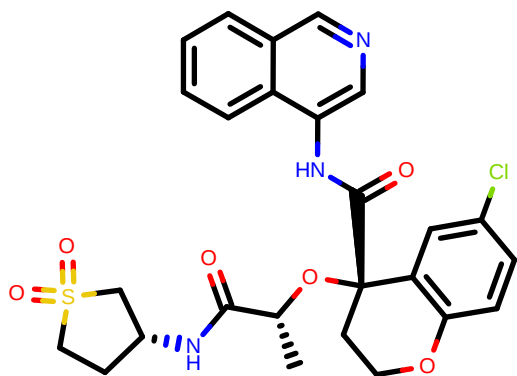
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.32

EN300-23318_1_2



CID: EN300-23318_1_2

SMILES:

C[C@H](Cl)=O)[C@@H](CCS(=O)(=O)C1O[C@H](CCOC3C2C(=O)C3)C1=O)N4CCCC5CCCC5

RUN:

RUN477

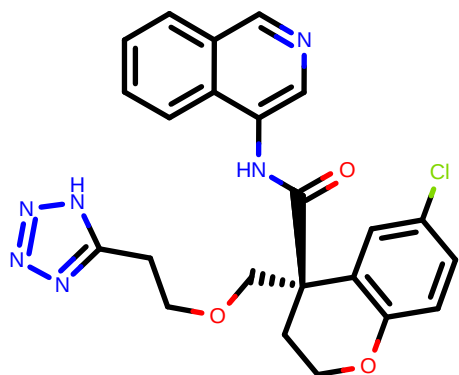
DDG (kcal/mol):

-0.17

dDDG (kcal/mol):

0.31

EN300-183231_2_1



CID: EN300-183231_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H](CCOC3C2C(=O)C3)C1=O)N4CCCC5CCCC5

RUN:

RUN1518

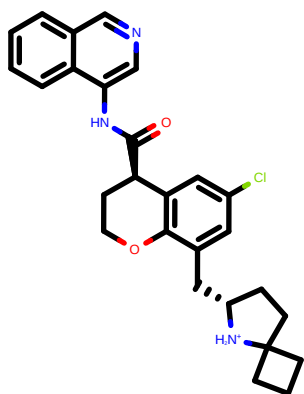
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

0.37

DAR-DIA-23e5a6a0-6_1



CID: DAR-DIA-23e5a6a0-6_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H](CCOC3C2C(=O)C3)C1=O)N4CCCC5CCCC5

RUN:

RUN132

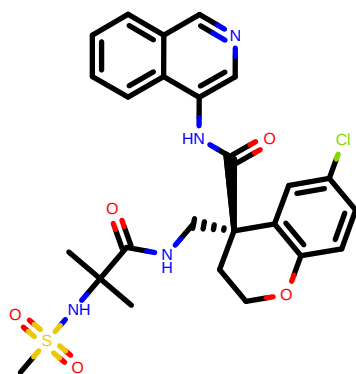
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

0.30

EN300-85849_2_1



CID: EN300-85849_2_1

SMILES:

CC(C)(C(=O)NC[C@H](CCOC2C1C(=O)C2)C1=O)N4CCCC5CCCC5

RUN:

RUN637

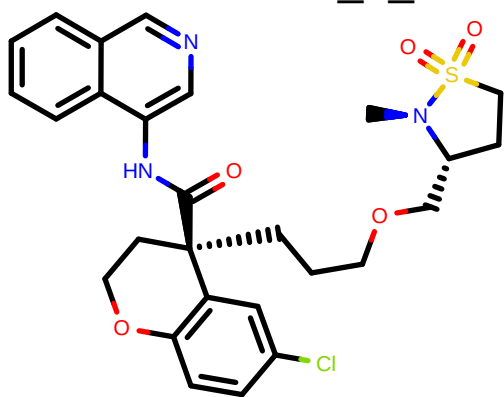
DDG (kcal/mol):

-0.16

dDDG (kcal/mol):

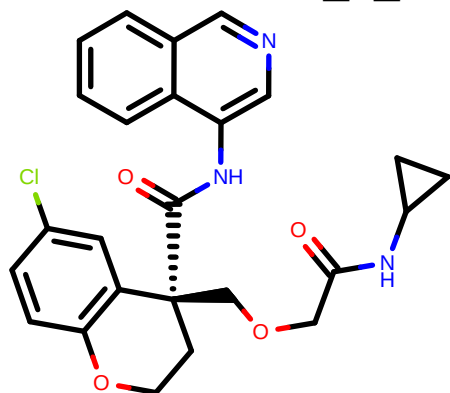
0.35

EN300-393148_4_2



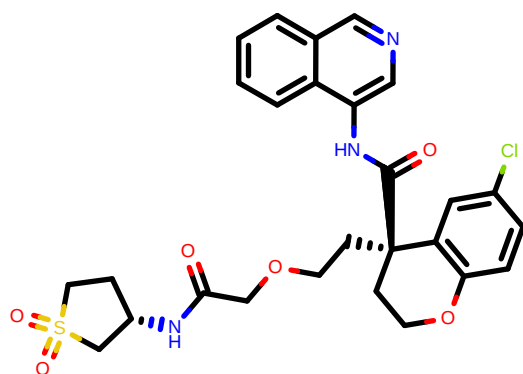
CID:	EN300-393148_4_2
SMILES:	<chem>C[N+]([O-])1[C@H](CCS1(=O)=O)C(=O)COC[C@]2(C)C(=O)C3C2C(C3)C(C(=O)Nc4cnc5c4cccc5</chem>
RUN:	RUN745
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.31

EN300-1253178_2_1



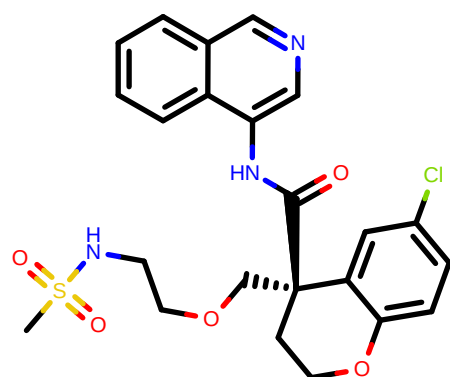
CID:	EN300-1253178_2_1
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(=O)C4C3C(C4)C(C(=O)Nc5ccccc5</chem>
RUN:	RUN1094
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.23

EN300-05512_3_2



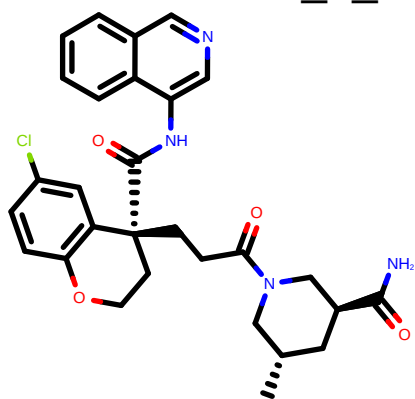
CID:	EN300-05512_3_2
SMILES:	<chem>c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)C(=O)C4C3C(C4)C(C(=O)Nc5ccccc5</chem>
RUN:	RUN1276
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.33

EN300-1238839_2_1



CID:	EN300-1238839_2_1
SMILES:	<chem>CS(=O)(=O)NCCOC[C@]1(C)C(=O)C2C1C(C2)C(C(=O)Nc3cnc4c3cccc4</chem>
RUN:	RUN283
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.39

EN300-1724086_2_2



CID:

EN300-1724086_2_2

SMILES:

C[C@H]1C[C@@H](CN(C1)C(=O)C[C@H]2(CCOc3c2cc(cc3)C(=O)Nc4nc5c6cccc5)C1=O)N

RUN:

