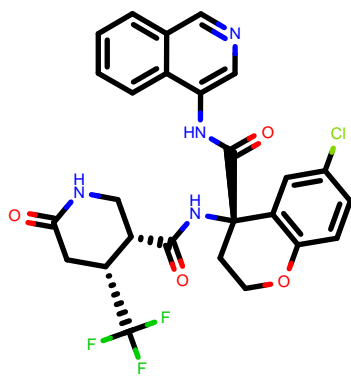


EN300-208959_1_2



CID: EN300-208959_1_2

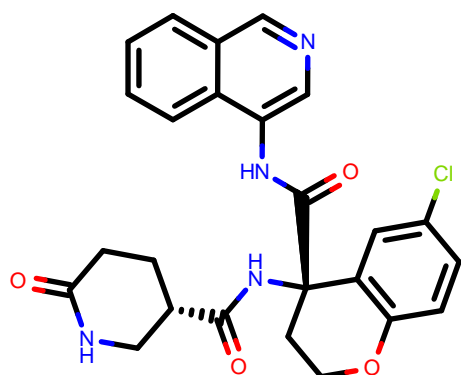
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)NC(=O)[C@H]5CNC(=O)C[C@@H]5C(F)(F)F

RUN: RUN8813

DDG (kcal/mol): -5.88

dDDG (kcal/mol): 0.15

EN300-42819_1_2



CID: EN300-42819_1_2

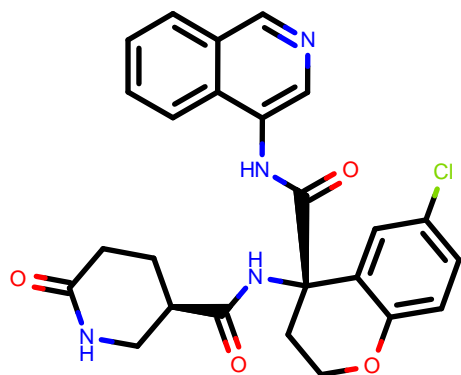
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)C)NC(=O)[C@H]5CCCC(=O)NCS

RUN: RUN4946

DDG (kcal/mol): -5.63

dDDG (kcal/mol): 0.25

EN300-42819_1_1



CID: EN300-42819_1_1

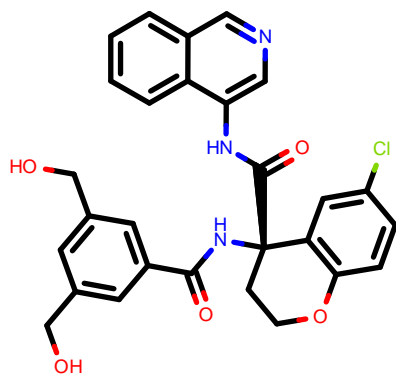
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)C)NC(=O)[C@H]5CCCC(=O)NCS

RUN: RUN4702

DDG (kcal/mol): -5.38

dDDG (kcal/mol): 0.27

EN300-211158_1_1



CID: EN300-211158_1_1

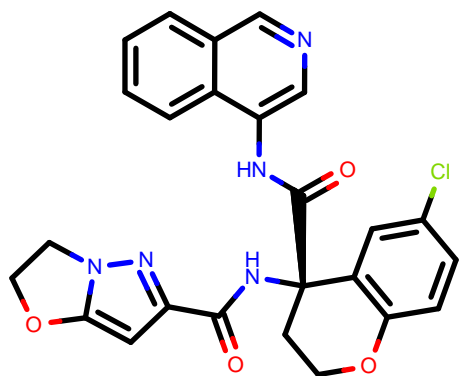
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)C)NC(=O)c5ccc(O)c(O)c5

RUN: RUN291

DDG (kcal/mol): -4.90

dDDG (kcal/mol): 0.25

EN300-181688_1_1



CID: EN300-181688_1_1

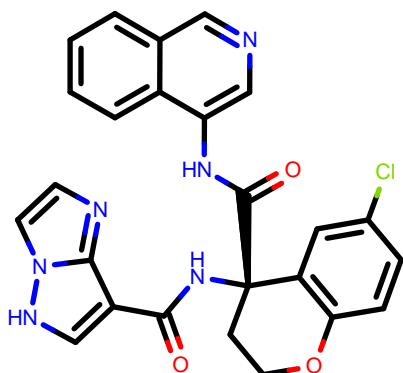
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6n(n5)CCO6

RUN: RUN2837

DDG (kcal/mol): -4.76

dDDG (kcal/mol): 0.18

EN300-135238_1_1



CID: EN300-135238_1_1

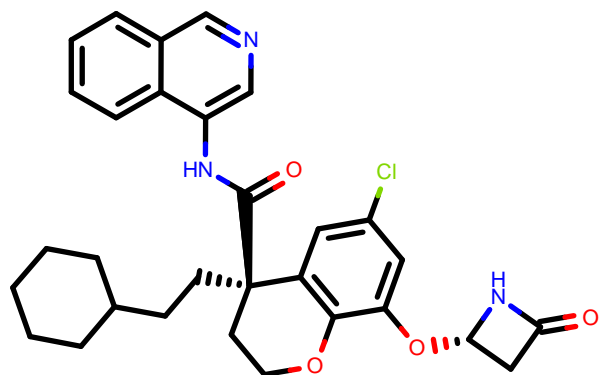
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]n6c5nc6

RUN: RUN4978

DDG (kcal/mol): -4.57

dDDG (kcal/mol): 0.20

VLA-UCB-50c39ae8-9_2



CID: VLA-UCB-50c39ae8-9_2

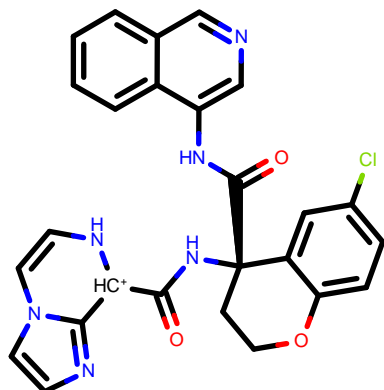
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)[H]5CC(=O)N5)C)COC6CCCC6

RUN: RUN8

DDG (kcal/mol): -4.51

dDDG (kcal/mol): 0.27

EN300-225012_1_1



CID: EN300-225012_1_1

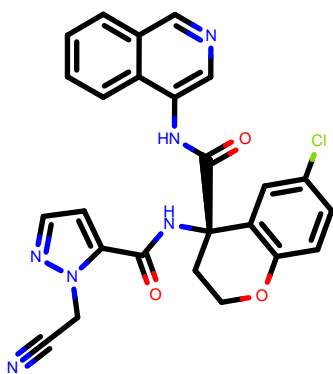
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6nccn6ccn5

RUN: RUN7040

DDG (kcal/mol): -4.43

dDDG (kcal/mol): 0.20

EN300-373791_1_1



CID: EN300-373791_1_1

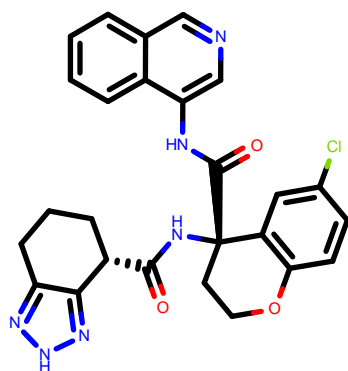
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn5CC#N

RUN: RUN7136

DDG (kcal/mol): -4.31

dDDG (kcal/mol): 0.20

EN300-208236_1_2



CID: EN300-208236_1_2

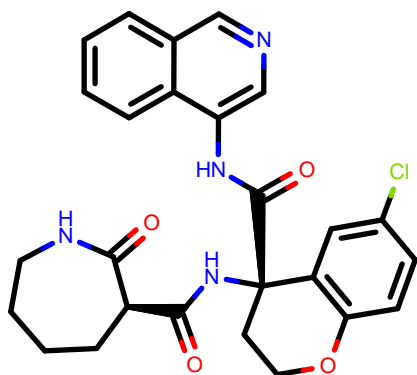
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6c5n[nH]6

RUN: RUN8913

DDG (kcal/mol): -4.30

dDDG (kcal/mol): 0.24

EN300-6737762_1_2



CID: EN300-6737762_1_2

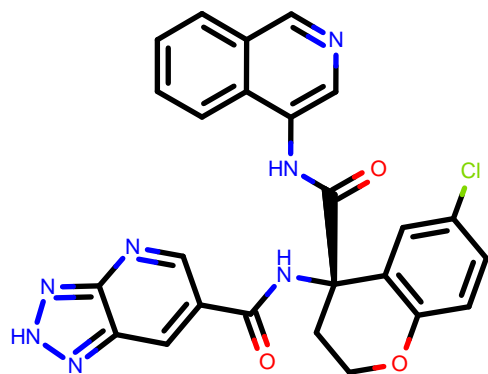
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCCCNC5=O

RUN: RUN523

DDG (kcal/mol): -4.28

dDDG (kcal/mol): 0.20

EN300-124555_1_1



CID: EN300-124555_1_1

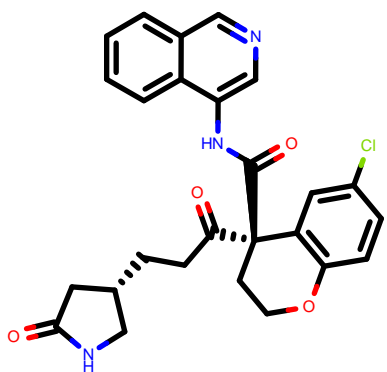
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6c(nc5)n[nH]6

RUN: RUN4302

DDG (kcal/mol): -4.22

dDDG (kcal/mol): 0.18

VLA-UCB-34f3ed0c-21_2



CID: VLA-UCB-34f3ed0c-21_2

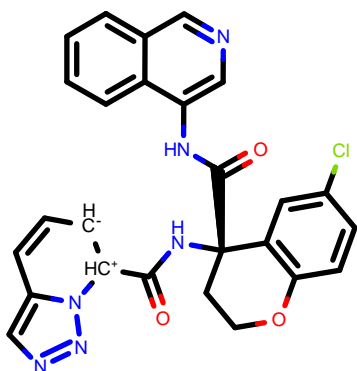
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NCS

RUN: RUN38

DDG (kcal/mol): -4.18

dDDG (kcal/mol): 0.26

EN300-2010167_1_1



CID: EN300-2010167_1_1

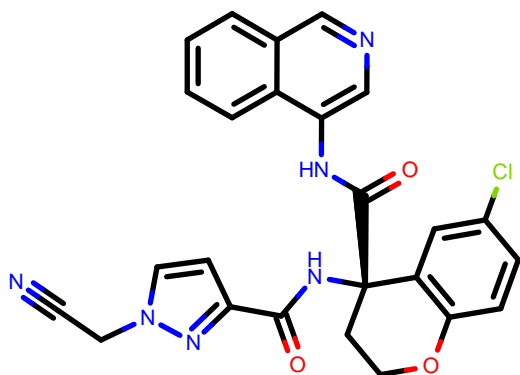
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6n5nnc6

RUN: RUN1289

DDG (kcal/mol): -4.17

dDDG (kcal/mol): 0.23

EN300-1251424_1_1



CID: EN300-1251424_1_1

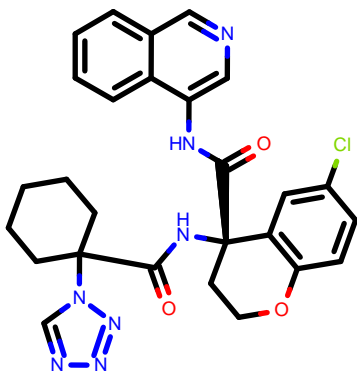
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(n5)CC#N

RUN: RUN5622

DDG (kcal/mol): -4.13

dDDG (kcal/mol): 0.20

EN300-186536_1_1



CID: EN300-186536_1_1

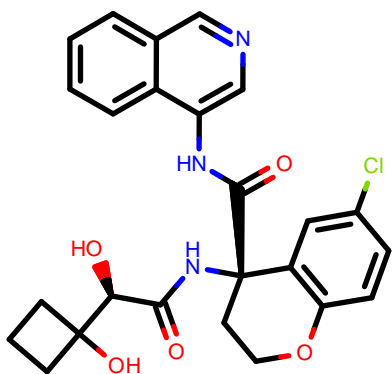
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCCC5)n6nncn6

RUN: RUN7500

DDG (kcal/mol): -4.12

dDDG (kcal/mol): 0.25

EN300-1073320_1_1



CID: EN300-1073320_1_1

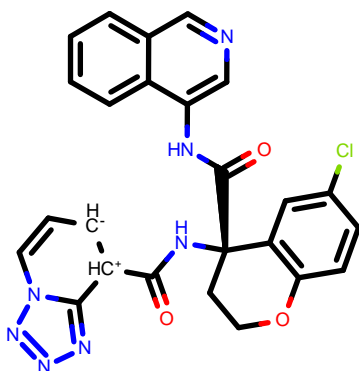
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN2344

DDG (kcal/mol): -4.11

dDDG (kcal/mol): 0.25

EN300-305984_1_1



CID: EN300-305984_1_1

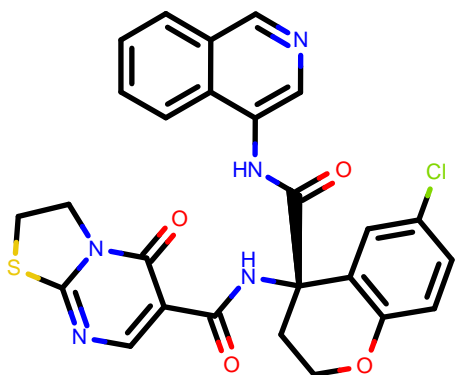
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnnc5nm6

RUN: RUN1353

DDG (kcal/mol): -4.09

dDDG (kcal/mol): 0.23

EN300-14405_1_1



CID: EN300-14405_1_1

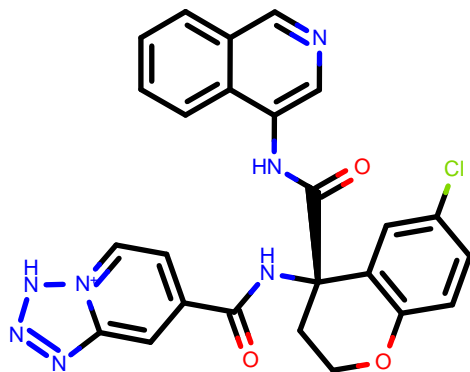
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncn6(c5=O)CCS6

RUN: RUN4934

DDG (kcal/mol): -4.05

dDDG (kcal/mol): 0.22

EN300-305567_1_1



CID: EN300-305567_1_1

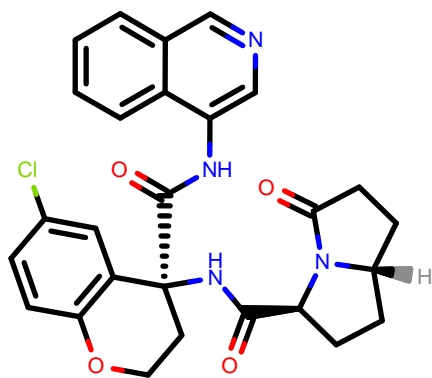
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn6(c5)nm6

RUN: RUN5374

DDG (kcal/mol): -3.99

dDDG (kcal/mol): 0.22

EN300-6479181_1_1



CID: EN300-6479181_1_1

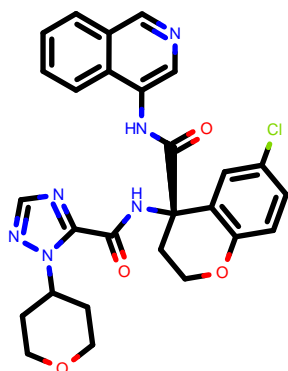
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@@H5CC[C@@H]6NSC(=O)CC6

RUN: RUN8761

DDG (kcal/mol): -3.98

dDDG (kcal/mol): 0.31

EN300-6732590_1_1



CID: EN300-6732590_1_1

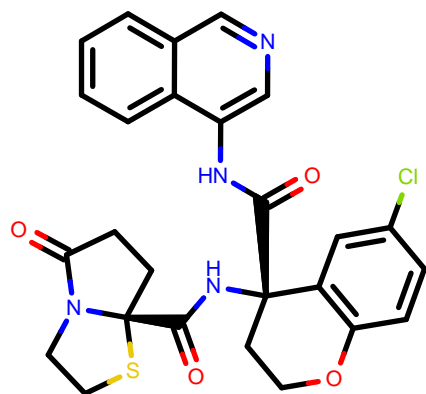
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nncn5C6CCOCC6

RUN: RUN9549

DDG (kcal/mol): -3.92

dDDG (kcal/mol): 0.22

EN300-10334_1_2



CID: EN300-10334_1_2

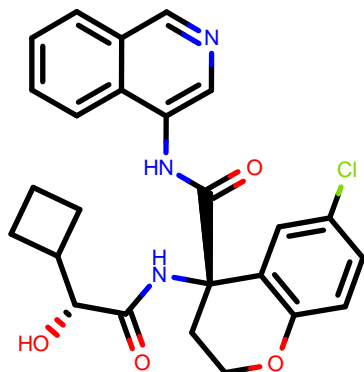
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@]56CCCC(=O)N5CCS6

RUN: RUN8156

DDG (kcal/mol): -3.90

dDDG (kcal/mol): 0.29

EN300-249764_1_1



CID: EN300-249764_1_1

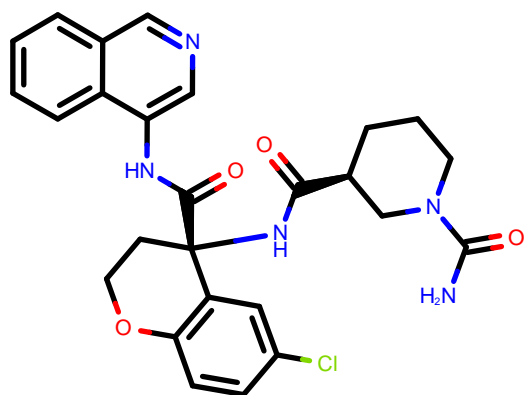
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C5CC5)O

RUN: RUN6070

DDG (kcal/mol): -3.89

dDDG (kcal/mol): 0.24

EN300-14767_1_2



CID: EN300-14767_1_2

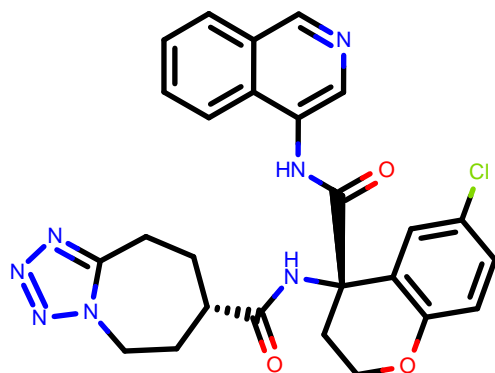
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCN(C5)C(=O)N

RUN: RUN6277

DDG (kcal/mol): -3.84

dDDG (kcal/mol): 0.25

EN300-253571_1_2



CID: EN300-253571_1_2

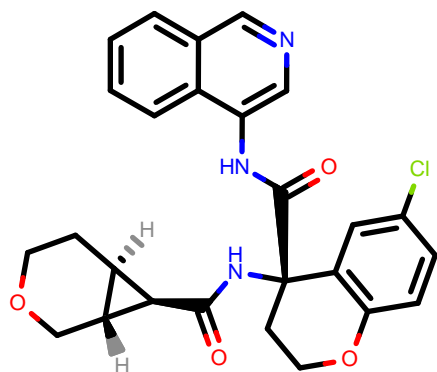
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC6C6nnn6CC5

RUN: RUN8685

DDG (kcal/mol): -3.83

dDDG (kcal/mol): 0.24

EN300-1644723_1_7



CID: EN300-1644723_1_7

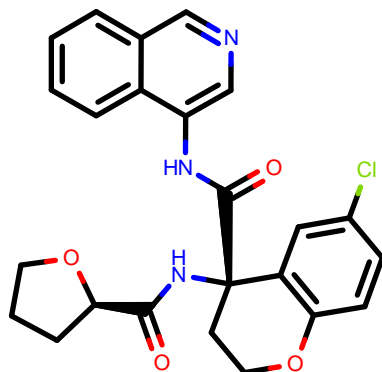
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H]6[C@H]5CCO6

RUN: RUN8829

DDG (kcal/mol): -3.77

dDDG (kcal/mol): 0.24

EN300-21009_1_2



CID: EN300-21009_1_2

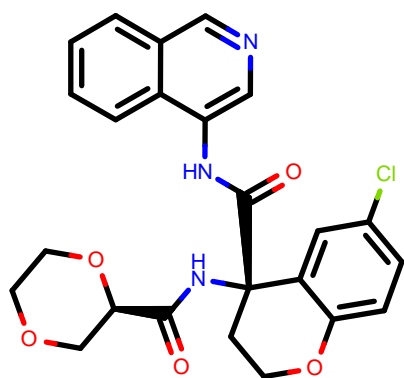
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC5

RUN: RUN4990

DDG (kcal/mol): -3.75

dDDG (kcal/mol): 0.20

EN300-36158_1_2



CID: EN300-36158_1_2

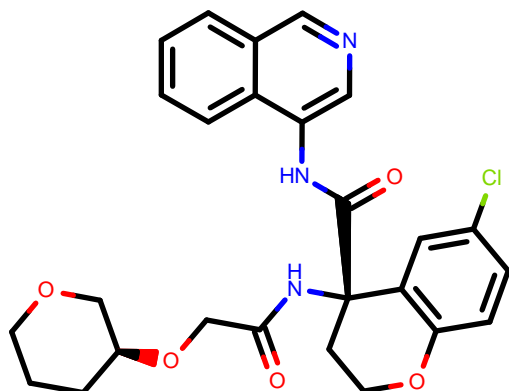
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COCOC5

RUN: RUN5850

DDG (kcal/mol): -3.75

dDDG (kcal/mol): 0.19

EN300-1627945_1_2



CID: EN300-1627945_1_2

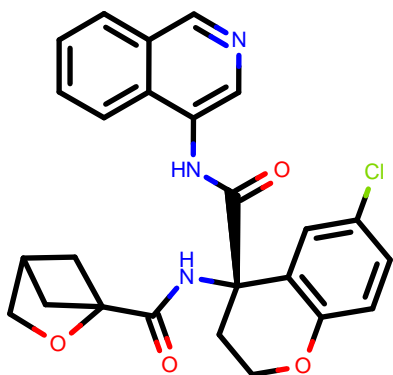
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@H]5COCOC5

RUN: RUN1201

DDG (kcal/mol): -3.75

dDDG (kcal/mol): 0.21

EN300-2007648_1_1



CID: EN300-2007648_1_1

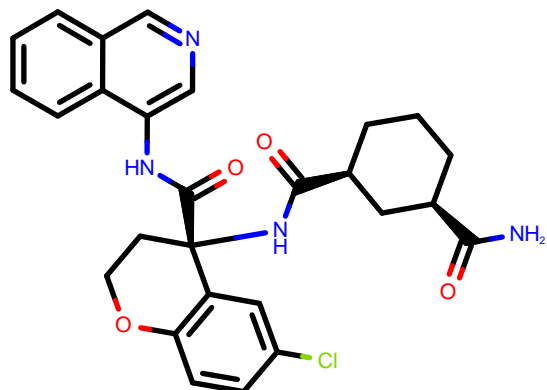
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(C5)CO6

RUN: RUN2512

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.21

EN300-90142_1_4



CID: EN300-90142_1_4

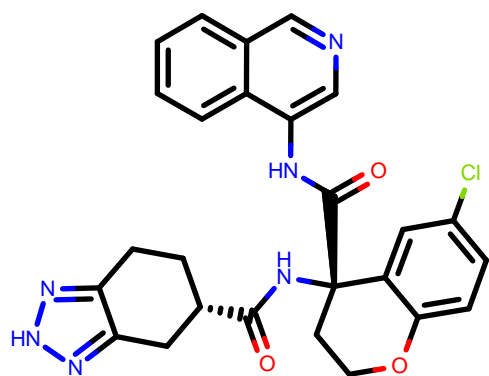
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](C5)C(=O)N

RUN: RUN5414

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.33

EN300-185729_1_1



CID: EN300-185729_1_1

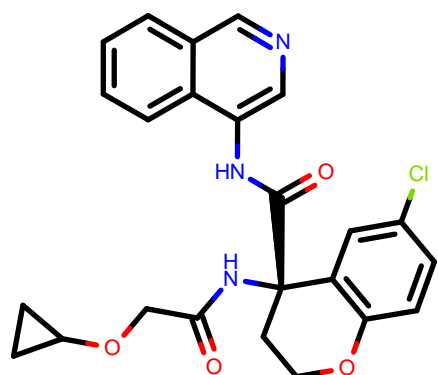
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6c(n[nH]6)C5

RUN: RUN3566

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.22

EN300-378373_1_1



CID: EN300-378373_1_1

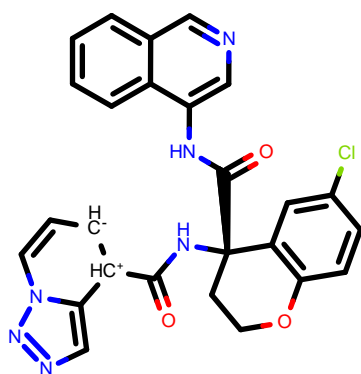
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)COC5CC5

RUN: RUN3286

DDG (kcal/mol): -3.74

dDDG (kcal/mol): 0.18

EN300-1074262_1_1



CID: EN300-1074262_1_1

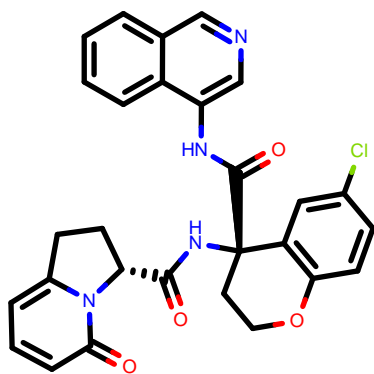
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc[nH5]n6

RUN: RUN1417

DDG (kcal/mol): -3.73

dDDG (kcal/mol): 0.20

EN300-332002_1_2



CID: EN300-332002_1_2

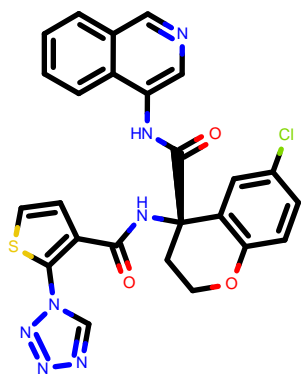
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6n5c(=O)ccc6

RUN: RUN9751

DDG (kcal/mol): -3.72

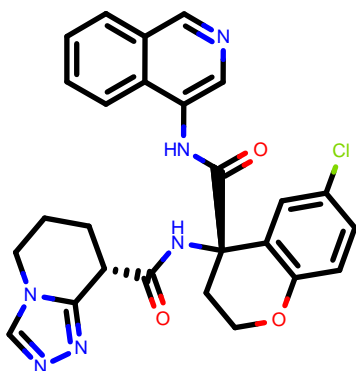
dDDG (kcal/mol): 0.29

EN300-6744029_1_1



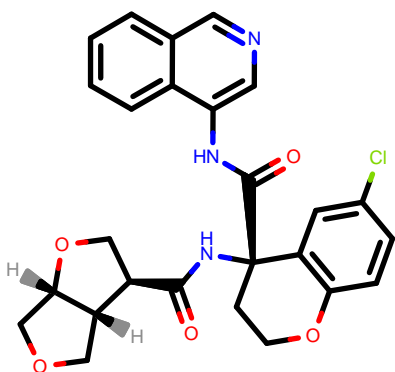
CID:	EN300-6744029_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccsc5n6nmn6</chem>
RUN:	RUN2386
DDG (kcal/mol):	-3.72
dDDG (kcal/mol):	0.20

EN300-748981_1_2



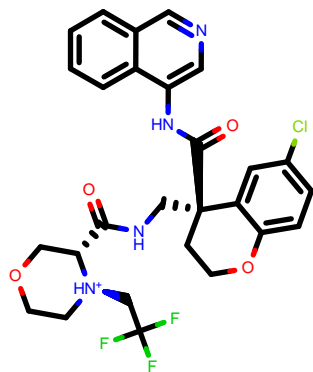
CID:	EN300-748981_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCc6n6c5nm6</chem>
RUN:	RUN8713
DDG (kcal/mol):	-3.70
dDDG (kcal/mol):	0.26

EN300-6482296_1_7



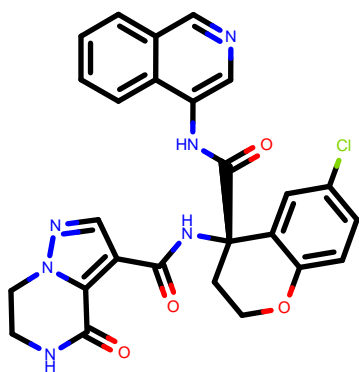
CID:	EN300-6482296_1_7
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5SC[C@@]5H5C[C@@]6H5C[C@@]6</chem>
RUN:	RUN5730
DDG (kcal/mol):	-3.64
dDDG (kcal/mol):	0.24

EN300-201551_2_4



CID:	EN300-201551_2_4
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5C[C@@]5N8[C@@]5C(F)(F)F</chem>
RUN:	RUN7717
DDG (kcal/mol):	-3.64
dDDG (kcal/mol):	0.27

EN300-6526669_1_1



CID: EN300-6526669_1_1

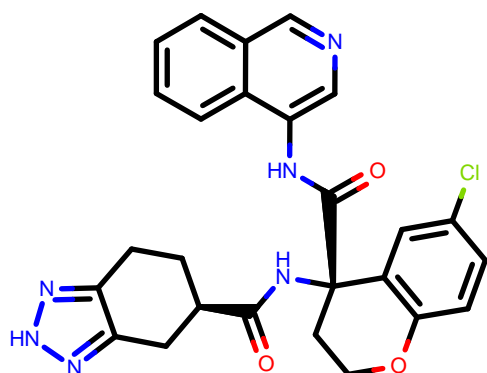
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5enn6c5C(=O)NCC6

RUN: RUN5034

DDG (kcal/mol): -3.60

dDDG (kcal/mol): 0.19

EN300-185729_1_2



CID: EN300-185729_1_2

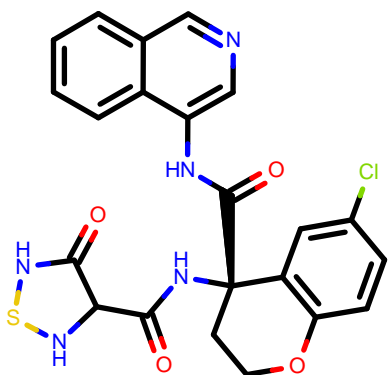
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5COCc6c(n[nH]n6)C5

RUN: RUN2111

DDG (kcal/mol): -3.58

dDDG (kcal/mol): 0.22

EN300-261859_1_1



CID: EN300-261859_1_1

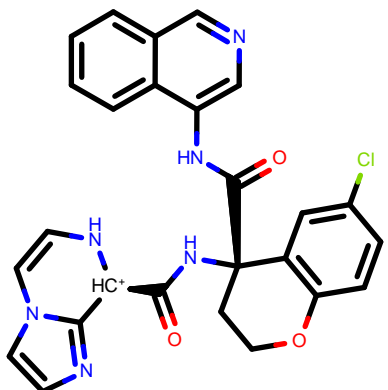
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(=O)[nH]sn5

RUN: RUN1761

DDG (kcal/mol): -3.58

dDDG (kcal/mol): 0.18

EN300-225012_1_1



CID: EN300-225012_1_1

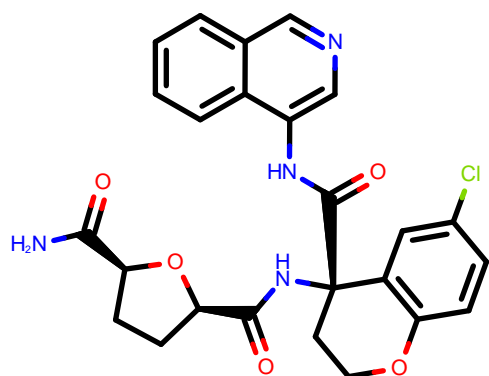
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6nccn6ccn5

RUN: RUN7044

DDG (kcal/mol): -3.58

dDDG (kcal/mol): 0.19

EN300-315238_1_1



CID: EN300-315238_1_1

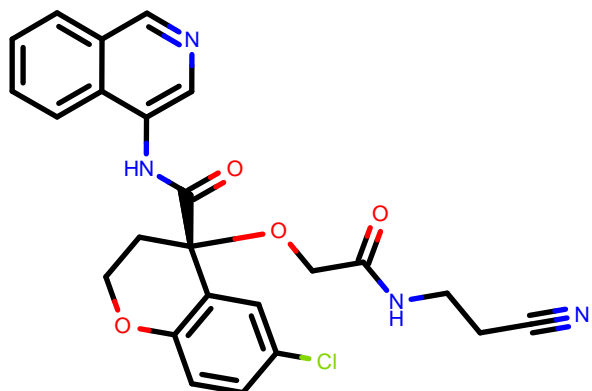
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](O5)C(=O)N

RUN: RUN8621

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.21

EN300-10895_1_1



CID: EN300-10895_1_1

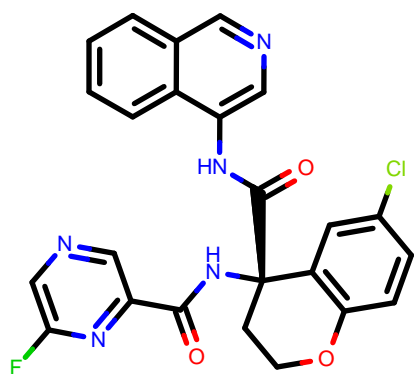
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCC#N

RUN: RUN967

DDG (kcal/mol): -3.57

dDDG (kcal/mol): 0.20

EN300-373552_1_1



CID: EN300-373552_1_1

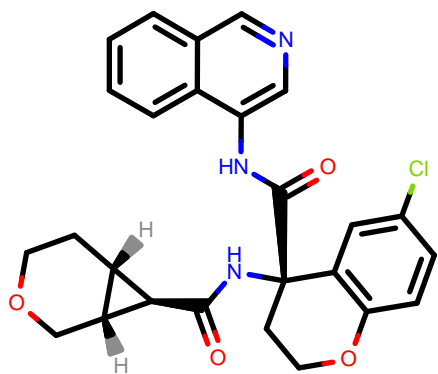
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncc(n5)F

RUN: RUN2802

DDG (kcal/mol): -3.53

dDDG (kcal/mol): 0.19

EN300-1644723_1_5



CID: EN300-1644723_1_5

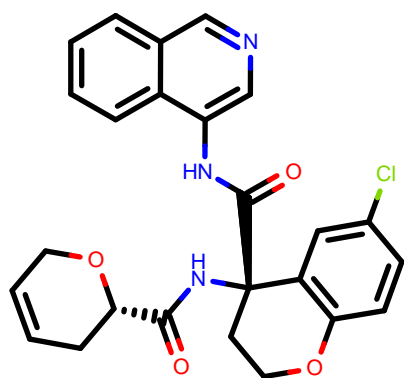
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](O5)C(=O)N

RUN: RUN4898

DDG (kcal/mol): -3.53

dDDG (kcal/mol): 0.21

EN300-378044_1_1



CID: EN300-378044_1_1

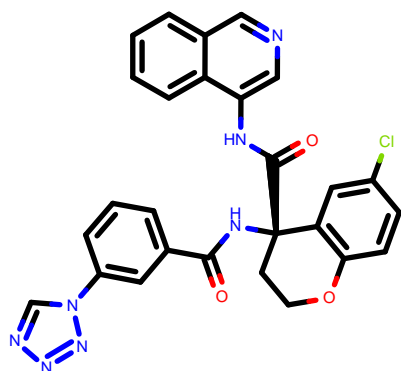
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC=CCO5

RUN: RUN7312

DDG (kcal/mol): -3.52

dDDG (kcal/mol): 0.21

EN300-09239_1_1



CID: EN300-09239_1_1

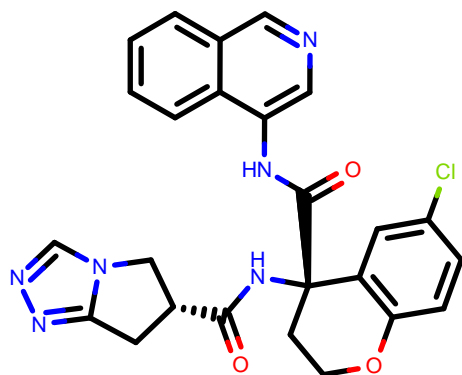
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5n6cnm6

RUN: RUN2827

DDG (kcal/mol): -3.51

dDDG (kcal/mol): 0.23

EN300-6745453_1_1



CID: EN300-6745453_1_1

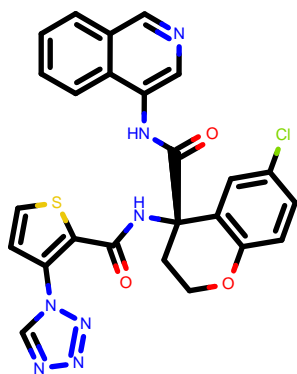
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C6c6nnm6C5

RUN: RUN9509

DDG (kcal/mol): -3.50

dDDG (kcal/mol): 0.23

EN300-36731_1_1



CID: EN300-36731_1_1

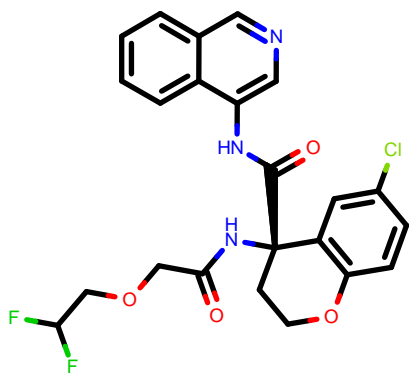
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(csc5)n6cnm6

RUN: RUN1026

DDG (kcal/mol): -3.48

dDDG (kcal/mol): 0.20

EN300-315792_1_1



CID: EN300-315792_1_1

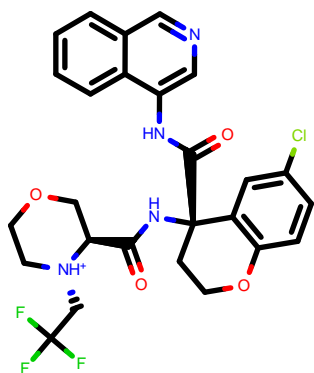
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F

RUN: RUN5290

DDG (kcal/mol): -3.45

dDDG (kcal/mol): 0.20

EN300-201551_1_1



CID: EN300-201551_1_1

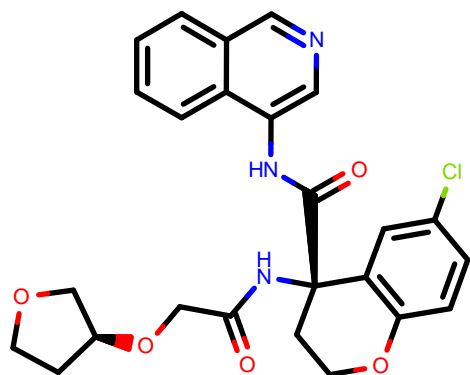
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5COC(F)F

RUN: RUN8100

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.28

EN300-99391_1_2



CID: EN300-99391_1_2

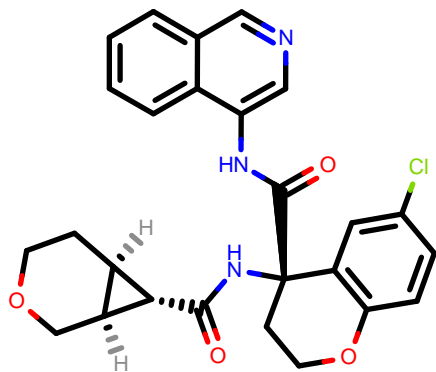
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@H]5COC(=O)C5

RUN: RUN2526

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.20

EN300-1644723_1_4



CID: EN300-1644723_1_4

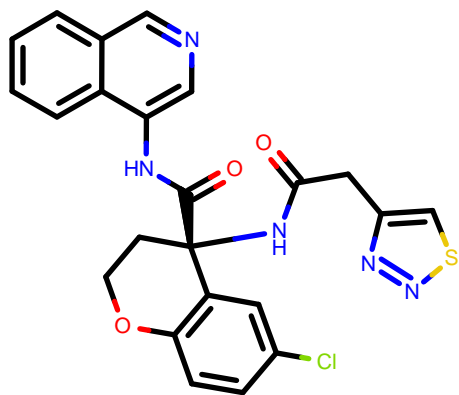
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5C@HC@H5COC(=O)C5

RUN: RUN4878

DDG (kcal/mol): -3.43

dDDG (kcal/mol): 0.23

EN300-300519_1_1



CID: EN300-300519_1_1

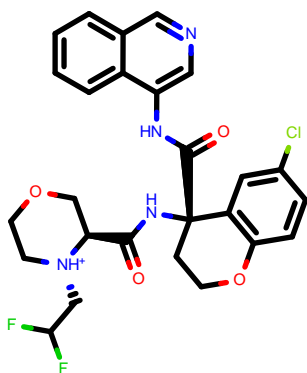
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5csnn5

RUN: RUN5130

DDG (kcal/mol): -3.42

dDDG (kcal/mol): 0.20

EN300-140582_1_3



CID: EN300-140582_1_3

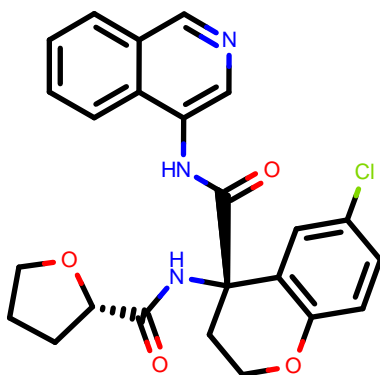
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5COCQ1N@H5CC(F)F

RUN: RUN6700

DDG (kcal/mol): -3.41

dDDG (kcal/mol): 0.23

EN300-104395_1_1



CID: EN300-104395_1_1

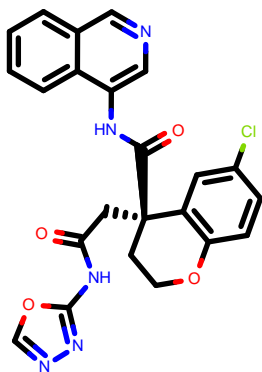
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CCOC5

RUN: RUN6456

DDG (kcal/mol): -3.40

dDDG (kcal/mol): 0.19

EN300-101637_1_1



CID: EN300-101637_1_1

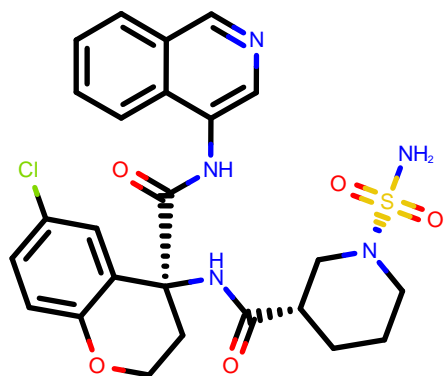
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnco5

RUN: RUN11839

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.16

EN300-219496_1_4



CID: EN300-219496_1_4

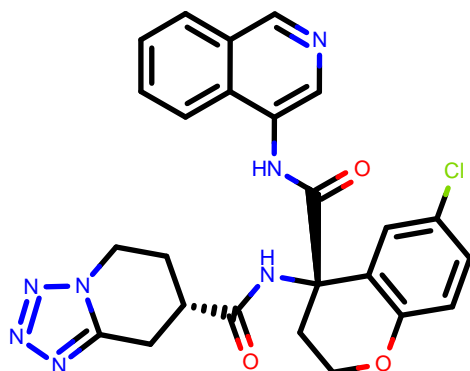
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCN5(C)S(=O)(=O)N

RUN: RUN6936

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.33

EN300-1653482_1_1



CID: EN300-1653482_1_1

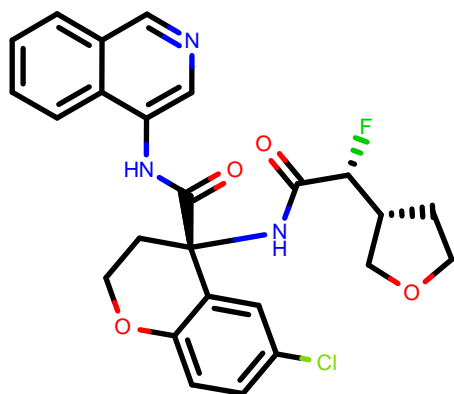
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCN6C(NN)C5

RUN: RUN6042

DDG (kcal/mol): -3.39

dDDG (kcal/mol): 0.23

EN300-783124_1_1



CID: EN300-783124_1_1

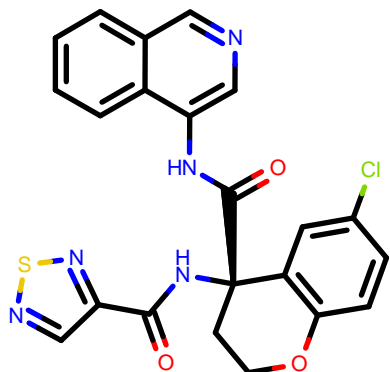
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@@H]5CCOC5)F

RUN: RUN5314

DDG (kcal/mol): -3.38

dDDG (kcal/mol): 0.23

EN300-42270_1_1



CID: EN300-42270_1_1

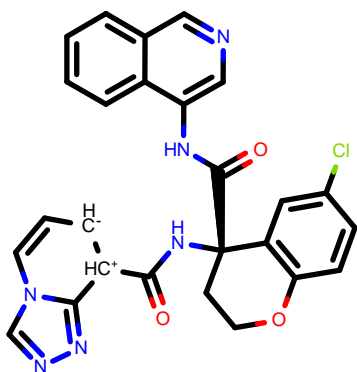
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nsn5

RUN: RUN5634

DDG (kcal/mol): -3.37

dDDG (kcal/mol): 0.18

EN300-1726153_1_1



CID: EN300-1726153_1_1

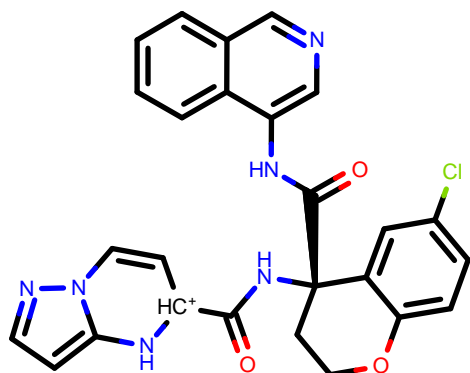
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)C4)NC(=O)C5CC6C=C5N6

RUN: RUN1305

DDG (kcal/mol): -3.36

dDDG (kcal/mol): 0.20

EN300-323327_1_1



CID: EN300-323327_1_1

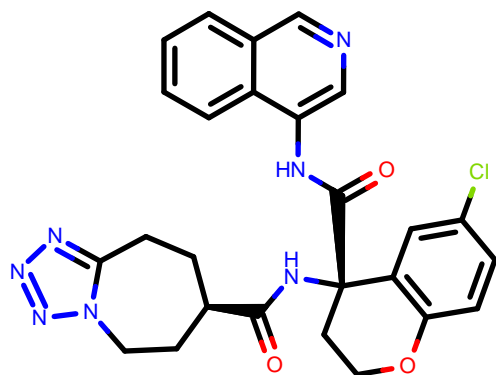
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)C4)NC(=O)C5CC6C(=N5)C6

RUN: RUN4798

DDG (kcal/mol): -3.33

dDDG (kcal/mol): 0.18

EN300-253571_1_1



CID: EN300-253571_1_1

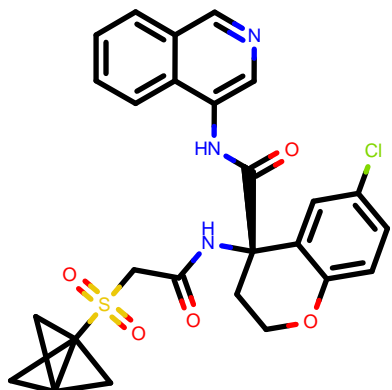
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)C4)NC(=O)[C@@]5C6C=C6N6C5

RUN: RUN8741

DDG (kcal/mol): -3.31

dDDG (kcal/mol): 0.23

EN300-6763072_1_1



CID: EN300-6763072_1_1

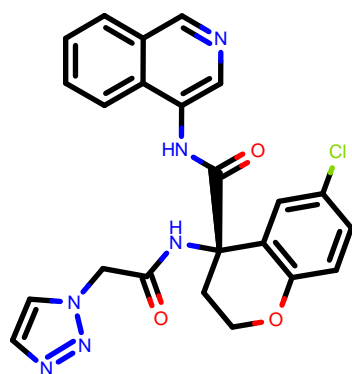
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)C4)NC(=O)CS(=O)(=O)C5C6C=C5C6

RUN: RUN7692

DDG (kcal/mol): -3.30

dDDG (kcal/mol): 0.21

EN300-100467_1_1



CID: EN300-100467_1_1

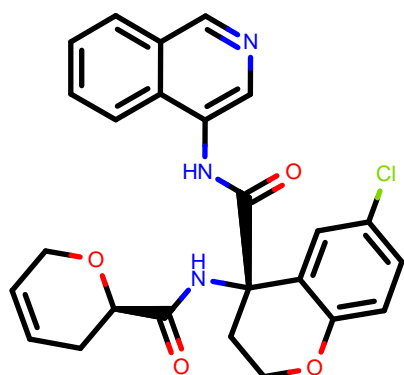
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnn5

RUN: RUN8316

DDG (kcal/mol): -3.29

dDDG (kcal/mol): 0.21

EN300-378044_1_2



CID: EN300-378044_1_2

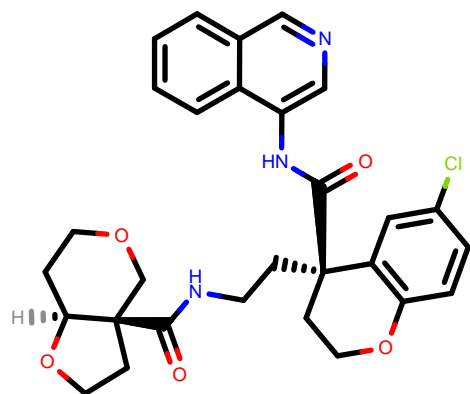
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5CC=CCO5

RUN: RUN5602

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.20

EN300-341337_3_4



CID: EN300-341337_3_4

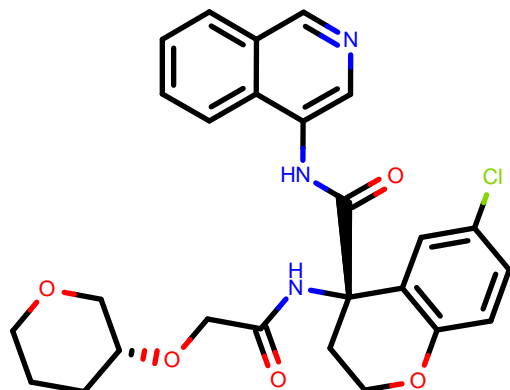
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H56CCO[C@@H]5CCO6

RUN: RUN13920

DDG (kcal/mol): -3.28

dDDG (kcal/mol): 0.26

EN300-1627945_1_1



CID: EN300-1627945_1_1

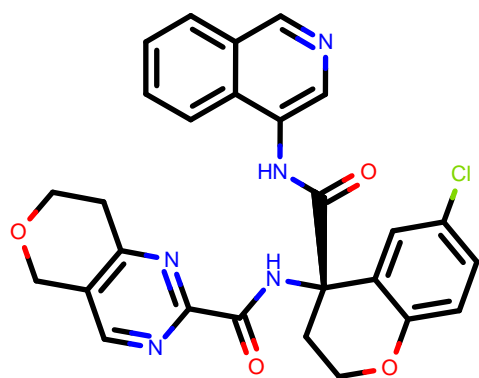
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@H]5CCOCC5

RUN: RUN4130

DDG (kcal/mol): -3.27

dDDG (kcal/mol): 0.20

EN300-7435929_1_1



CID: EN300-7435929_1_1

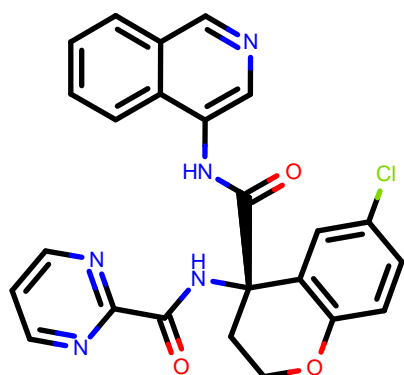
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6c(n5)CCOC6

RUN: RUN6664

DDG (kcal/mol): -3.26

dDDG (kcal/mol): 0.20

EN300-80230_1_1



CID: EN300-80230_1_1

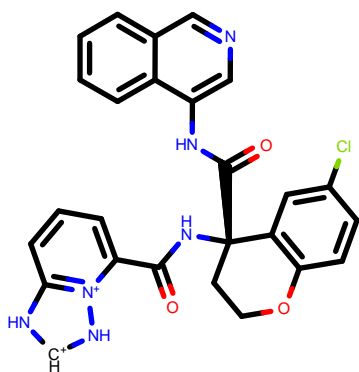
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccc5

RUN: RUN4590

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.17

EN300-129441_1_1



CID: EN300-129441_1_1

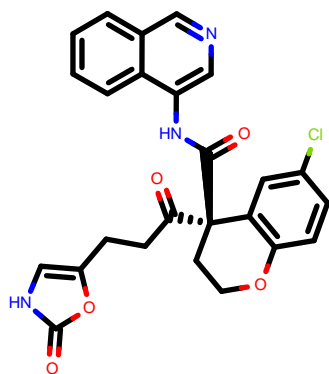
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6n5nc6

RUN: RUN3362

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-9_1



CID: VLA-UCB-34f3ed0c-9_1

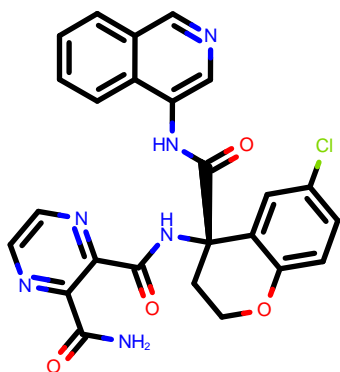
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5

RUN: RUN33

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.19

EN300-21200_1_1



CID: EN300-21200_1_1

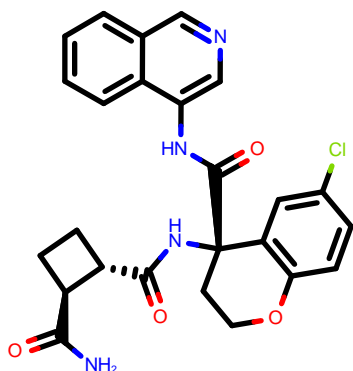
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ncn5)C(=O)N

RUN: RUN6592

DDG (kcal/mol): -3.24

dDDG (kcal/mol): 0.22

EN300-217107_1_4



CID: EN300-217107_1_4

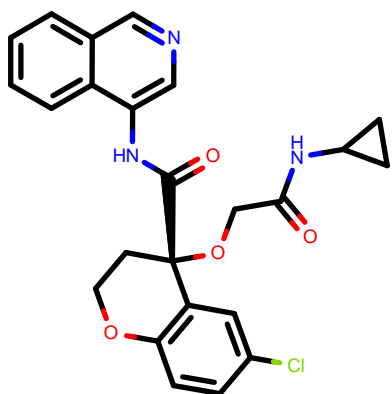
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H]5C(=O)N

RUN: RUN5342

DDG (kcal/mol): -3.23

dDDG (kcal/mol): 0.25

EN300-1253178_1_1



CID: EN300-1253178_1_1

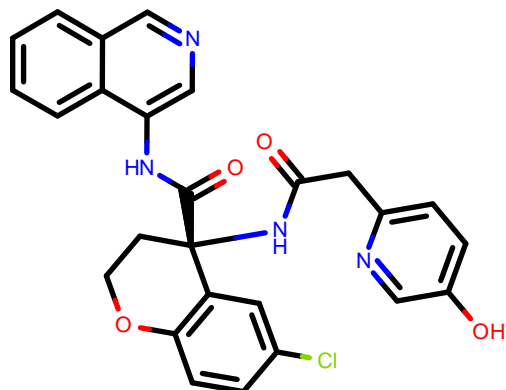
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5

RUN: RUN1253

DDG (kcal/mol): -3.22

dDDG (kcal/mol): 0.20

EN300-188341_1_1



CID: EN300-188341_1_1

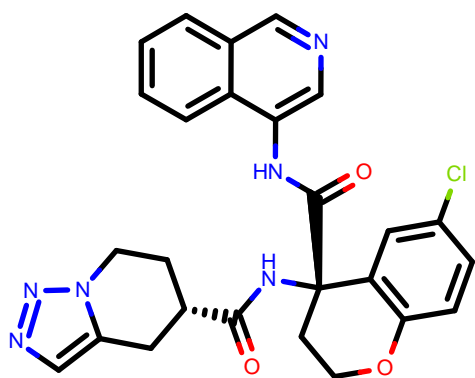
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(en5)O

RUN: RUN9221

DDG (kcal/mol): -3.21

dDDG (kcal/mol): 0.22

EN300-7430501_1_1



CID: EN300-7430501_1_1

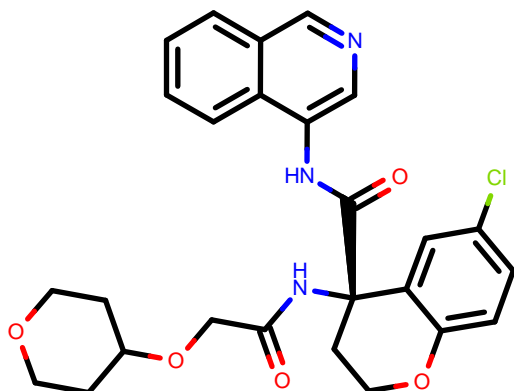
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCn6c(cnn6)C5

RUN: RUN7532

DDG (kcal/mol): -3.20

dDDG (kcal/mol): 0.20

EN300-77520_1_1



CID: EN300-77520_1_1

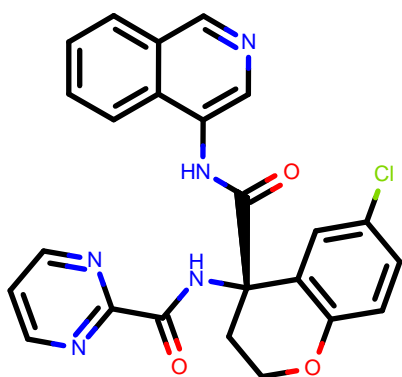
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC5CCOCC5

RUN: RUN2852

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.20

EN300-80230_1_1



CID: EN300-80230_1_1

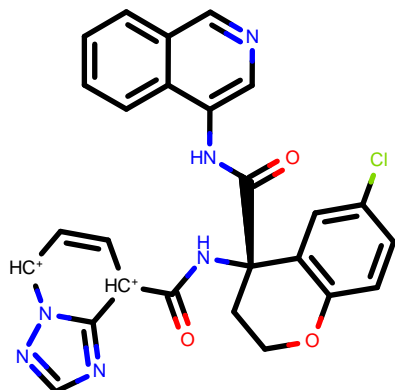
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccc5

RUN: RUN4594

DDG (kcal/mol): -3.19

dDDG (kcal/mol): 0.16

EN300-366857_1_1



CID: EN300-366857_1_1

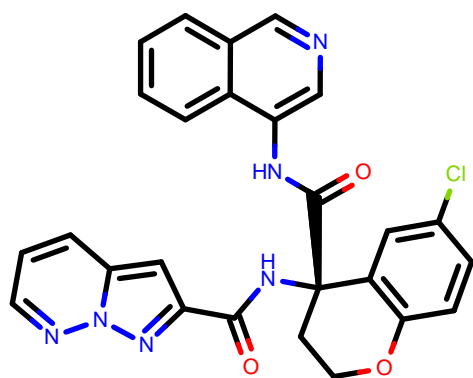
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6c5[n+]6

RUN: RUN3430

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.24

EN300-6473108_1_1



CID: EN300-6473108_1_1

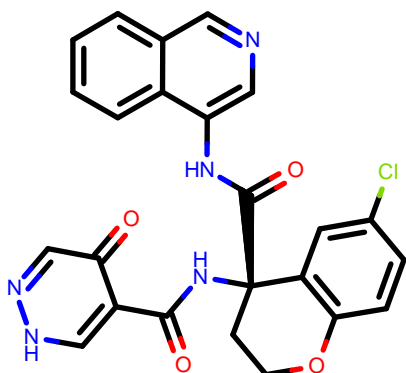
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6ccocn6n5

RUN: RUN1888

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.17

EN300-243828_1_1



CID: EN300-243828_1_1

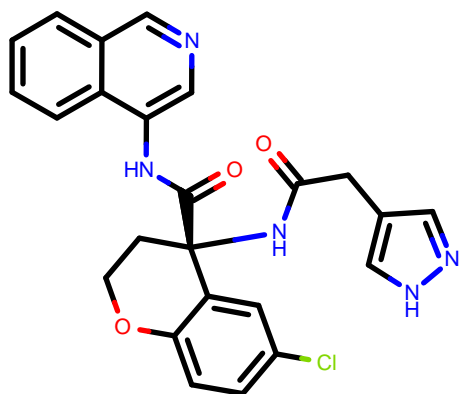
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]nc5=O

RUN: RUN3350

DDG (kcal/mol): -3.18

dDDG (kcal/mol): 0.31

EN300-1589101_1_1



CID: EN300-1589101_1_1

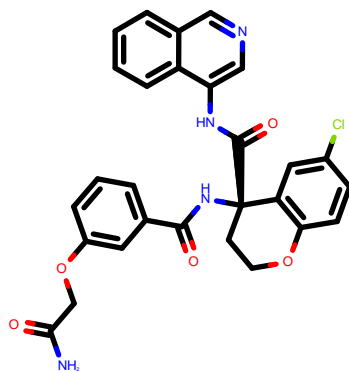
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5c[nH]nc5

RUN: RUN8605

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.25

EN300-30687_1_1



CID: EN300-30687_1_1

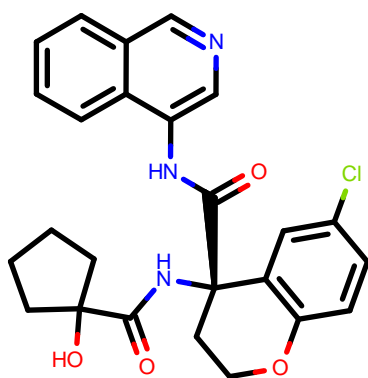
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(cc5)OC(=O)N

RUN: RUN275

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.22

EN300-25960_1_1



CID: EN300-25960_1_1

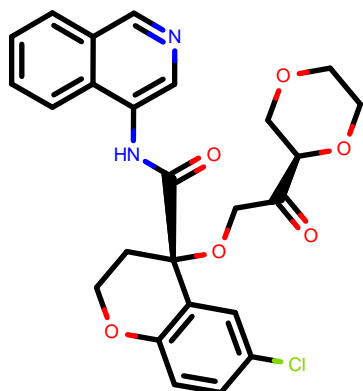
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCCC5)O

RUN: RUN2659

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.24

EN300-6238494_1_2



CID: EN300-6238494_1_2

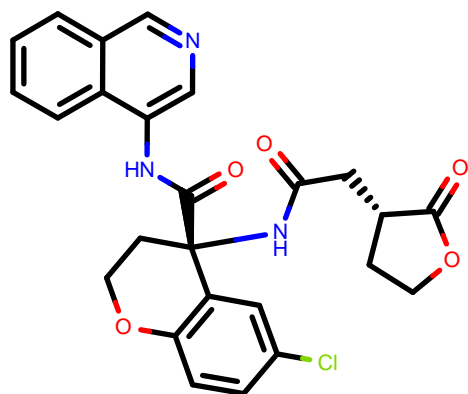
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)[C@H]5COCC5=O

RUN: RUN1213

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.24

EN300-1072972_1_1



CID: EN300-1072972_1_1

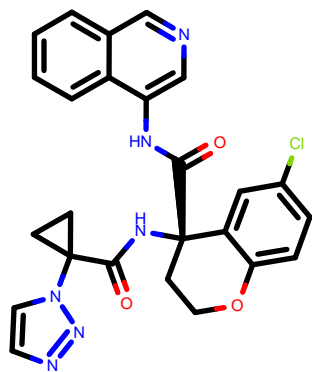
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@H]5COCC5=O

RUN: RUN2449

DDG (kcal/mol): -3.16

dDDG (kcal/mol): 0.27

EN300-658559_1_1



CID: EN300-658559_1_1

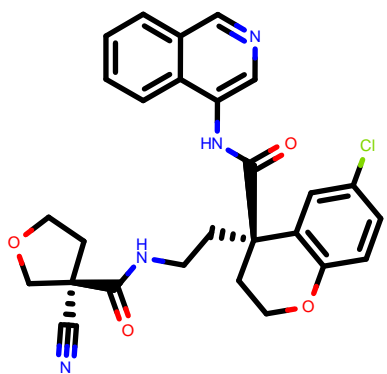
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)n6cnn6

RUN: RUN2183

DDG (kcal/mol): -3.15

dDDG (kcal/mol): 0.21

EN300-261210_3_2



CID: EN300-261210_3_2

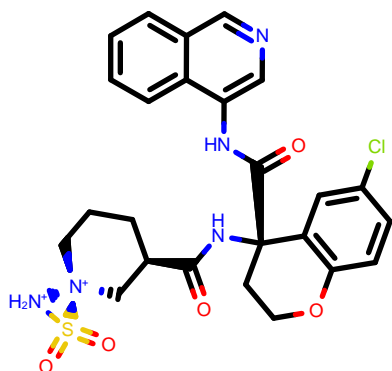
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(COCOC5)C#N

RUN: RUN7335

DDG (kcal/mol): -3.15

dDDG (kcal/mol): 0.25

EN300-219496_1_1



CID: EN300-219496_1_1

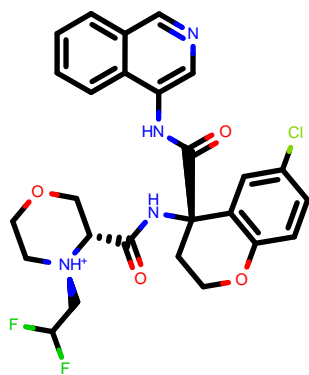
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(C)S(=O)(=O)N

RUN: RUN4586

DDG (kcal/mol): -3.14

dDDG (kcal/mol): 0.37

EN300-140582_1_2



CID: EN300-140582_1_2

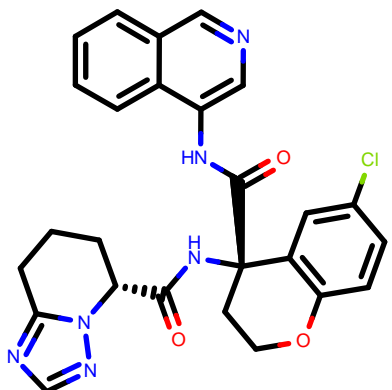
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(C)COC(F)F

RUN: RUN9413

DDG (kcal/mol): -3.12

dDDG (kcal/mol): 0.27

EN300-1273016_1_2



CID: EN300-1273016_1_2

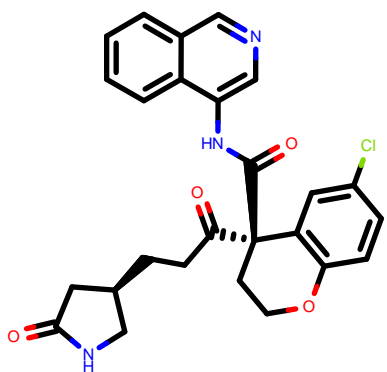
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(C)CCc6n5ncn6

RUN: RUN9141

DDG (kcal/mol): -3.10

dDDG (kcal/mol): 0.25

VLA-UCB-34f3ed0c-21_1



CID: VLA-UCB-34f3ed0c-21_1

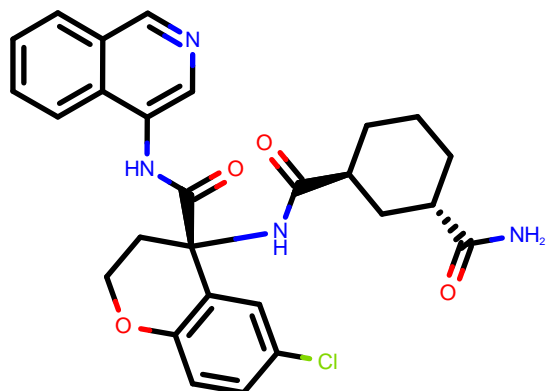
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NCS

RUN: RUN22

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.26

EN300-90142_1_2



CID: EN300-90142_1_2

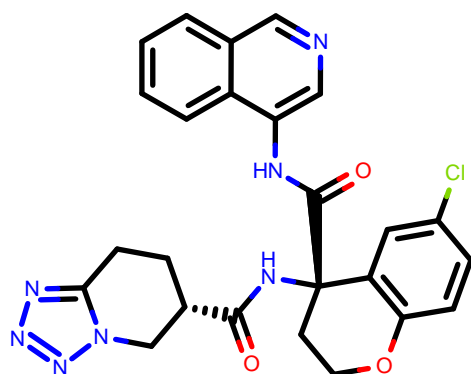
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)[C@@H]5CC[C@@H]5Cl=O

RUN: RUN9557

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.30

EN300-269453_1_2



CID: EN300-269453_1_2

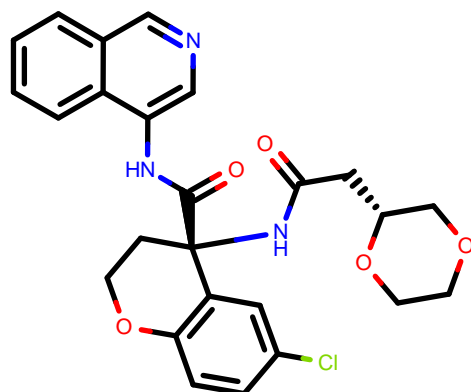
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)[C@@H]5CC6Nnnc6CS

RUN: RUN5094

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.21

EN300-731622_1_2



CID: EN300-731622_1_2

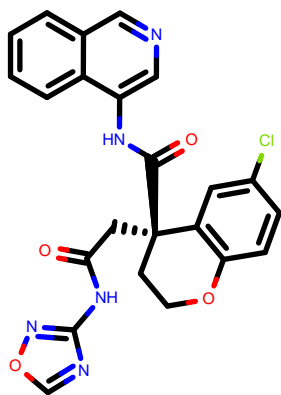
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)[C@@H]5CCOC6O5

RUN: RUN1960

DDG (kcal/mol): -3.09

dDDG (kcal/mol): 0.23

EN300-117222_1_1



CID: EN300-117222_1_1

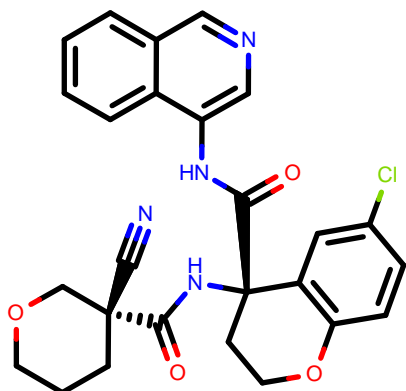
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncon5

RUN: RUN11855

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.17

EN300-301925_1_2



CID: EN300-301925_1_2

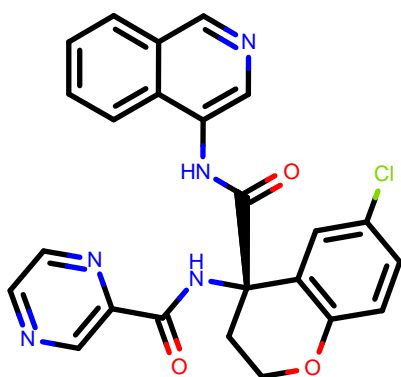
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN4370

DDG (kcal/mol): -3.06

dDDG (kcal/mol): 0.25

EN300-19900_1_1



CID: EN300-19900_1_1

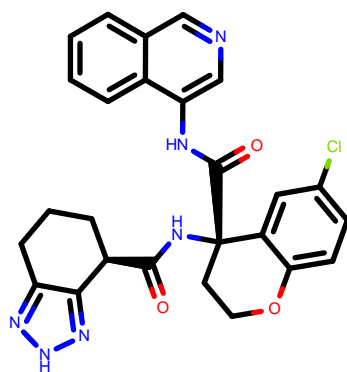
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccn5

RUN: RUN2752

DDG (kcal/mol): -3.05

dDDG (kcal/mol): 0.17

EN300-208236_1_1



CID: EN300-208236_1_1

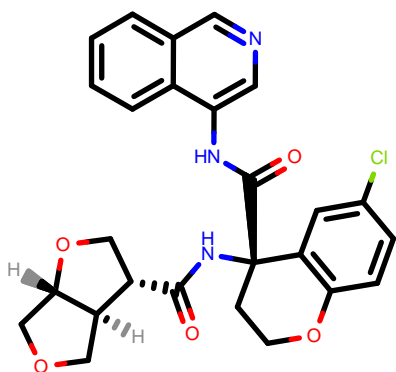
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCc6c5n[nH]n6

RUN: RUN9385

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.24

EN300-6482296_1_4



CID: EN300-6482296_1_4

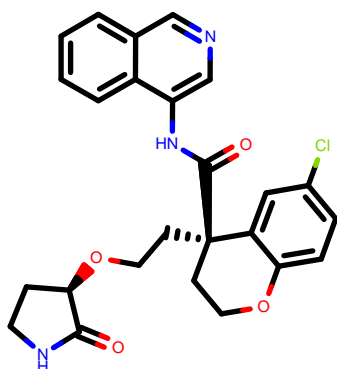
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)C@@H5CO[C@@H]5COC=O

RUN: RUN8476

DDG (kcal/mol): -3.04

dDDG (kcal/mol): 0.23

EN300-6736413_3_2



CID: EN300-6736413_3_2

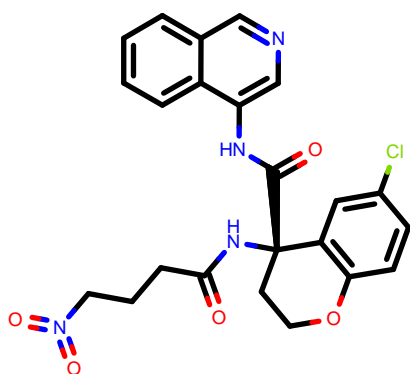
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)C@@H5CCNC5=O

RUN: RUN1776

DDG (kcal/mol): -3.02

dDDG (kcal/mol): 0.21

EN300-143449_1_1



CID: EN300-143449_1_1

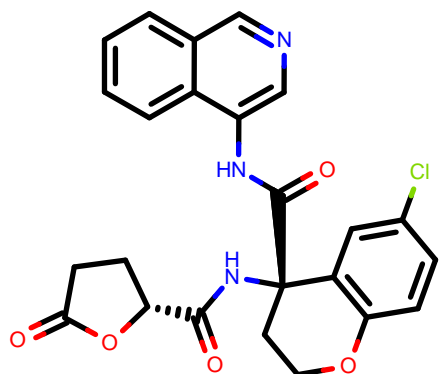
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCN(=O)=O

RUN: RUN5638

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.24

EN300-332606_1_1



CID: EN300-332606_1_1

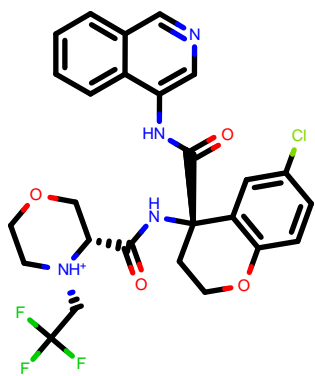
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)O5

RUN: RUN3494

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.22

EN300-201551_1_2



CID: EN300-201551_1_2

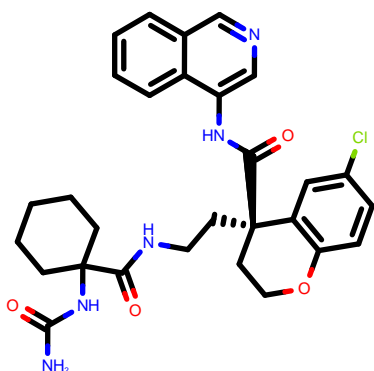
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COCC[N@]5CC(F)(F)F

RUN: RUN4686

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.24

EN300-78368_3_1



CID: EN300-78368_3_1

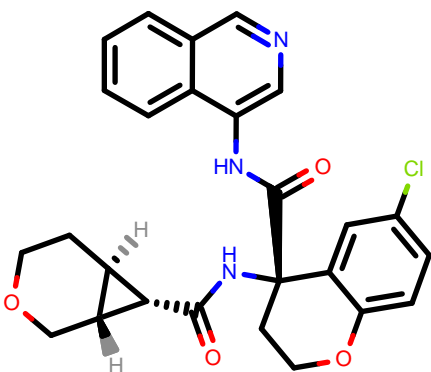
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCCOC5)NC(=O)N

RUN: RUN14116

DDG (kcal/mol): -3.01

dDDG (kcal/mol): 0.37

EN300-1644723_1_8



CID: EN300-1644723_1_8

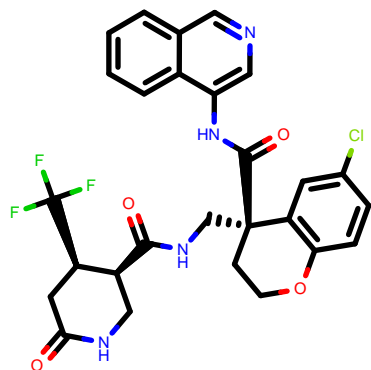
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]6[C@@H]5COCC6

RUN: RUN8953

DDG (kcal/mol): -3.00

dDDG (kcal/mol): 0.21

EN300-208959_2_2



CID: EN300-208959_2_2

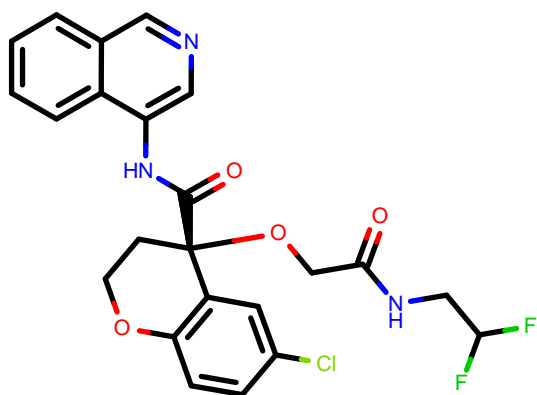
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CNC(=O)[C@H]5C(F)(F)F

RUN: RUN3759

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.17

EN300-120586_1_1



CID: EN300-120586_1_1

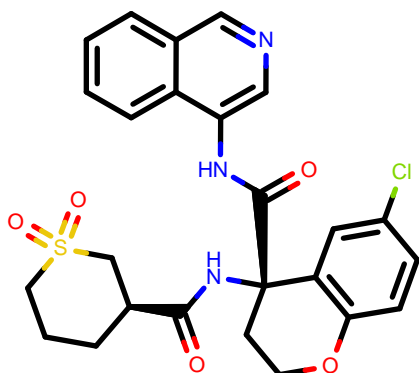
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CC(=O)NCC(F)F

RUN: RUN1181

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.19

EN300-77778_1_2



CID: EN300-77778_1_2

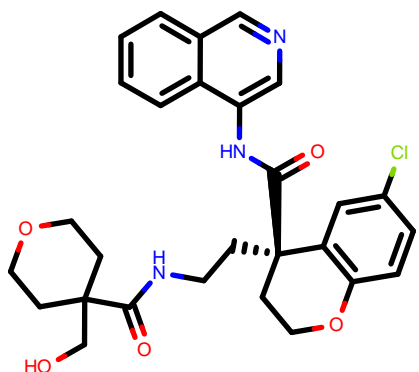
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)NC(=O)C@H5CCCS(=O)(=O)C5

RUN: RUN2930

DDG (kcal/mol): -2.99

dDDG (kcal/mol): 0.24

EN300-244909_3_1



CID: EN300-244909_3_1

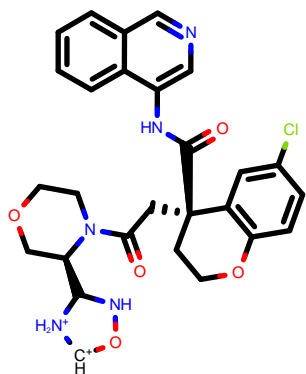
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CCNC(=O)C5(CCOCC5)CO

RUN: RUN14864

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.32

EN300-122849_1_2



CID: EN300-122849_1_2

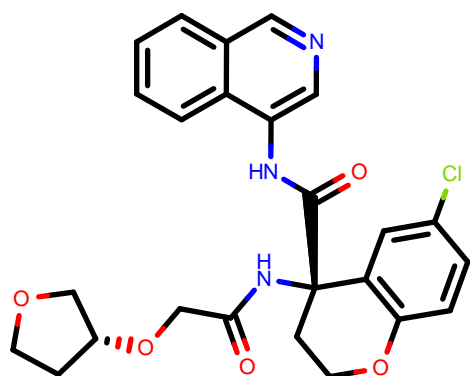
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CC(=O)N5CCOC[C@@]H5c6ncon6

RUN: RUN9588

DDG (kcal/mol): -2.98

dDDG (kcal/mol): 0.26

EN300-99391_1_1



CID: EN300-99391_1_1

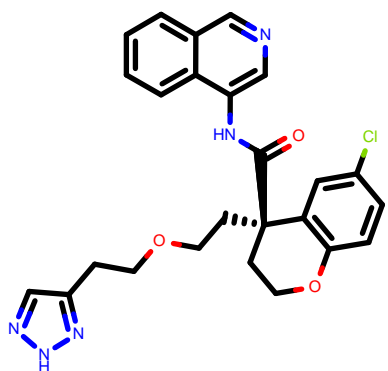
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@]5HJ5CCOC5

RUN: RUN3986

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.20

EN300-222357_3_1



CID: EN300-222357_3_1

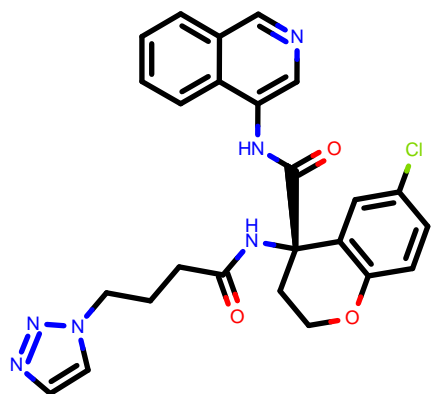
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5c[nH]n5

RUN: RUN1983

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.22

EN300-124301_1_1



CID: EN300-124301_1_1

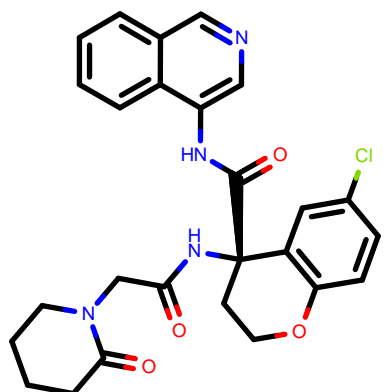
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5

RUN: RUN6928

DDG (kcal/mol): -2.97

dDDG (kcal/mol): 0.21

EN300-36111_1_1



CID: EN300-36111_1_1

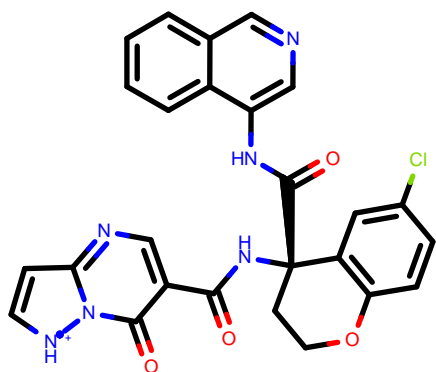
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O

RUN: RUN8769

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.24

EN300-220228_1_1



CID: EN300-220228_1_1

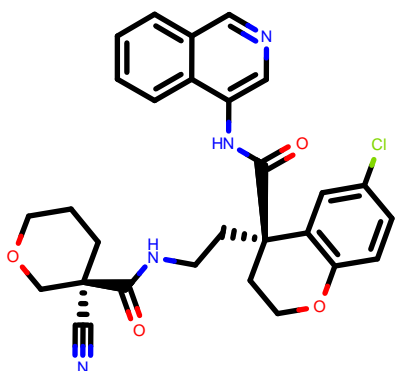
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6ccc[nH]n6c5=O

RUN: RUN2071

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.22

EN300-301925_3_2



CID: EN300-301925_3_2

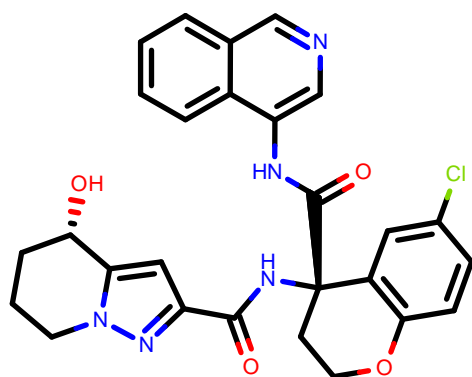
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN13854

DDG (kcal/mol): -2.96

dDDG (kcal/mol): 0.26

EN300-399606_1_1



CID: EN300-399606_1_1

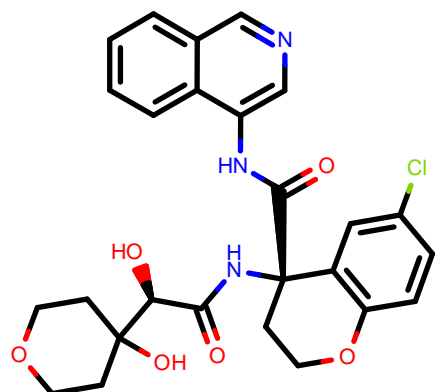
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CC[C@@]3H6O