RUN679

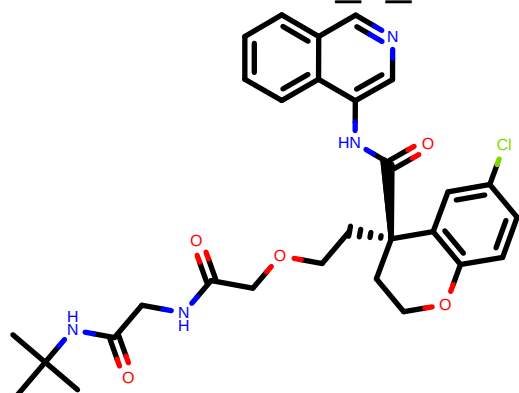
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

0.20

EN300-48760_3_1



CID:

EN300-48760_3_1

SMILES:

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

RUN:

RUN1164

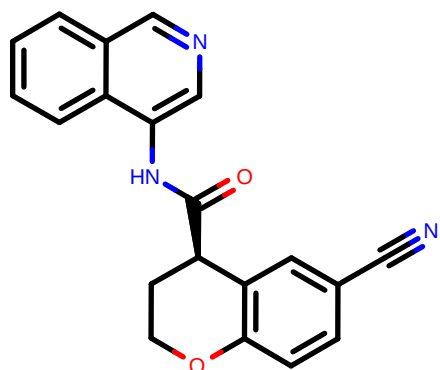
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

0.45

DAR-DIA-6a508060-3_1



CID:

DAR-DIA-6a508060-3_1

SMILES:

c1ccc2c(c1)nccc2NC(=O)[C@@H](C@H)3CCOC4c3cc(cc4)C#N

RUN:

RUN26

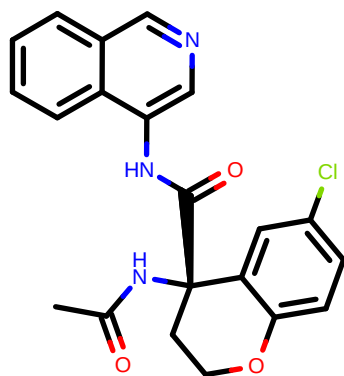
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

0.05

EN300-18074_1_1



CID:

EN300-18074_1_1

SMILES:

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

RUN:

RUN633

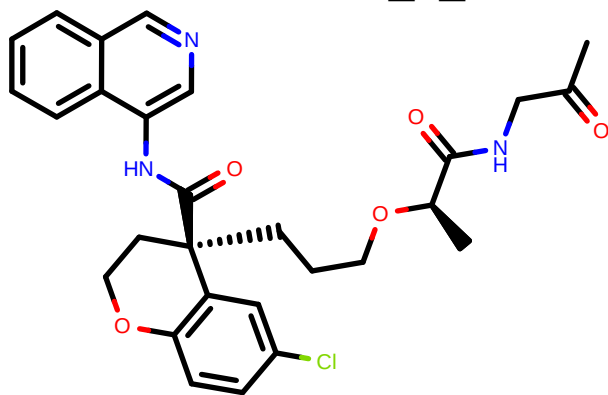
DDG (kcal/mol):

-0.15

dDDG (kcal/mol):

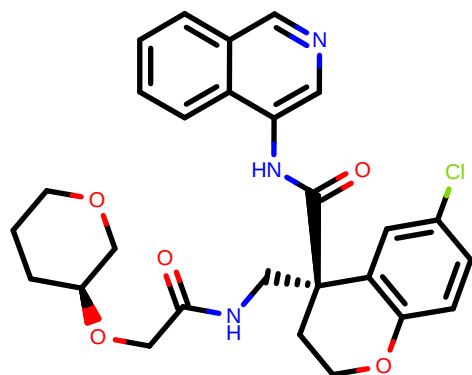
0.18

EN300-131093_4_2



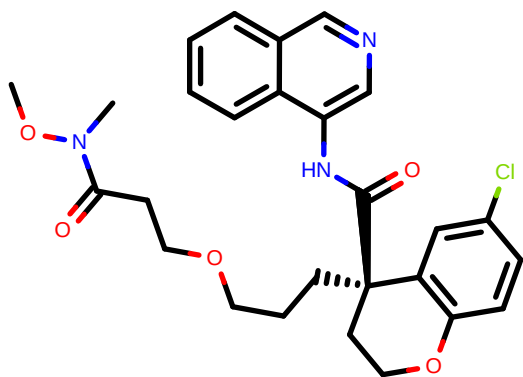
CID:	EN300-131093_4_2
SMILES:	<chem>CC(=O)N[C@@H](C(=O)NCC(=O)C)OCC[C@]1(C)C(=O)C2=CC(=CC=C2)C1C(=O)Nc3ncoc4c3ccoc4</chem>
RUN:	RUN1223
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.31

EN300-1627945_2_2



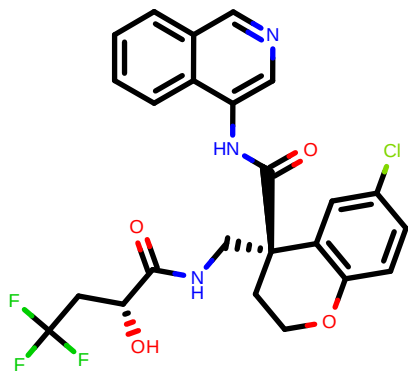
CID:	EN300-1627945_2_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4=CC(=CC=C4)C1CNC(=O)CO[C@H]5CCOC5</chem>
RUN:	RUN786
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.30

EN300-174603_4_1



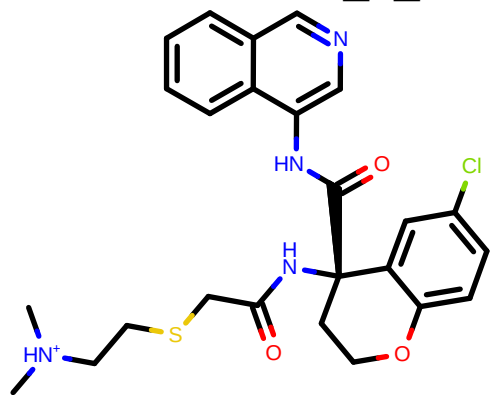
CID:	EN300-174603_4_1
SMILES:	<chem>CN(C(=O)CCOCC[C@]1(C)C(=O)C2=CC(=CC=C2)C1C(=O)Nc3ncoc4c3ccoc4)OC</chem>
RUN:	RUN967
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.31

EN300-1932013_2_1



CID:	EN300-1932013_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(=O)C4=CC(=CC=C4)C1CNC(=O)[C@@H](C(F)(F)F)O</chem>
RUN:	RUN1728
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.46

EN300-1708620_1_1



CID: EN300-1708620_1_1

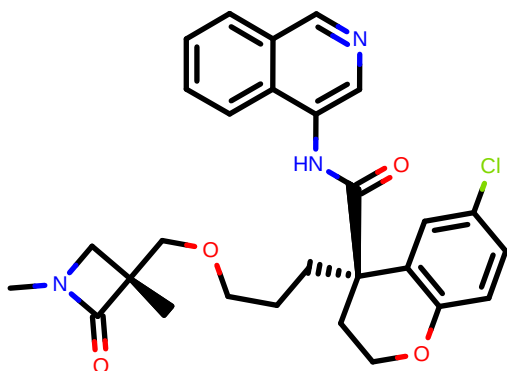
SMILES: C[NH+](C)CCSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN1109