RUN: RUN307

DDG (kcal/mol): -2.95

dDDG (kcal/mol): 0.19

EN300-749499_1_1



CID: EN300-749499_1_1

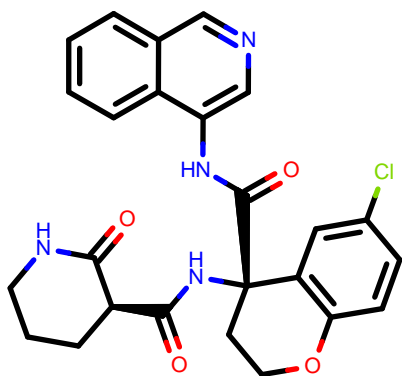
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(C5(CCCOC5)O)O

RUN: RUN6968

DDG (kcal/mol): -2.95

dDDG (kcal/mol): 0.24

EN300-82616_1_2



CID: EN300-82616_1_2

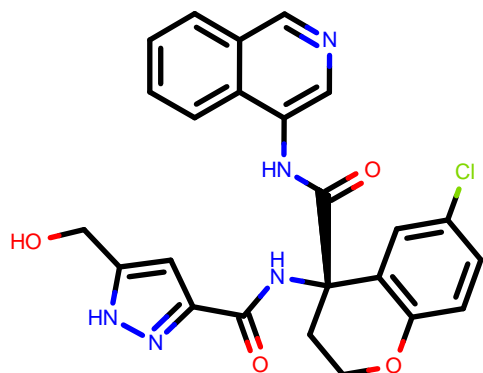
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCNC5=O

RUN: RUN1705

DDG (kcal/mol): -2.94

dDDG (kcal/mol): 0.28

EN300-658865_1_1



CID: EN300-658865_1_1

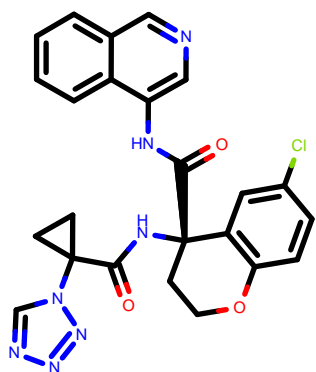
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc[nH]n5CO

RUN: RUN1393

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.19

EN300-263085_1_1



CID: EN300-263085_1_1

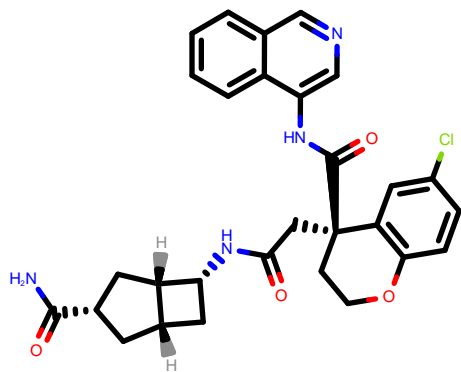
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5n6cnn6

RUN: RUN6424

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.22

EN300-1268016_1_7



CID: EN300-1268016_1_7

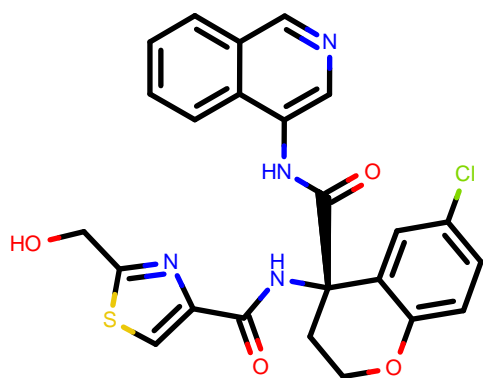
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5(C)C[C@@H]6[C@H](C)C[C@H]6C1=O

RUN: RUN6435

DDG (kcal/mol): -2.93

dDDG (kcal/mol): 0.26

EN300-250112_1_1



CID: EN300-250112_1_1

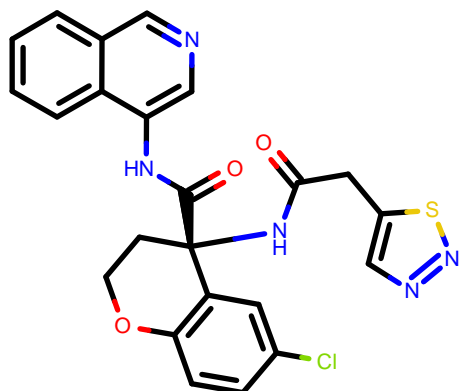
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5scn(n5)CO

RUN: RUN1297

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.21

EN300-260152_1_1



CID: EN300-260152_1_1

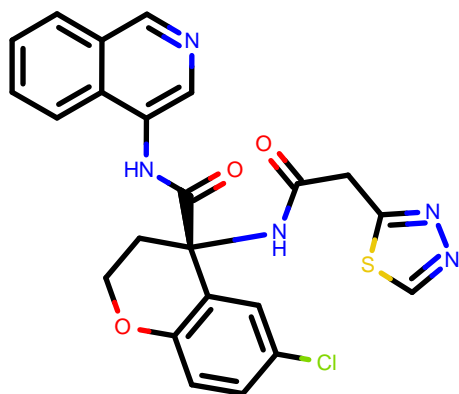
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnns5

RUN: RUN8060

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.20

EN300-6488240_1_1



CID: EN300-6488240_1_1

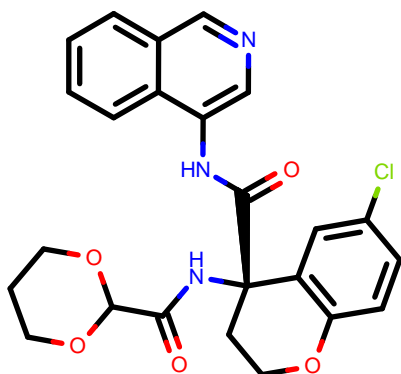
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnncs5

RUN: RUN8304

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.19

EN300-170985_1_1



CID: EN300-170985_1_1

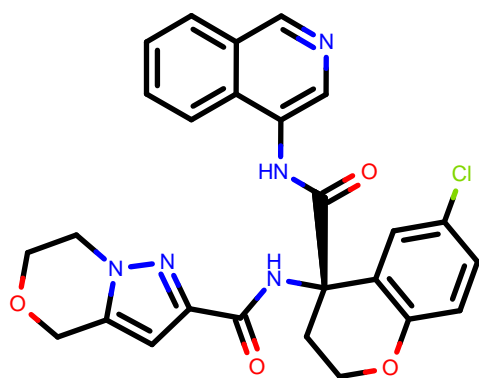
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCCO5

RUN: RUN7548

DDG (kcal/mol): -2.91

dDDG (kcal/mol): 0.19

EN300-244278_1_1



CID: EN300-244278_1_1

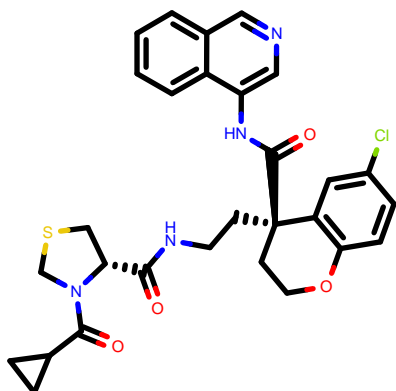
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6n(n5)CCOC6

RUN: RUN1649

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.17

EN300-18928_3_2



CID: EN300-18928_3_2

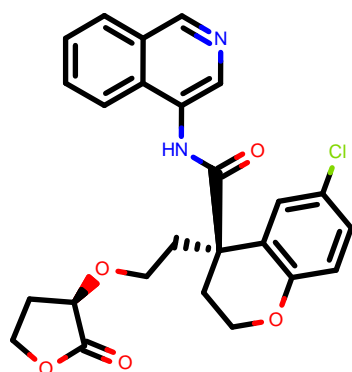
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CSCN5C1=O)C6COC6

RUN: RUN10968

DDG (kcal/mol): -2.90

dDDG (kcal/mol): 0.30

EN300-20496_3_2



CID: EN300-20496_3_2

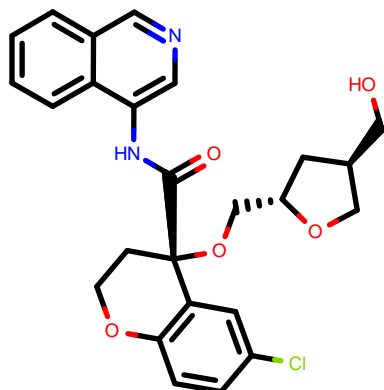
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@@H]5CCOC5=O

RUN: RUN1528

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.24

EN300-6494158_1_4



CID: EN300-6494158_1_4

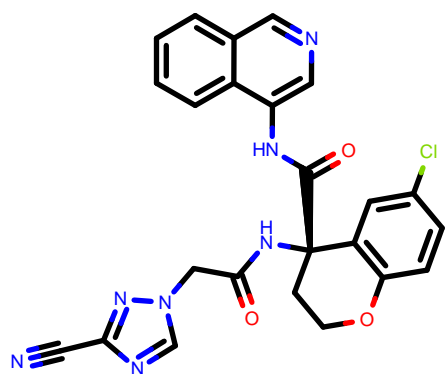
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5C[C@@H](CO)C5O

RUN: RUN2123

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.24

EN300-111863_1_1



CID: EN300-111863_1_1

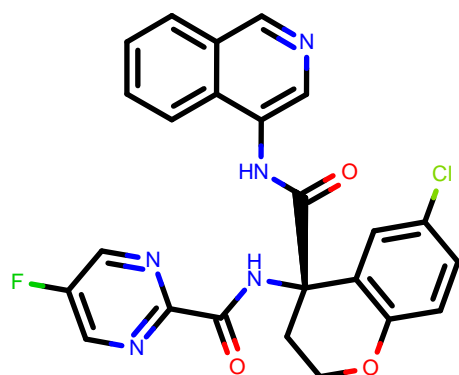
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ncnc5C#N

RUN: RUN9373

DDG (kcal/mol): -2.89

dDDG (kcal/mol): 0.20

EN300-149296_1_1



CID: EN300-149296_1_1

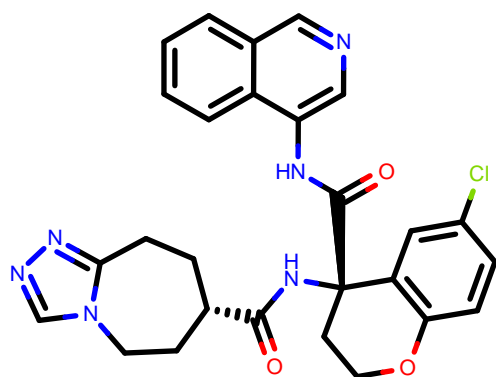
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncc(F)c5

RUN: RUN5834

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.19

EN300-366687_1_2



CID: EN300-366687_1_2

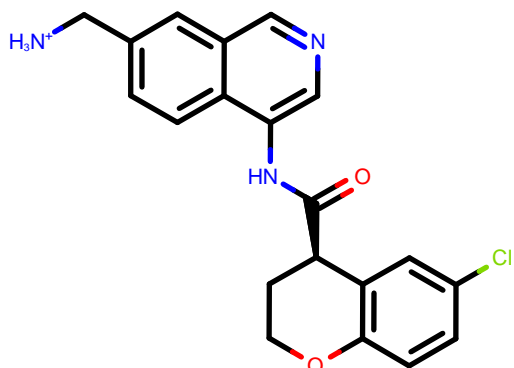
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC6Nnnc6CC5

RUN: RUN8204

DDG (kcal/mol): -2.88

dDDG (kcal/mol): 0.24

MAK-UNK-8be7dca9-5_1



CID: MAK-UNK-8be7dca9-5_1

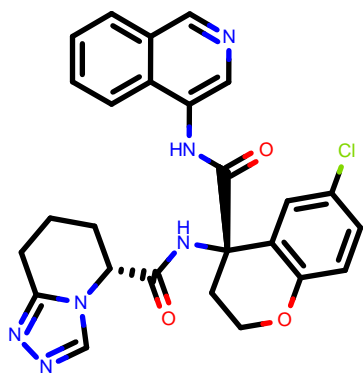
SMILES: c1cc2c(cc1C[NH3+])ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN91

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.10

EN300-6478631_1_2



CID: EN300-6478631_1_2

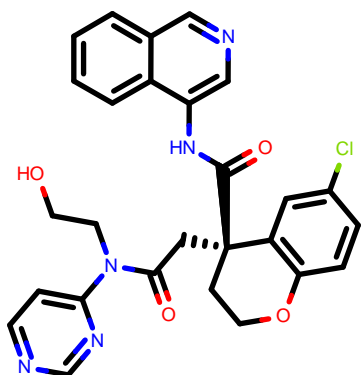
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCc6n5cnn6

RUN: RUN8588

DDG (kcal/mol): -2.87

dDDG (kcal/mol): 0.24

EN300-256174_1_1



CID: EN300-256174_1_1

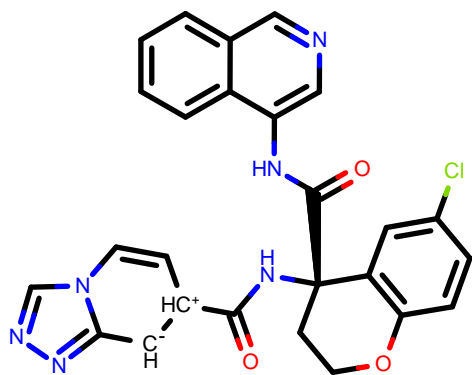
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5cnnn5

RUN: RUN12360

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.29

EN300-7537194_1_1



CID: EN300-7537194_1_1

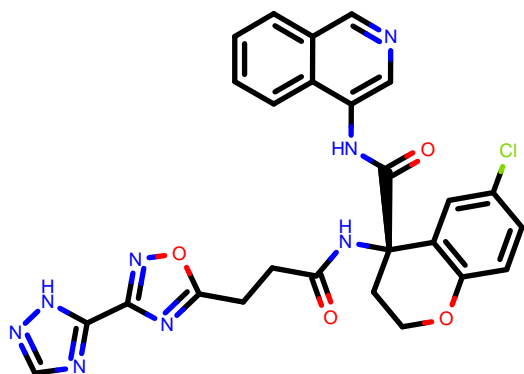
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6cnn65

RUN: RUN5282

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.22

EN300-61140_1_1



CID: EN300-61140_1_1

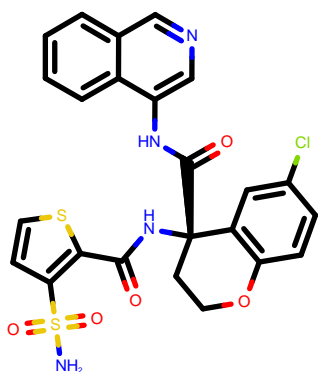
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5nc(n5)c6[nH]n6

RUN: RUN4890

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.25

EN300-24419_1_1



CID: EN300-24419_1_1

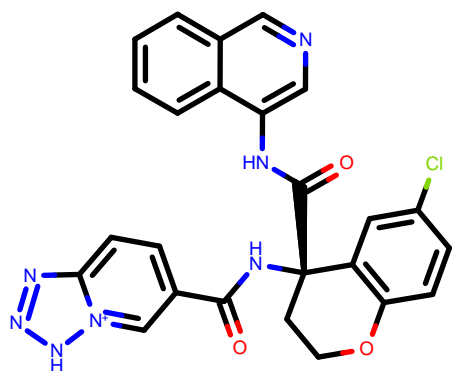
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ccs5)S(=O)(=O)N

RUN: RUN6852

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.29

EN300-102853_1_1



CID: EN300-102853_1_1

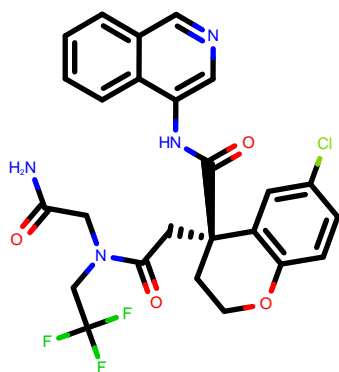
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6nnn6c5

RUN: RUN4202

DDG (kcal/mol): -2.86

dDDG (kcal/mol): 0.21

EN300-138676_1_1



CID: EN300-138676_1_1

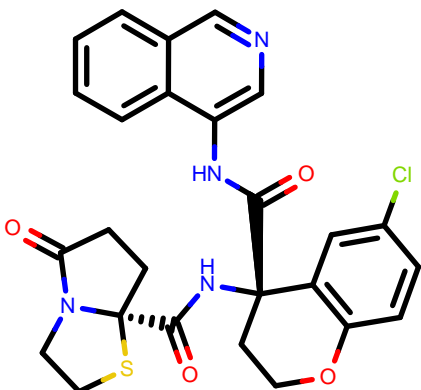
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)CC(F)(F)F

RUN: RUN1447

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.25

EN300-10334_1_1



CID: EN300-10334_1_1

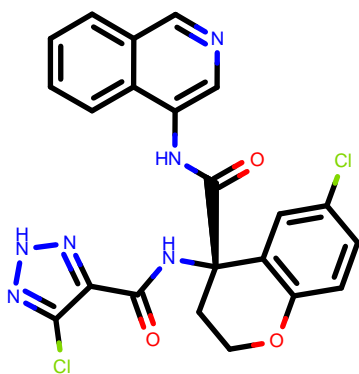
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCCC(=O)N5CCS6

RUN: RUN8749

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.28

EN300-149013_1_1



CID: EN300-149013_1_1

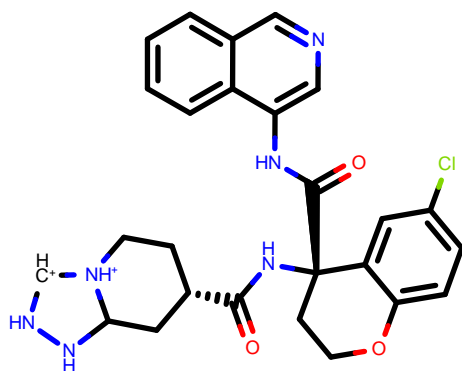
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(n[nH]n5)Cl

RUN: RUN6078

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.18

EN300-6474341_1_1



CID: EN300-6474341_1_1

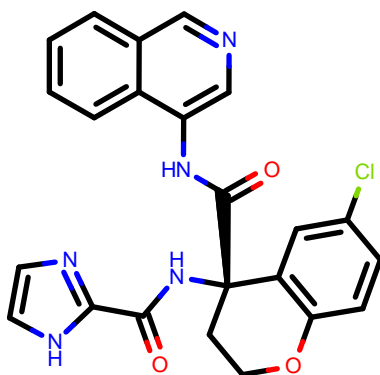
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CN6cnc6C5

RUN: RUN9706

DDG (kcal/mol): -2.85

dDDG (kcal/mol): 0.23

EN300-315836_1_1



CID: EN300-315836_1_1

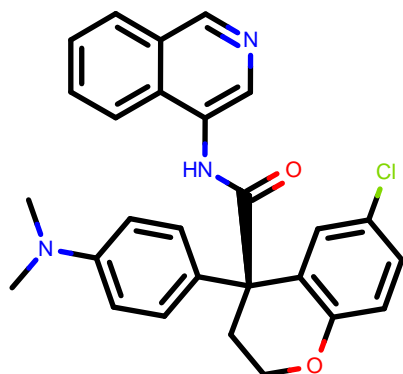
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]jcn5

RUN: RUN2635

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.17

VLA-UCB-551c2366-1_1



CID: VLA-UCB-551c2366-1_1

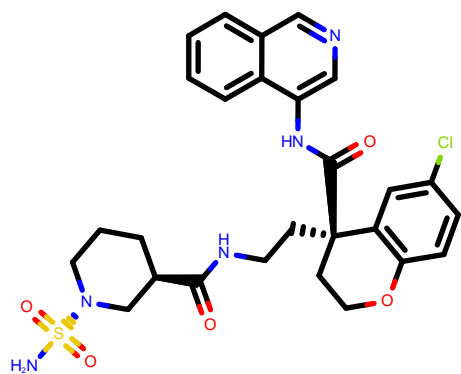
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4ccc5

RUN: RUN62

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.17

EN300-219496_3_3



CID: EN300-219496_3_3

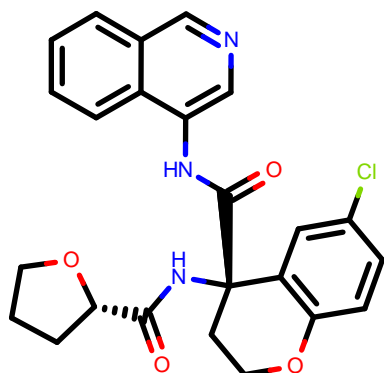
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3ccc4O)CCNC(=O)C@H5CCCC[NH]C5(S(=O)(=O)N

RUN: RUN697

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.60

EN300-104395_1_1



CID: EN300-104395_1_1

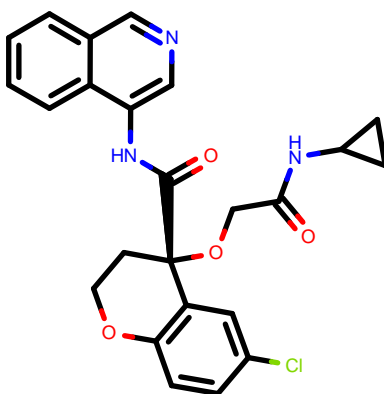
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3ccc(cc4)O)NC(=O)[C@@H]5CCOC5

RUN: RUN6460

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.21

EN300-1253178_1_1



CID: EN300-1253178_1_1

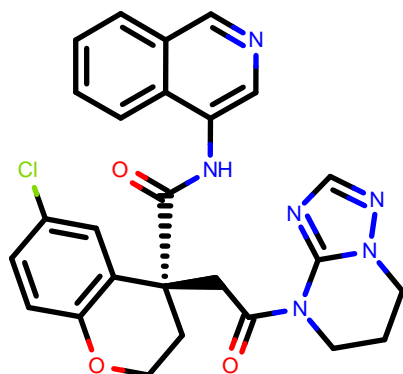
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3ccc(cc4)O)OCC(=O)NC5C5

RUN: RUN1261

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.19

EN300-54588_1_1



CID: EN300-54588_1_1

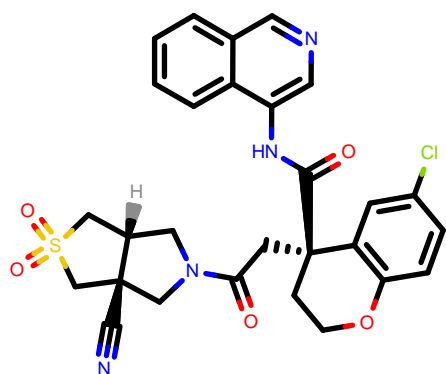
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4c3ccc(cc4)O)CC(=O)N5CCNc6c5ncn6

RUN: RUN6863

DDG (kcal/mol): -2.84

dDDG (kcal/mol): 0.20

EN300-701244_1_1



CID: EN300-701244_1_1

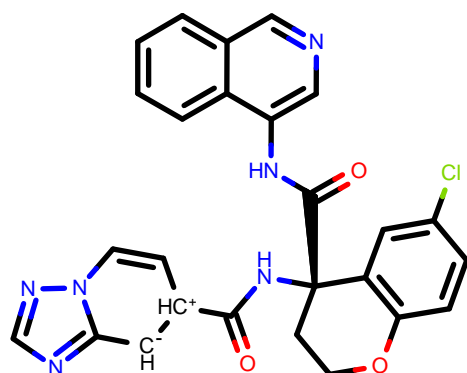
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CS(=O)(=O)C[C@]6(C)S5#N

RUN: RUN7931

DDG (kcal/mol): -2.83

dDDG (kcal/mol): 0.32

EN300-192893_1_1



CID: EN300-192893_1_1

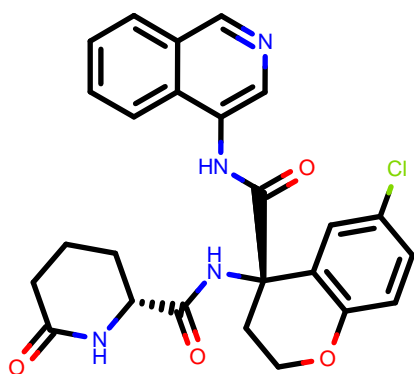
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6c(c5)n[nH+]6

RUN: RUN5526

DDG (kcal/mol): -2.82

dDDG (kcal/mol): 0.20

EN300-146491_1_1



CID: EN300-146491_1_1

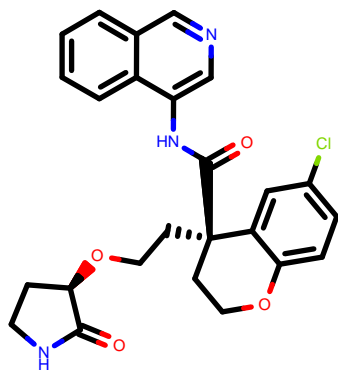
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN3658

DDG (kcal/mol): -2.82

dDDG (kcal/mol): 0.21

EN300-6736413_3_2



CID: EN300-6736413_3_2

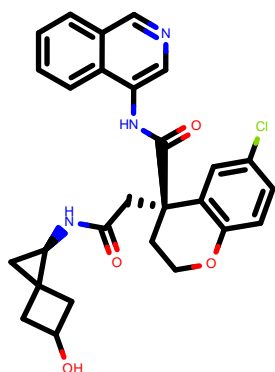
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCNC5=O

RUN: RUN1768

DDG (kcal/mol): -2.82

dDDG (kcal/mol): 0.20

EN300-624143_1_1



CID: EN300-624143_1_1

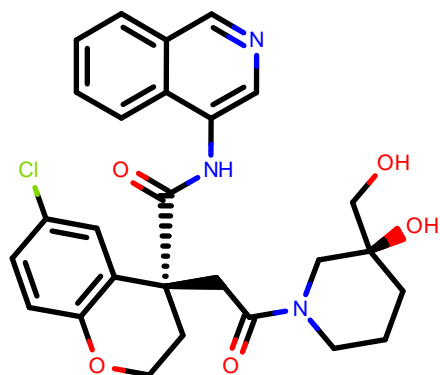
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CC(=O)N[C@@H]5CC56CC(C6)O

RUN: RUN3057

DDG (kcal/mol): -2.82

dDDG (kcal/mol): 0.26

EN300-251396_1_2



CID: EN300-251396_1_2

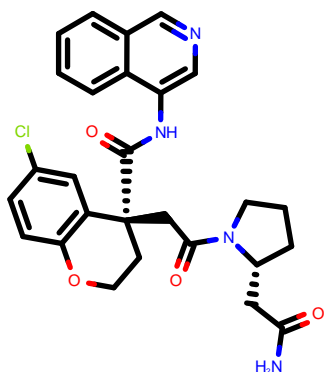
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CC(=O)N5CCC[C@]3(C5)(CO)O

RUN: RUN9540

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.33

EN300-124652_1_1



CID: EN300-124652_1_1

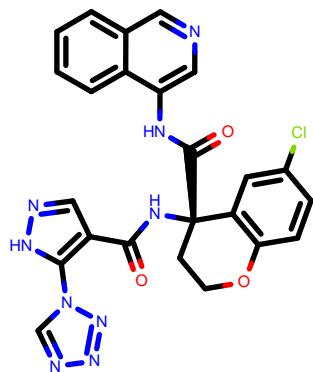
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)CC(=O)N5CCC[C@]3(H)5CC(=O)N

RUN: RUN5149

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.24

EN300-7549839_1_1



CID: EN300-7549839_1_1

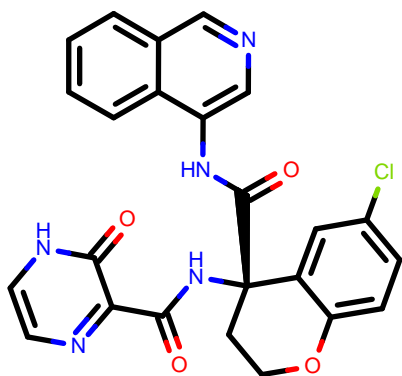
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOC4c3cc(cc4)C)NC(=O)c5cn[nH]5n6cn6

RUN: RUN2970

DDG (kcal/mol): -2.81

dDDG (kcal/mol): 0.22

EN300-97055_1_1



CID: EN300-97055_1_1

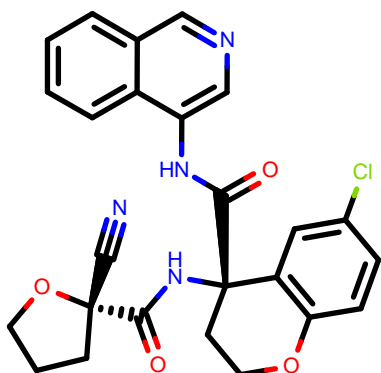
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)c5c[nH]cn5

RUN: RUN3202

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.19

EN300-3710141_1_2



CID: EN300-3710141_1_2

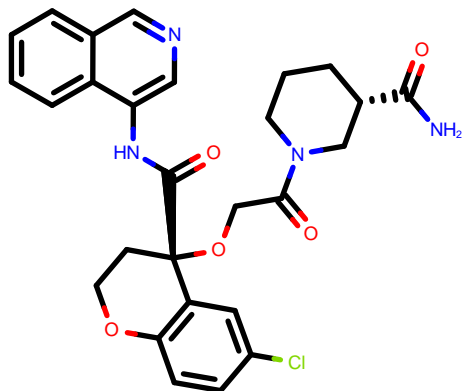
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)[C@@]5(CCCO5)C#N

RUN: RUN4550

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.21

EN300-22880_1_1



CID: EN300-22880_1_1

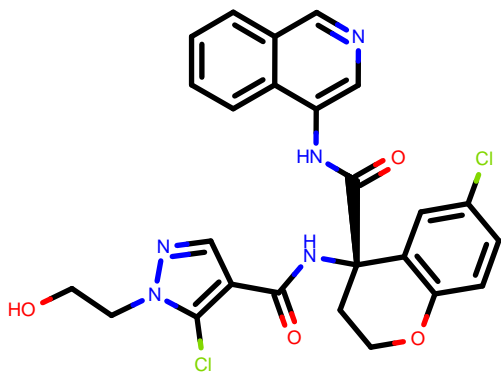
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)OCC(=O)N5CCCC[C@@H](C5)C(=O)N

RUN: RUN303

DDG (kcal/mol): -2.80

dDDG (kcal/mol): 0.27

EN300-333468_1_1



CID: EN300-333468_1_1

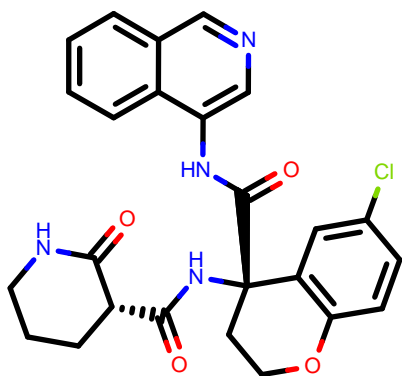
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)NC(=O)c5nn(c5Cl)CCO

RUN: RUN7168

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.24

EN300-82616_1_1



CID: EN300-82616_1_1

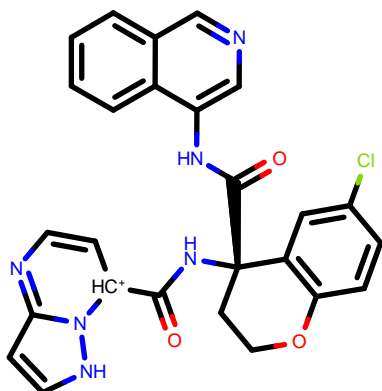
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CCNC5=O

RUN: RUN3426

DDG (kcal/mol): -2.79

dDDG (kcal/mol): 0.25

EN300-322100_1_1



CID: EN300-322100_1_1

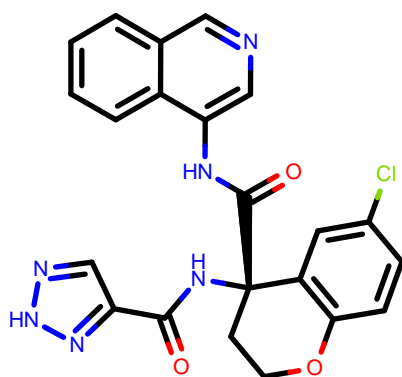
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6n5nc6

RUN: RUN3550

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.22

EN300-31998_1_1



CID: EN300-31998_1_1

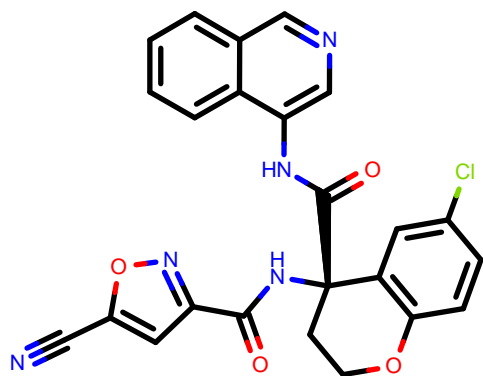
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]n5

RUN: RUN3186

DDG (kcal/mol): -2.78

dDDG (kcal/mol): 0.16

EN300-1178005_1_1



CID: EN300-1178005_1_1

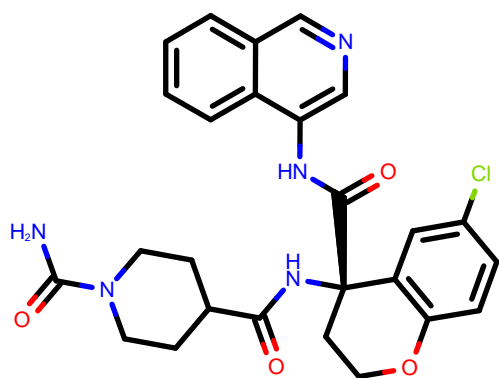
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)n5C#N

RUN: RUN3034

DDG (kcal/mol): -2.77

dDDG (kcal/mol): 0.18

EN300-13489_1_1



CID: EN300-13489_1_1

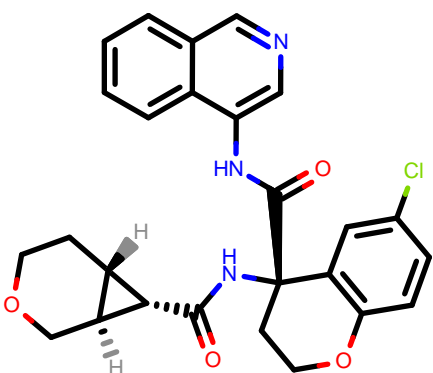
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CCN(CC5)C(=O)N

RUN: RUN8032

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.26

EN300-1644723_1_2



CID: EN300-1644723_1_2

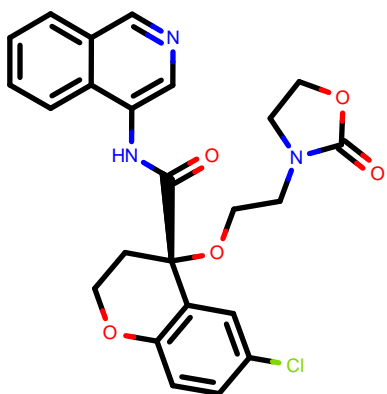
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]6[C@H]5COC6

RUN: RUN8528

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.21

EN300-370967_1_1



CID: EN300-370967_1_1

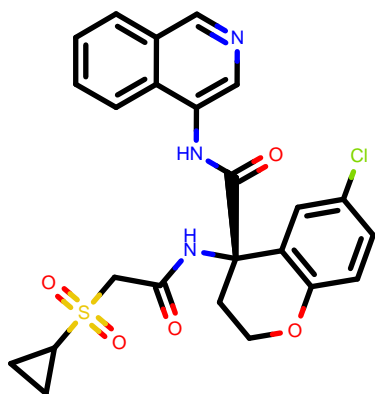
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCN5CCOC5=O

RUN: RUN2035

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.28

EN300-248618_1_1



CID: EN300-248618_1_1

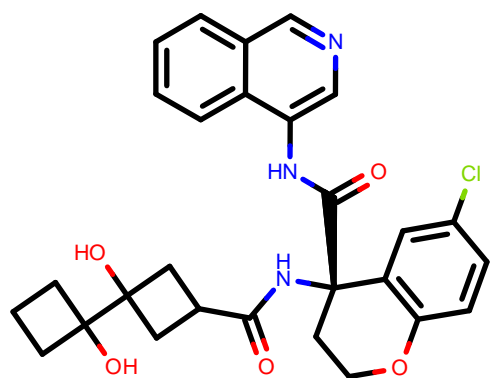
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS(=O)(=O)C5CC5

RUN: RUN6816

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.20

EN300-7459768_1_1



CID: EN300-7459768_1_1

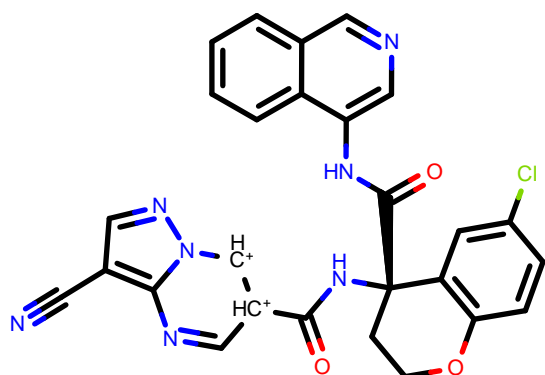
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(C5)(C6(CCC6)O)O

RUN: RUN8452

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.29

EN300-1697480_1_1



CID: EN300-1697480_1_1

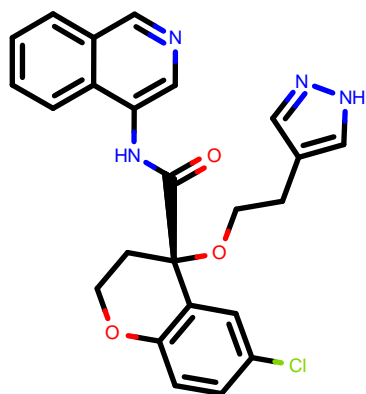
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6c(cnn6c5)C#N

RUN: RUN9874

DDG (kcal/mol): -2.76

dDDG (kcal/mol): 0.28

EDJ-MED-28ec730d-5_1



CID: EDJ-MED-28ec730d-5_1

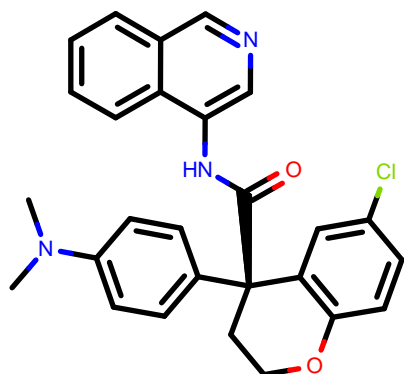
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5

RUN: RUN103

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.20

VLA-UCB-551c2366-1_1



CID: VLA-UCB-551c2366-1_1

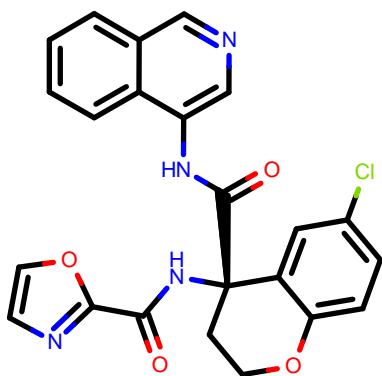
SMILES: CN(C)c1ccc(cc1)[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cnc5c4cccc5

RUN: RUN63

DDG (kcal/mol): -2.75

dDDG (kcal/mol): 0.17

EN300-318344_1_1



CID: EN300-318344_1_1

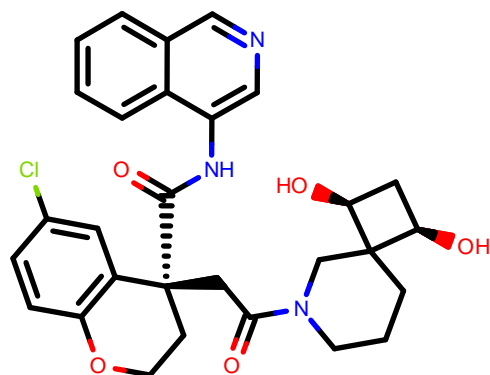
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncco5

RUN: RUN5234

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.17

EN300-7445890_1_1



CID: EN300-7445890_1_1

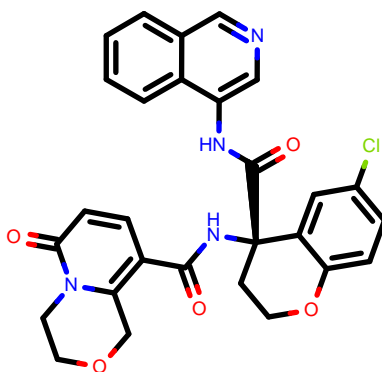
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC6(C5)C@H]C[C@@H]6O

RUN: RUN9876

DDG (kcal/mol): -2.74

dDDG (kcal/mol): 0.29

EN300-7538678_1_1



CID: EN300-7538678_1_1

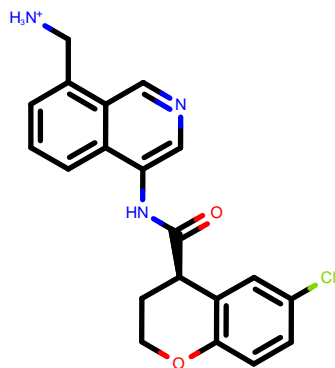
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(=O)n6c5OCCC6

RUN: RUN5226

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.25

MAK-UNK-8be7dca9-6_1



CID: MAK-UNK-8be7dca9-6_1

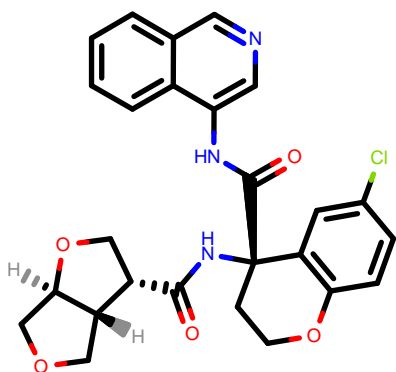
SMILES: c1cc(c2cncc(c2c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C)[NH3+]

RUN: RUN136

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.10

EN300-6482296_1_6



CID: EN300-6482296_1_6

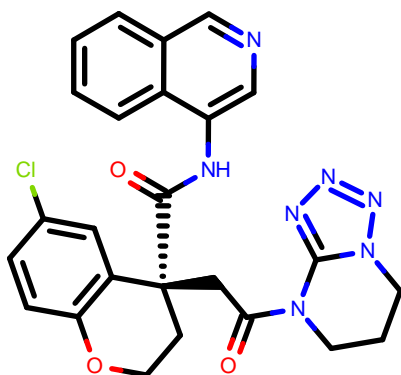
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)C)N(C1=O)C@H5CQ[C@@H]6C@H5COC6

RUN: RUN9485

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.21

EN300-217416_1_1



CID: EN300-217416_1_1

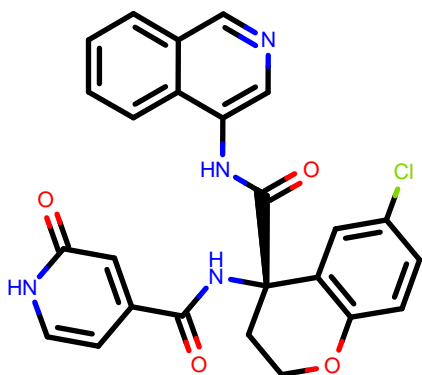
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)C)CC(=O)N5CCn6c5mnr6

RUN: RUN10541

DDG (kcal/mol): -2.73

dDDG (kcal/mol): 0.19

EN300-97661_1_1



CID: EN300-97661_1_1

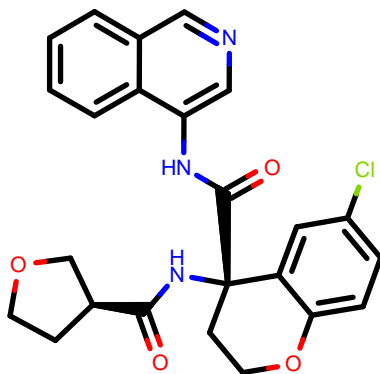
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)C)N(C1=O)c5cc[nH]c1=O)c5

RUN: RUN5382

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.21

EN300-53423_1_2



CID: EN300-53423_1_2

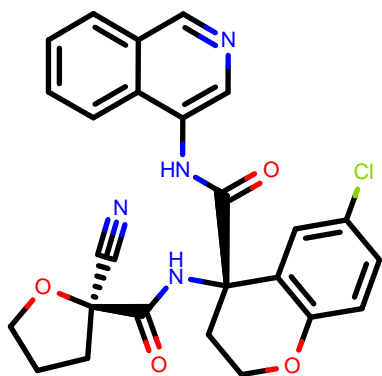
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)C)N(C1=O)[C@H]5CCOC5

RUN: RUN4790

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.22

EN300-3710141_1_1



CID: EN300-3710141_1_1

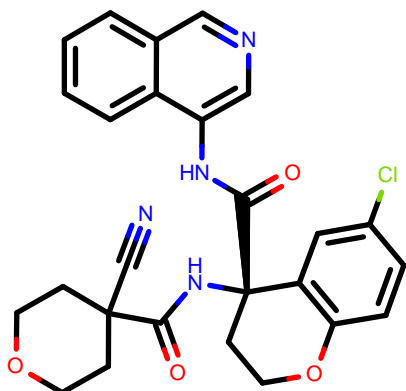
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN4362

DDG (kcal/mol): -2.72

dDDG (kcal/mol): 0.23

EN300-74089_1_1



CID: EN300-74089_1_1

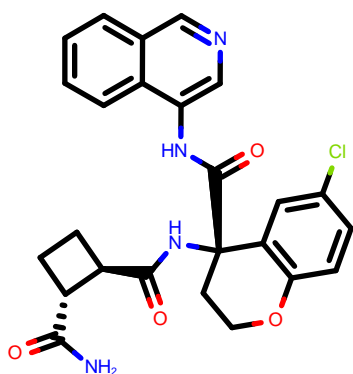
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN8124

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.23

EN300-217107_1_1



CID: EN300-217107_1_1

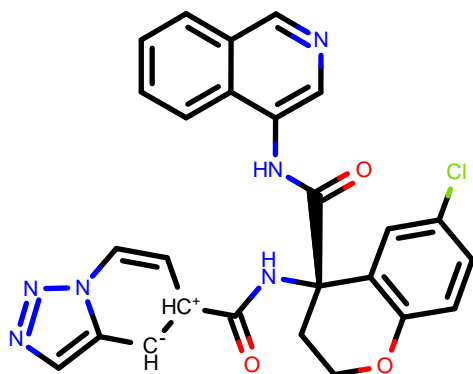
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(C)C#N

RUN: RUN5878

DDG (kcal/mol): -2.71

dDDG (kcal/mol): 0.22

EN300-6743433_1_1



CID: EN300-6743433_1_1

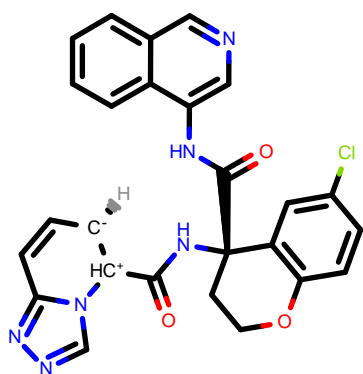
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5c5cn6c(c5)cn6

RUN: RUN4158

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.19

EN300-6488157_1_1



CID: EN300-6488157_1_1

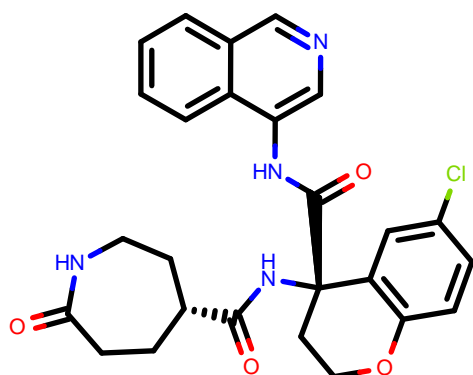
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5n6

RUN: RUN1313

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.20

EN300-152337_1_1



CID: EN300-152337_1_1

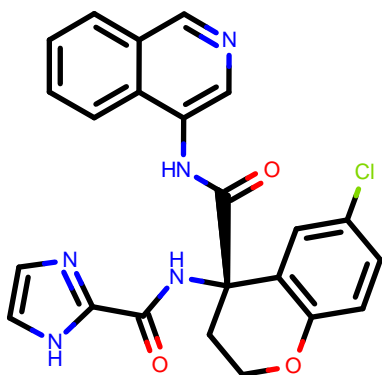
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCCC(=O)NC5

RUN: RUN3442

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.19

EN300-315836_1_1



CID: EN300-315836_1_1

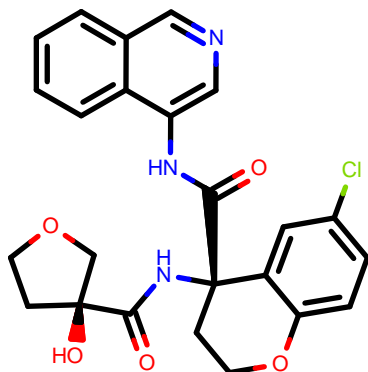
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]cnc5

RUN: RUN2641

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.18

EN300-148421_1_1



CID: EN300-148421_1_1

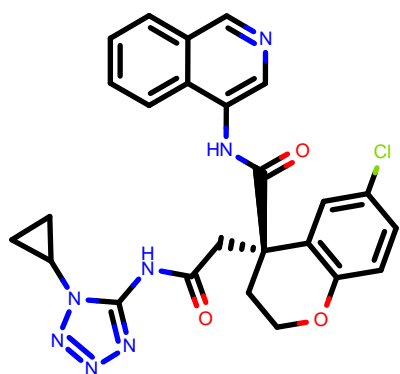
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCOCS)O

RUN: RUN7384

DDG (kcal/mol): -2.70

dDDG (kcal/mol): 0.22

EN300-225786_1_1



CID: EN300-225786_1_1

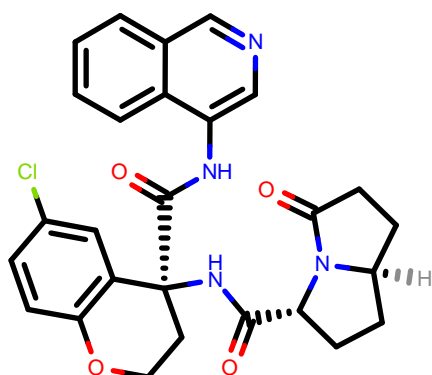
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnn5C6CC6

RUN: RUN13430

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.24

EN300-6479181_1_4



CID: EN300-6479181_1_4

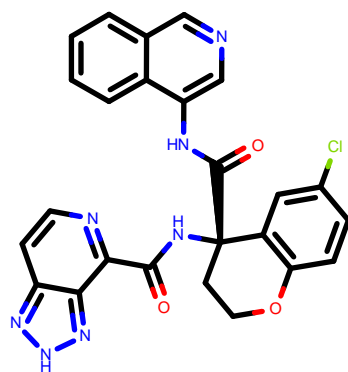
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5CC[C@H]6N5C=O)CC6

RUN: RUN9580

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.29

EN300-7426383_1_1



CID: EN300-7426383_1_1

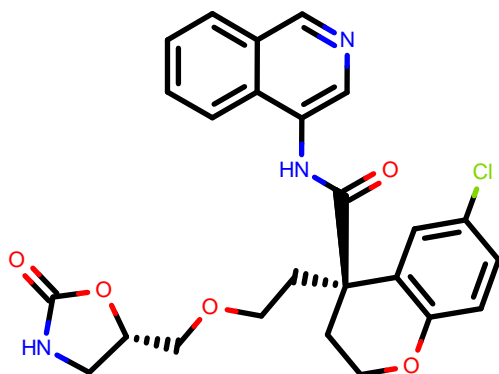
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c(ccn5)n[nH]6

RUN: RUN3242

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.18

EN300-203293_3_2



CID: EN300-203293_3_2

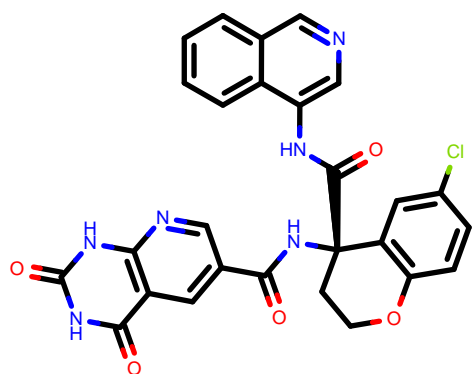
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]4H5CNC(=O)O5

RUN: RUN882

DDG (kcal/mol): -2.69

dDDG (kcal/mol): 0.24

EN300-42131_1_1



CID: EN300-42131_1_1

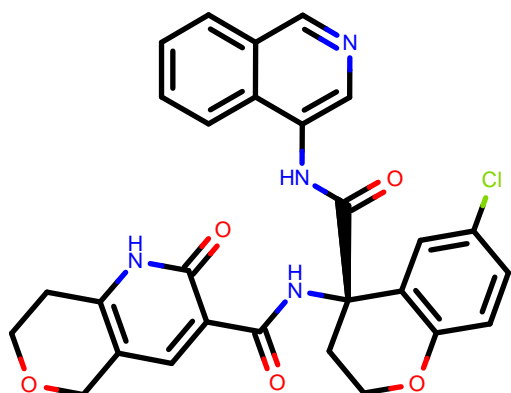
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c([nH]c(=O)[nH]c6=O)nc5

RUN: RUN9919

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.22

EN300-383824_1_1



CID: EN300-383824_1_1

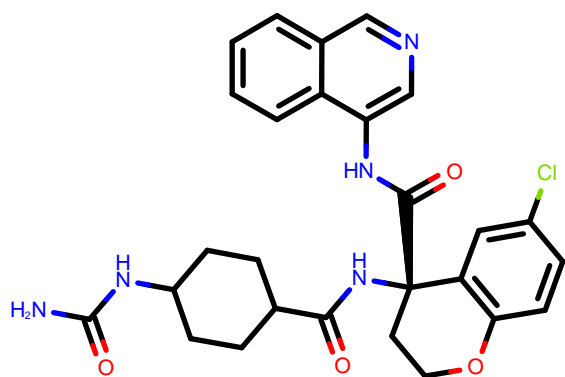
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c([nH]c5=O)CCOC6

RUN: RUN7292

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.26

EN300-53591_1_1



CID: EN300-53591_1_1

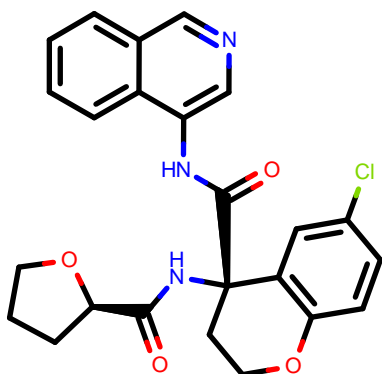
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CCCC(C5)NC(=O)N

RUN: RUN8805

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.28

EN300-21009_1_2



CID: EN300-21009_1_2

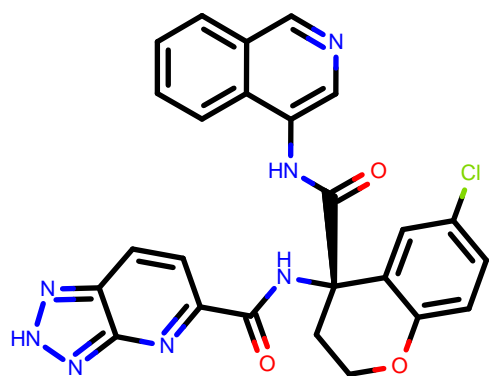
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCOC5

RUN: RUN4986

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.19

EN300-133058_1_1



CID: EN300-133058_1_1

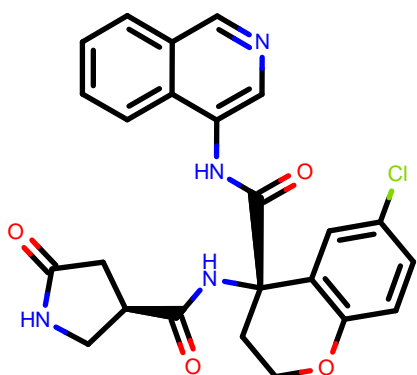
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)n[nH]6

RUN: RUN1241

DDG (kcal/mol): -2.68

dDDG (kcal/mol): 0.18

EN300-59487_1_1



CID: EN300-59487_1_1

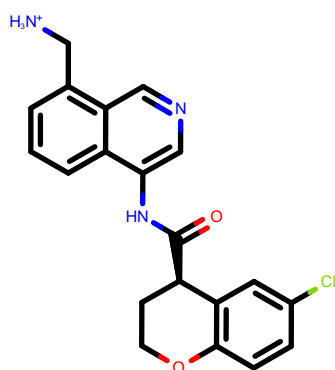
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4HJ5C(=O)NCS

RUN: RUN7812

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.19

MAK-UNK-8be7dca9-6_1



CID: MAK-UNK-8be7dca9-6_1

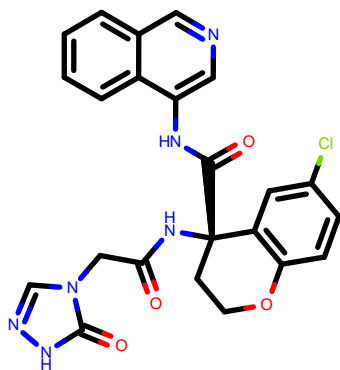
SMILES: c1cc(c2cnc(c2c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C)[NH3+]

RUN: RUN137

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.11

EN300-120820_1_1



CID: EN300-120820_1_1

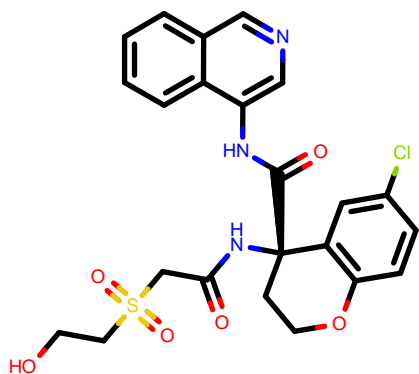
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cn[nH]5=O

RUN: RUN9205

DDG (kcal/mol): -2.67

dDDG (kcal/mol): 0.20

EN300-4293814_1_1



CID: EN300-4293814_1_1

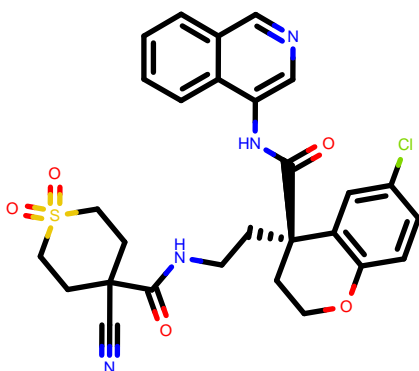
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS(=O)(=O)CCO

RUN: RUN1864

DDG (kcal/mol): -2.66

dDDG (kcal/mol): 0.40

EN300-73967_3_1



CID: EN300-73967_3_1

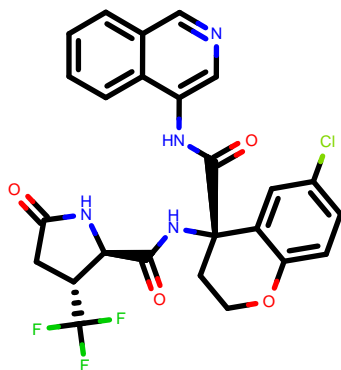
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCS(=O)(=O)CC5)C#N

RUN: RUN15076

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.30

EN300-169955_1_4



CID: EN300-169955_1_4

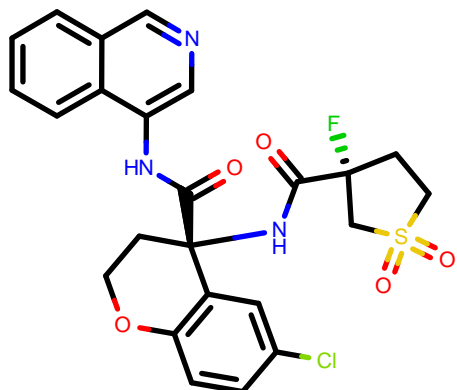
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5(C#C(F)(F)F)CC1(O)N5C(F)F

RUN: RUN6648

DDG (kcal/mol): -2.65

dDDG (kcal/mol): 0.22

EN300-311920_1_2



CID: EN300-311920_1_2

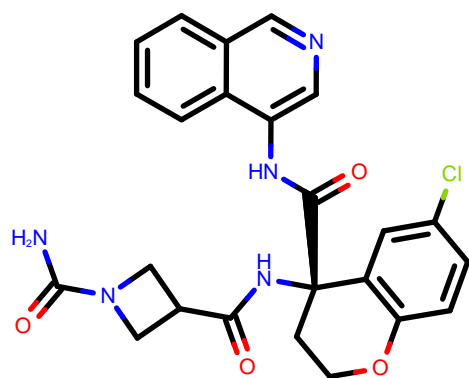
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@]5(C)S(CCS(=O)(=O)C5)F

RUN: RUN8312

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.27

EN300-1248250_1_1



CID: EN300-1248250_1_1

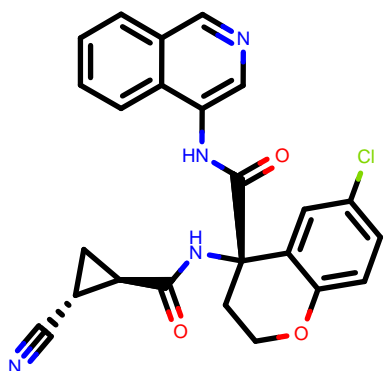
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)NC(=O)C5CN(C5)C(=O)N

RUN: RUN3590

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.20

EN300-1588617_1_1



CID: EN300-1588617_1_1

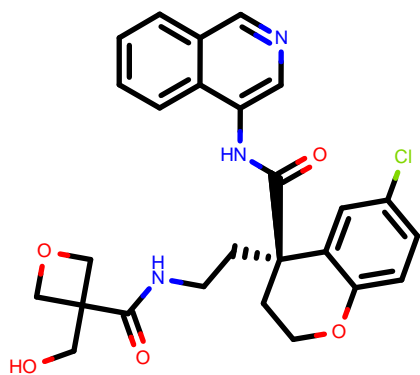
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)NC(=O)[C@@]5C[C@H]5C#N

RUN: RUN5918

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.19

EN300-105693_3_1



CID: EN300-105693_3_1

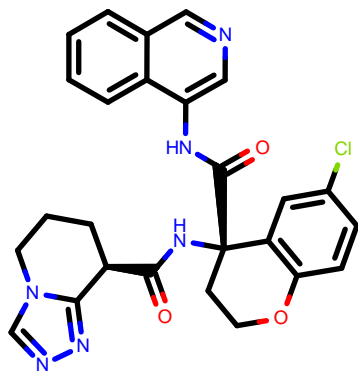
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)CCNC(=O)C5(COC5)CO

RUN: RUN4385

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.26

EN300-748981_1_1



CID: EN300-748981_1_1

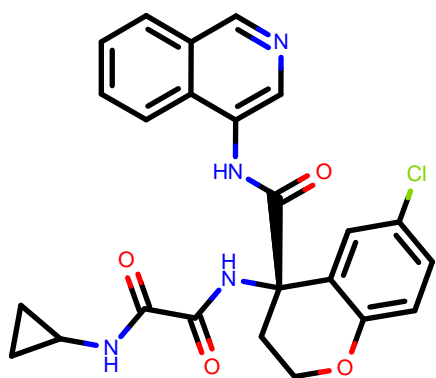
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)NC(=O)[C@@]5C[C@H]5CCN6C6N5

RUN: RUN8817

DDG (kcal/mol): -2.64

dDDG (kcal/mol): 0.22

EN300-78135_1_1



CID: EN300-78135_1_1

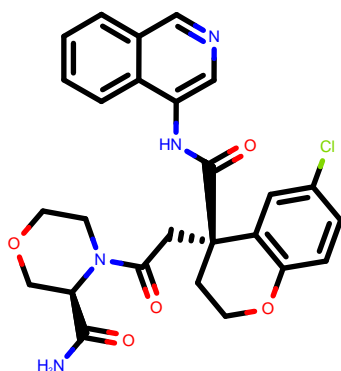
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NC5CC5

RUN: RUN2602

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.17

EN300-124383_1_2



CID: EN300-124383_1_2

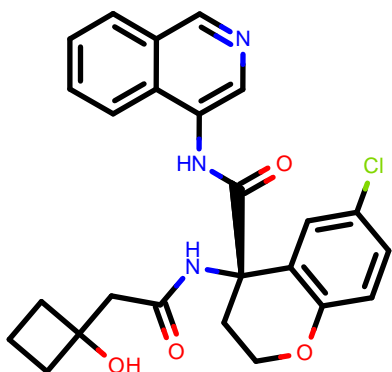
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCOC[C@@]H5C(=O)N

RUN: RUN6252

DDG (kcal/mol): -2.63

dDDG (kcal/mol): 0.24

EN300-246423_1_1



CID: EN300-246423_1_1

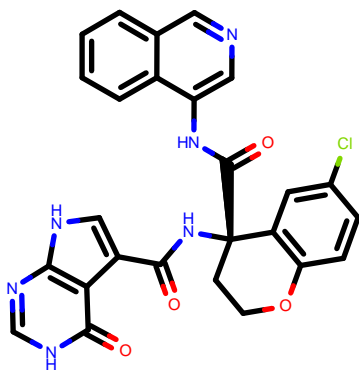
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5(CCC5)O

RUN: RUN779

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.22

EN300-746311_1_1



CID: EN300-746311_1_1

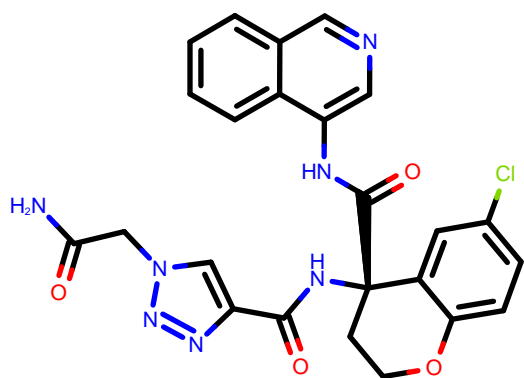
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH]c6c5c(=O)[nH]n6

RUN: RUN8717

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.20

EN300-52380_1_1



CID: EN300-52380_1_1

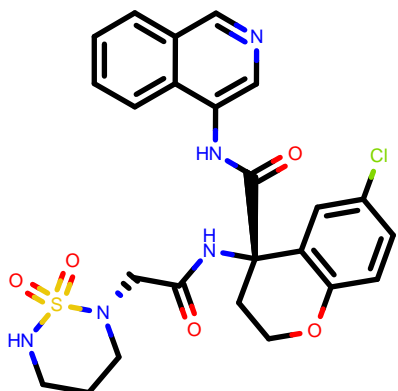
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)CC(=O)N

RUN: RUN3962

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.20

EN300-4726186_1_1



CID: EN300-4726186_1_1

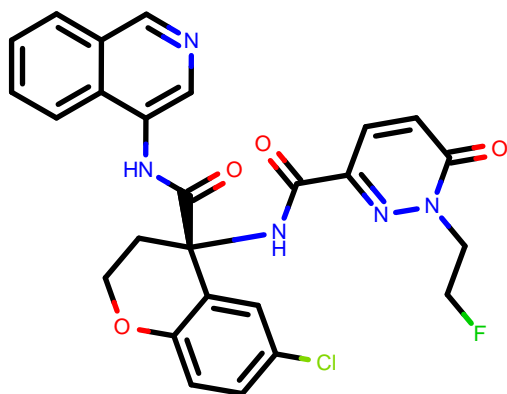
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[N@]5CCCCNS5(=O)=O

RUN: RUN2365

DDG (kcal/mol): -2.62

dDDG (kcal/mol): 0.36

EN300-263456_1_1



CID: EN300-263456_1_1

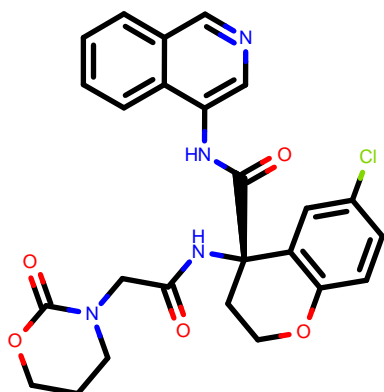
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(=O)n(n5)CCF

RUN: RUN2718

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.23

EN300-103638_1_1



CID: EN300-103638_1_1

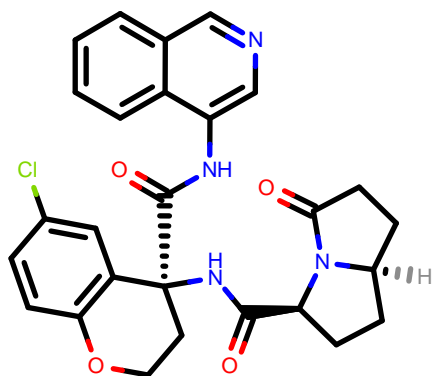
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5CCCCO5=O

RUN: RUN9401

DDG (kcal/mol): -2.61

dDDG (kcal/mol): 0.23

EN300-6479181_1_3



CID: EN300-6479181_1_3

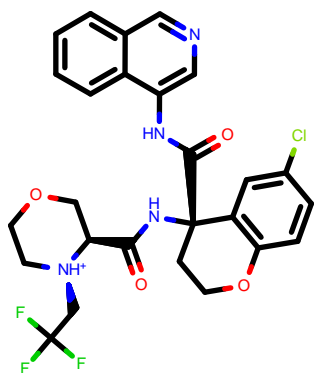
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COC(=O)C3)NC(=O)C@@H5CC[C@@H]5NC(=O)C6

RUN: RUN8568

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.20

EN300-201551_1_3



CID: EN300-201551_1_3

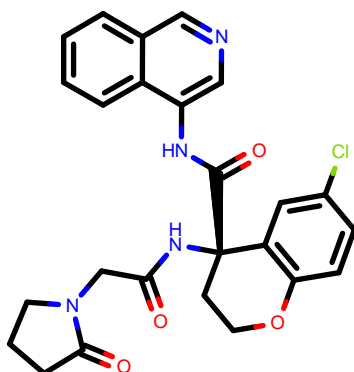
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COC(=O)C3)NC(=O)C@@H5CC[C@@H]5C(F)(F)F

RUN: RUN9185

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.23

EN300-11934_1_1



CID: EN300-11934_1_1

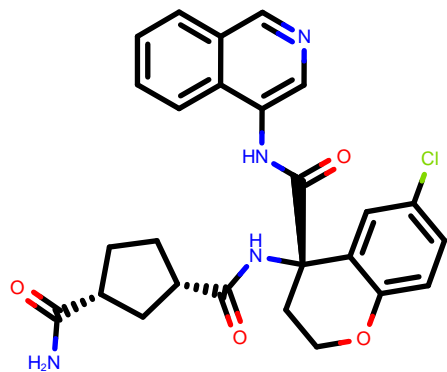
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COC(=O)C3)NC(=O)CN5CCCC5=O

RUN: RUN9169

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.23

EN300-370753_1_1



CID: EN300-370753_1_1

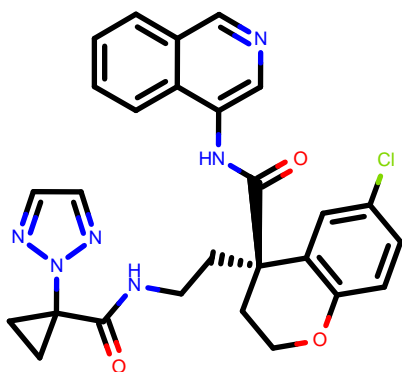
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](COC(=O)C3)NC(=O)C@H[C@@H]5C(=O)N

RUN: RUN9369

DDG (kcal/mol): -2.60

dDDG (kcal/mol): 0.32

EN300-1722017_3_1



CID: EN300-1722017_3_1

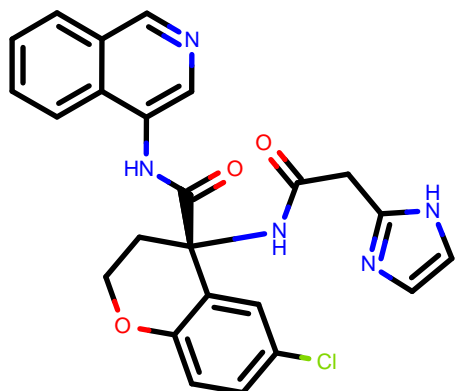
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5[nH]nccn6

RUN: RUN11361

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.24

EN300-220527_1_1



CID: EN300-220527_1_1

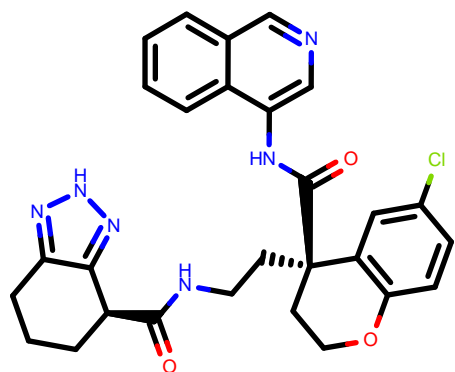
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5[nH]nccn5

RUN: RUN6476

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.20

EN300-208236_3_2



CID: EN300-208236_3_2

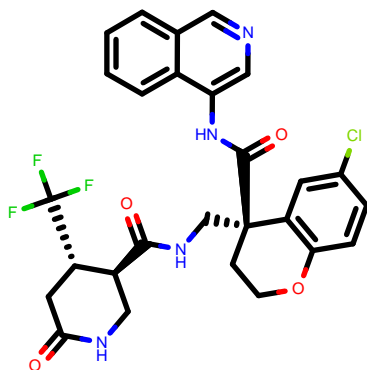
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CCNC(=O)C@H5CCc6c5n[nH]n6

RUN: RUN15268

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.26

EN300-208959_2_4



CID: EN300-208959_2_4

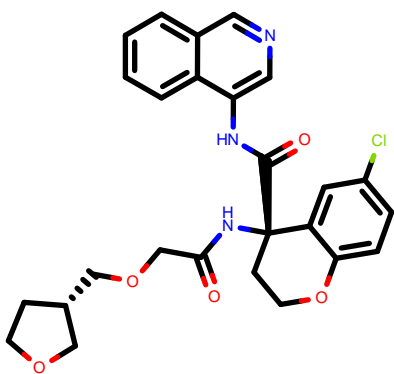
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@@3(CCOc4c3cc(cc4)C)CNC(=O)C@H5CNC(=O)C@H5C(F)F(F)F

RUN: RUN3519

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.27

EN300-80522_1_2



CID: EN300-80522_1_2

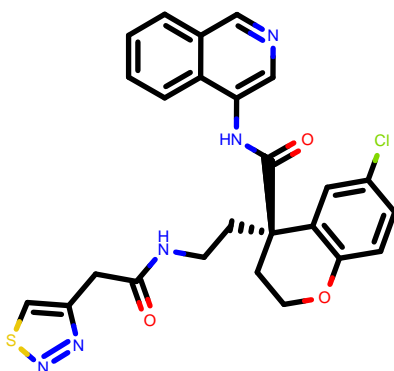
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCOC5

RUN: RUN7304

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.22

EN300-300519_3_1



CID: EN300-300519_3_1

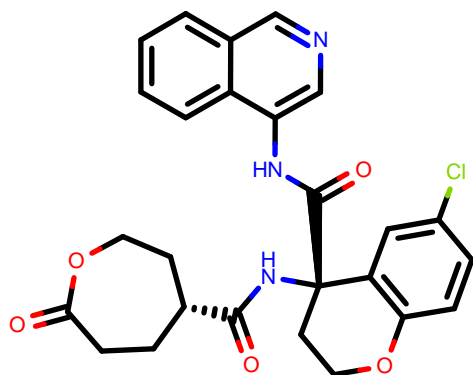
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5csnn5

RUN: RUN15308

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.24

EN300-2011083_1_1



CID: EN300-2011083_1_1

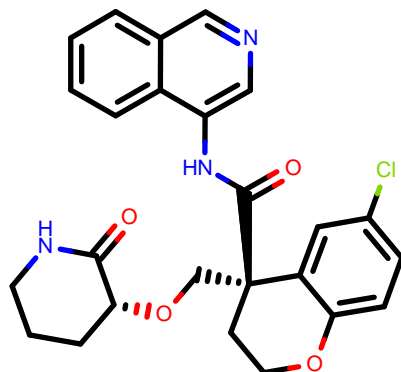
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)OCC5

RUN: RUN6788

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.23

EN300-107267_2_2



CID: EN300-107267_2_2

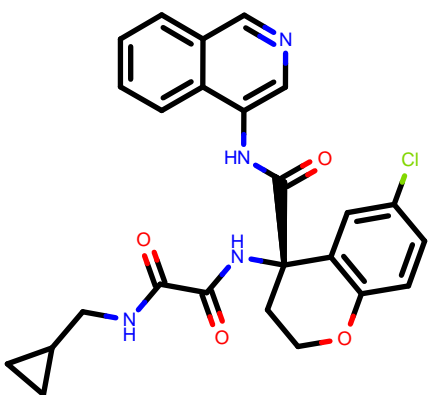
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCCNCS=O

RUN: RUN1386

DDG (kcal/mol): -2.59

dDDG (kcal/mol): 0.22

EN300-173216_1_1



CID: EN300-173216_1_1

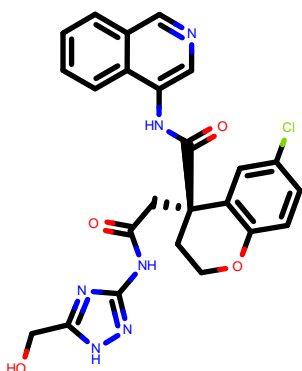
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NCC5CC5

RUN: RUN2463

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.19

EN300-96013_1_1



CID: EN300-96013_1_1

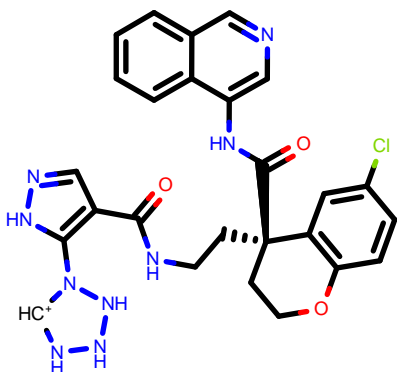
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5nc([nH]n5)CO

RUN: RUN4553

DDG (kcal/mol): -2.58

dDDG (kcal/mol): 0.17

EN300-7549839_3_1



CID: EN300-7549839_3_1

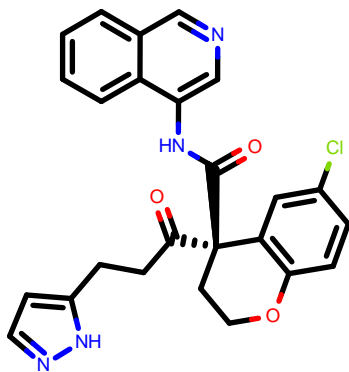
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cn([nH]c5n6cnn6

RUN: RUN14522

DDG (kcal/mol): -2.57

dDDG (kcal/mol): 0.26

VLA-UCB-34f3ed0c-8_1



CID: VLA-UCB-34f3ed0c-8_1

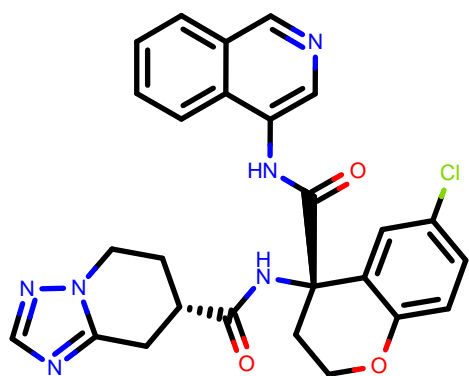
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)CCc5ccn[nH]5

RUN: RUN34

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.21

EN300-1448674_1_1



CID: EN300-1448674_1_1

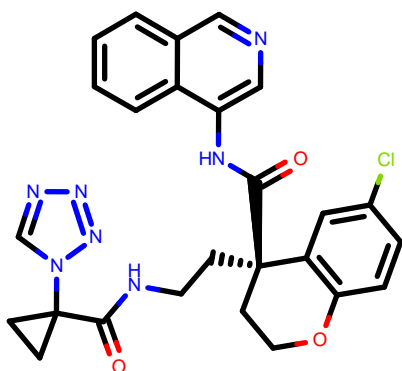
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5Cn6c(ncn6)C5

RUN: RUN6026

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.21

EN300-263085_3_1



CID: EN300-263085_3_1

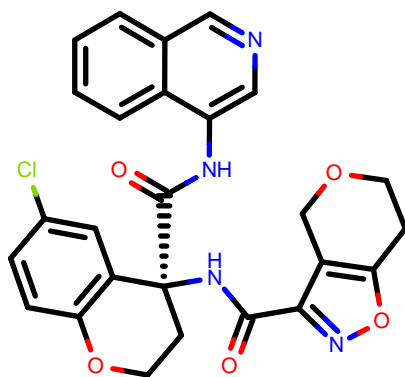
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5n6cncn6

RUN: RUN2811

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.25

EN300-88819_1_1



CID: EN300-88819_1_1

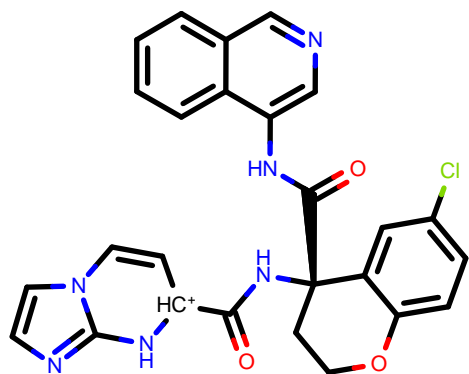
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6c(nc5)CCOC6

RUN: RUN2910

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.19

EN300-6499719_1_1



CID: EN300-6499719_1_1

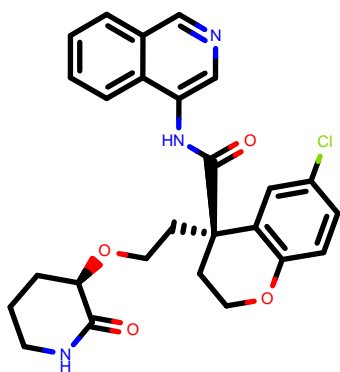
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc6cnc6[nH+]5

RUN: RUN5630

DDG (kcal/mol): -2.56

dDDG (kcal/mol): 0.21

EN300-107267_3_2



CID: EN300-107267_3_2

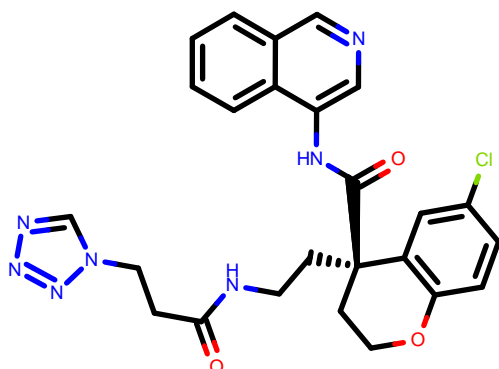
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@@]5H5CCNCNS=O

RUN: RUN1520

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.22

EN300-191904_3_1



CID: EN300-191904_3_1

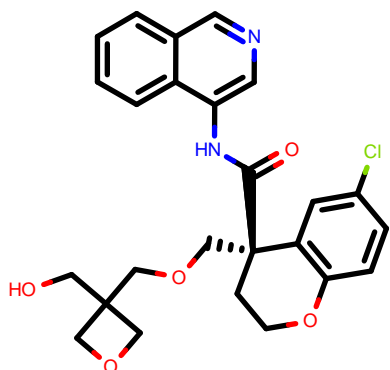
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5nnn5

RUN: RUN3793

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.23

EN300-102347_2_1



CID: EN300-102347_2_1

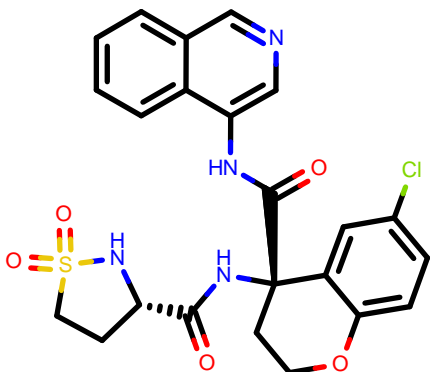
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(C)COC(C)C

RUN: RUN812

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.22

EN300-45049_1_1



CID: EN300-45049_1_1

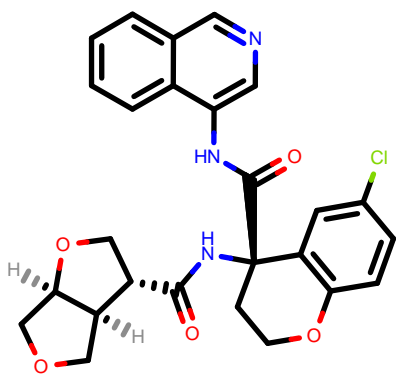
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5H5SCCS(=O)(=O)N5

RUN: RUN1697

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.27

EN300-6482296_1_2



CID: EN300-6482296_1_2

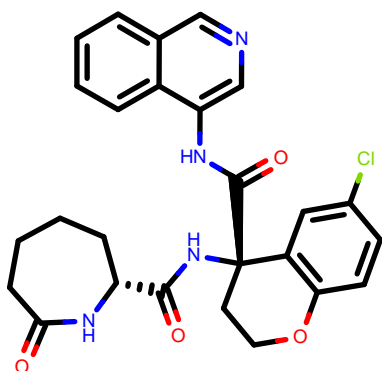
SMILES: c1ccc2c(c1)nccc2NC(=O)C@@3(CCOc4c3ccc4)C(NC(=O)C@H)C@H5COC6

RUN: RUN3482

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.21

EN300-80083_1_2



CID: EN300-80083_1_2

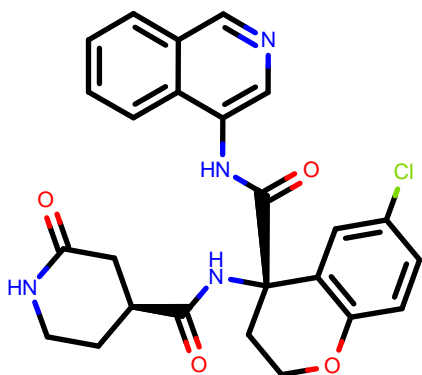
SMILES: c1ccc2c(c1)nccc2NC(=O)C@@3(CCOc4c3ccc(cc4)C)NC(=O)C@H)C@H5CCCCC(=O)N5