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.39

EN300-1273362_4_1



CID: EN300-1273362_4_1

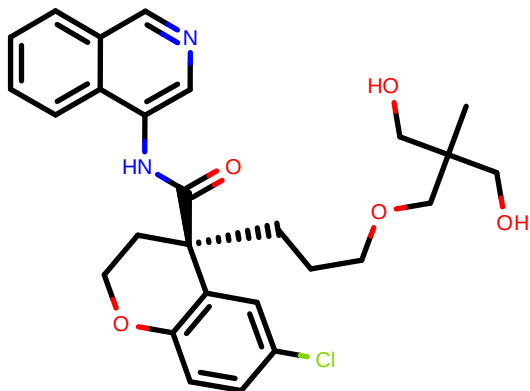
SMILES: C[C@@]1(CN(C1=O)C)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1471

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.46

EN300-218116_4_1



CID: EN300-218116_4_1

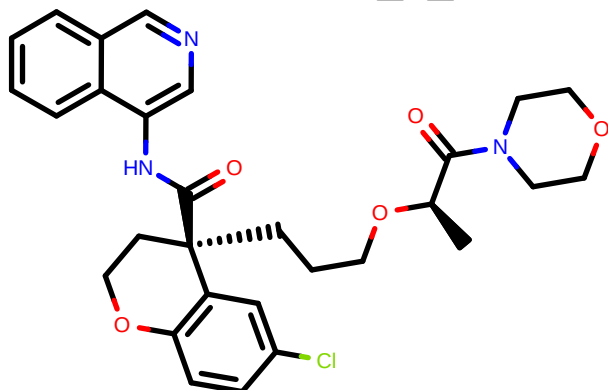
SMILES: CC(CO)(CO)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccccc4

RUN: RUN348

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.39

EN300-05754_4_2



CID: EN300-05754_4_2

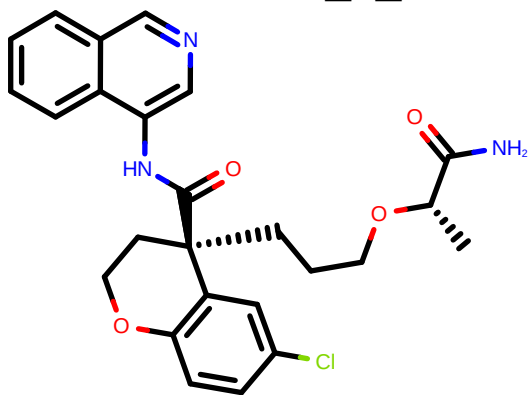
SMILES: C[C@H](C(=O)N1CCOCC1)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4ccccc5

RUN: RUN1263

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.41

EN300-17381_4_1



CID: EN300-17381_4_1

SMILES:

C[C@@H](C(=O)N)OCCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccoc4

RUN:

RUN1087

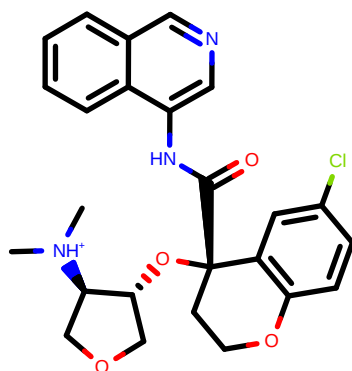
DDG (kcal/mol):

-0.14

dDDG (kcal/mol):

0.32

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)Nc4ncc5c4ccoc5

RUN:

RUN1336

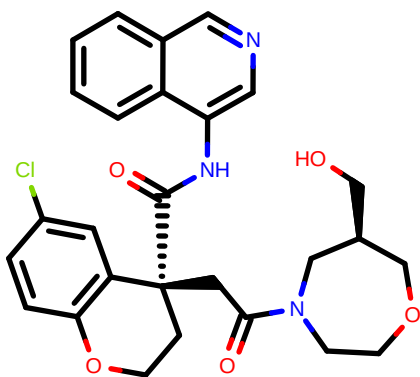
DDG (kcal/mol):

-0.13

dDDG (kcal/mol):

0.32

EN300-6478054_1_1



CID: EN300-6478054_1_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)CO

RUN:

RUN399

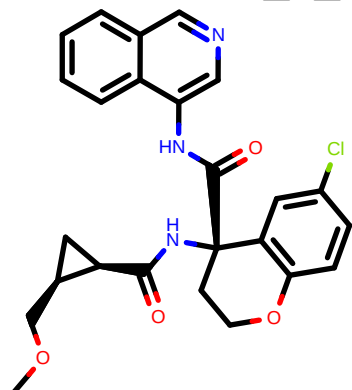
DDG (kcal/mol):

-0.13

dDDG (kcal/mol):

0.38

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)Nc4ncc5c4ccoc5

RUN:

RUN1692

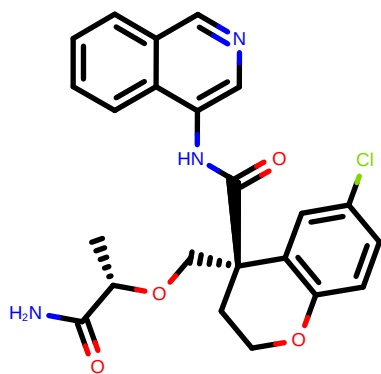
DDG (kcal/mol):

-0.13

dDDG (kcal/mol):

0.26

EN300-17381_2_1



CID: EN300-17381_2_1

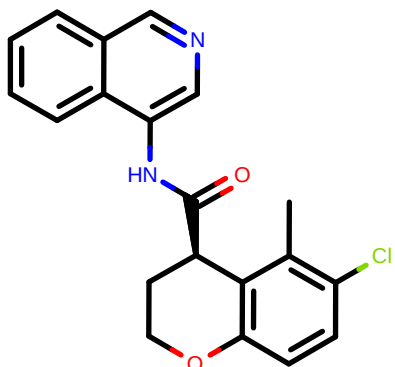
SMILES: C[C@@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN886

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.23

EDJ-MED-e4b030d8-8_1



CID: EDJ-MED-e4b030d8-8_1

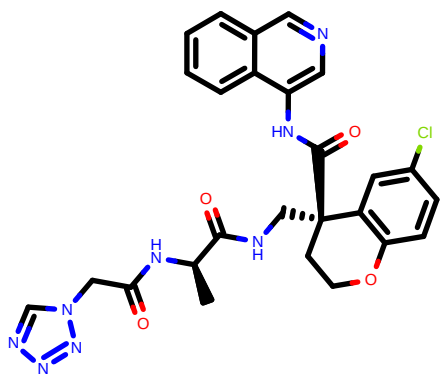
SMILES: Cc1c(ccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN44

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.07

EN300-649743_2_1



CID: EN300-649743_2_1

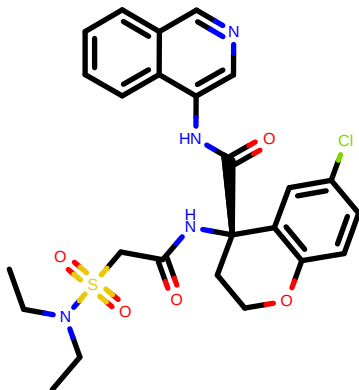
SMILES: C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)Cn5cnmn5

RUN: RUN1161

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.41

EN300-75819_1_1



CID: EN300-75819_1_1

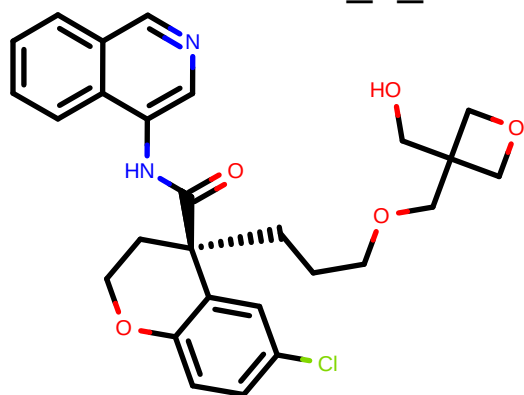
SMILES: CCN(CC)S(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN665