RUN: RUN803

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.25

EN300-107493_1_1



CID: EN300-107493_1_1

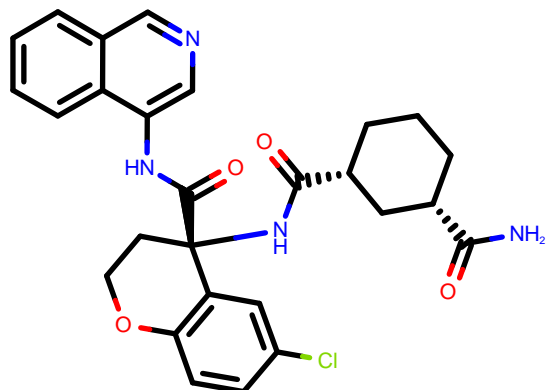
SMILES: c1ccc2c(c1)nccc2NC(=O)C@@3(CCOc4c3ccc(cc4)C)NC(=O)C@H)C@H5CCNC(=O)C5

RUN: RUN3074

DDG (kcal/mol): -2.55

dDDG (kcal/mol): 0.24

EN300-90142_1_1



CID: EN300-90142_1_1

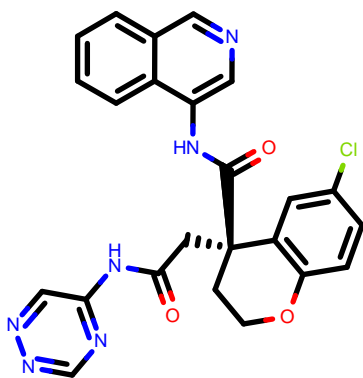
SMILES: c1ccc2c(c1)nccc2NC(=O)C@@3(CCOc4c3ccc4)C(NC(=O)C@H)C@H5CCC(C)C@H)C5(C)C(=O)N

RUN: RUN5790

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.26

EN300-110325_1_1



CID: EN300-110325_1_1

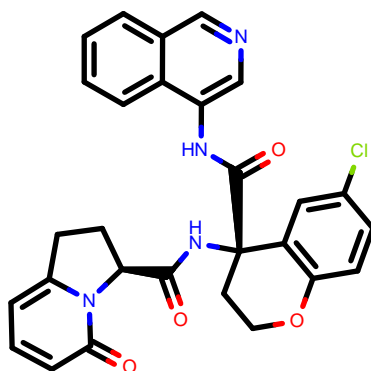
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nncn5

RUN: RUN14828

DDG (kcal/mol): -2.54

dDDG (kcal/mol): 0.25

EN300-332002_1_1



CID: EN300-332002_1_1

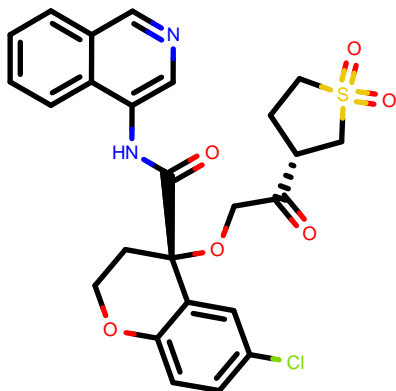
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4H5CCc6n5c(=O)ccc6

RUN: RUN9049

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.21

EN300-226314_1_1



CID: EN300-226314_1_1

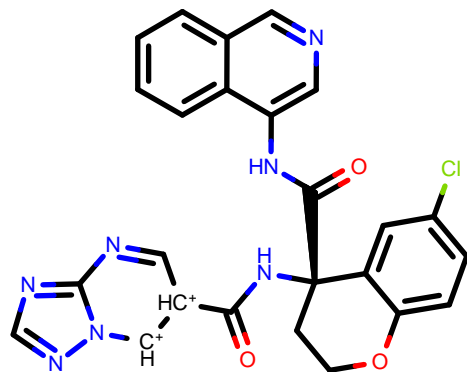
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@]4H5CCS(=O)(=O)C5

RUN: RUN903

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.30

EN300-7540875_1_1



CID: EN300-7540875_1_1

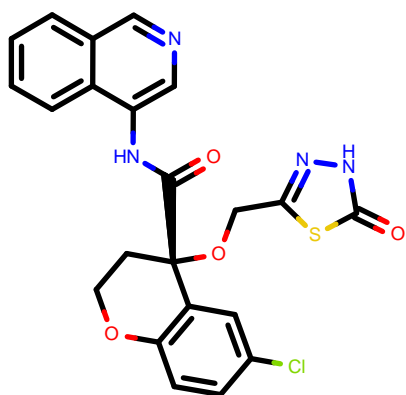
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6nncn6c5

RUN: RUN5746

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.19

EN300-171766_1_1



CID: EN300-171766_1_1

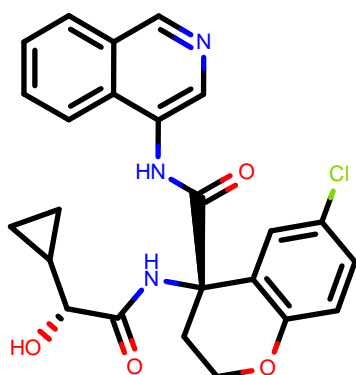
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5n[nH]c(=O)s5

RUN: RUN1757

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.17

EN300-72211_1_1



CID: EN300-72211_1_1

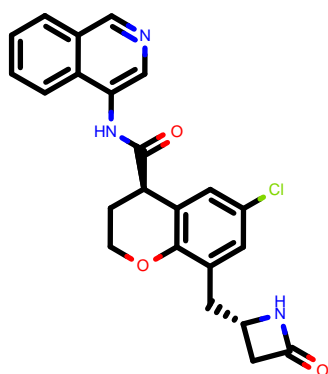
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5CC5)O

RUN: RUN2922

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.21

DAR-DIA-6a508060-5_1



CID: DAR-DIA-6a508060-5_1

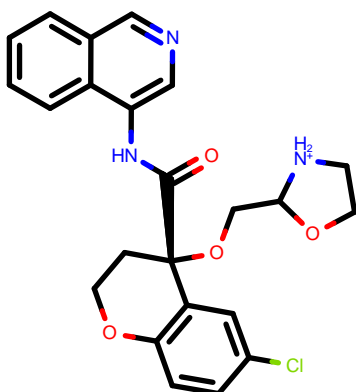
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[C@H]5CC(=O)N5Cl

RUN: RUN192

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.20

EN300-317555_1_1



CID: EN300-317555_1_1

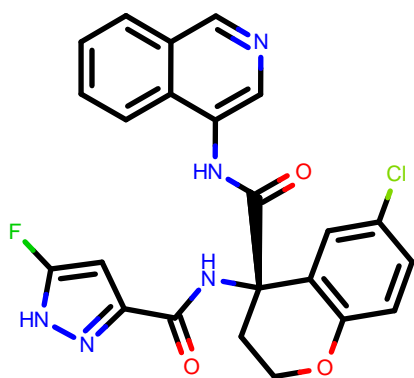
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5

RUN: RUN2382

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.15

EN300-150212_1_1



CID: EN300-150212_1_1

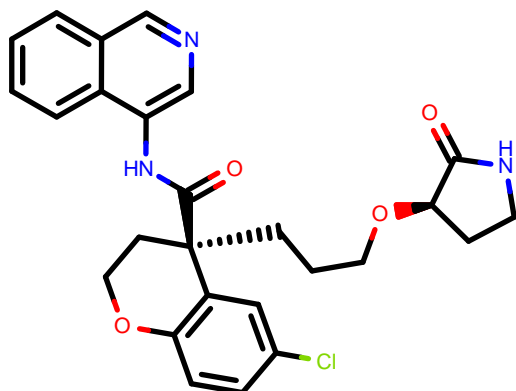
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc[nH]n5F

RUN: RUN3030

DDG (kcal/mol): -2.53

dDDG (kcal/mol): 0.17

EN300-6736413_4_2



CID: EN300-6736413_4_2

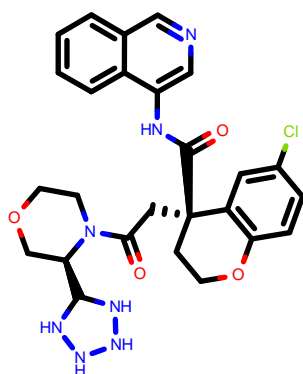
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN677

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.21

EN300-239825_1_2



CID: EN300-239825_1_2

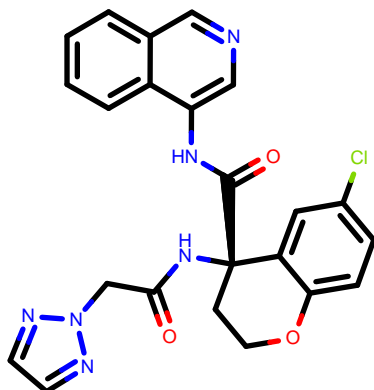
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5c6[nH]n6

RUN: RUN9675

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.28

EN300-100916_1_1



CID: EN300-100916_1_1

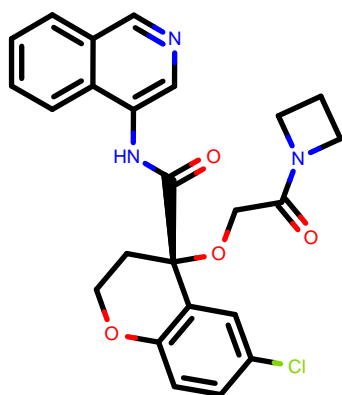
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5nccn5

RUN: RUN7372

DDG (kcal/mol): -2.52

dDDG (kcal/mol): 0.20

EN300-11195_1_1



CID: EN300-11195_1_1

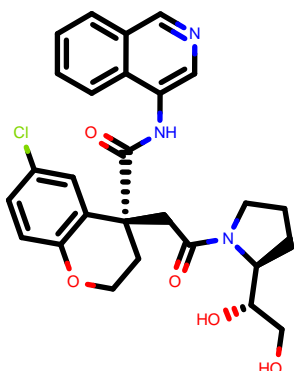
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCC(=O)N5CCCC5

RUN: RUN1533

DDG (kcal/mol): -2.51

dDDG (kcal/mol): 0.19

EN300-7459540_1_4



CID: EN300-7459540_1_4

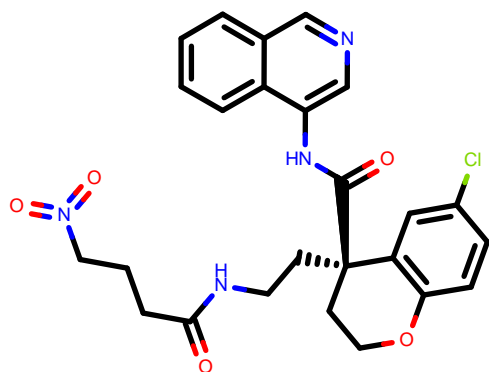
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)CC(=O)N5CCCC[C@@H]5[C@@H](CO)O

RUN: RUN9684

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.37

EN300-143449_3_1



CID: EN300-143449_3_1

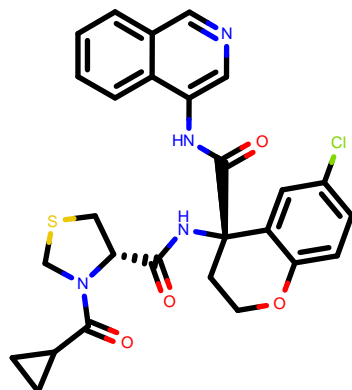
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)O)CCNC(=O)CCCN(=O)=O

RUN: RUN14154

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.22

EN300-18928_1_2



CID: EN300-18928_1_2

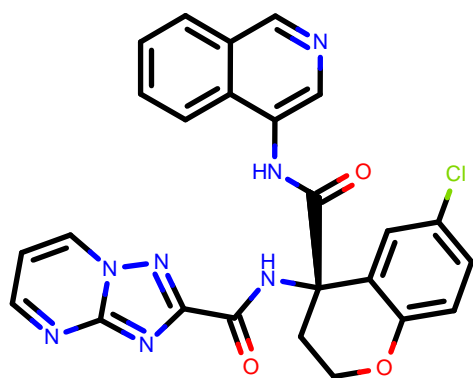
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)N)C(=O)[C@@H]5CSCN5C(=O)C6CC6

RUN: RUN8512

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.24

EN300-83529_1_1



CID: EN300-83529_1_1

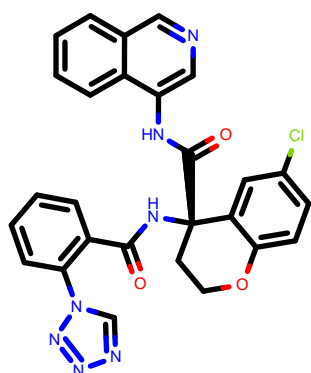
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nc6nccn6n5

RUN: RUN3666

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.17

EN300-09325_1_1



CID: EN300-09325_1_1

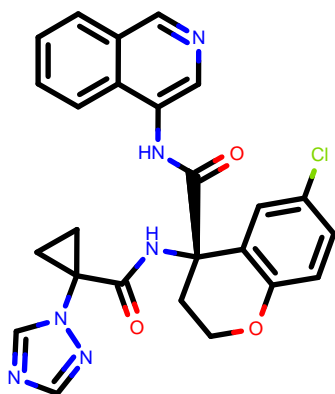
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5n6cnn6

RUN: RUN2435

DDG (kcal/mol): -2.50

dDDG (kcal/mol): 0.25

EN300-246440_1_1



CID: EN300-246440_1_1

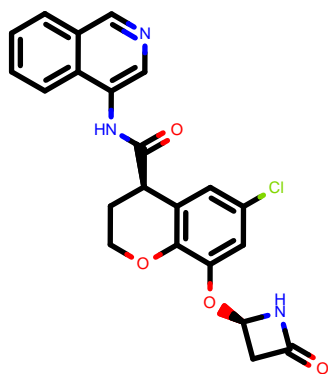
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5n6cnn6

RUN: RUN6432

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.22

VLA-UCB-50c39ae8-8_1



CID: VLA-UCB-50c39ae8-8_1

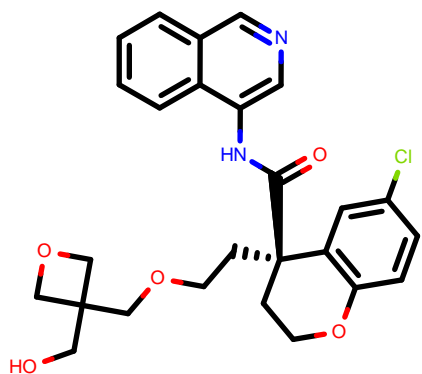
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOc4c3cc(cc4)O[C@@H]5CC(=O)N5Cl

RUN: RUN12

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.21

EN300-102347_3_1



CID: EN300-102347_3_1

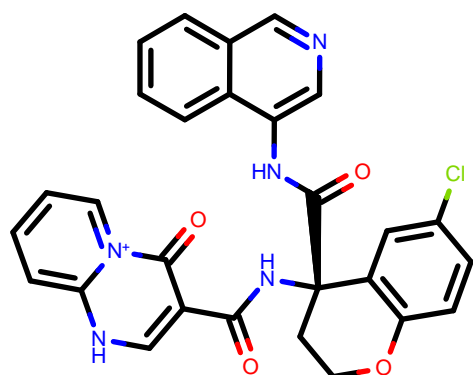
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC5(COC5)CO

RUN: RUN954

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.24

EN300-35781_1_1



CID: EN300-35781_1_1

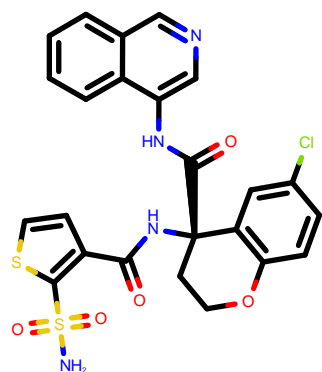
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc6ccccc6s5=O

RUN: RUN2151

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.26

EN300-294602_1_1



CID: EN300-294602_1_1

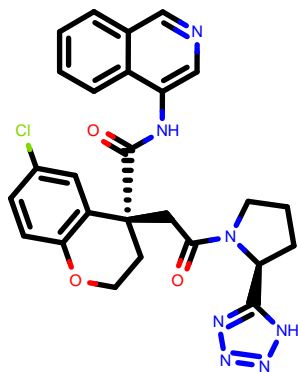
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc6S(=O)(=O)N6

RUN: RUN6808

DDG (kcal/mol): -2.49

dDDG (kcal/mol): 0.27

EN300-2908043_1_1



CID: EN300-2908043_1_1

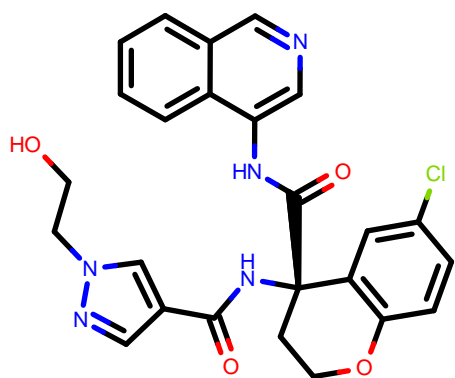
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC[C@H]5c6n[nH]n6

RUN: RUN9947

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.28

EN300-761209_1_1



CID: EN300-761209_1_1

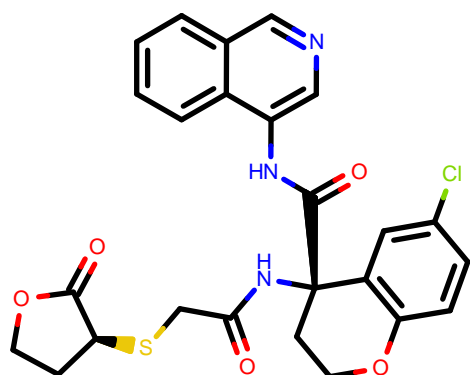
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn(c5)CO

RUN: RUN5474

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.18

EN300-113218_1_1



CID: EN300-113218_1_1

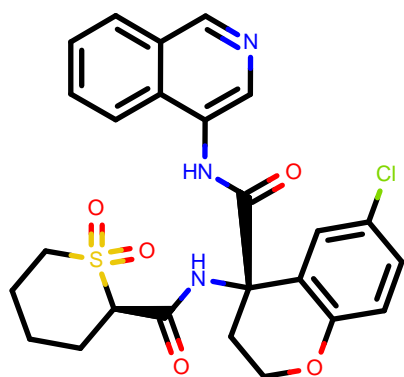
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@H]5COCS=O

RUN: RUN2736

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.24

EN300-107435_1_2



CID: EN300-107435_1_2

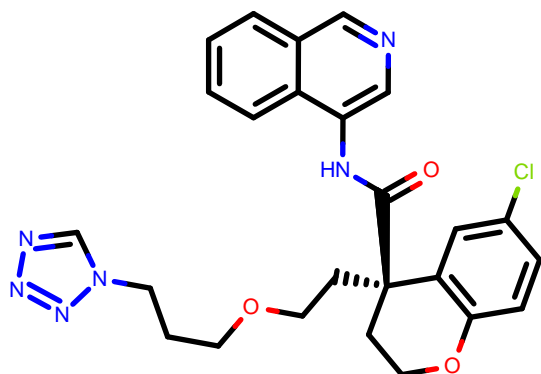
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5SCCSCS(=O)=O

RUN: RUN8448

DDG (kcal/mol): -2.48

dDDG (kcal/mol): 0.30

EN300-1696962_3_1



CID: EN300-1696962_3_1

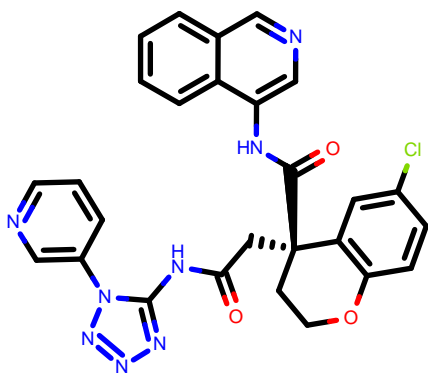
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCn5cnn5

RUN: RUN1688

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.25

EN300-1704428_1_1



CID: EN300-1704428_1_1

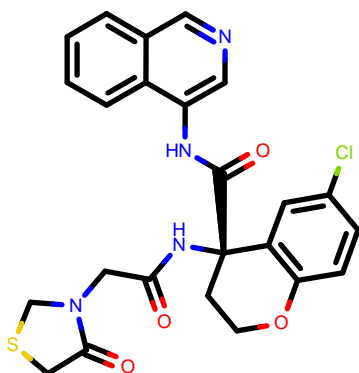
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnn5c6ccccc6

RUN: RUN14692

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.24

EN300-10747_1_1



CID: EN300-10747_1_1

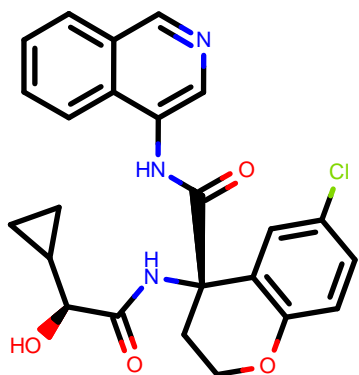
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5SCC5=O

RUN: RUN9085

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.21

EN300-72211_1_2



CID: EN300-72211_1_2

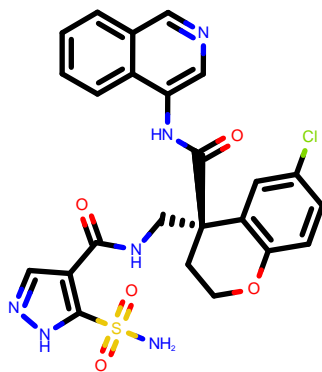
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]1C5CC5=O

RUN: RUN1034

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.27

EN300-144606_2_1



CID: EN300-144606_2_1

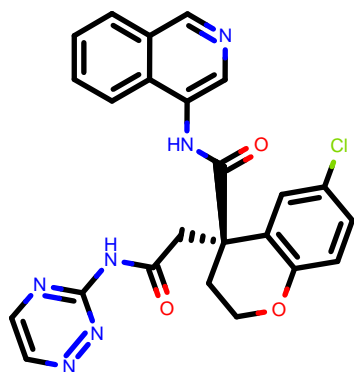
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5n[nH]c5S(=O)(=O)N

RUN: RUN8662

DDG (kcal/mol): -2.47

dDDG (kcal/mol): 0.28

EN300-20363_1_1



CID: EN300-20363_1_1

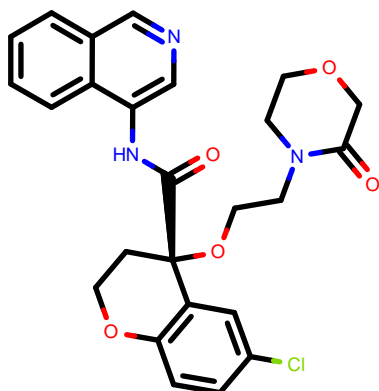
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nccnn5

RUN: RUN11226

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.18

EN300-219330_1_1



CID: EN300-219330_1_1

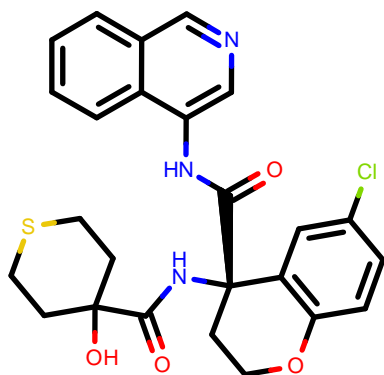
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOCC5=O

RUN: RUN2794

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.25

EN300-122340_1_1



CID: EN300-122340_1_1

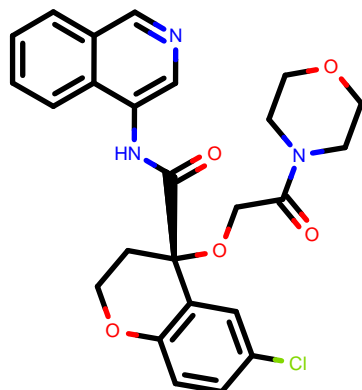
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCS)CC5=O

RUN: RUN2609

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.25

EN300-1241327_1_1



CID: EN300-1241327_1_1

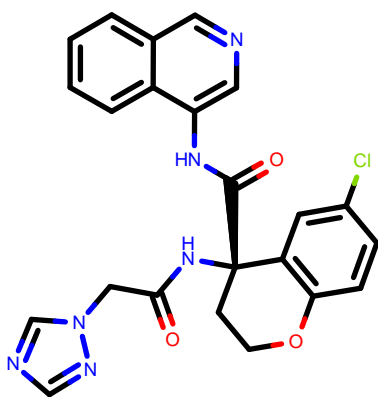
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCOCC5

RUN: RUN2494

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.20

EN300-06654_1_1



CID: EN300-06654_1_1

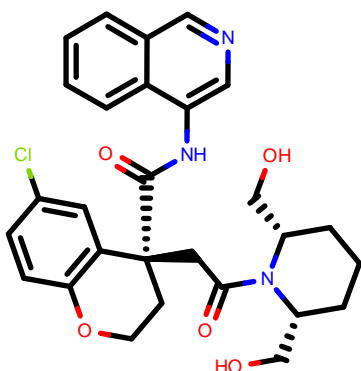
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncn5

RUN: RUN3670

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.19

EN300-6472771_1_1



CID: EN300-6472771_1_1

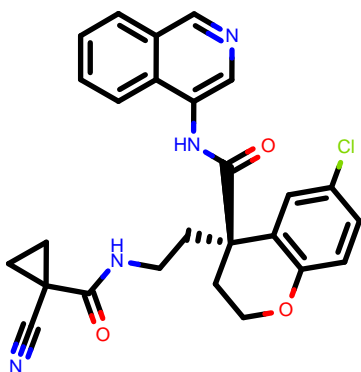
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5[C@H](CCC[C@H]5CO)CO

RUN: RUN12148

DDG (kcal/mol): -2.46

dDDG (kcal/mol): 0.33

EN300-114082_3_1



CID: EN300-114082_3_1

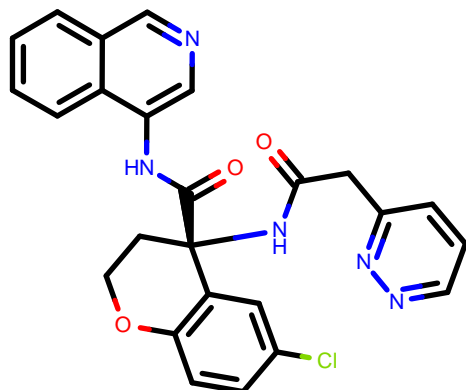
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(C)C5#N

RUN: RUN4701

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.20

EN300-7456948_1_1



CID: EN300-7456948_1_1

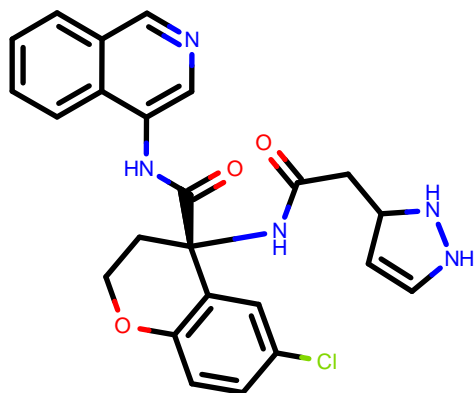
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccnnc5

RUN: RUN8997

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.21

VLA-UCB-34f3ed0c-4_1



CID: VLA-UCB-34f3ed0c-4_1

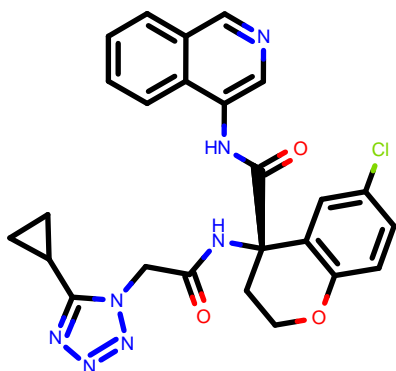
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cn[nH]5

RUN: RUN6417

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.20

EN300-872798_1_1



CID: EN300-872798_1_1

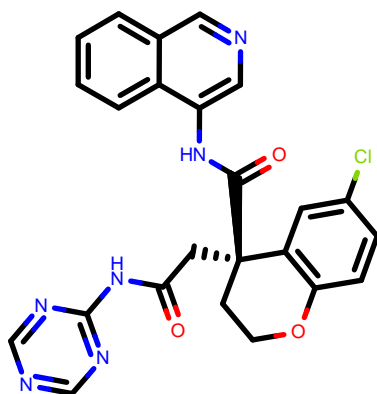
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(mn5)C6C66

RUN: RUN2547

DDG (kcal/mol): -2.45

dDDG (kcal/mol): 0.26

EN300-342082_1_1



CID: EN300-342082_1_1

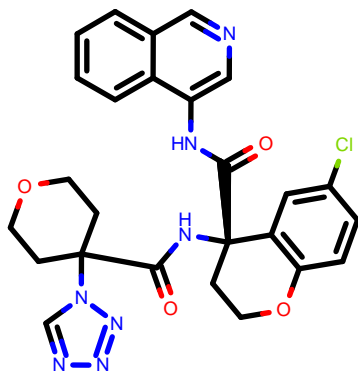
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nncn5

RUN: RUN12008

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.16

EN300-254908_1_1



CID: EN300-254908_1_1

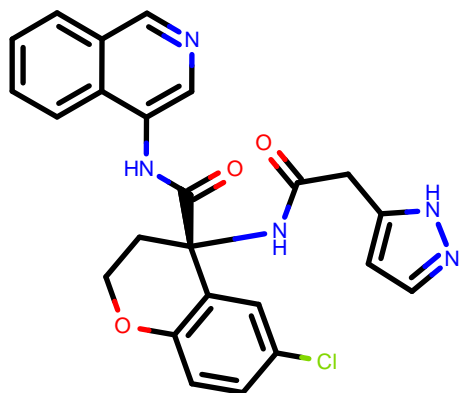
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)n6n6n6

RUN: RUN8697

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

VLA-UCB-34f3ed0c-4_1



CID: VLA-UCB-34f3ed0c-4_1

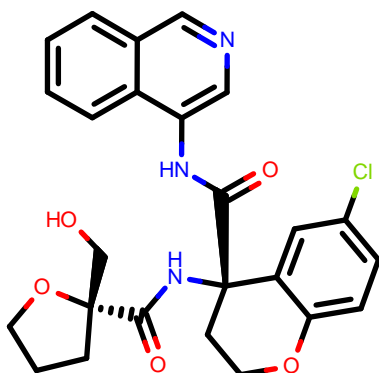
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cc[nH]5

RUN: RUN233

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.24

EN300-1425677_1_2



CID: EN300-1425677_1_2

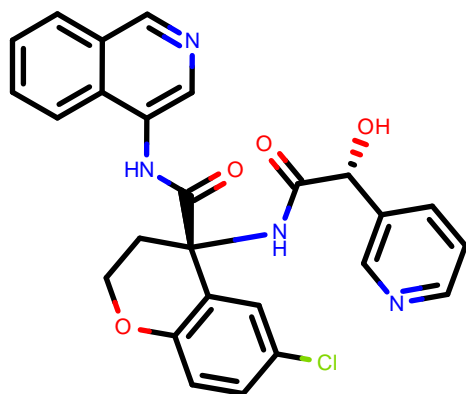
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOc5)CO

RUN: RUN1281

DDG (kcal/mol): -2.44

dDDG (kcal/mol): 0.27

EN300-134855_1_2



CID: EN300-134855_1_2

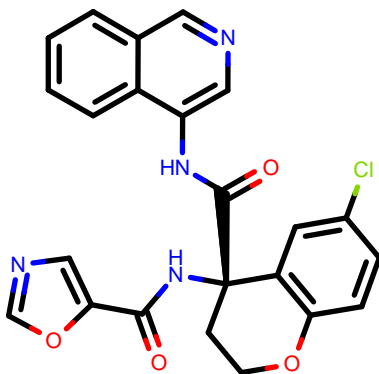
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C=CNc5O

RUN: RUN7556

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.23

EN300-25446_1_1



CID: EN300-25446_1_1

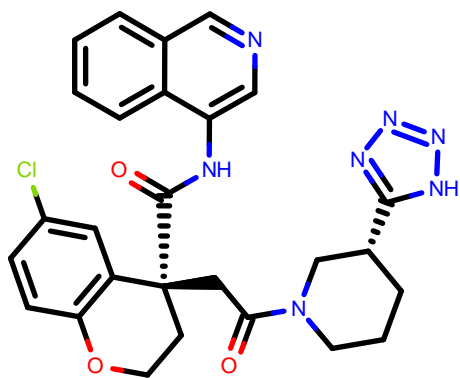
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncn5

RUN: RUN5390

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.16

EN300-115760_1_2



CID: EN300-115760_1_2

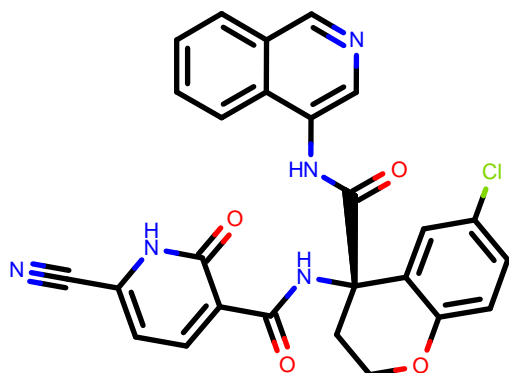
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H](C5)c6n[n-]n6

RUN: RUN9939

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.32

EN300-640698_1_1



CID: EN300-640698_1_1

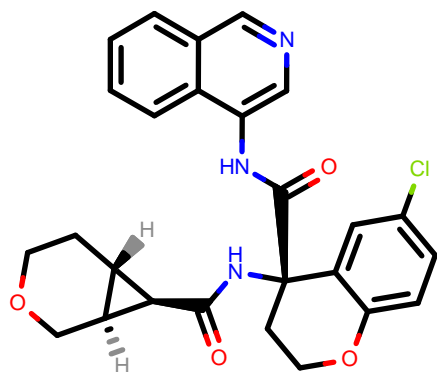
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc([nH]c5=O)C#N

RUN: RUN739

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.25

EN300-1644723_1_1



CID: EN300-1644723_1_1

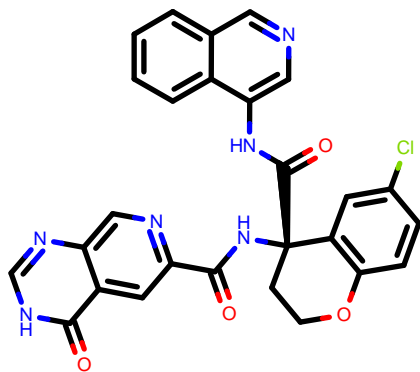
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H]6C[C@H]5OCC6

RUN: RUN8328

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.20

EN300-151756_1_1



CID: EN300-151756_1_1

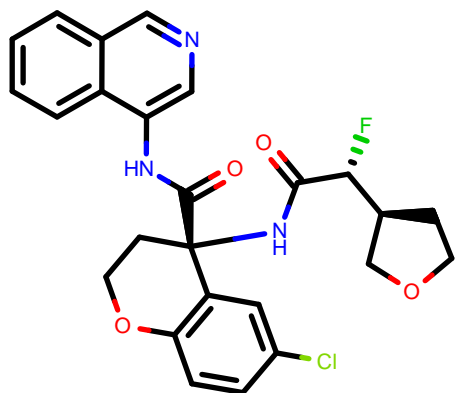
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(en5)nd[nH]6=O

RUN: RUN2087

DDG (kcal/mol): -2.43

dDDG (kcal/mol): 0.17

EN300-783124_1_3



CID: EN300-783124_1_3

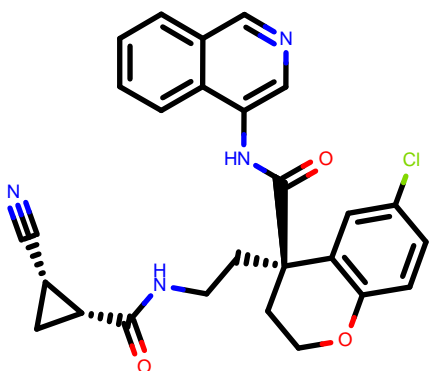
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]([C@H]5CCOC5)F

RUN: RUN4014

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.23

EN300-1600363_3_1



CID: EN300-1600363_3_1

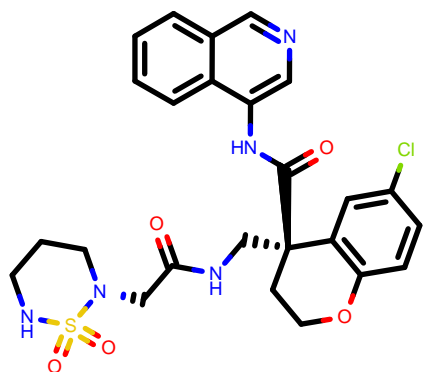
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[C@H]5CN

RUN: RUN15197

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.20

EN300-4726186_2_2



CID: EN300-4726186_2_2

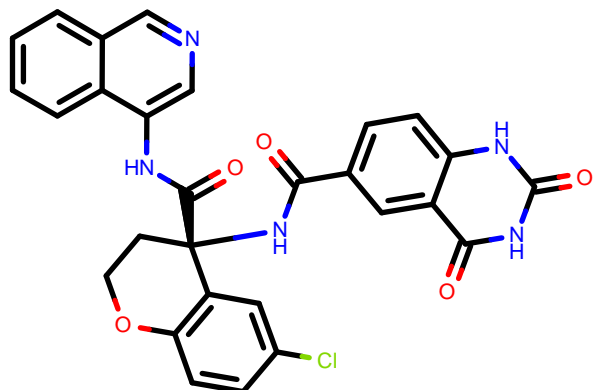
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[N@@]5SCCNS5(=O)=O

RUN: RUN1156

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.33

EN300-1723214_1_1



CID: EN300-1723214_1_1

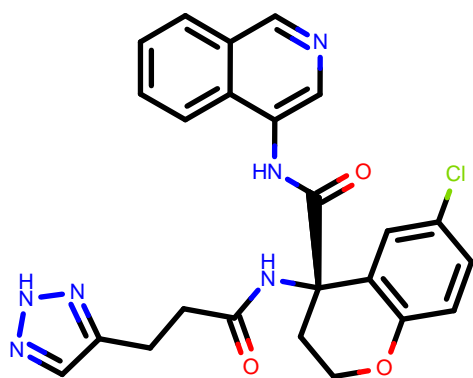
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6c(c5)c(-O)H5(-O)H96

RUN: RUN9916

DDG (kcal/mol): -2.42

dDDG (kcal/mol): 0.26

EN300-244947_1_1



CID: EN300-244947_1_1

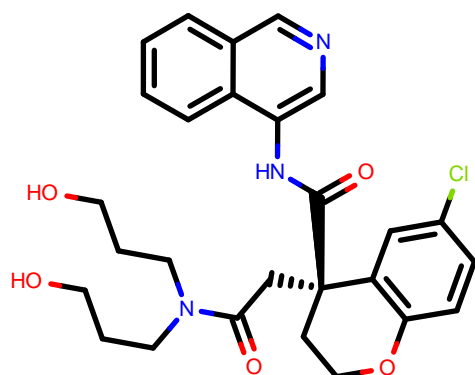
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5cn[nH]n5

RUN: RUN8284

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.20

EN300-141457_1_1



CID: EN300-141457_1_1

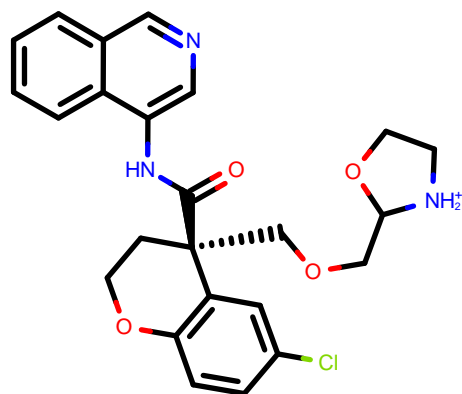
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCCO)CCO

RUN: RUN9392

DDG (kcal/mol): -2.41

dDDG (kcal/mol): 0.30

EN300-317555_2_1



CID: EN300-317555_2_1

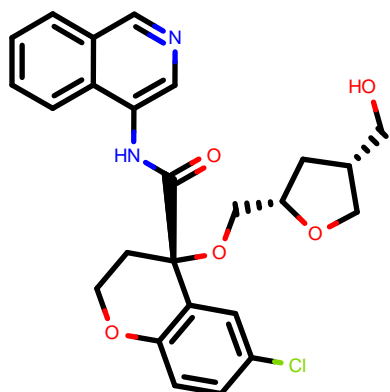
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5=NCCO5

RUN: RUN1857

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.17

EN300-6494158_1_2



CID: EN300-6494158_1_2

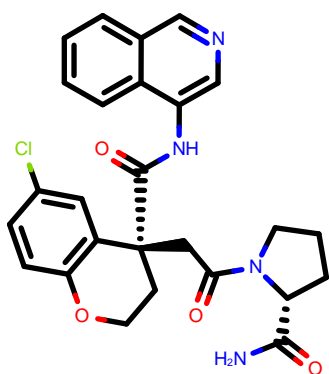
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5(CO)COC5

RUN: RUN1868

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.27

EN300-07127_1_2



CID: EN300-07127_1_2

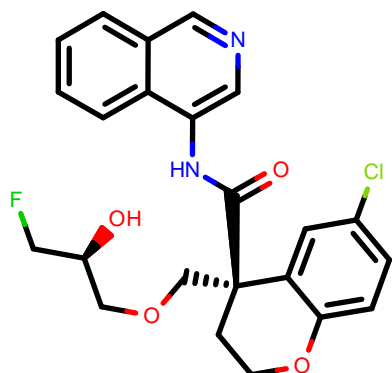
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN5517

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.21

EN300-1968342_2_1



CID: EN300-1968342_2_1

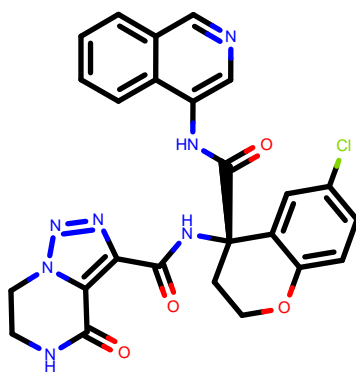
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O

RUN: RUN1825

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.23

EN300-176023_1_1



CID: EN300-176023_1_1

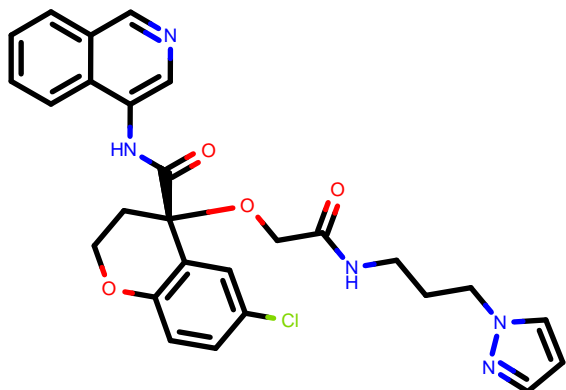
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6n(nm5)CCNCC6=O

RUN: RUN8949

DDG (kcal/mol): -2.40

dDDG (kcal/mol): 0.21

EN300-47500_1_1



CID: EN300-47500_1_1

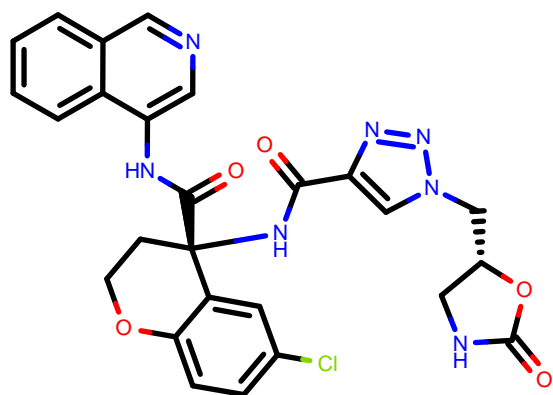
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCN5CCCN5

RUN: RUN2326

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.26

EN300-379219_1_1



CID: EN300-379219_1_1

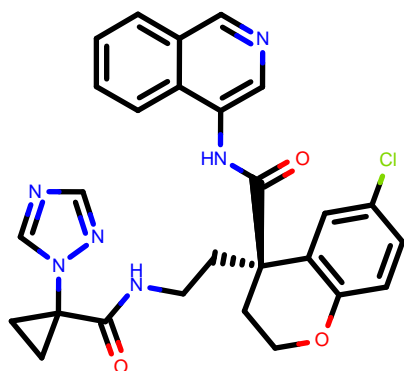
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)C[C@@H]6CNC(=O)O6

RUN: RUN1465

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.24

EN300-246440_3_1



CID: EN300-246440_3_1

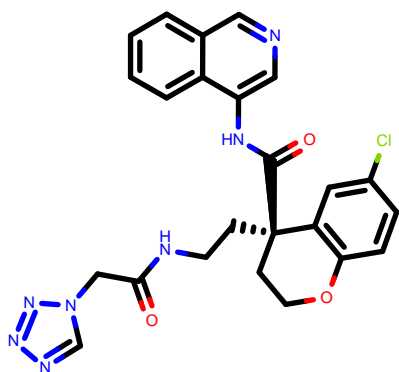
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5n6cn6

RUN: RUN9108

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.23

EN300-20980_3_1



CID: EN300-20980_3_1

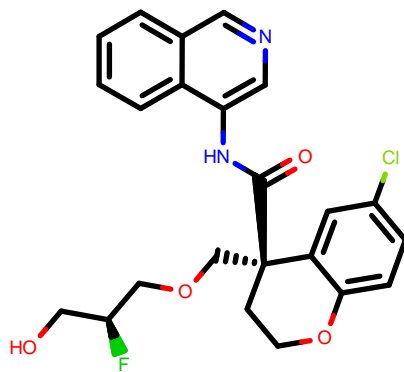
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cn5

RUN: RUN15154

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.19

EN300-1600517_2_1



CID: EN300-1600517_2_1

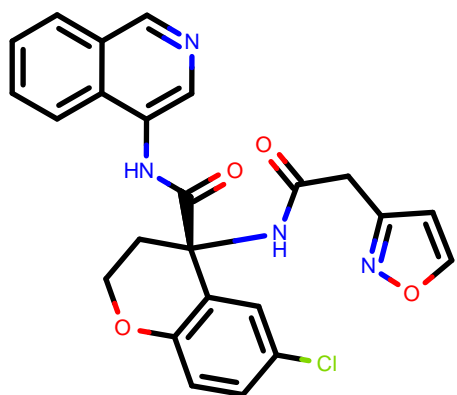
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@H](CO)F

RUN: RUN796

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.24

EN300-82037_1_1



CID: EN300-82037_1_1

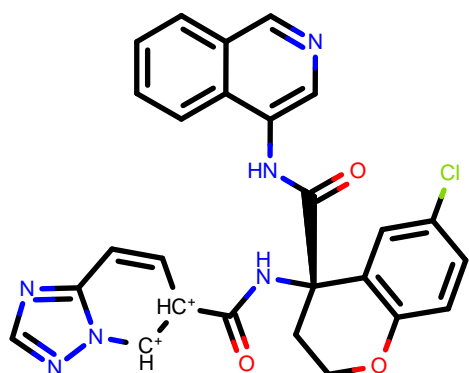
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5ccon5

RUN: RUN8280

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.20

EN300-1592151_1_1



CID: EN300-1592151_1_1

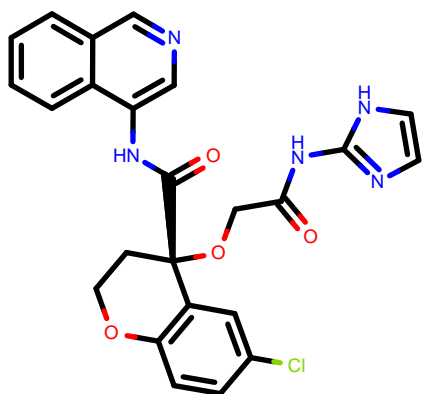
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn6nn6c5

RUN: RUN4266

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.19

EN300-331993_1_1



CID: EN300-331993_1_1

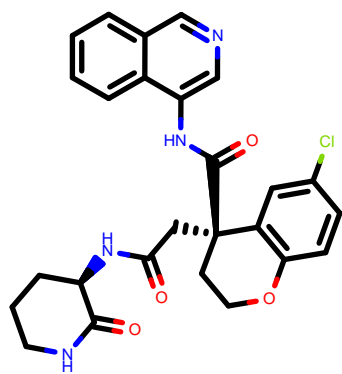
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)Nc5[nH]cn5

RUN: RUN1733

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.19

EN300-60035_1_2



CID: EN300-60035_1_2

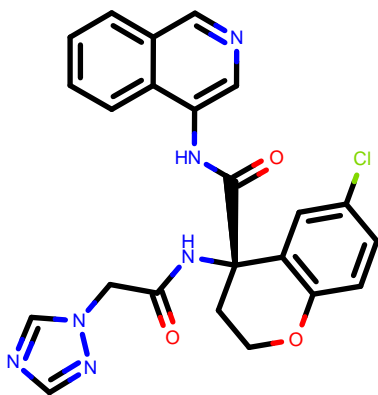
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]4H5CCNCC5=O

RUN: RUN12022

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.21

EN300-06654_1_1



CID: EN300-06654_1_1

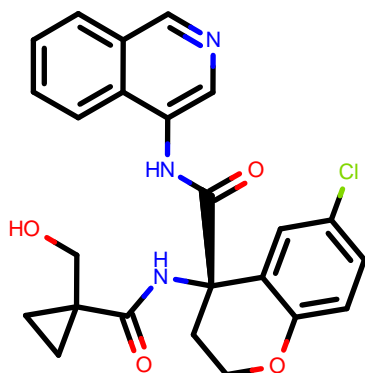
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncn5

RUN: RUN3674

DDG (kcal/mol): -2.39

dDDG (kcal/mol): 0.20

EN300-146174_1_1



CID: EN300-146174_1_1

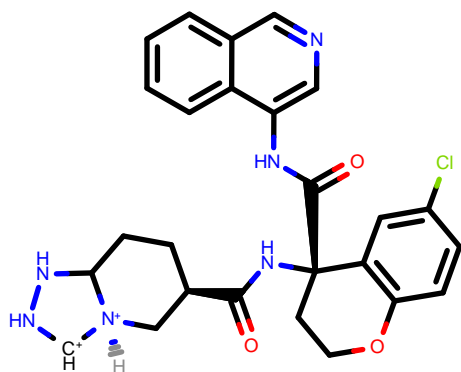
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)CO

RUN: RUN1002

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.20

EN300-51350_1_1



CID: EN300-51350_1_1

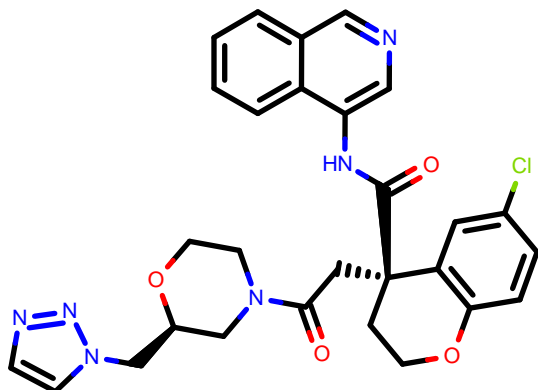
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNC6NCCN6C5

RUN: RUN5038

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.21

EN300-307567_1_1



CID: EN300-307567_1_1

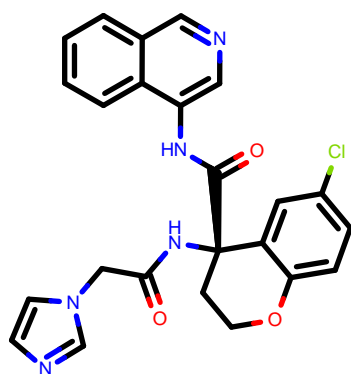
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]5(C)Cn6cncn6

RUN: RUN9396

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.30

EN300-38979_1_1



CID: EN300-38979_1_1

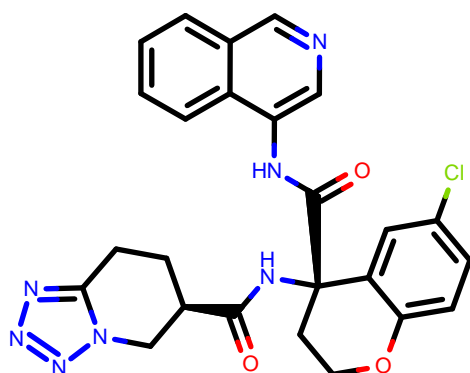
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5

RUN: RUN8520

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.20

EN300-269453_1_1



CID: EN300-269453_1_1

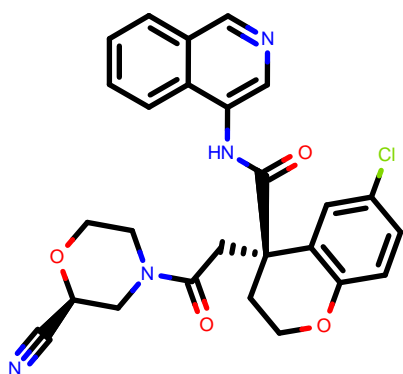
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5Cn6nnn6C5

RUN: RUN9670

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.24

EN300-70489_1_2



CID: EN300-70489_1_2

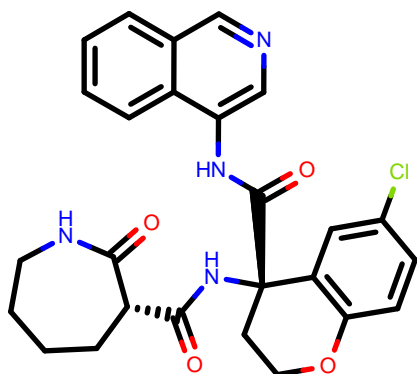
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]5(C)C#N

RUN: RUN10687

DDG (kcal/mol): -2.38

dDDG (kcal/mol): 0.25

EN300-6737762_1_1



CID: EN300-6737762_1_1

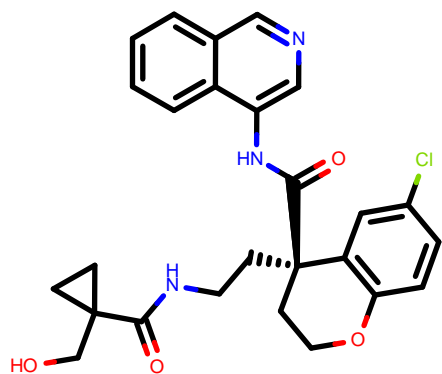
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CCCCN5=O

RUN: RUN1617

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.20

EN300-146174_3_1



CID: EN300-146174_3_1

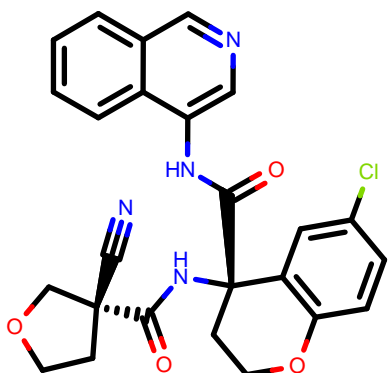
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)CO

RUN: RUN2284

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.22

EN300-261210_1_2



CID: EN300-261210_1_2

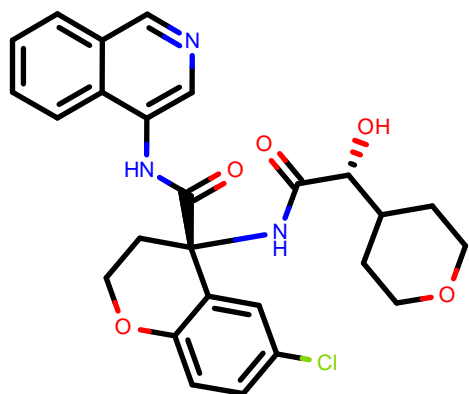
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOCC5)C#N

RUN: RUN6892

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.26

EN300-7443878_1_1



CID: EN300-7443878_1_1

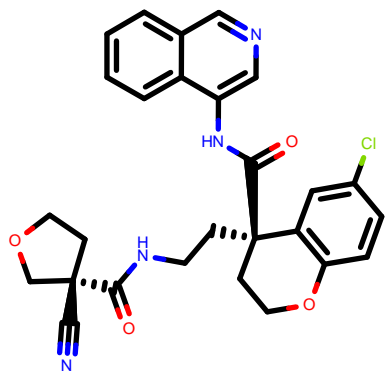
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H[C5(COCC5)O]

RUN: RUN3786

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.23

EN300-261210_3_1



CID: EN300-261210_3_1

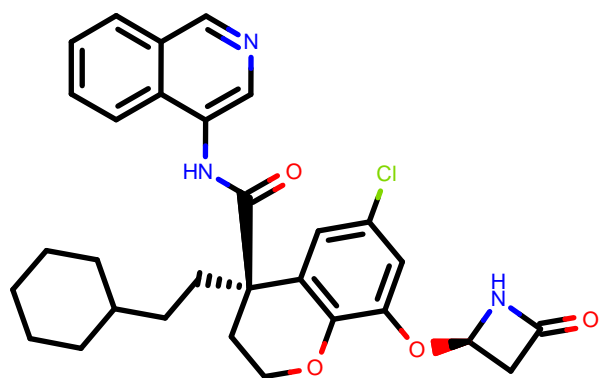
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOCC5)C#N

RUN: RUN8840

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.25

VLA-UCB-50c39ae8-9_1



CID: VLA-UCB-50c39ae8-9_1

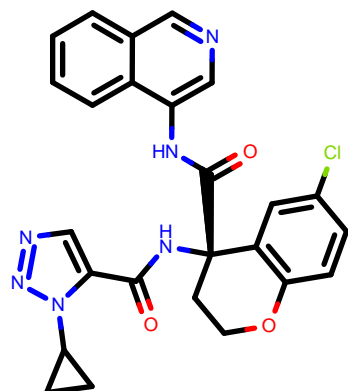
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)C1CCC6CCCC6

RUN: RUN142

DDG (kcal/mol): -2.37

dDDG (kcal/mol): 0.38

EN300-1718675_1_1



CID: EN300-1718675_1_1

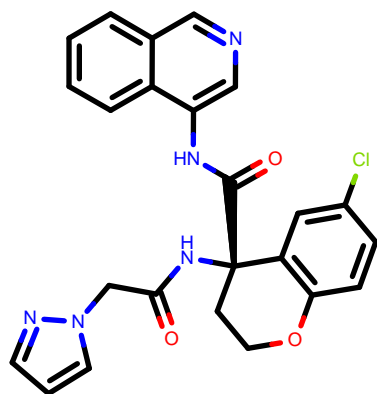
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn5C6CC6

RUN: RUN8556

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.21

EN300-23942_1_1



CID: EN300-23942_1_1

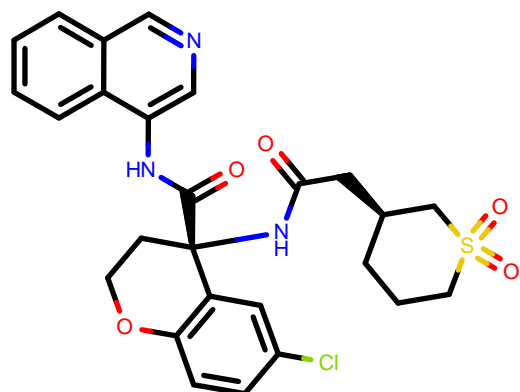
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5cccn5

RUN: RUN7940

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.22

EN300-220676_1_1



CID: EN300-220676_1_1

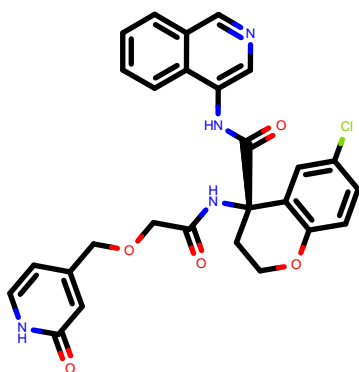
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5SCCS(=O)(=O)C5

RUN: RUN9081

DDG (kcal/mol): -2.36

dDDG (kcal/mol): 0.36

EN300-316258_1_1



CID: EN300-316258_1_1

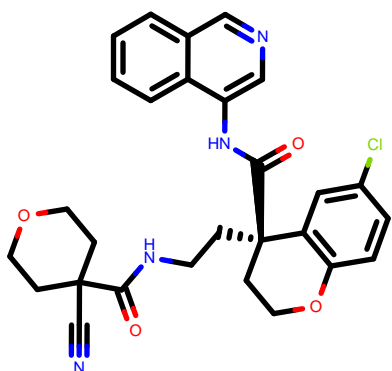
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COCc5cc[nH]c5=O

RUN: RUN7456

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.26

EN300-74089_3_1



CID: EN300-74089_3_1

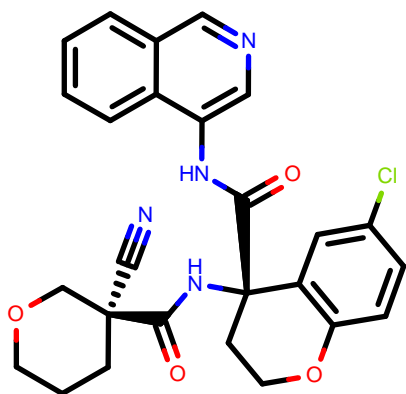
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCOCC5)C#N

RUN: RUN8756

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.27

EN300-301925_1_1



CID: EN300-301925_1_1

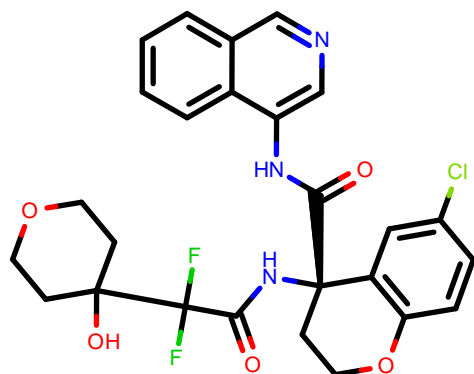
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCCOC5)C#N

RUN: RUN8264

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.25

EN300-706065_1_1



CID: EN300-706065_1_1

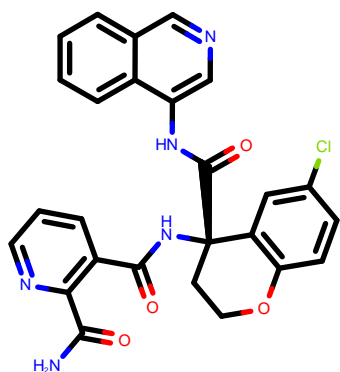
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(C5(CCOCC5)O)(F)F

RUN: RUN7560

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.27

EN300-135530_1_1



CID: EN300-135530_1_1

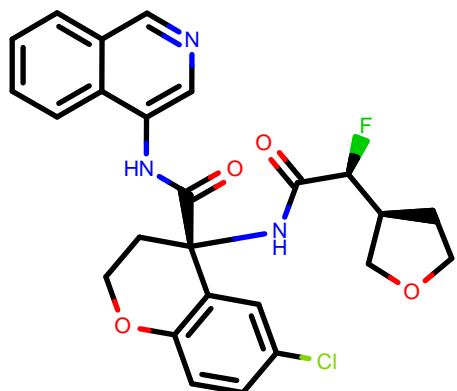
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5C(=O)N

RUN: RUN6500

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.20

EN300-783124_1_4



CID: EN300-783124_1_4

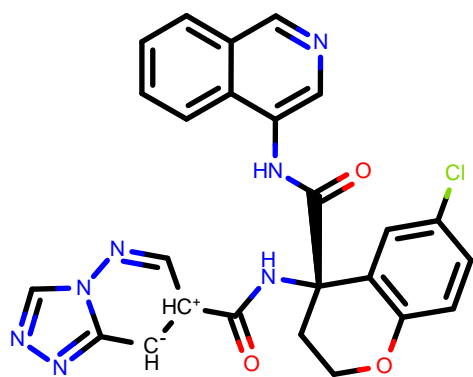
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@H]5CCOC5)F

RUN: RUN2477

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.23

EN300-7438185_1_1



CID: EN300-7438185_1_1

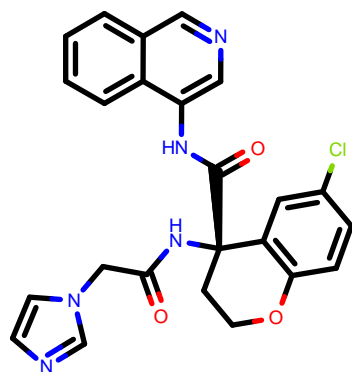
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6nnnc6n5

RUN: RUN5434

DDG (kcal/mol): -2.35

dDDG (kcal/mol): 0.20

EN300-38979_1_1



CID: EN300-38979_1_1

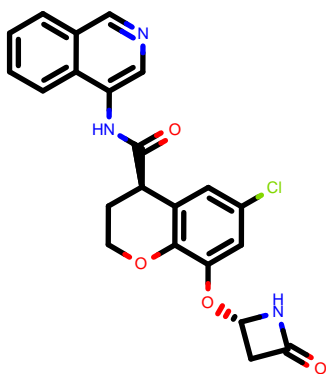
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5

RUN: RUN8516

DDG (kcal/mol): -2.35

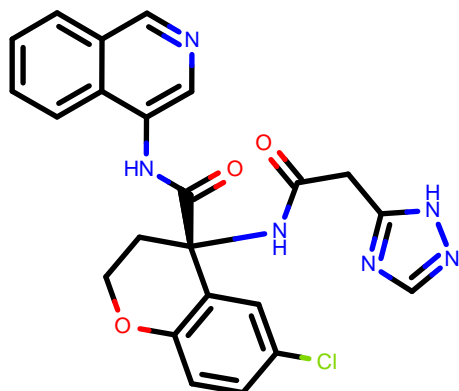
dDDG (kcal/mol): 0.21

VLA-UCB-50c39ae8-8_2



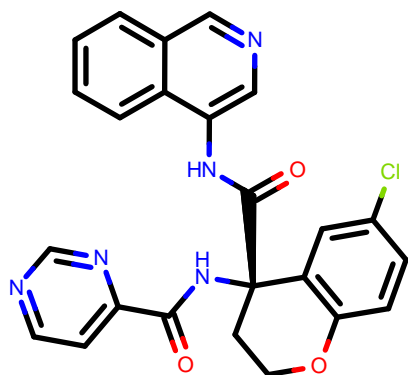
CID:	VLA-UCB-50c39ae8-8_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOC4c3cc(cc4O)[C@H]5CC(=O)N5Cl</chem>
RUN:	RUN25
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.15

EN300-96159_1_1



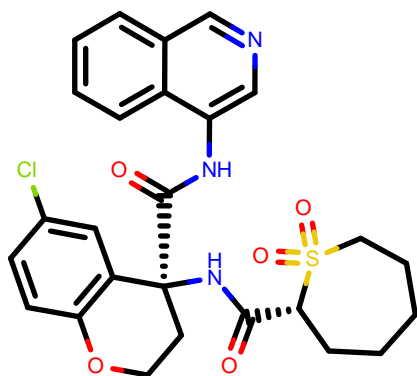
CID:	EN300-96159_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C5[nH]n5</chem>
RUN:	RUN6102
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.19

EN300-111006_1_1



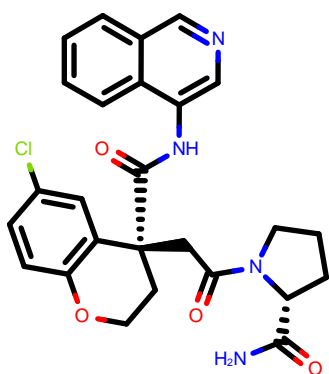
CID:	EN300-111006_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cncn5</chem>
RUN:	RUN3138
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.17

EN300-6499531_1_2



CID:	EN300-6499531_1_2
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@H]5CCCCCS5(=O)=O</chem>
RUN:	RUN6401
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.25

EN300-07127_1_2



CID: EN300-07127_1_2

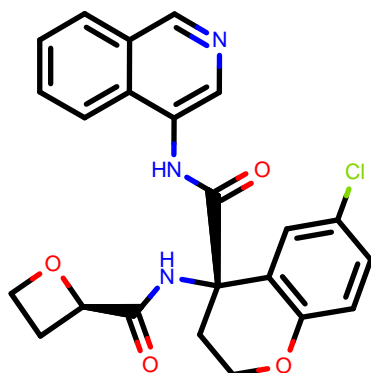
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN5521

DDG (kcal/mol): -2.34

dDDG (kcal/mol): 0.24

EN300-85760_1_2



CID: EN300-85760_1_2

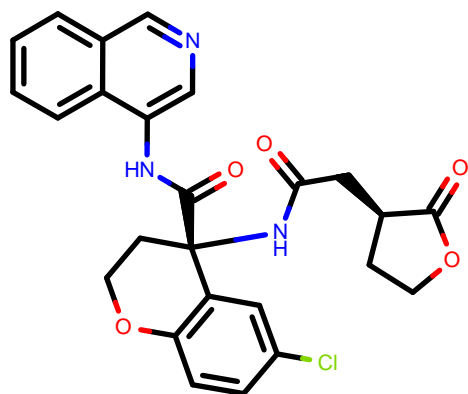
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC5

RUN: RUN5858

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.18

EN300-1072972_1_2



CID: EN300-1072972_1_2

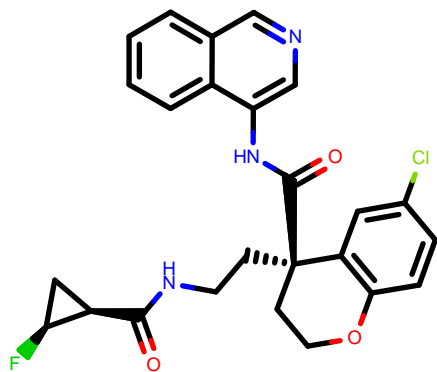
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC5=O

RUN: RUN3714

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.31

EN300-4698402_3_1



CID: EN300-4698402_3_1

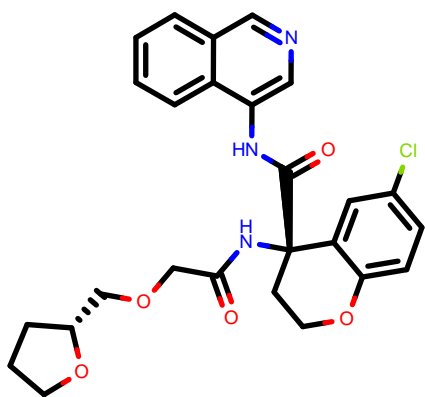
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN8996

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.21

EN300-60033_1_1



CID: EN300-60033_1_1

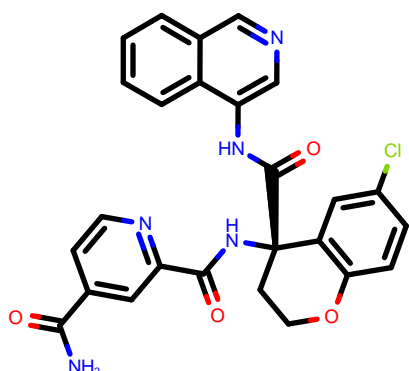
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCCO5

RUN: RUN7036

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.24

EN300-131051_1_1



CID: EN300-131051_1_1

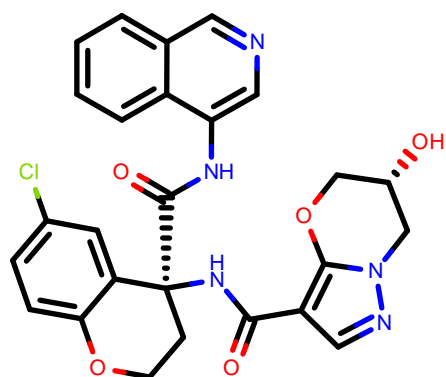
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccncc5C(=O)N

RUN: RUN1337

DDG (kcal/mol): -2.33

dDDG (kcal/mol): 0.17

EN300-6497444_1_2



CID: EN300-6497444_1_2

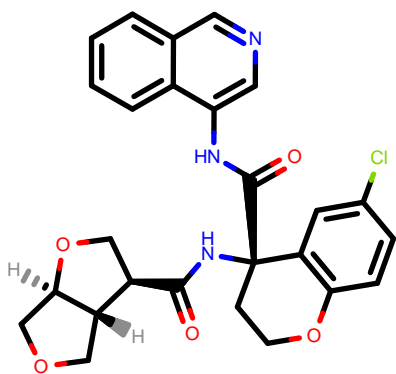
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5OC[C@@H](C6)O

RUN: RUN7600

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.23

EN300-6482296_1_5



CID: EN300-6482296_1_5

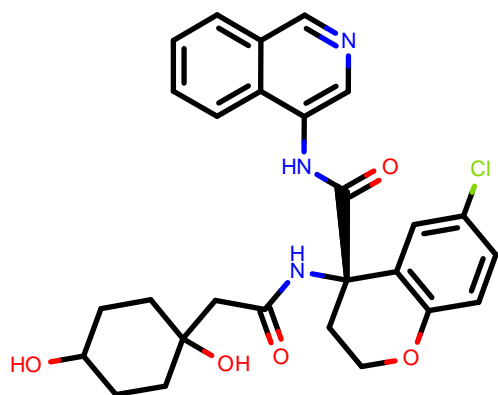
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CO[C@@H]6C[C@@H]5CO6

RUN: RUN3538

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.22

EN300-181558_1_1



CID: EN300-181558_1_1

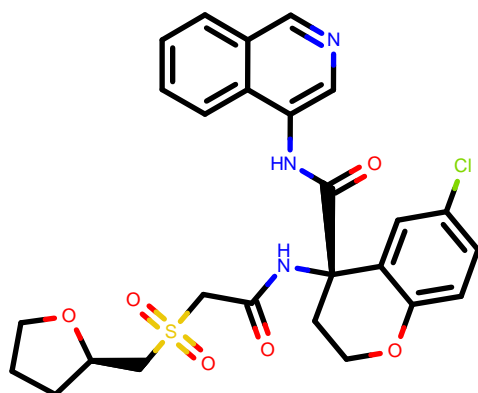
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCC(C)C5)O

RUN: RUN6640

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.29

EN300-67023_1_1



CID: EN300-67023_1_1

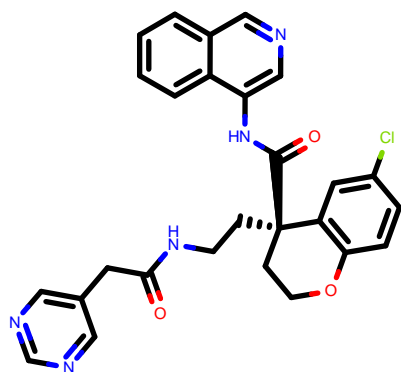
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)CC

RUN: RUN7740

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.35

EN300-185751_3_1



CID: EN300-185751_3_1

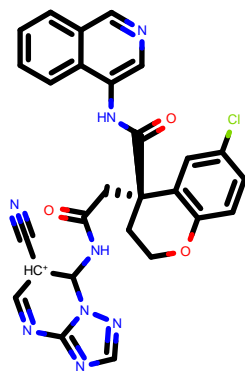
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5cncnc5

RUN: RUN9260

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.23

EN300-6472316_1_1



CID: EN300-6472316_1_1

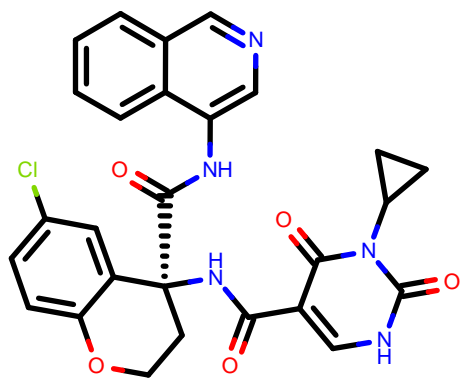
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5c6ncn5n6C#N

RUN: RUN8764

DDG (kcal/mol): -2.32

dDDG (kcal/mol): 0.22

EN300-7433864_1_1



CID: EN300-7433864_1_1

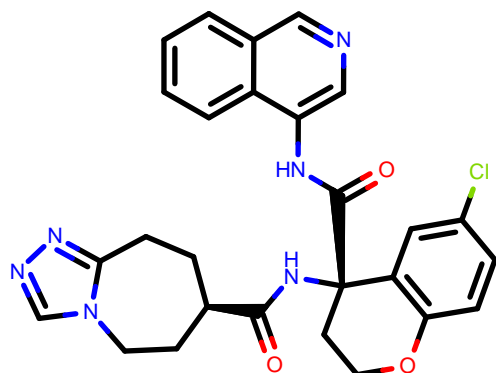
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c1c(=O)n(c5=O)C6CC6

RUN: RUN7968

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.27

EN300-366687_1_1



CID: EN300-366687_1_1

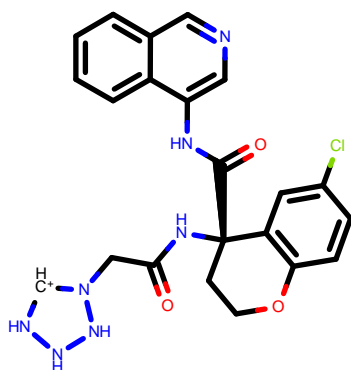
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5CC6c6nnc6CC5

RUN: RUN8416

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.20

EN300-20980_1_1



CID: EN300-20980_1_1

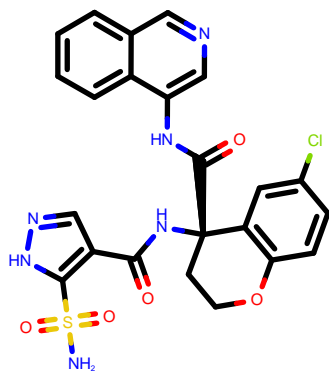
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnnn5

RUN: RUN7256

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.19

EN300-144606_1_1



CID: EN300-144606_1_1

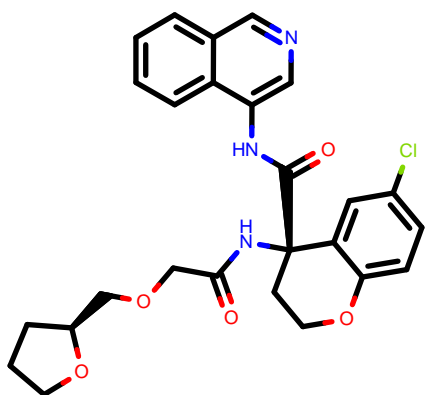
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c5S1(=O)=O)N

RUN: RUN8108

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.26

EN300-60033_1_2



CID: EN300-60033_1_2

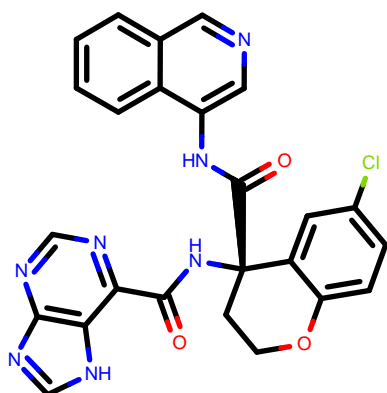
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCCO5

RUN: RUN6656

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.23

EN300-252018_1_1



CID: EN300-252018_1_1

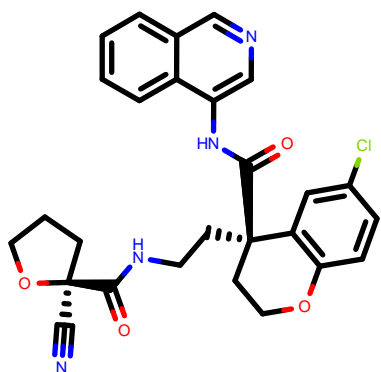
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c(nc[nH]6)ncn5

RUN: RUN4430

DDG (kcal/mol): -2.31

dDDG (kcal/mol): 0.18

EN300-3710141_3_2



CID: EN300-3710141_3_2

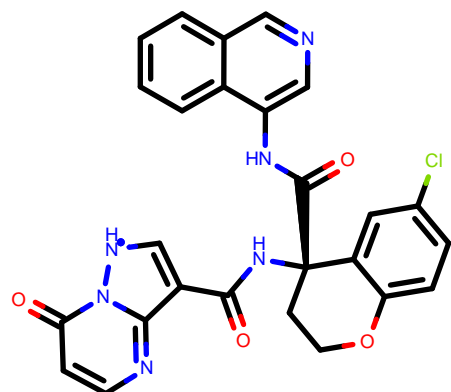
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN11994

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.27

EN300-203940_1_1



CID: EN300-203940_1_1

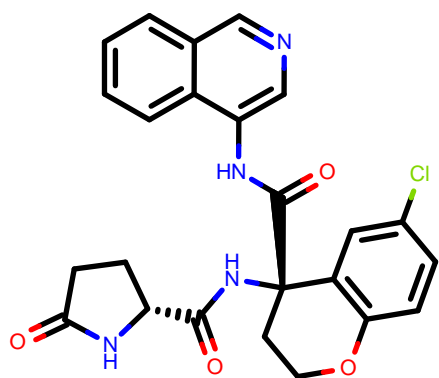
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]6c5ncnc6=O

RUN: RUN2316

DDG (kcal/mol): -2.30

dDDG (kcal/mol): 0.21

EN300-54541_1_1



CID: EN300-54541_1_1

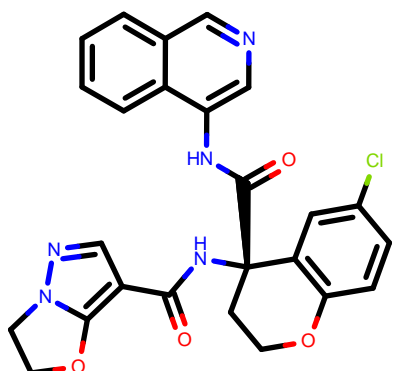
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC[C@@]5O

RUN: RUN7920

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.21

EN300-303519_1_1



CID: EN300-303519_1_1

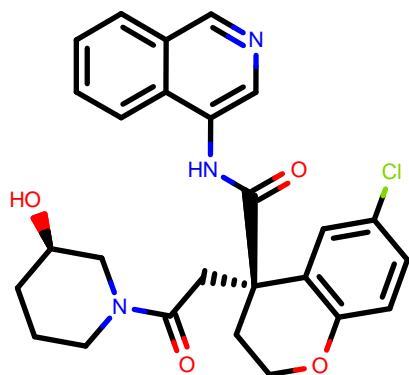
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nnc6c5OCC6

RUN: RUN3146

DDG (kcal/mol): -2.29

dDDG (kcal/mol): 0.20

EN300-266117_1_1



CID: EN300-266117_1_1

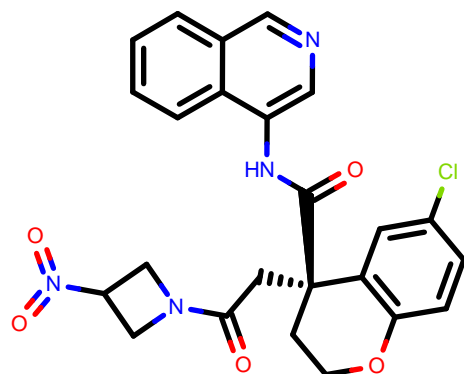
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)O

RUN: RUN5285

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.23

EN300-7461023_1_1



CID: EN300-7461023_1_1

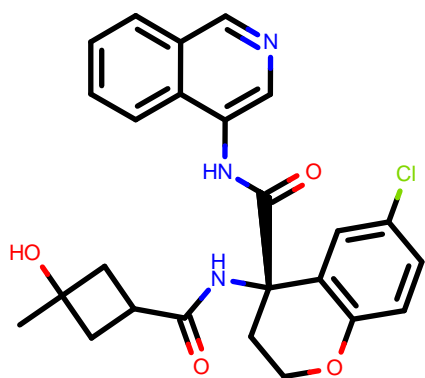
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)N(=O)=O

RUN: RUN12790

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.19

EN300-7183657_1_1



CID: EN300-7183657_1_1

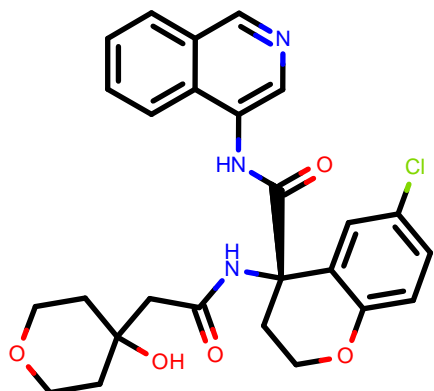
SMILES: C[C@]1[C[C@@H](C1C(=O)N[C@@]2(c3c(ccc(c3)Cl)OCC2)C(=O)Nc4c5c(cnc4)ccoc5)O

RUN: RUN2135

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.22

EN300-151423_1_1



CID: EN300-151423_1_1

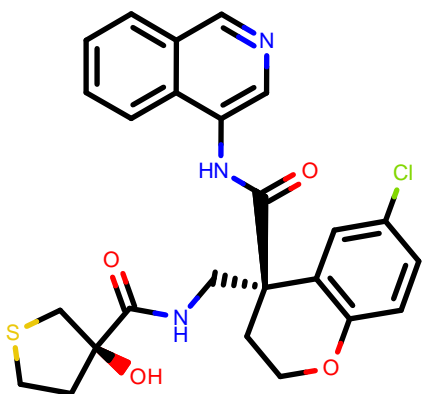
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)NC(=O)CC5(CCOCC5)O

RUN: RUN7056

DDG (kcal/mol): -2.28

dDDG (kcal/mol): 0.24

EN300-122656_2_1



CID: EN300-122656_2_1

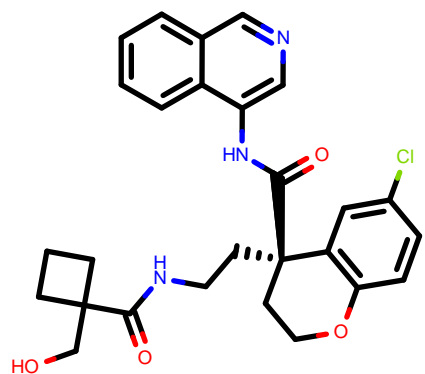
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CNC(=O)[C@@]5(CCCS5)O