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.44

EN300-102347_4_1



CID:

EN300-102347_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCOC(C5COC5)CO

RUN:

RUN1095

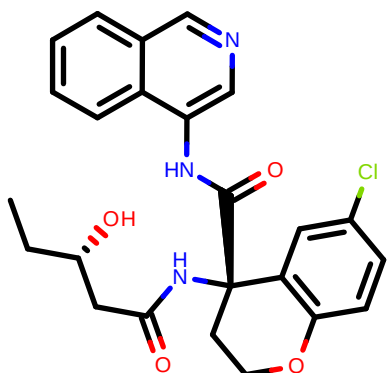
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

0.41

EN300-224741_1_1



CID:

EN300-224741_1_1

SMILES:

CC[C@@H](CC(=O)N[C@@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3ccccc4)O

RUN:

RUN1125

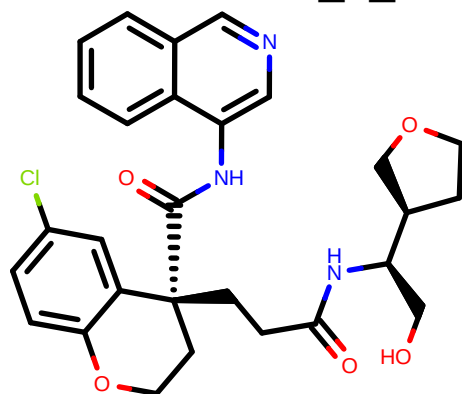
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

0.24

EN300-104493_2_2



CID:

EN300-104493_2_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)[C@@H]5COC5

RUN:

RUN1339

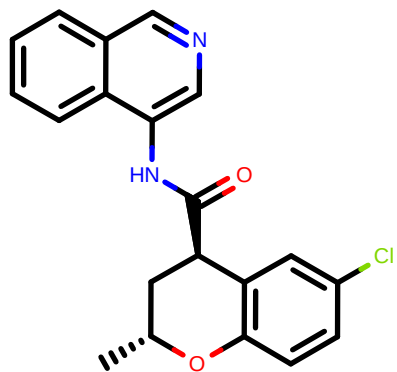
DDG (kcal/mol):

-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)Nc3cncnc4c3ccccc4

RUN:

RUN38

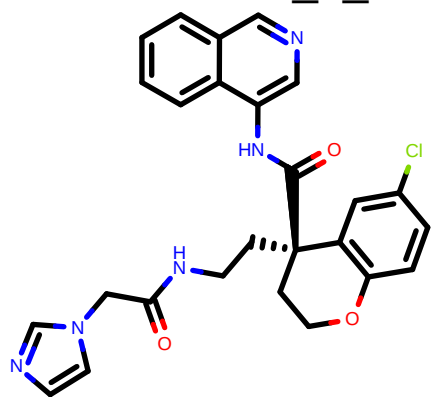
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

0.05

EN300-38979_3_1



CID:

EN300-38979_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cnc5

RUN:

RUN1394

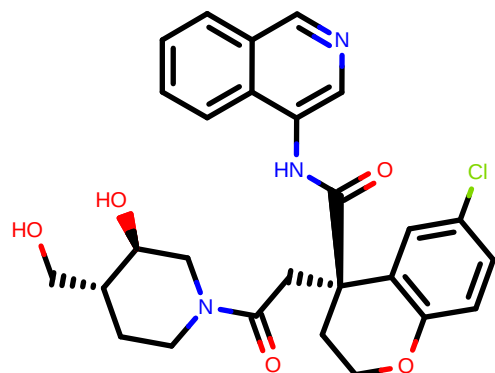
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

0.24

EN300-95639_1_3



CID:

EN300-95639_1_3

SMILES:

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

RUN:

RUN447

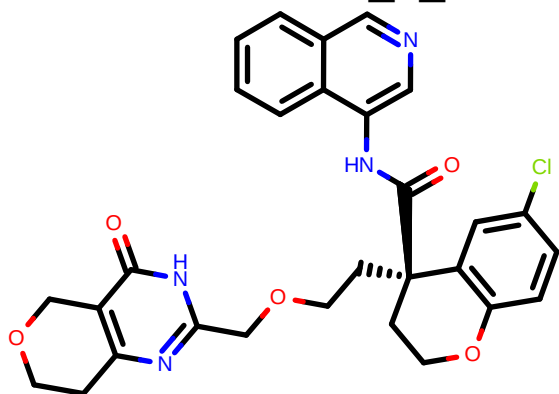
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

0.40

EN300-343103_3_1



CID:

EN300-343103_3_1

SMILES:

c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCc5[nH]c(=O)c6c(n5)CCOC6

RUN:

RUN1779

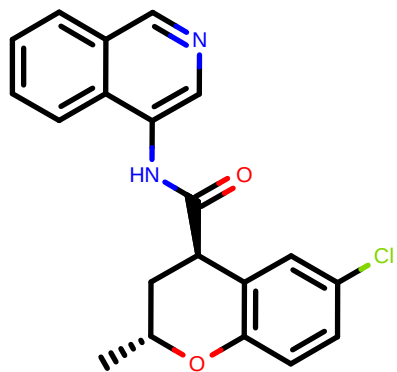
DDG (kcal/mol):

-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)C)C(=O)Nc3cnc4c3ccccc4

RUN:

RUN37

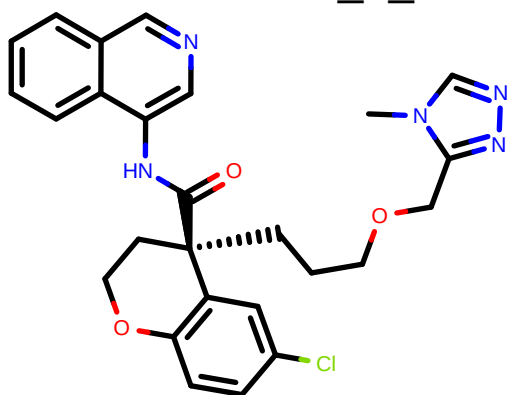
DDG (kcal/mol):

-0.12

dDDG (kcal/mol):

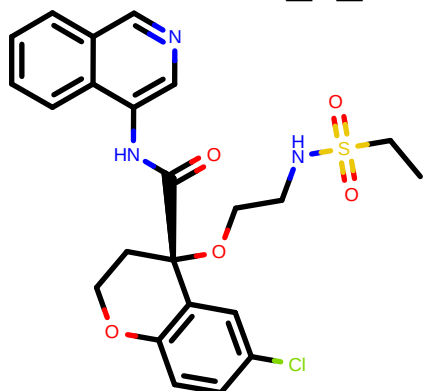
0.04

EN300-113112_4_1



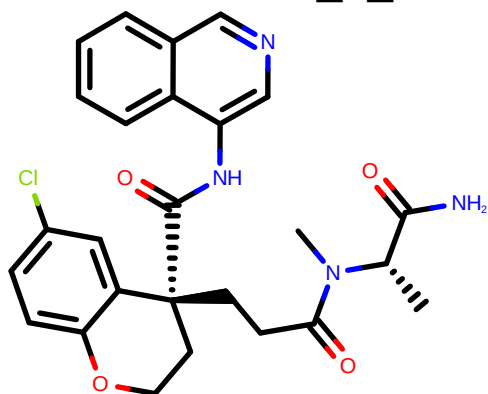
CID:	EN300-113112_4_1
SMILES:	<chem>Cn1ennc1COCCC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN824
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.37