RUN: RUN4875

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.47

EN300-149975_3_1



CID: EN300-149975_3_1

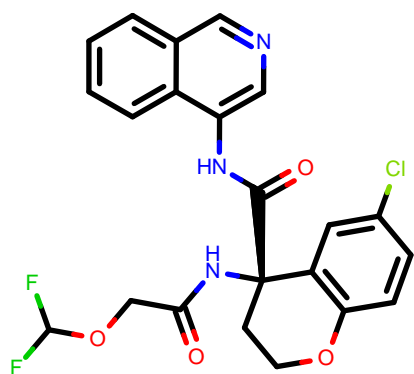
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCNC(=O)C5(CCC5)CO

RUN: RUN12840

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.24

EN300-179091_1_1



CID: EN300-179091_1_1

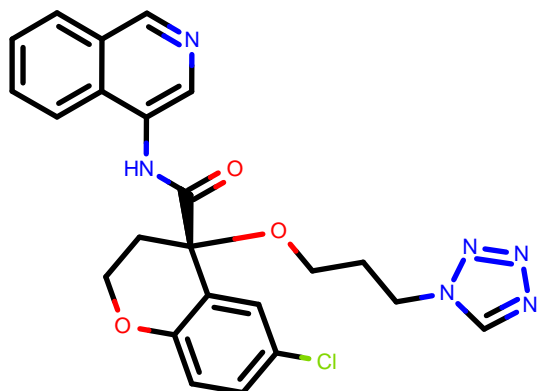
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(F)F

RUN: RUN5270

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.20

EN300-1696962_1_1



CID: EN300-1696962_1_1

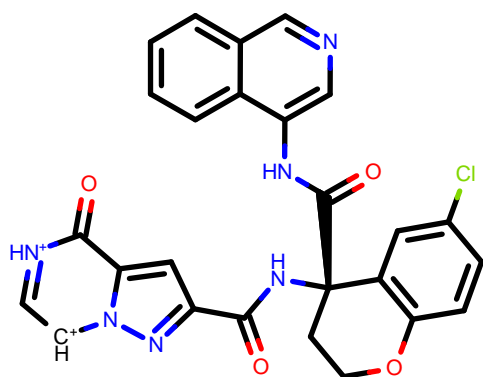
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cnnn5

RUN: RUN775

DDG (kcal/mol): -2.27

dDDG (kcal/mol): 0.19

EN300-393121_1_1



CID: EN300-393121_1_1

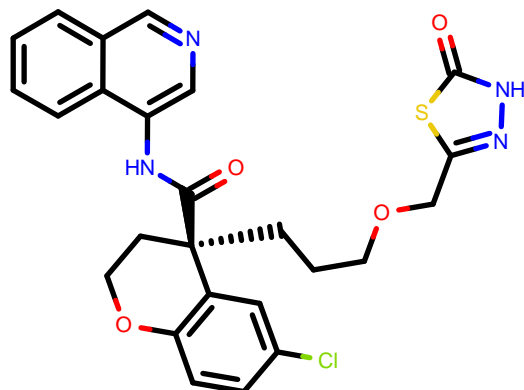
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(=O)[nH]cnn65

RUN: RUN1817

DDG (kcal/mol): -2.26

dDDG (kcal/mol): 0.18

EN300-171766_4_1



CID: EN300-171766_4_1

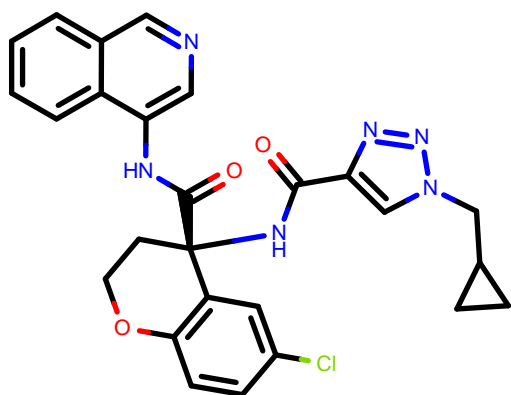
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5n[nH]c(=O)s5

RUN: RUN1419

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.20

EN300-247428_1_1



CID: EN300-247428_1_1

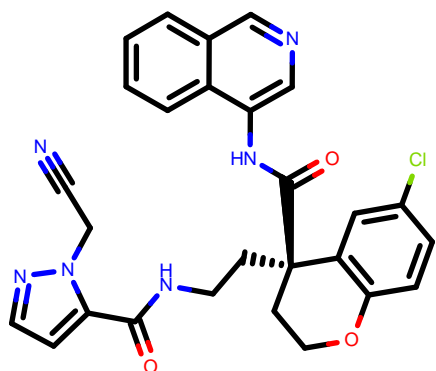
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(nn5)CC6CC6

RUN: RUN3090

DDG (kcal/mol): -2.25

dDDG (kcal/mol): 0.20

EN300-373791_3_1



CID: EN300-373791_3_1

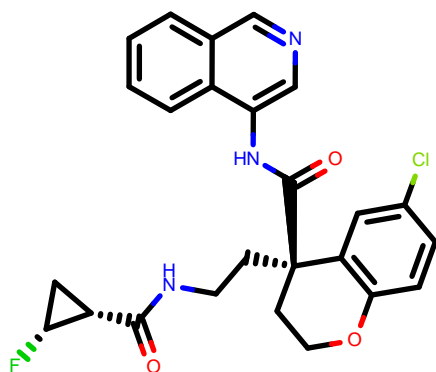
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cnnc5C#N

RUN: RUN14008

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.27

EN300-97300_3_2



CID: EN300-97300_3_2

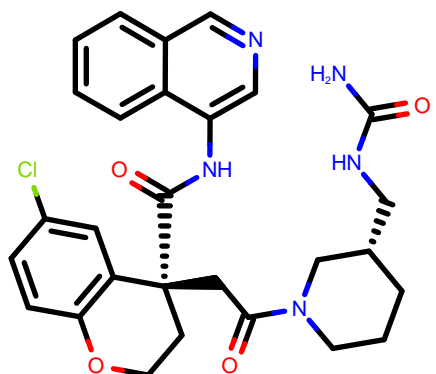
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C[C@H]5F

RUN: RUN15001

DDG (kcal/mol): -2.24

dDDG (kcal/mol): 0.17

EN300-42195_1_2



CID: EN300-42195_1_2

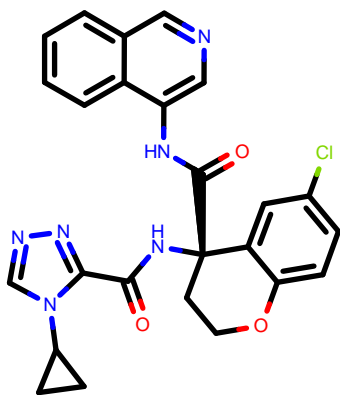
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@H](C5)CNC(=O)N

RUN: RUN10615

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.31

EN300-6745581_1_1



CID: EN300-6745581_1_1

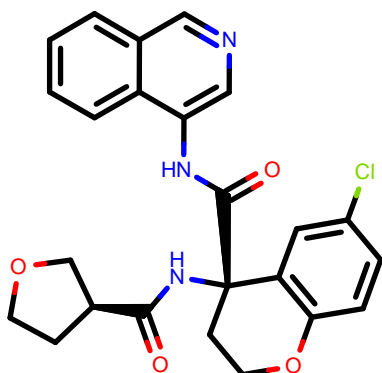
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nncn5C6CC6

RUN: RUN7888

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.20

EN300-53423_1_2



CID: EN300-53423_1_2

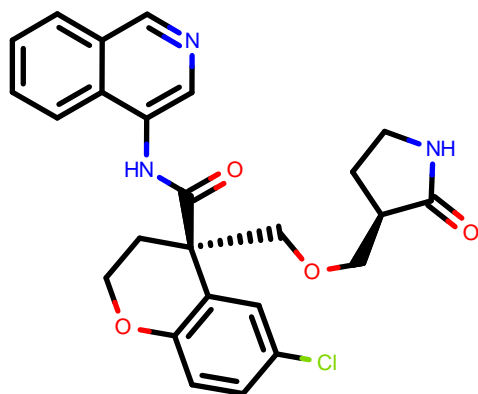
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCOC5

RUN: RUN4794

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.21

EN300-246248_2_1



CID: EN300-246248_2_1

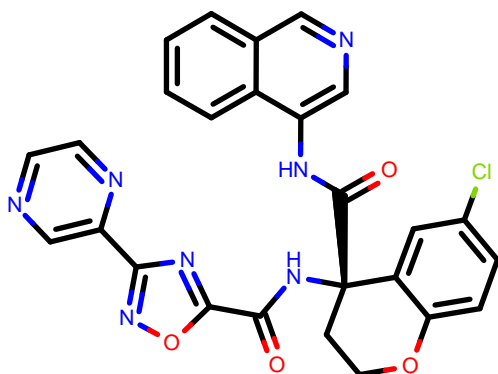
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@H]5CCNC5=O

RUN: RUN1290

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.21

EN300-239219_1_1



CID: EN300-239219_1_1

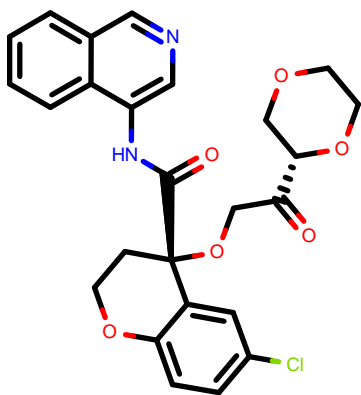
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nc(ncn5)c6nccn6

RUN: RUN3506

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.21

EN300-6238494_1_1



CID: EN300-6238494_1_1

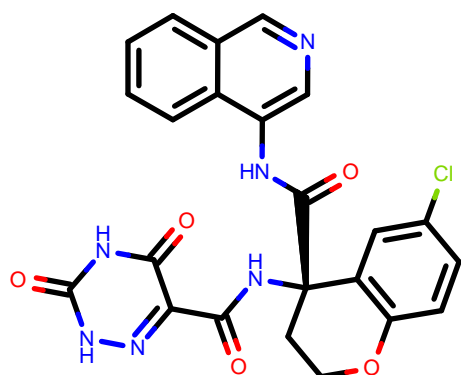
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COCOC5

RUN: RUN1085

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.27

EN300-122319_1_1



CID: EN300-122319_1_1

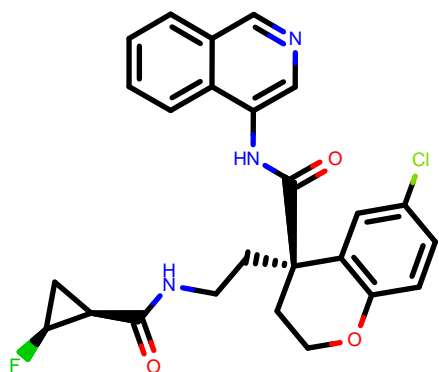
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(=O)[nH]c(=O)[nH]n5

RUN: RUN3410

DDG (kcal/mol): -2.23

dDDG (kcal/mol): 0.20

EN300-4698402_3_1



CID: EN300-4698402_3_1

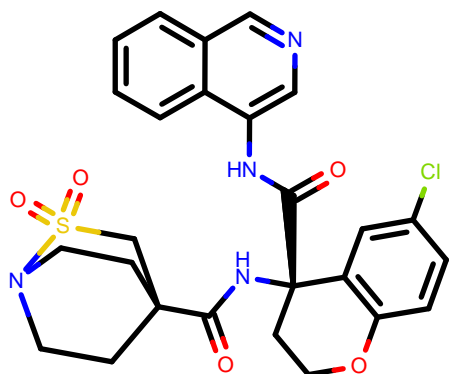
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN9000

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.19

EN300-6731334_1_1



CID: EN300-6731334_1_1

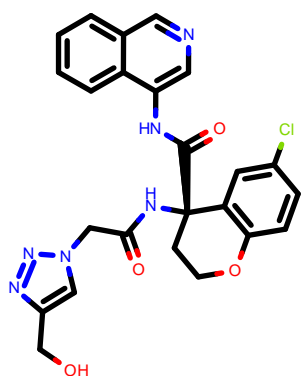
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CCN(CC5)S(=O)(=O)C6

RUN: RUN5774

DDG (kcal/mol): -2.22

dDDG (kcal/mol): 0.33

EN300-108236_1_1



CID: EN300-108236_1_1

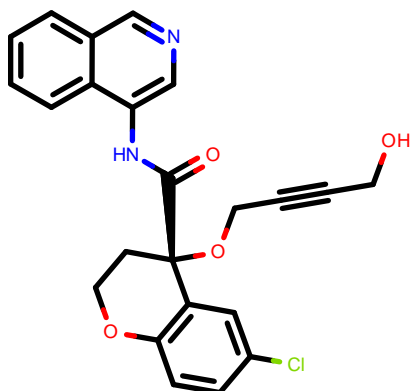
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ccn5CO

RUN: RUN8909

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.22

EN300-83766_1_1



CID: EN300-83766_1_1

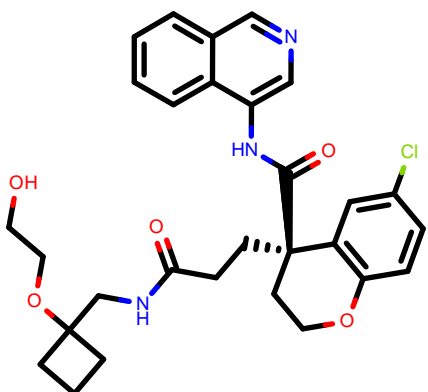
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC#CCO

RUN: RUN2361

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.15

EN300-171481_2_1



CID: EN300-171481_2_1

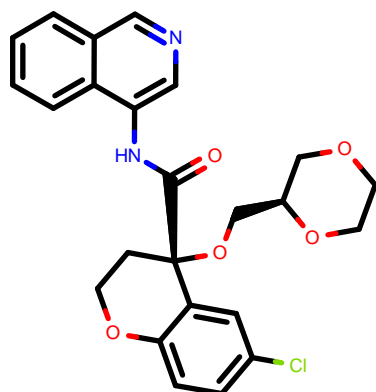
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCC5(CCC5)OCCO

RUN: RUN5828

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.33

EN300-139167_1_1



CID: EN300-139167_1_1

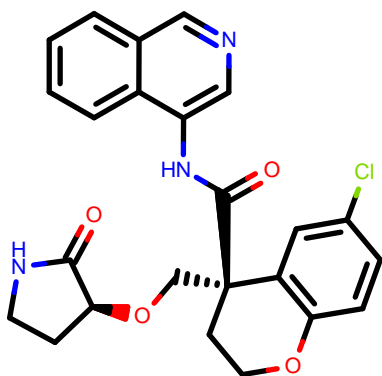
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5COCCO5

RUN: RUN2703

DDG (kcal/mol): -2.21

dDDG (kcal/mol): 0.22

EN300-6736413_2_1



CID: EN300-6736413_2_1

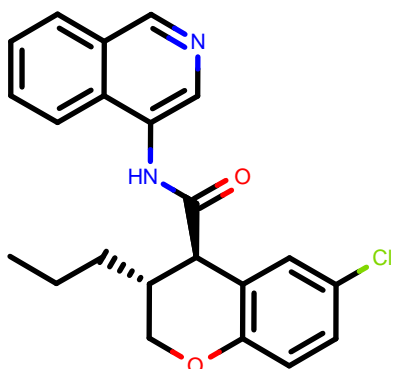
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O

RUN: RUN2520

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.19

EDJ-MED-e4b030d8-6_1



CID: EDJ-MED-e4b030d8-6_1

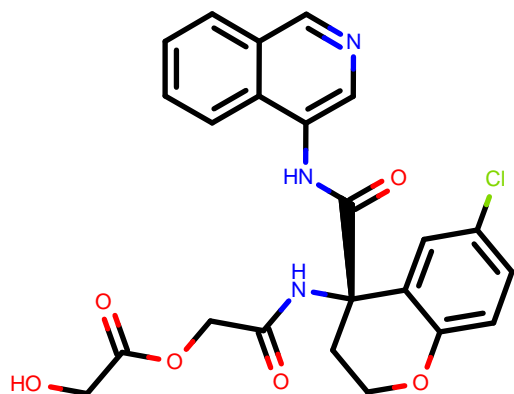
SMILES: CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3nccc4c3ccc4)Cl

RUN: RUN72

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.10

EN300-7459916_1_1



CID: EN300-7459916_1_1

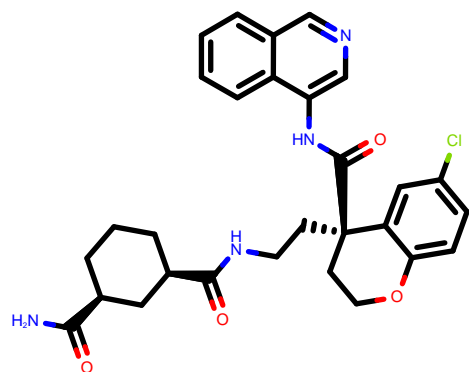
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)NC(=O)COC(=O)CO

RUN: RUN315

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.22

EN300-90142_3_1



CID: EN300-90142_3_1

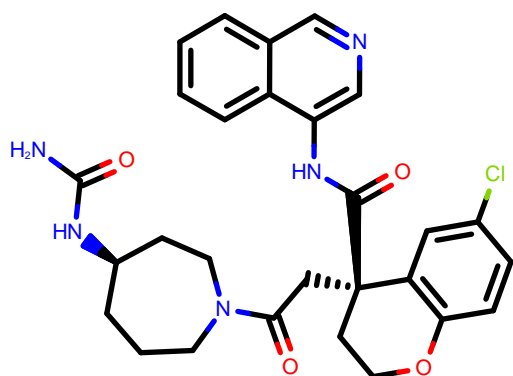
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOCc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC[C@@H]5(C)C(=O)N

RUN: RUN15127

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.28

EN300-6759972_1_2



CID: EN300-6759972_1_2

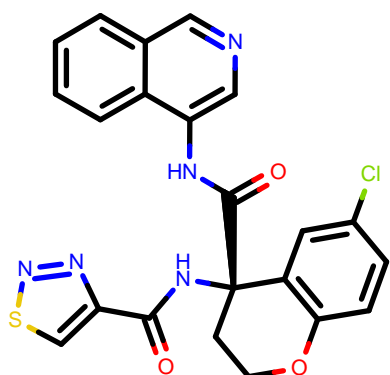
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H](CC5)NC(=O)N

RUN: RUN3161

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.26

EN300-24297_1_1



CID: EN300-24297_1_1

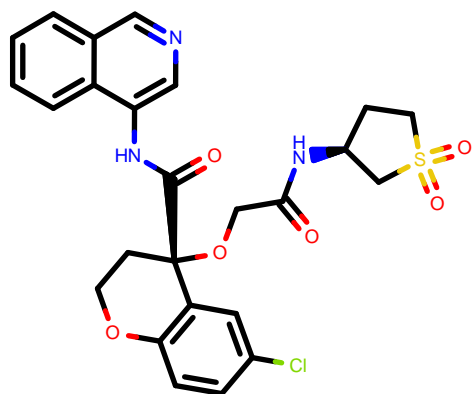
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5csnn5

RUN: RUN2918

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.20

EN300-05512_1_2



CID: EN300-05512_1_2

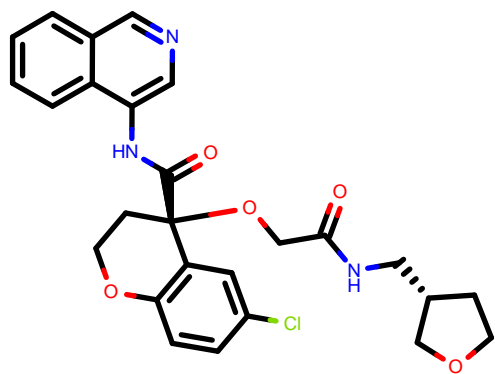
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@H]5CCS(=O)(=O)C5

RUN: RUN767

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.31

EN300-46832_1_1



CID: EN300-46832_1_1

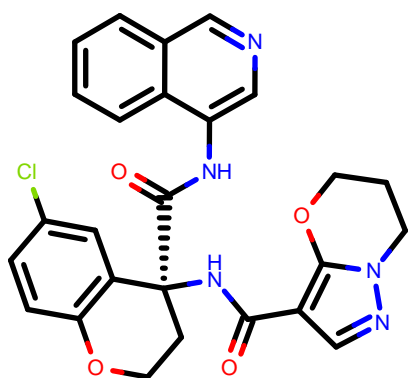
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@H]5CCOC5

RUN: RUN647

DDG (kcal/mol): -2.20

dDDG (kcal/mol): 0.27

EN300-103722_1_1



CID: EN300-103722_1_1

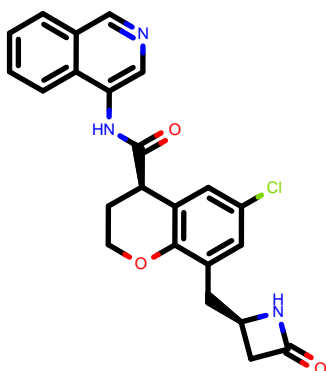
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn6c5OCC6

RUN: RUN7904

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.22

DAR-DIA-6a508060-5_3



CID: DAR-DIA-6a508060-5_3

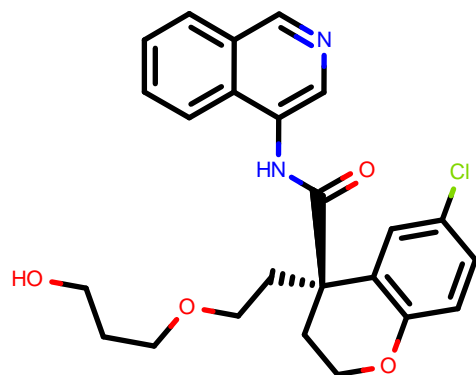
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)N5C

RUN: RUN190

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.17

EN300-221518_3_1



CID: EN300-221518_3_1

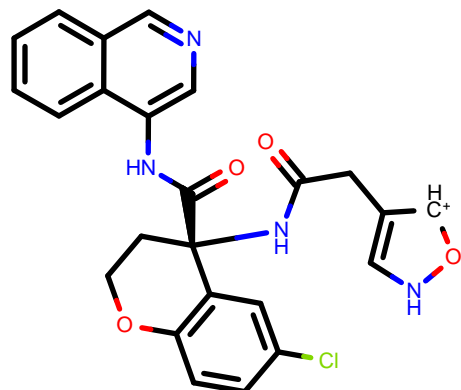
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCO

RUN: RUN1072

DDG (kcal/mol): -2.19

dDDG (kcal/mol): 0.20

EN300-315963_1_1



CID: EN300-315963_1_1

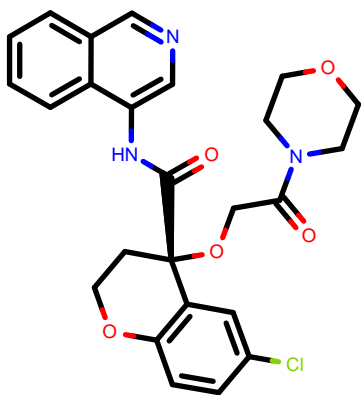
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5cnc5

RUN: RUN8308

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.21

EN300-1241327_1_1



CID: EN300-1241327_1_1

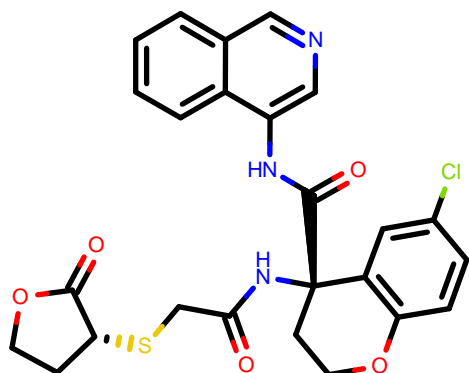
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCOCC5

RUN: RUN2501

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.19

EN300-113218_1_2



CID: EN300-113218_1_2

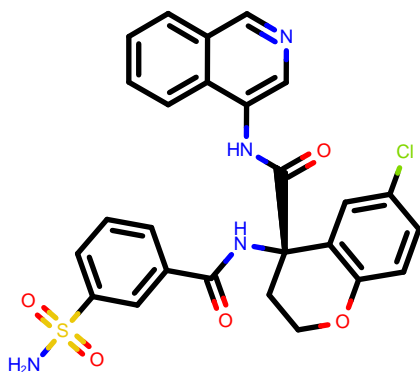
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS[C@@H]5CCOCC5=O

RUN: RUN3966

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.23

EN300-04520_1_1



CID: EN300-04520_1_1

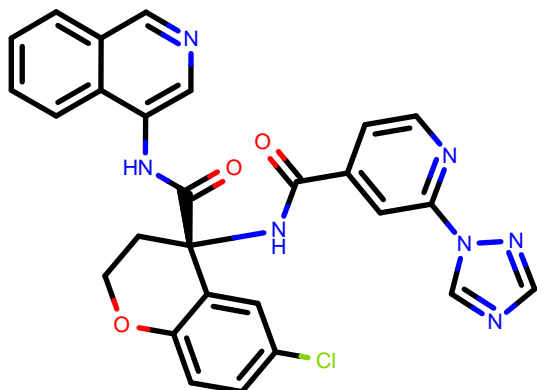
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(c5)S(=O)(=O)N

RUN: RUN467

DDG (kcal/mol): -2.18

dDDG (kcal/mol): 0.24

EN300-58433_1_1



CID: EN300-58433_1_1

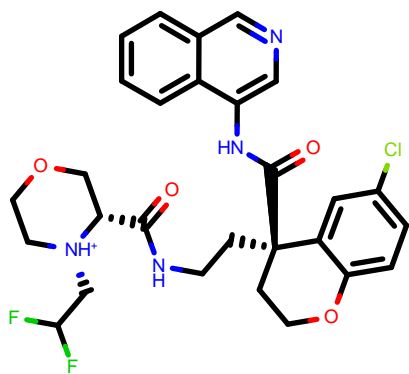
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnc(c5)n6cncn6

RUN: RUN4546

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.24

EN300-140582_3_2



CID: EN300-140582_3_2

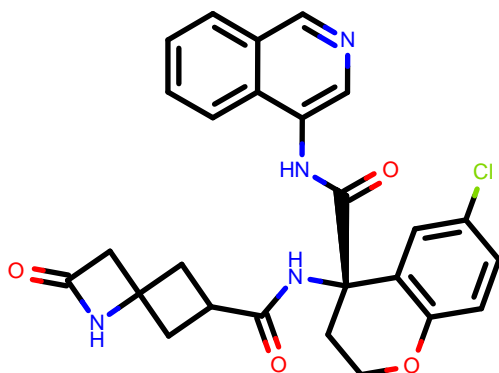
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCC(N@)5CC(F)F

RUN: RUN11327

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.29

EN300-1700760_1_1



CID: EN300-1700760_1_1

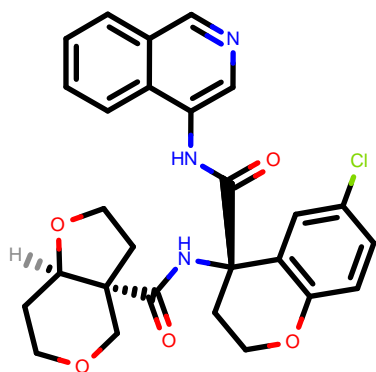
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN9445

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.20

EN300-341337_1_2



CID: EN300-341337_1_2

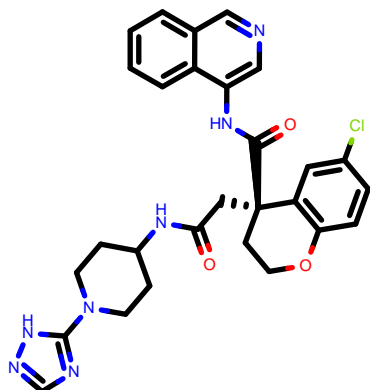
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]56CCO[C@]5(H)CCO6

RUN: RUN8132

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.31

EN300-6474740_1_1



CID: EN300-6474740_1_1

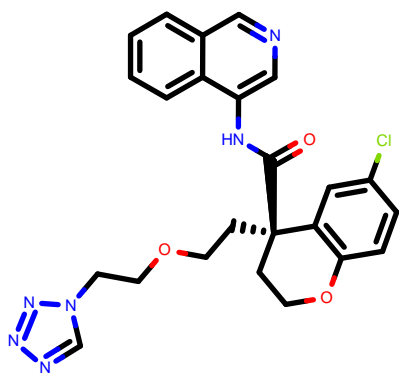
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CCN(CC5)c6[nH]nc6

RUN: RUN15315

DDG (kcal/mol): -2.17

dDDG (kcal/mol): 0.30

EN300-364679_3_1



CID: EN300-364679_3_1

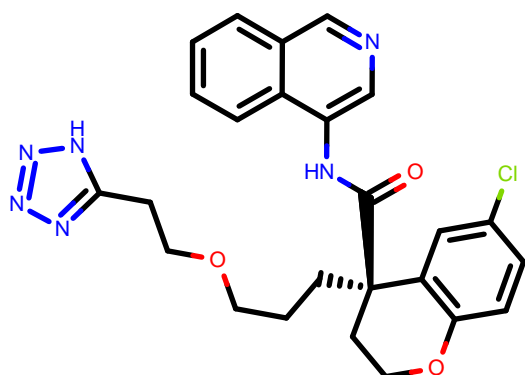
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnnn5

RUN: RUN1823

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.24

EN300-183231_4_1



CID: EN300-183231_4_1

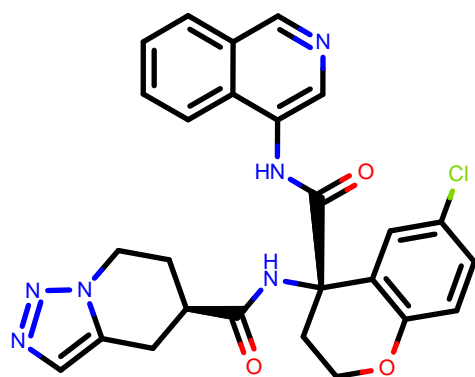
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5[nH]n5

RUN: RUN333

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.24

EN300-7430501_1_2



CID: EN300-7430501_1_2

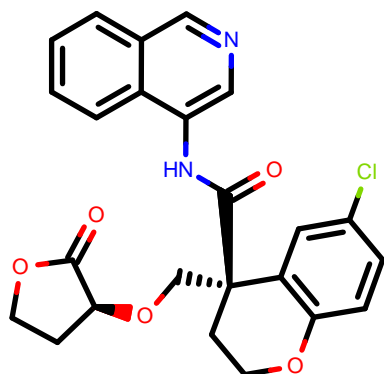
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5Cn6cnc6c5

RUN: RUN5978

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.20

EN300-20496_2_1



CID: EN300-20496_2_1

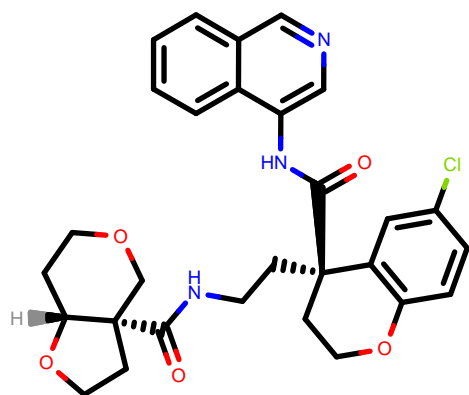
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@]5COC(=O)C5=O

RUN: RUN2589

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.18

EN300-341337_3_1



CID: EN300-341337_3_1

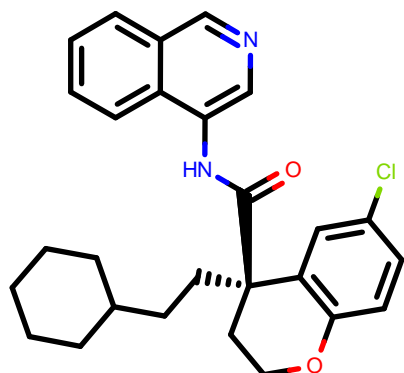
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C@56CCO[C@@H]5CCOOC6

RUN: RUN9080

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.24

VLA-UCB-50c39ae8-10_1



CID: VLA-UCB-50c39ae8-10_1

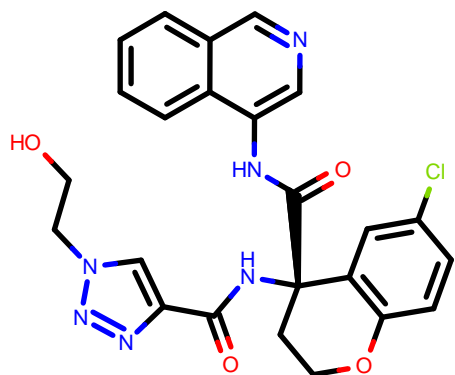
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5CCCCC5

RUN: RUN36

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.18

EN300-52193_1_1



CID: EN300-52193_1_1

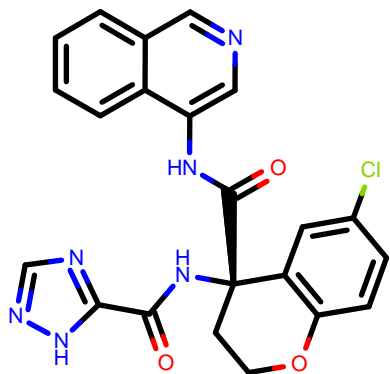
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn[nH]c5CO

RUN: RUN2706

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.17

EN300-100741_1_1



CID: EN300-100741_1_1

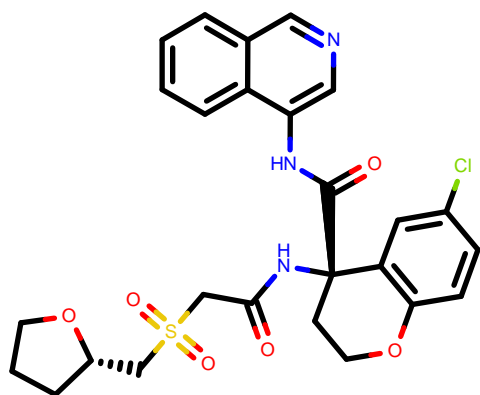
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5[nH]ncn5

RUN: RUN2777

DDG (kcal/mol): -2.16

dDDG (kcal/mol): 0.18

EN300-67023_1_2



CID: EN300-67023_1_2

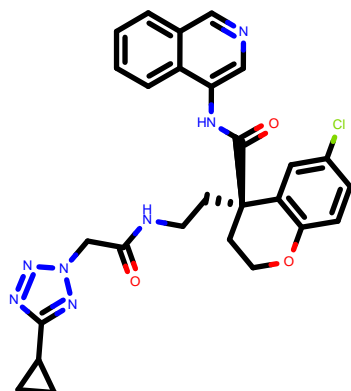
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS(=O)(=O)C[C@@]H5CCOC5

RUN: RUN7948

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.36

EN300-1719432_3_1



CID: EN300-1719432_3_1

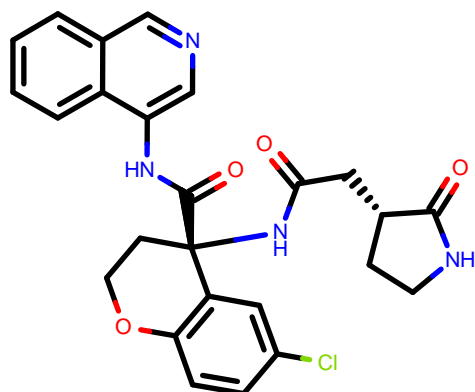
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5nc(n5)C6CC6

RUN: RUN11895

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.28

EN300-343474_1_1



CID: EN300-343474_1_1

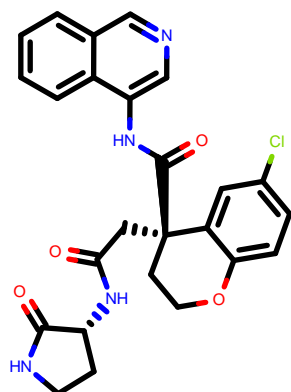
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]H5CCNC5=O

RUN: RUN2491

DDG (kcal/mol): -2.15

dDDG (kcal/mol): 0.24

EN300-307333_1_1



CID: EN300-307333_1_1

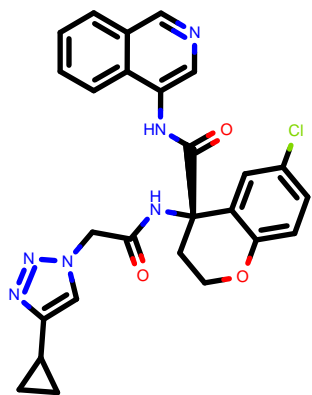
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]H5CCNC5=O

RUN: RUN5505

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.23

EN300-107892_1_1



CID: EN300-107892_1_1

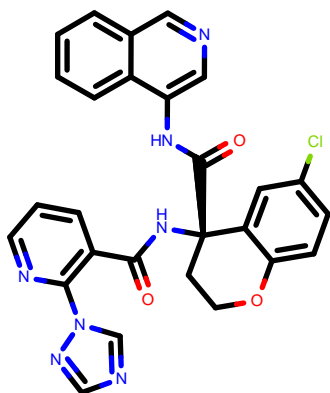
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5cc(mn5)C6C66

RUN: RUN9077

DDG (kcal/mol): -2.14

dDDG (kcal/mol): 0.23

EN300-28571_1_1



CID: EN300-28571_1_1

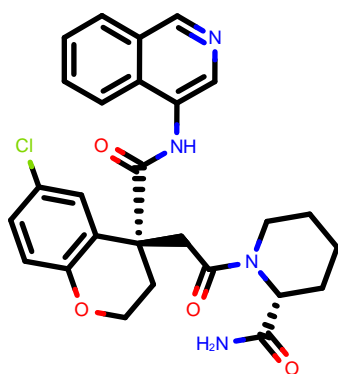
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccncc5n6cn6

RUN: RUN3798

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.22

EN300-34542_1_2



CID: EN300-34542_1_2

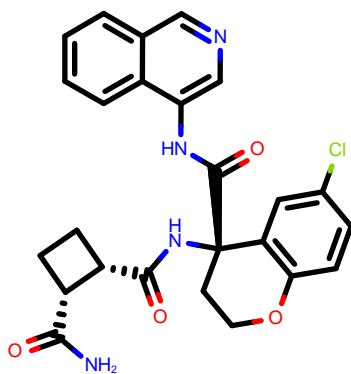
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@]3HJ5C(=O)N

RUN: RUN10259

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.22

EN300-217107_1_2



CID: EN300-217107_1_2

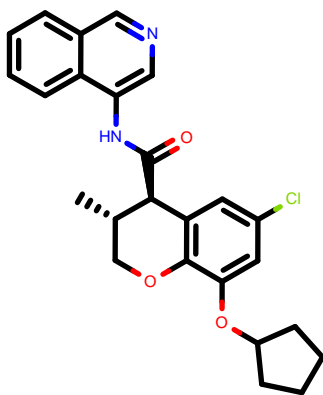
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]3HJ5CC[C@@]3HJ5C(=O)N

RUN: RUN8432

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.22

DAR-DIA-0d514e7d-4_1



CID: DAR-DIA-0d514e7d-4_1

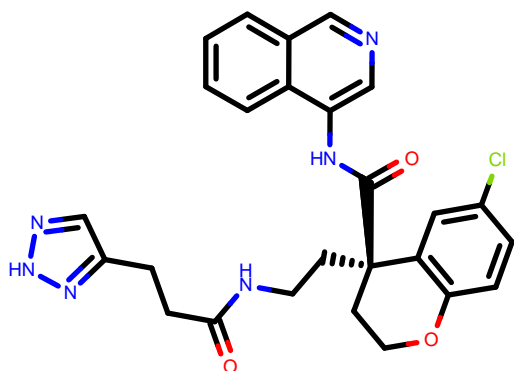
SMILES: C[C@H]1COc2c(cc2OC3CCCC3)Cl[C@@H]1C(=O)Nc4cnc5c4cccc5

RUN: RUN168

DDG (kcal/mol): -2.13

dDDG (kcal/mol): 0.20

EN300-244947_3_1



CID: EN300-244947_3_1

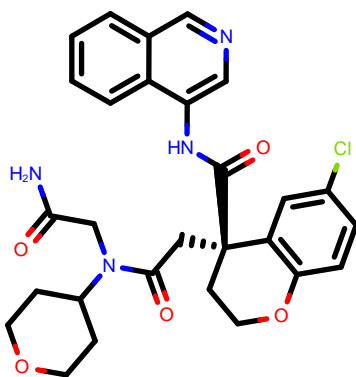
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5cn[nH]5

RUN: RUN9136

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.27

EN300-373584_1_1



CID: EN300-373584_1_1

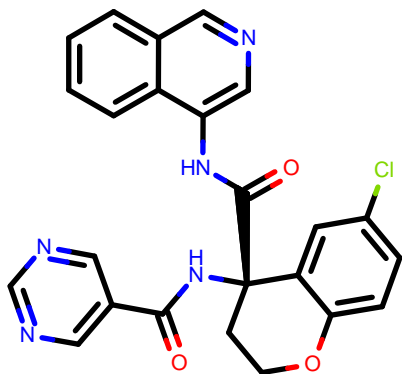
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)C5COCC5

RUN: RUN2292

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.39

EN300-64297_1_1



CID: EN300-64297_1_1

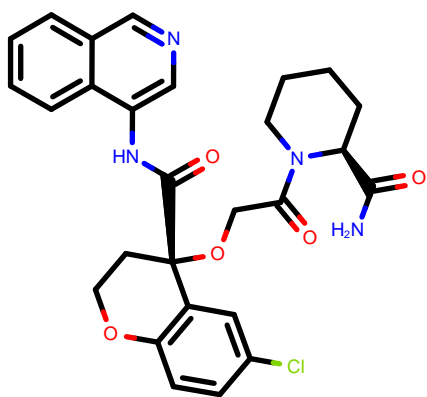
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncnc5

RUN: RUN5462

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.19

EN300-22879_1_1



CID: EN300-22879_1_1

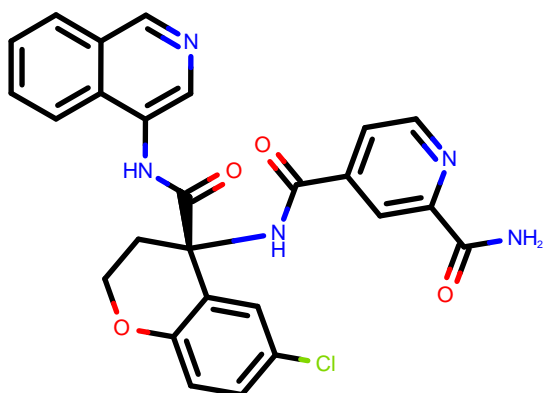
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN2466

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.28

EN300-102071_1_1



CID: EN300-102071_1_1

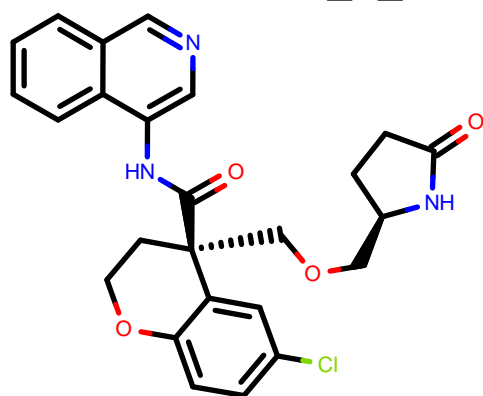
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccncc5C(=O)N