EN300-73582_1_1



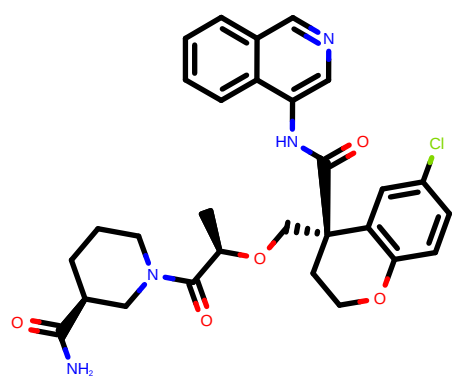
CID:	EN300-73582_1_1
SMILES:	<chem>CCS(=O)(=O)NCCO[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1080
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.40

EN300-125409_2_1



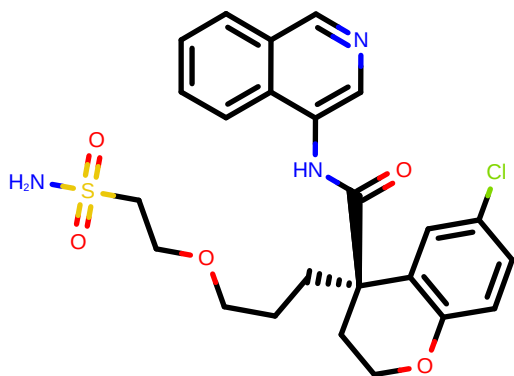
CID:	EN300-125409_2_1
SMILES:	<chem>C[C@]@H](C(=O)N)N(C)C(=O)CC[C@]1(CCOC2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN360
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.33

EN300-28177_2_2



CID:	EN300-28177_2_2
SMILES:	<chem>C[C@]H](C(=O)N)CCC[C@]@H](Cl)C(=O)NOC[C@]2(CCOC3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5</chem>
RUN:	RUN1302
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.44

EN300-270710_4_1



CID: EN300-270710_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)N

RUN:

RUN991

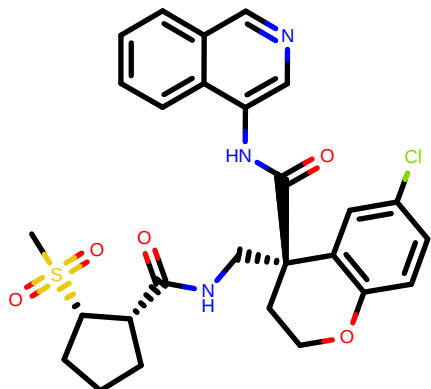
DDG (kcal/mol):

-0.10

dDDG (kcal/mol):

0.36

EN300-1387145_2_4



CID: EN300-1387145_2_4

SMILES:

CS(=O)(=O)[C@H]1CCC[C@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccccc5

RUN:

RUN1129

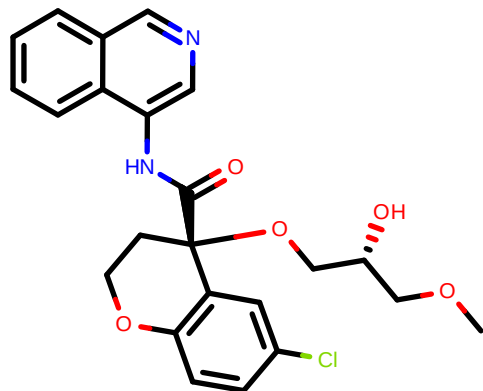
DDG (kcal/mol):

-0.10

dDDG (kcal/mol):

0.24

EN300-1915260_1_2



CID: EN300-1915260_1_2

SMILES:

COC[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3ccccc4)O

RUN:

RUN1480

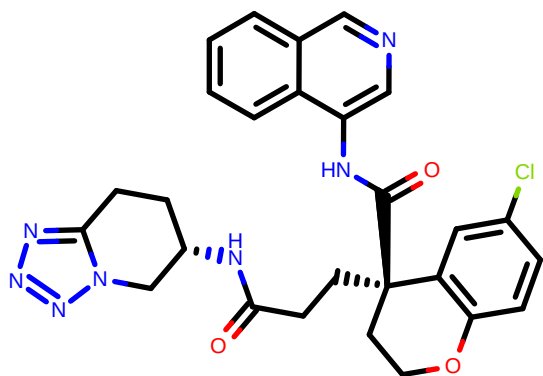
DDG (kcal/mol):

-0.10

dDDG (kcal/mol):

0.28

EN300-7444106_2_2



CID: EN300-7444106_2_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCc6nnnn6CS

RUN:

RUN1259

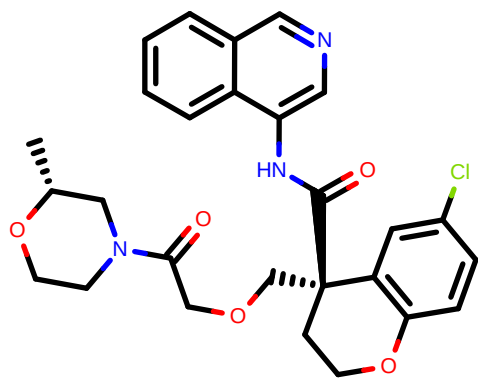
DDG (kcal/mol):

-0.10

dDDG (kcal/mol):

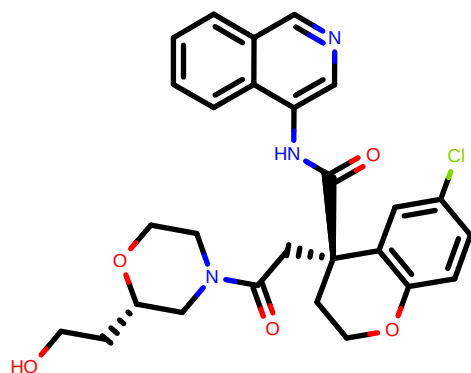
0.23

EN300-25572_2_1



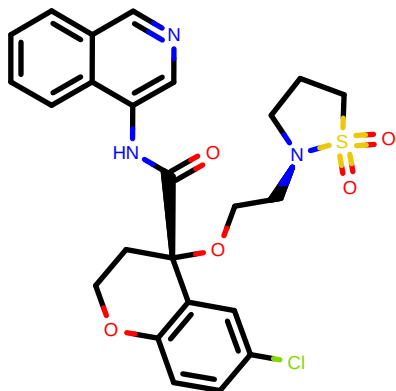
CID:	EN300-25572_2_1
SMILES:	<chem>C[C@@H]1CN(CCO1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4ccccc5</chem>
RUN:	RUN419
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.33

EN300-102007_1_2



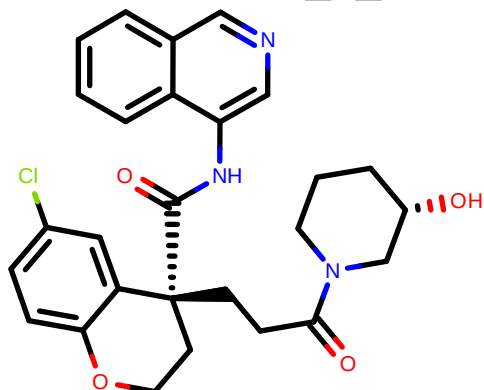
CID:	EN300-102007_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CCO</chem>
RUN:	RUN693
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.44

EN300-114134_1_1



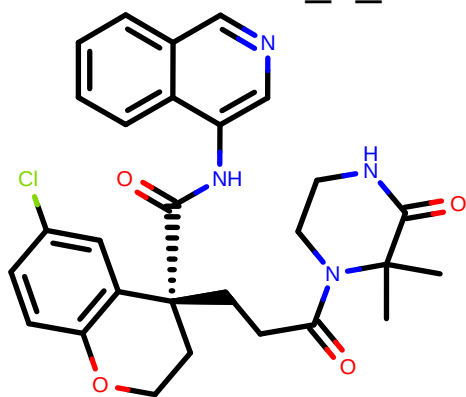
CID:	EN300-114134_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@]5SCC(=O)S(=O)(=O)O</chem>
RUN:	RUN856
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.27

EN300-20284_2_1



CID:	EN300-20284_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCC[C@H](C5)O</chem>
RUN:	RUN796
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.27

EN300-68882_2_1



CID: EN300-68882_2_1

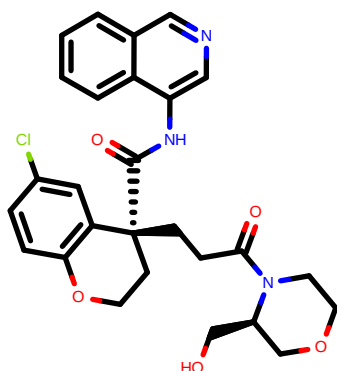
SMILES: CC1(C(=O)NCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncnc5c4cccc5)C

RUN: RUN804

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.35

EN300-173903_2_1



CID: EN300-173903_2_1

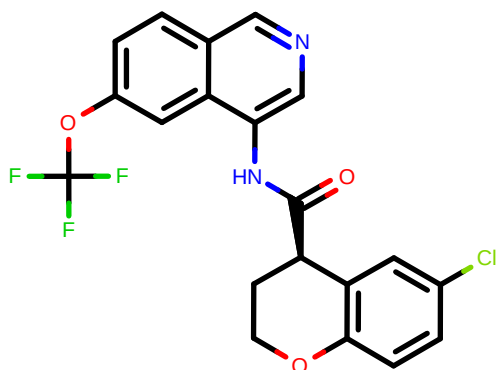
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@H]5CO

RUN: RUN1251

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.28

BEN-DND-c852c98b-2_1



CID: BEN-DND-c852c98b-2_1

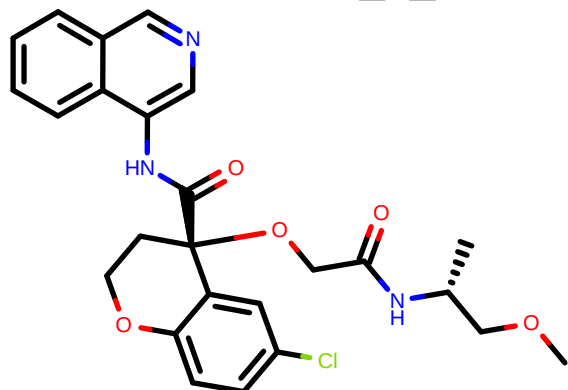
SMILES: c1cc2cncc(c2cc1OC(F)(F)F)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl

RUN: RUN61

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.07

EN300-02067_1_2



CID: EN300-02067_1_2

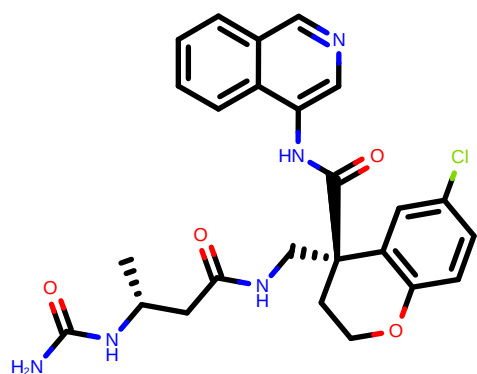
SMILES: C[C@H](COC)NC(=O)CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN1192

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.24

EN300-268198_2_2



CID: EN300-268198_2_2

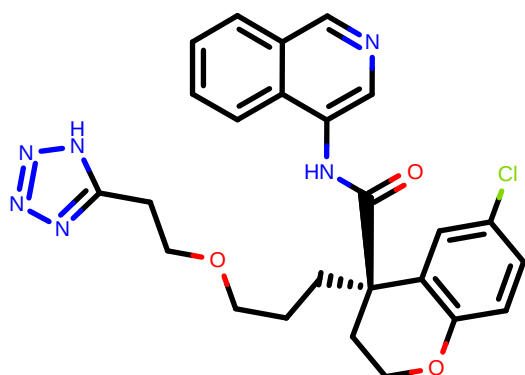
SMILES: C[C@H](CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ccc4c3ccc4NC(=O)N

RUN: RUN581

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.40

EN300-183231_4_1



CID: EN300-183231_4_1

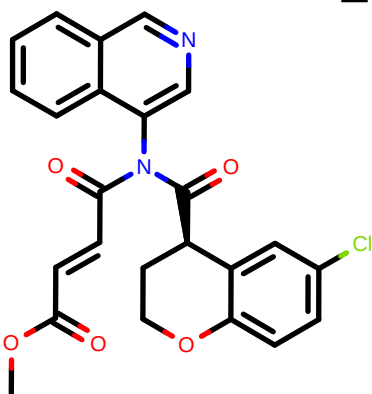
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5n[nH]n5

RUN: RUN1782

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.57

DAR-DIA-5ff57136-9_1



CID: DAR-DIA-5ff57136-9_1

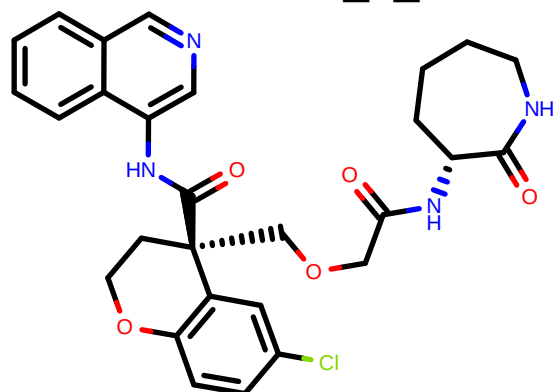
SMILES: COC(=O)/C=C/C(=O)N(c1cncc2c1ccc2)C(=O)[C@@H]3CCOCc4ccc(cc4)Cl

RUN: RUN256

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.26

EN300-37195_2_1



CID: EN300-37195_2_1

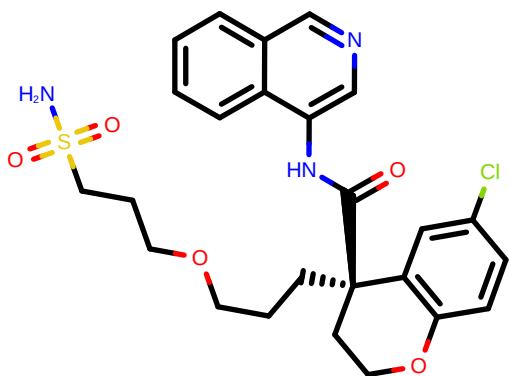
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN443

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.30

EN300-79588_4_1



CID:

EN300-79588_4_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](CCOC4C3CC(Cc4C)C)CCOC(=O)C(=O)N

RUN:

RUN539

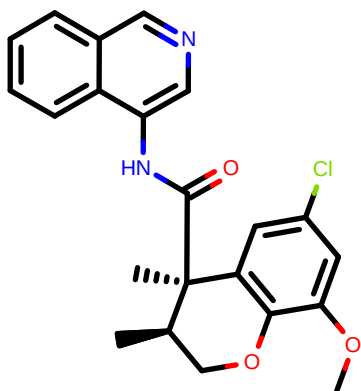
DDG (kcal/mol):

-0.06

dDDG (kcal/mol):

0.35

DAR-DIA-0d514e7d-26_1



CID:

DAR-DIA-0d514e7d-26_1

SMILES:

C[C@@H]1COC2C(Cc3cc(OC)Cl)[C@H]1(C)C(C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN215

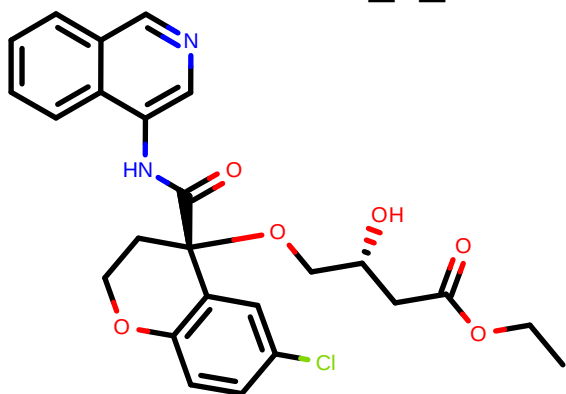
DDG (kcal/mol):

-0.06

dDDG (kcal/mol):

0.18

EN300-102988_1_1



CID:

EN300-102988_1_1

SMILES:

CCOC(=O)C[C@@H](C)[C@H]1COC2C1C(Cc3cc(OC)Cl)C(=O)Nc3ncnc4c3ccccc4O

RUN:

RUN968

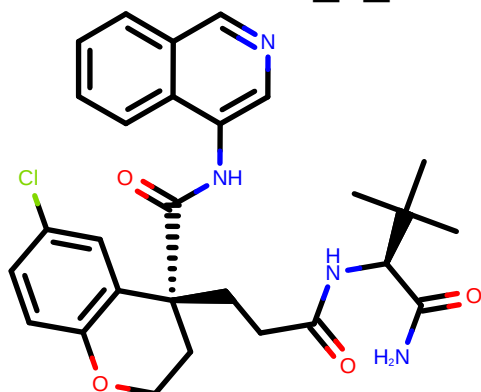
DDG (kcal/mol):

-0.06

dDDG (kcal/mol):

0.31

EN300-96001_2_1



CID:

EN300-96001_2_1

SMILES:

CC(C)(C)[C@@H](C(=O)N)NC(=O)CC[C@H]1C(COC2C1C(Cc3cc(OC)Cl)C(=O)Nc3ncnc4c3ccccc4

RUN:

RUN1027

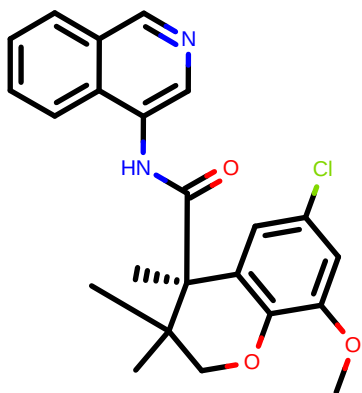
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

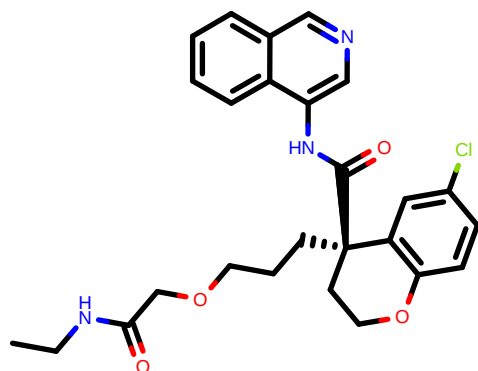
0.42

DAR-DIA-0d514e7d-27_1



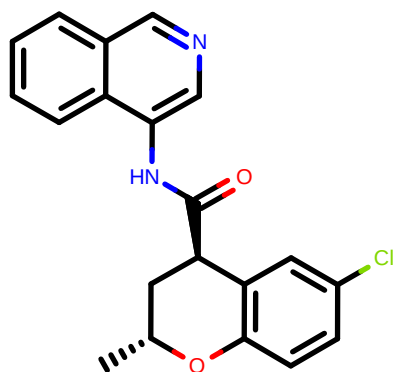
CID:	DAR-DIA-0d514e7d-27_1
SMILES:	<chem>C[C@@]1(c2cc(cc(c2OCC1(C)C)OC)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN172
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.19

EN300-7003350_4_1



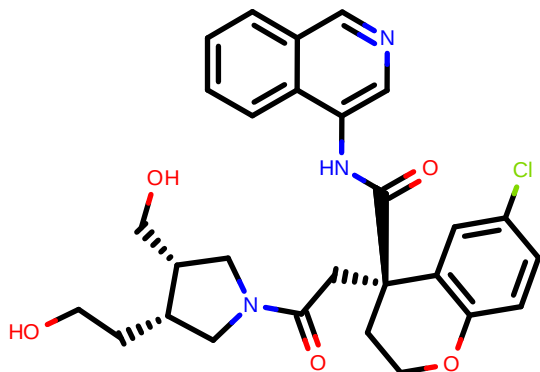
CID:	EN300-7003350_4_1
SMILES:	<chem>CCNC(=O)COCC[C@]1(c2cc(cc(c2OCC1(C)C)OC)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN1039
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

EDJ-MED-e4b030d8-2_1



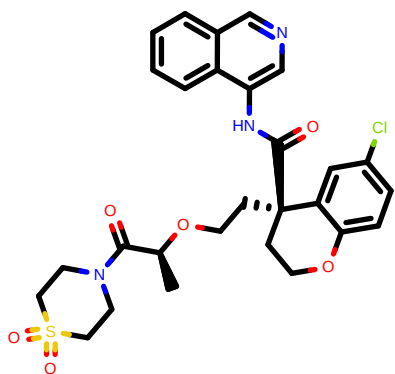
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN36
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.05

EN300-1425608_1_1



CID:	EN300-1425608_1_1
SMILES:	<chem>c1ccc2(c1)ncnc2N[C@@H]3C[C@@H](c4cc(ccc4OC)C)C(=O)N5C[C@@H]6[C@@H](C5)CO[C@H]6CO</chem>
RUN:	RUN375
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.38

EN300-1265949_3_1



CID:

EN300-1265949_3_1

SMILES:

C[C@@H](C(=O)N1CCS(=O)(=O)CC1)OC[C@H]2(COC3C2CC(=O)C3)C(=O)N4NCC5C4CCCC5

RUN:

RUN1188

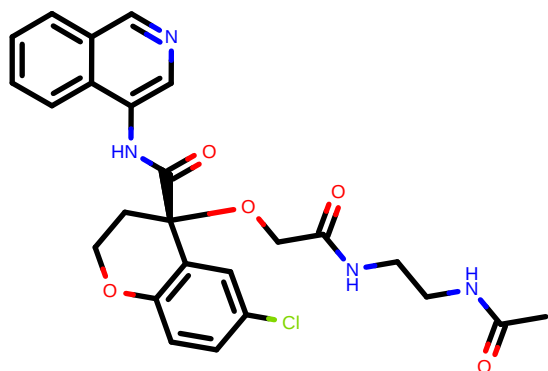
DDG (kcal/mol):

-0.05

dDDG (kcal/mol):

0.43

EN300-23129_1_1



CID:

EN300-23129_1_1

SMILES:

CC(=O)NCCNC(=O)CO[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN:

RUN1456

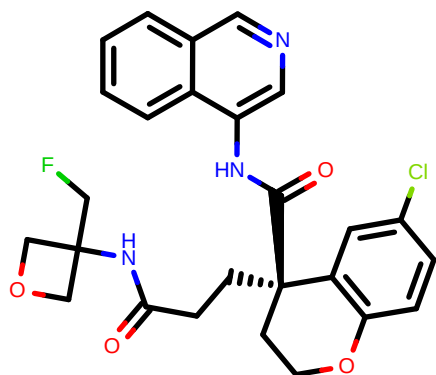
DDG (kcal/mol):

-0.04

dDDG (kcal/mol):

0.26

EN300-6970573_2_1



CID:

EN300-6970573_2_1

SMILES:

c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(COC5)CF

RUN:

RUN710

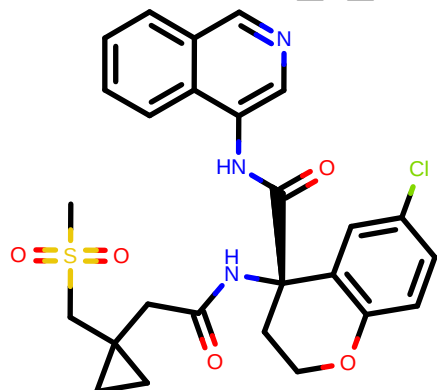
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

0.31

EN300-97904_1_1



CID:

EN300-97904_1_1

SMILES:

CS(=O)(=O)CC1(CC1)CC(=O)N[C@@H]2(CCOc3c2cc(cc3)Cl)C(=O)N4NCC5C4CCCC5

RUN:

RUN434

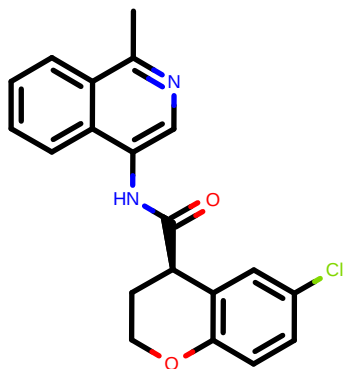
DDG (kcal/mol):

-0.03

dDDG (kcal/mol):

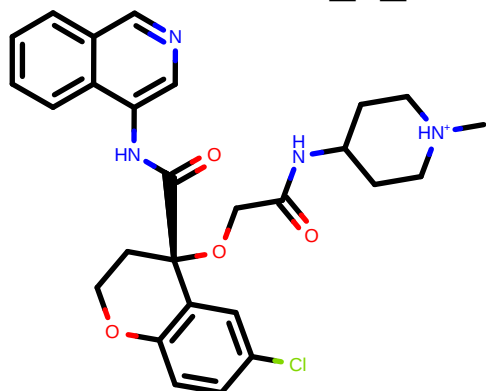
0.31

ADA-UCB-dc2b944c-12_1



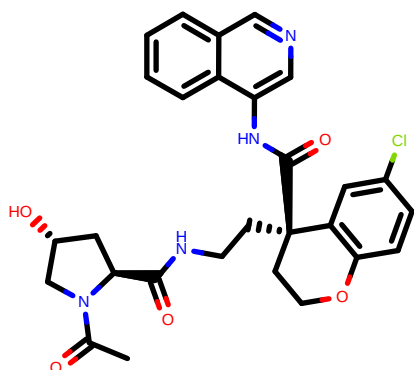
CID:	ADA-UCB-dc2b944c-12_1
SMILES:	<chem>Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl</chem>
RUN:	RUN64
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.08

EN300-342462_1_1



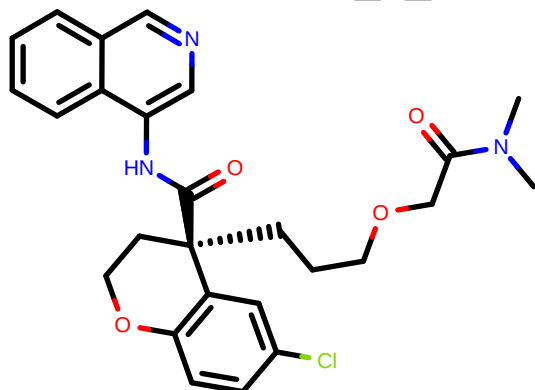
CID:	EN300-342462_1_1
SMILES:	<chem>C[NH+]1CCC(CC1)NC(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5</chem>
RUN:	RUN761
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.40

EN300-1703718_3_1



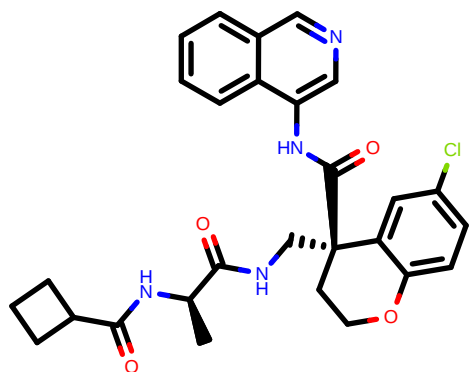
CID:	EN300-1703718_3_1
SMILES:	<chem>CC(=O)N1C[C@H](C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4nccc5c4cccc5O</chem>
RUN:	RUN740
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.31

EN300-216063_4_1



CID:	EN300-216063_4_1
SMILES:	<chem>CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3nccc4c3cccc4</chem>
RUN:	RUN635
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.32

EN300-66082_2_2



CID: EN300-66082_2_2

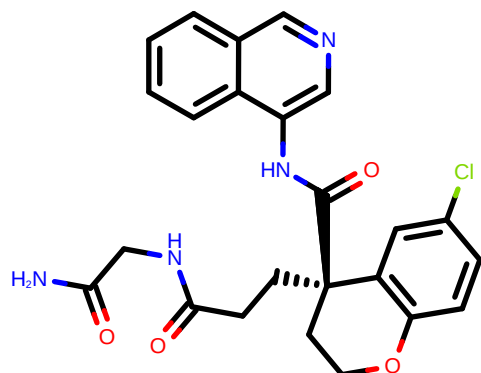
SMILES: C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)C)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCCS

RUN: RUN865

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.39

EN300-16216_2_1



CID: EN300-16216_2_1

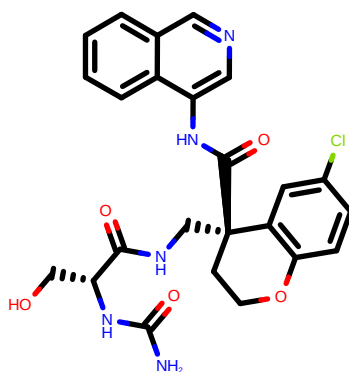
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(=O)N

RUN: RUN915

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.22

EN300-10170_2_1



CID: EN300-10170_2_1

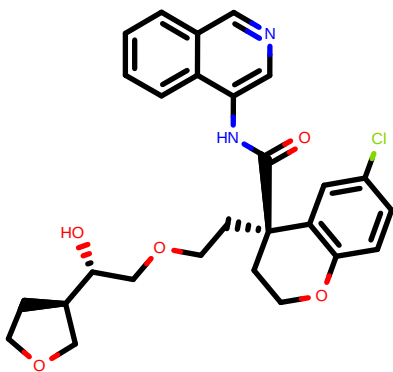
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](CO)NC(=O)N

RUN: RUN1449

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.33

EN300-1911992_3_2



CID: EN300-1911992_3_2

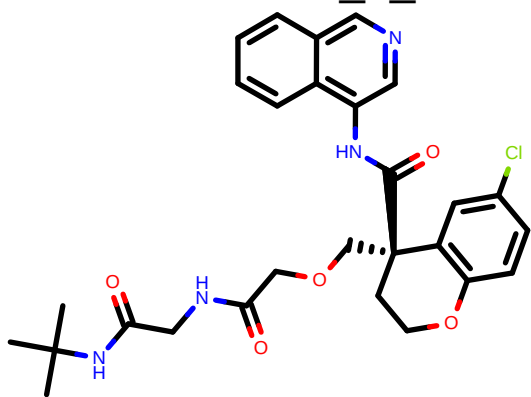
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)5CCOC5O

RUN: RUN337

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.34

EN300-48760_2_1



CID:	EN300-48760_2_1
SMILES:	<chem>CC(C)(C)NC(=O)CNC(=O)COC[C@H]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4</chem>
RUN:	RUN799
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.43