RUN: RUN4394

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.22

EN300-264301_2_1



CID: EN300-264301_2_1

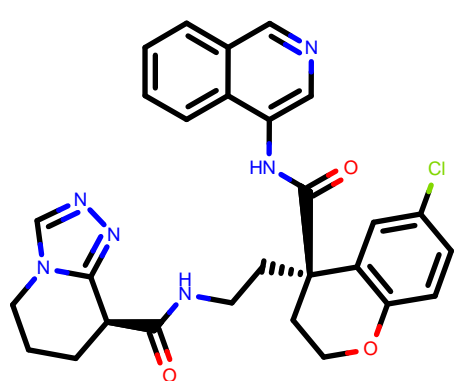
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNC(=O)N5

RUN: RUN876

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.25

EN300-748981_3_2



CID: EN300-748981_3_2

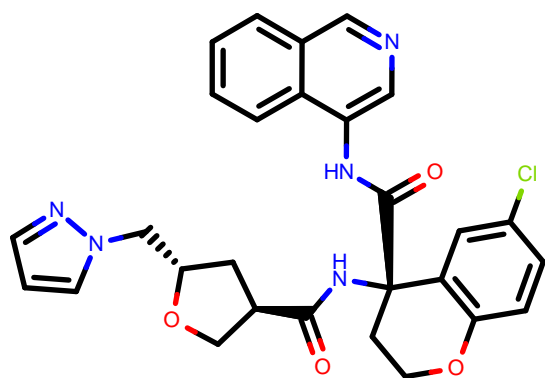
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCN6c5nc6

RUN: RUN5093

DDG (kcal/mol): -2.12

dDDG (kcal/mol): 0.30

EN300-6494859_1_1



CID: EN300-6494859_1_1

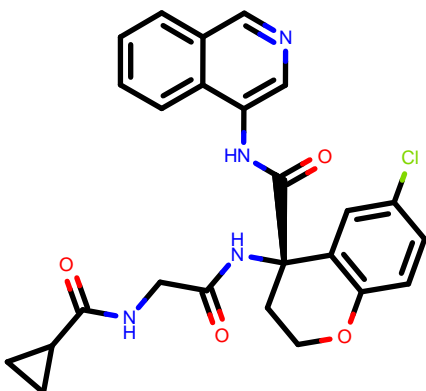
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C[C@H](O)C5

RUN: RUN8372

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.25

EN300-36522_1_1



CID: EN300-36522_1_1

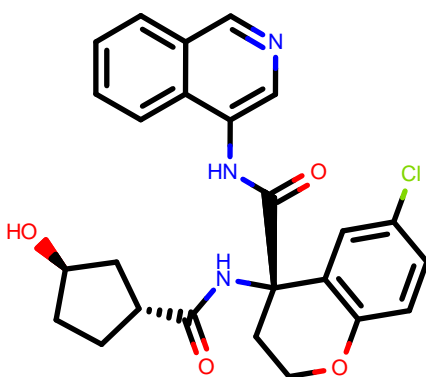
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)C5O5

RUN: RUN8765

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.23

EN300-321597_1_1



CID: EN300-321597_1_1

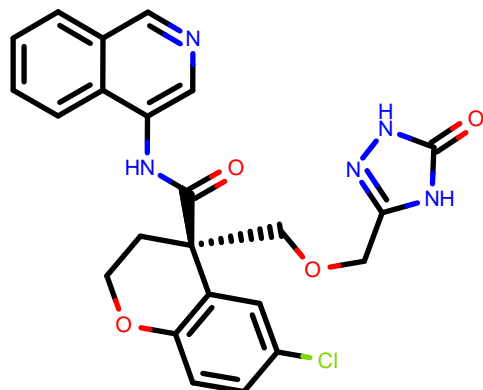
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC[C@H](C5)O

RUN: RUN3594

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.20

EN300-73772_2_1



CID: EN300-73772_2_1

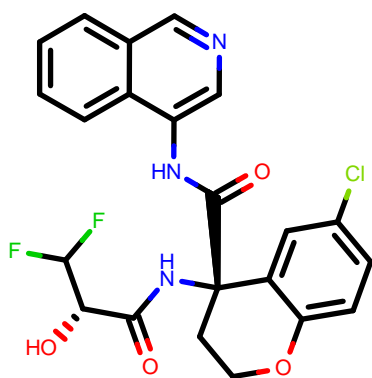
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCc5[nH]c(=O)[nH]5

RUN: RUN2422

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.19

EN300-1932780_1_1



CID: EN300-1932780_1_1

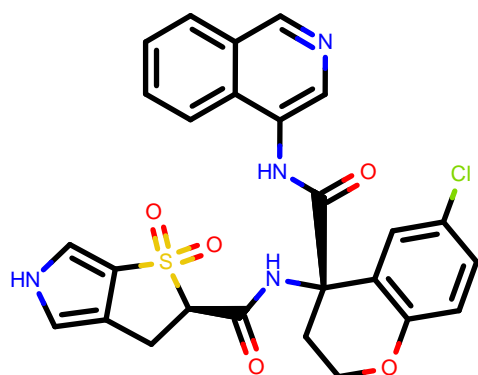
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C(F)F)O

RUN: RUN5938

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.25

EN300-7445396_1_2



CID: EN300-7445396_1_2

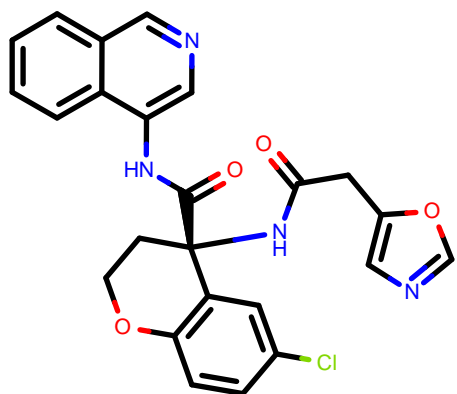
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C6c[nH]pc6S5(=O)=O

RUN: RUN395

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.33

EN300-6491117_1_1



CID: EN300-6491117_1_1

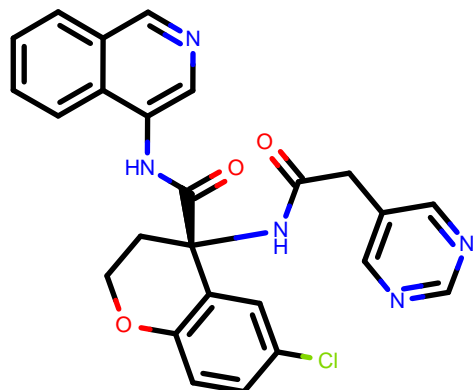
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cncc5

RUN: RUN7596

DDG (kcal/mol): -2.11

dDDG (kcal/mol): 0.18

EN300-185751_1_1



CID: EN300-185751_1_1

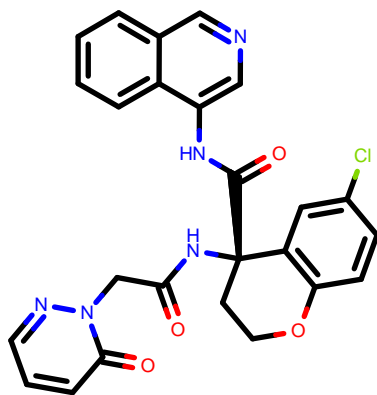
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cncc5

RUN: RUN9321

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.20

EN300-237561_1_1



CID: EN300-237561_1_1

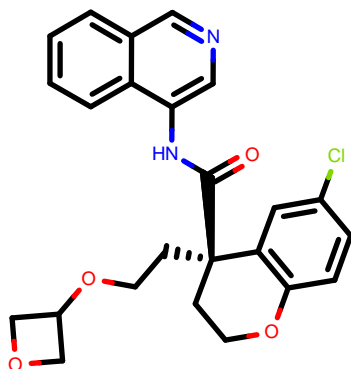
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c(=O)ocn5

RUN: RUN9165

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.26

EN300-317082_3_1



CID: EN300-317082_3_1

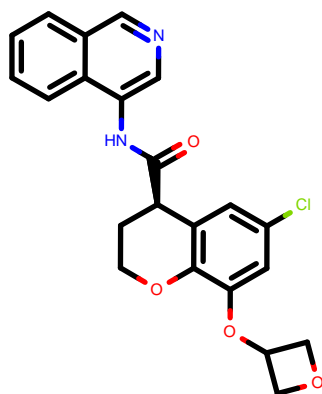
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOC5COC5

RUN: RUN1136

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.18

EDJ-MED-e4b030d8-4_1



CID: EDJ-MED-e4b030d8-4_1

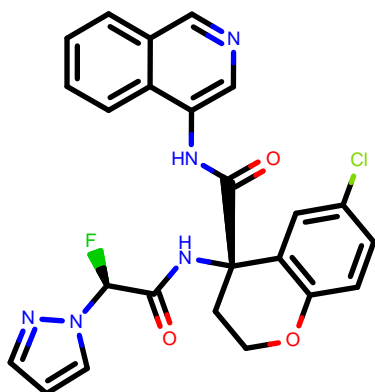
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)COC5COC5Cl

RUN: RUN156

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.21

EN300-1726277_1_1



CID: EN300-1726277_1_1

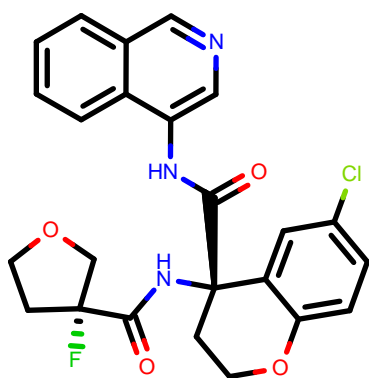
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4[C@@H](n5cccn5)F

RUN: RUN8040

DDG (kcal/mol): -2.10

dDDG (kcal/mol): 0.19

EN300-188356_1_2



CID: EN300-188356_1_2

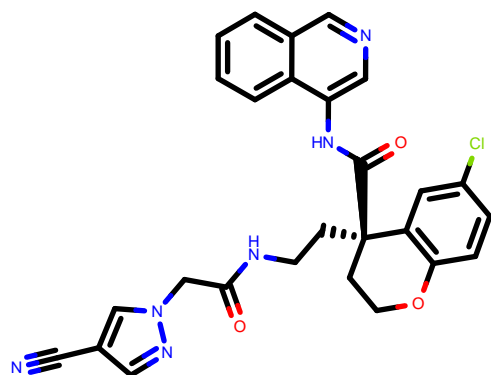
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)F

RUN: RUN7196

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.22

EN300-1590388_3_1



CID: EN300-1590388_3_1

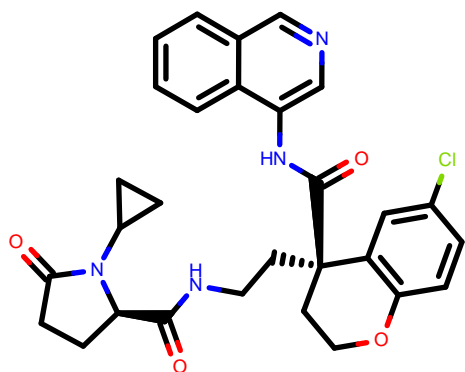
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn5C#N

RUN: RUN15187

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.26

EN300-3044054_3_2



CID: EN300-3044054_3_2

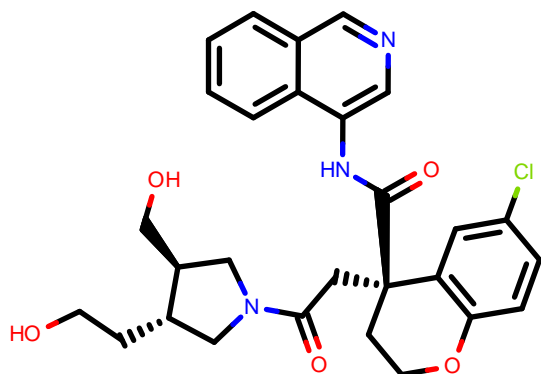
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCC(=O)N5)C6C6

RUN: RUN7911

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.27

EN300-1425608_1_1



CID: EN300-1425608_1_1

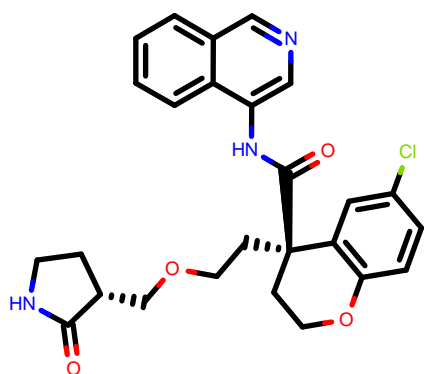
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C1=O)NSC[C@@]5(C)COCCO

RUN: RUN6344

DDG (kcal/mol): -2.09

dDDG (kcal/mol): 0.28

EN300-246248_3_1



CID: EN300-246248_3_1

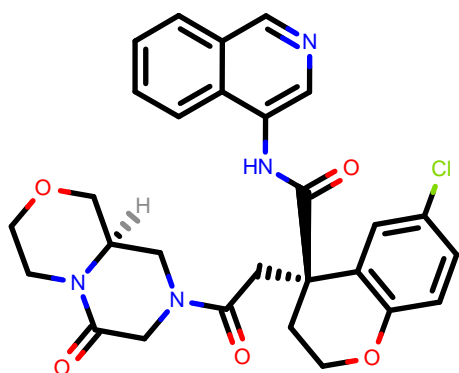
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CCNC5=O

RUN: RUN1720

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.26

EN300-6758891_1_1



CID: EN300-6758891_1_1

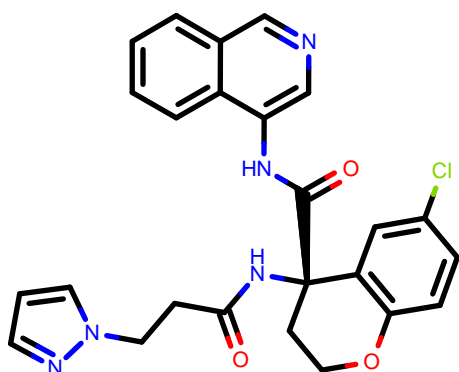
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)C(=O)N[C@@]5COC(=O)N[C@@]5C

RUN: RUN9500

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.22

EN300-25986_1_1



CID: EN300-25986_1_1

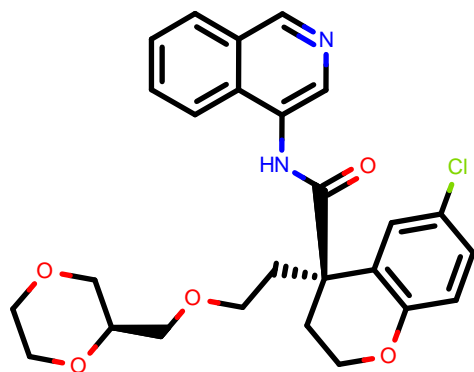
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5cccn5

RUN: RUN9249

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.21

EN300-139167_3_2



CID: EN300-139167_3_2

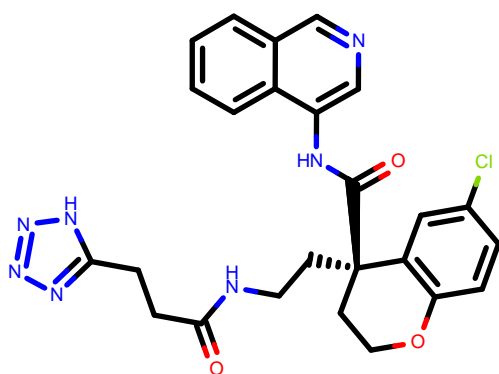
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5COCOC5

RUN: RUN1855

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.23

EN300-251851_3_1



CID: EN300-251851_3_1

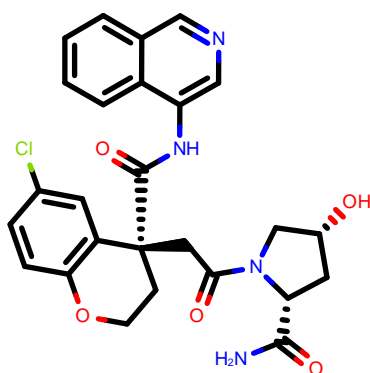
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5n[nH]n5

RUN: RUN13834

DDG (kcal/mol): -2.08

dDDG (kcal/mol): 0.27

EN300-07752_1_4



CID: EN300-07752_1_4

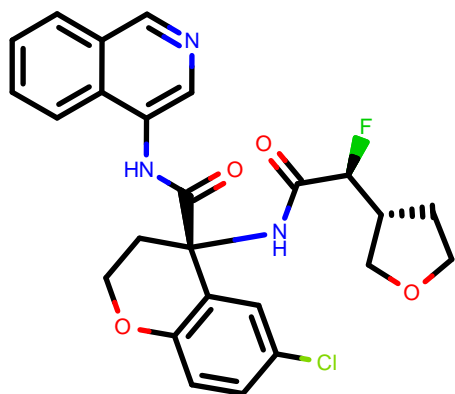
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(O)NC(=O)N

RUN: RUN6571

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.25

EN300-783124_1_2



CID: EN300-783124_1_2

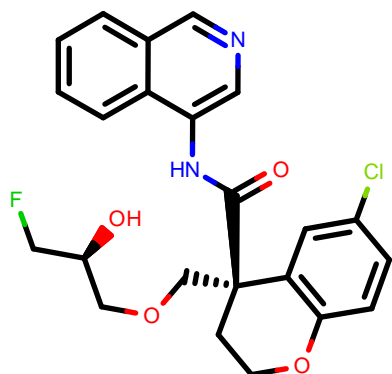
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]3COC(F)F

RUN: RUN1089

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.21

EN300-1968342_2_1



CID: EN300-1968342_2_1

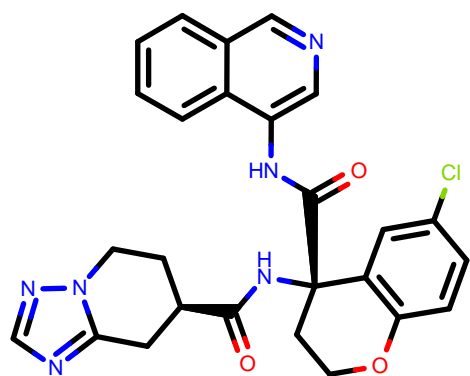
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]3(CF)O

RUN: RUN1833

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.23

EN300-1448674_1_2



CID: EN300-1448674_1_2

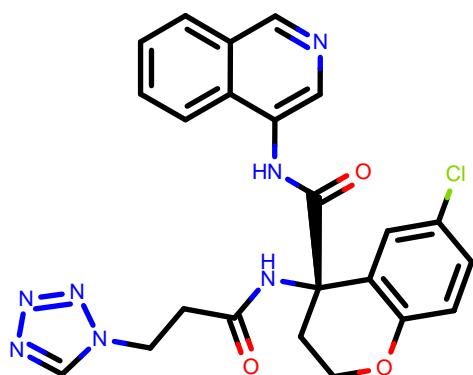
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C5Cn6cnc6)C5

RUN: RUN5930

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.20

EN300-191904_1_1



CID: EN300-191904_1_1

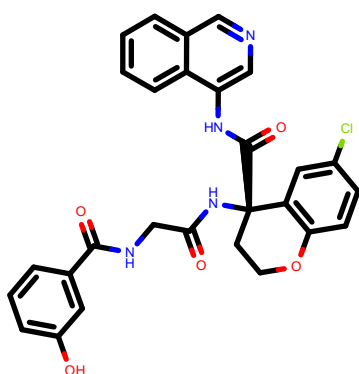
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cnn5

RUN: RUN8853

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.23

EN300-54417_1_1



CID: EN300-54417_1_1

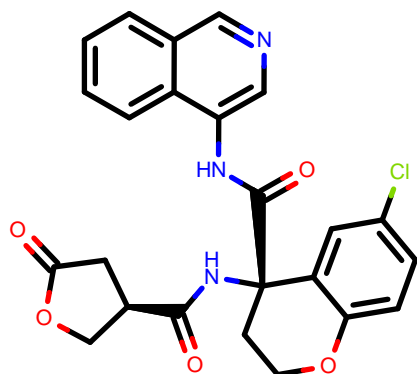
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5ccccc5O

RUN: RUN9598

DDG (kcal/mol): -2.07

dDDG (kcal/mol): 0.27

EN300-113234_1_1



CID: EN300-113234_1_1

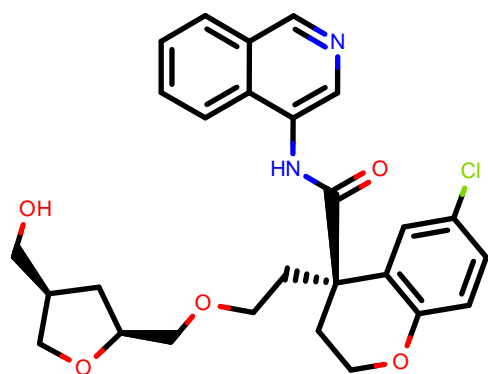
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C5C(=O)OC5

RUN: RUN4754

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.21

EN300-6494158_3_2



CID: EN300-6494158_3_2

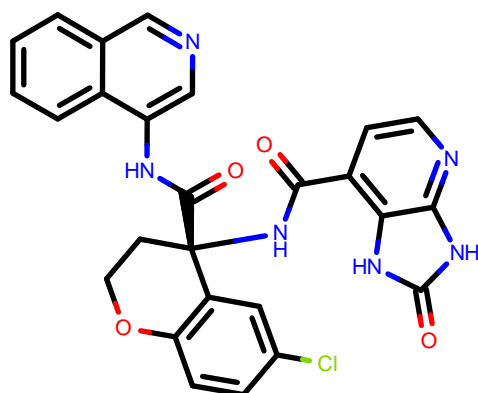
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]H5C[C@@]H(CO5)CO

RUN: RUN1368

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.31

EN300-189901_1_1



CID: EN300-189901_1_1

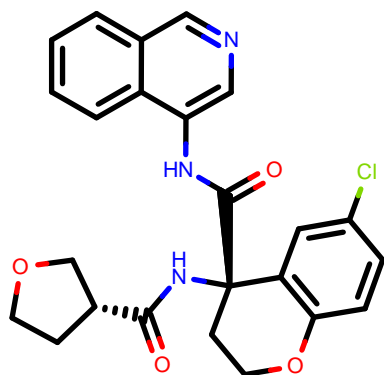
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6c5[nH]c1=O[nH]6

RUN: RUN7772

DDG (kcal/mol): -2.06

dDDG (kcal/mol): 0.20

EN300-53423_1_1



CID: EN300-53423_1_1

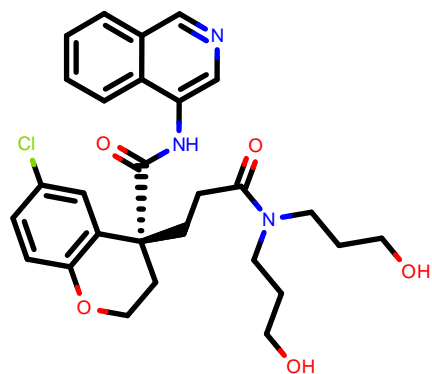
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5CCOC5

RUN: RUN4918

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.19

EN300-141457_2_1



CID: EN300-141457_2_1

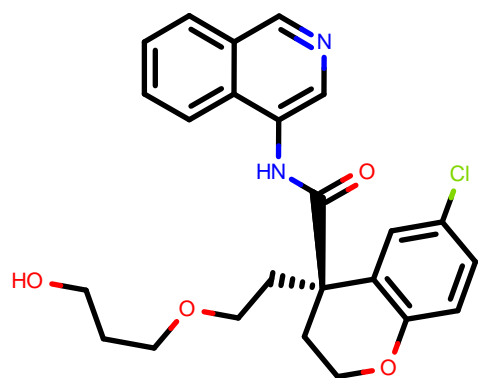
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N(CCCO)CCCO

RUN: RUN4316

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.27

EN300-221518_3_1



CID: EN300-221518_3_1

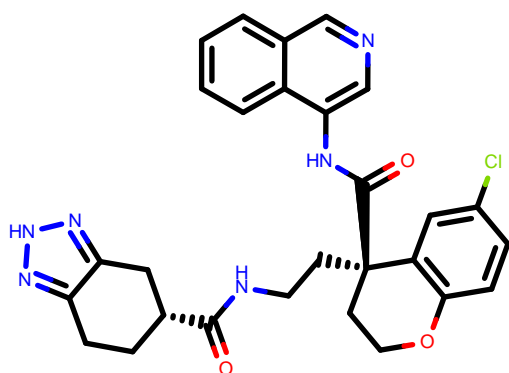
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)O)CCOCCCO

RUN: RUN1080

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.21

EN300-185729_3_2



CID: EN300-185729_3_2

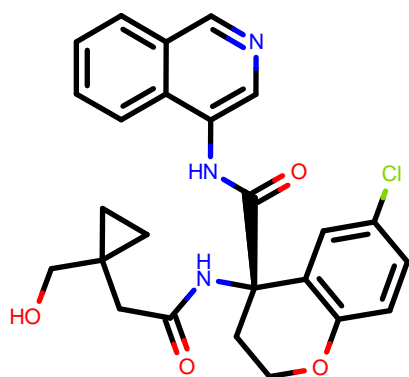
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)[C@@]4H5COC6=CN#N#N6C5

RUN: RUN15290

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.29

EN300-107048_1_1



CID: EN300-107048_1_1

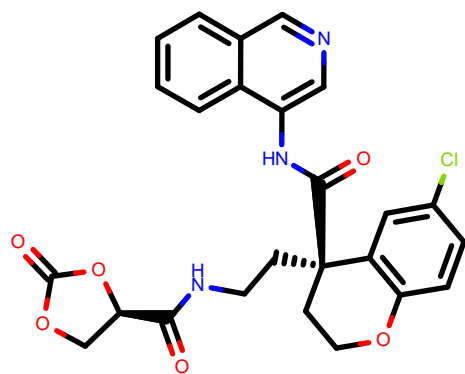
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)O)NC(=O)CC5(C)CC5CO

RUN: RUN3806

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.26

EN300-5253939_3_2



CID: EN300-5253939_3_2

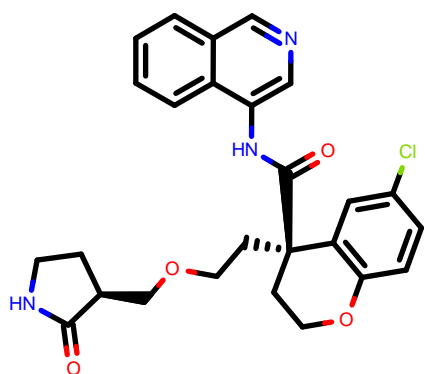
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)[C@@]4H5COC(=O)O5

RUN: RUN9192

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.22

EN300-246248_3_2



CID: EN300-246248_3_2

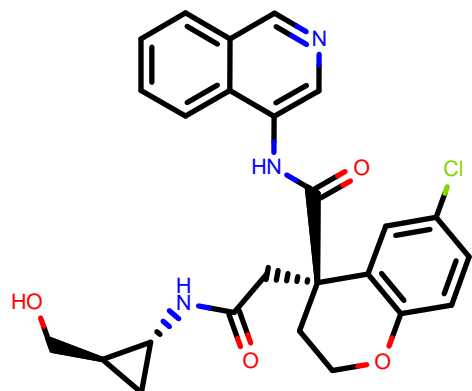
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN1792

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.23

EN300-399072_1_1



CID: EN300-399072_1_1

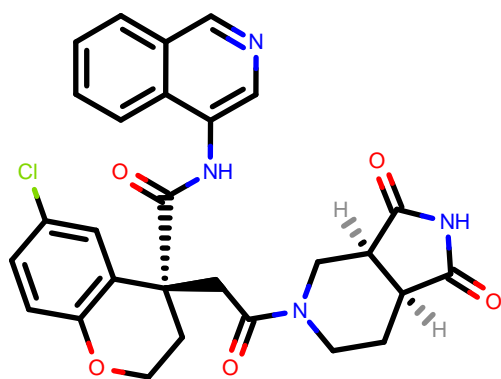
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]5CO

RUN: RUN281

DDG (kcal/mol): -2.05

dDDG (kcal/mol): 0.24

EN300-104029_1_4



CID: EN300-104029_1_4

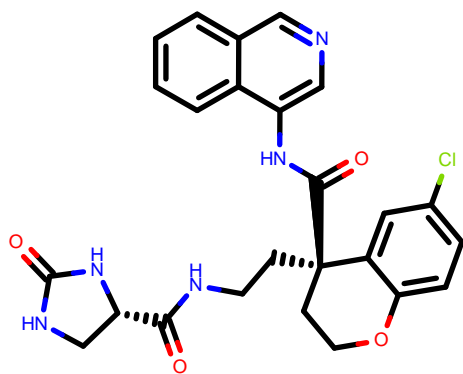
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5C[C@H]5C(=O)NC6=O

RUN: RUN4245

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.22

EN300-66461_3_1



CID: EN300-66461_3_1

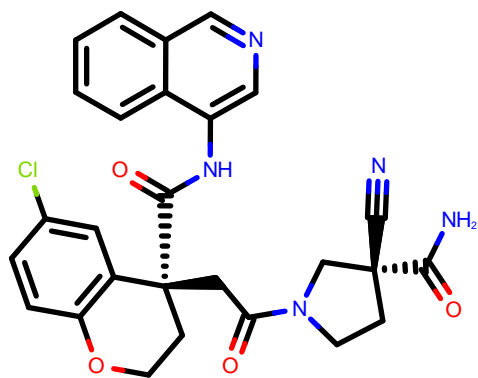
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CNC(=O)N5

RUN: RUN15389

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.22

EN300-1608992_1_1



CID: EN300-1608992_1_1

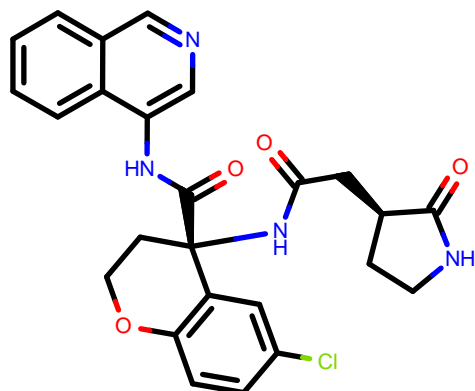
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(C#N)C(=O)N

RUN: RUN10011

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.25

EN300-343474_1_2



CID: EN300-343474_1_2

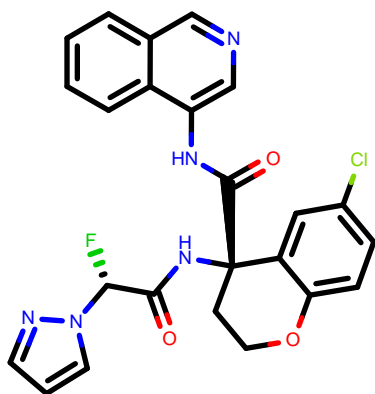
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCNC5=O

RUN: RUN3710

DDG (kcal/mol): -2.04

dDDG (kcal/mol): 0.27

EN300-1726277_1_2



CID: EN300-1726277_1_2

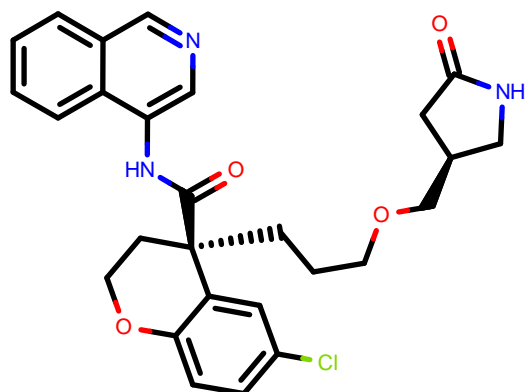
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](n5cccn5)F

RUN: RUN8500

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.19

EN300-246747_4_2



CID: EN300-246747_4_2

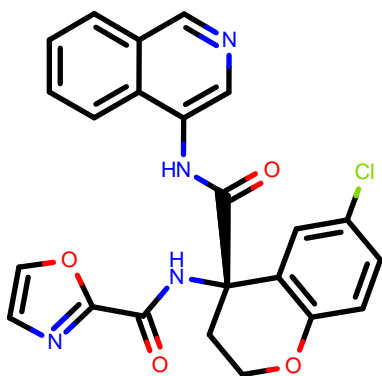
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5CC(=O)NCS

RUN: RUN1922

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.25

EN300-318344_1_1



CID: EN300-318344_1_1

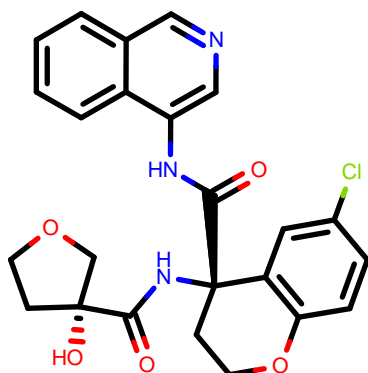
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncco5

RUN: RUN5238

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.19

EN300-148421_1_2



CID: EN300-148421_1_2

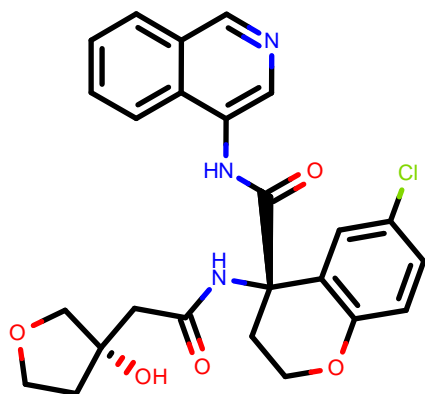
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)O

RUN: RUN2730

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.25

EN300-360157_1_2



CID: EN300-360157_1_2

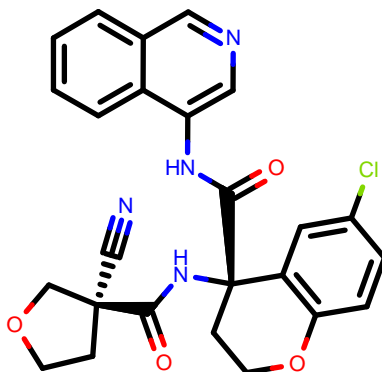
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)O

RUN: RUN6780

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.24

EN300-261210_1_1



CID: EN300-261210_1_1

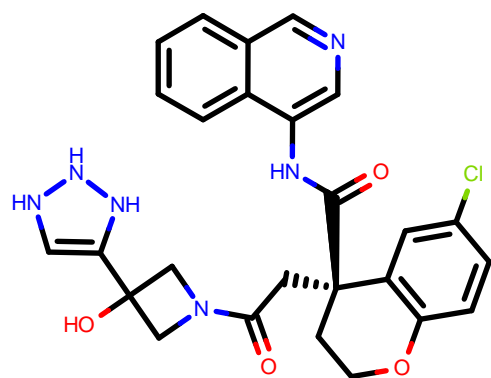
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOc5)C#N

RUN: RUN7460

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.27

EN300-384234_1_1



CID: EN300-384234_1_1

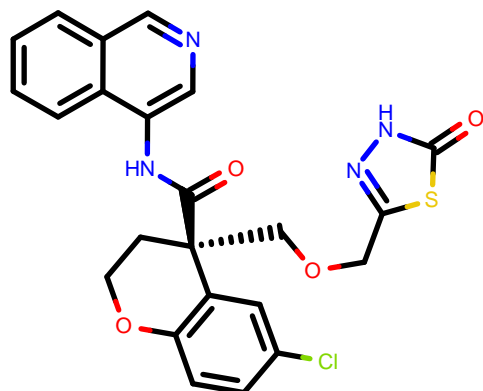
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cn[nH]n6)O

RUN: RUN6101

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.22

EN300-171766_2_1



CID: EN300-171766_2_1

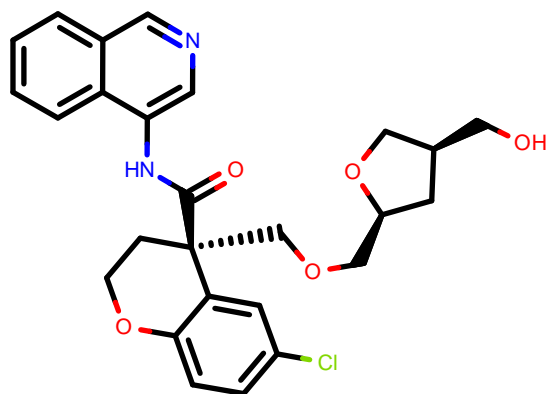
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5n[nH]c(=O)s5

RUN: RUN444

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.18

EN300-6494158_2_2



CID: EN300-6494158_2_2

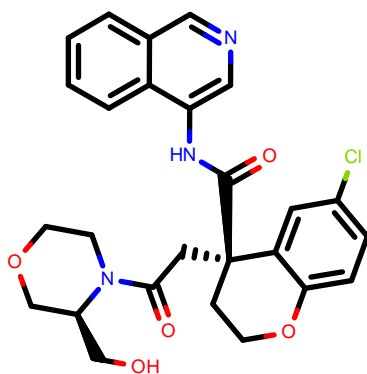
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C[C@@H](CO)CO

RUN: RUN1418

DDG (kcal/mol): -2.03

dDDG (kcal/mol): 0.24

EN300-154201_1_1



CID: EN300-154201_1_1

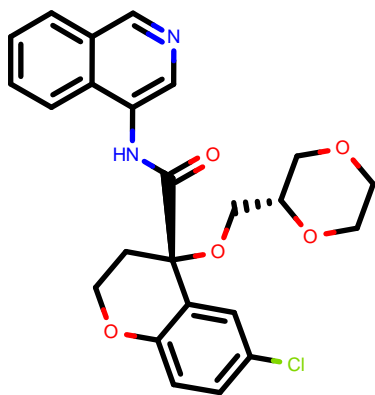
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN11461

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.26

EN300-139167_1_2



CID: EN300-139167_1_2

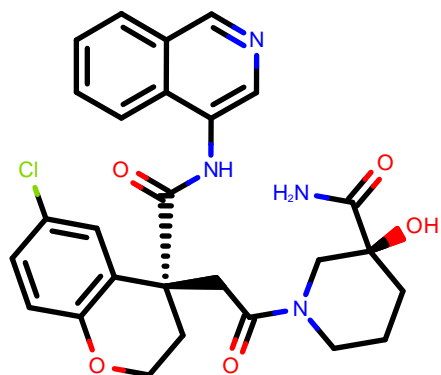
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COC(=O)5

RUN: RUN2091

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.23

EN300-210553_1_2



CID: EN300-210553_1_2

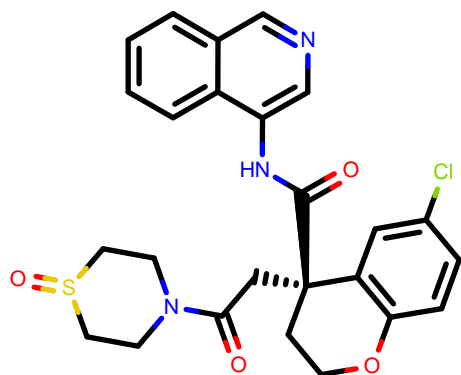
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H](C5)C(=O)NO

RUN: RUN5193

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.29

EN300-69588_1_1



CID: EN300-69588_1_1

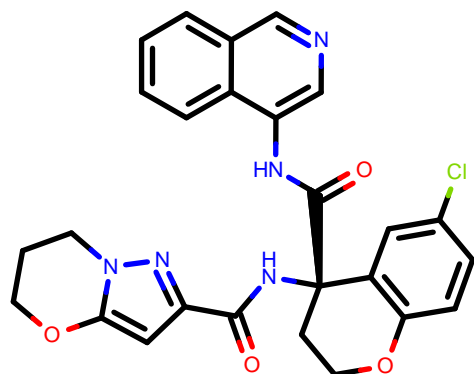
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)CC5

RUN: RUN9264

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.23

EN300-103720_1_1



CID: EN300-103720_1_1

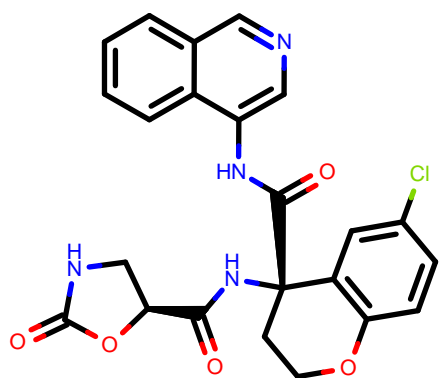
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCCO6

RUN: RUN675

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.21

EN300-244403_1_1



CID: EN300-244403_1_1

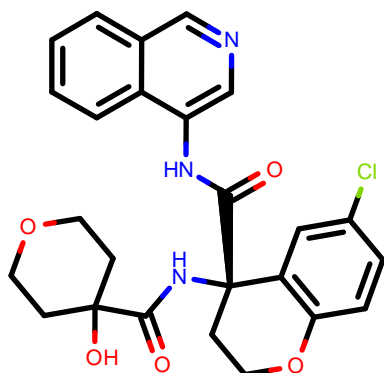
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5CNC(=O)O5

RUN: RUN5078

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.19

EN300-69368_1_1



CID: EN300-69368_1_1

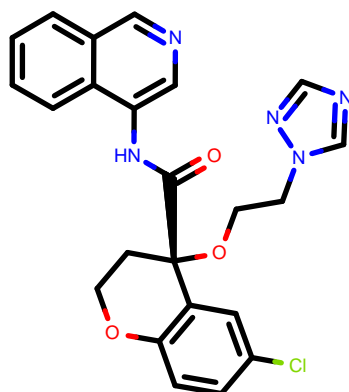
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)O

RUN: RUN2807

DDG (kcal/mol): -2.02

dDDG (kcal/mol): 0.23

EN300-6255179_1_1



CID: EN300-6255179_1_1

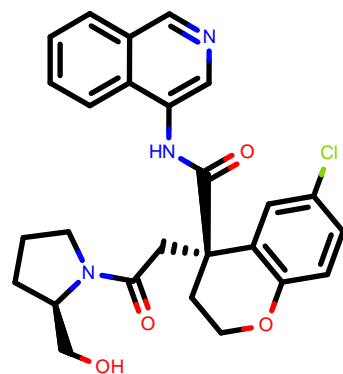
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5ncn5

RUN: RUN1133

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.20

EN300-54891_1_1



CID: EN300-54891_1_1

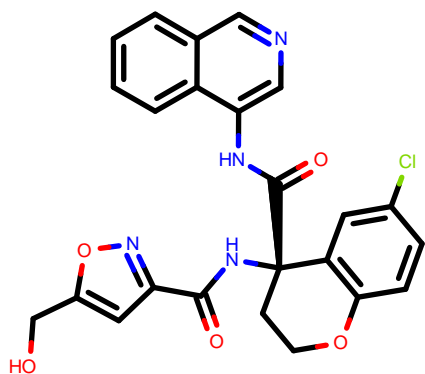
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]H5CO

RUN: RUN3237

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.20

EN300-95507_1_1



CID: EN300-95507_1_1

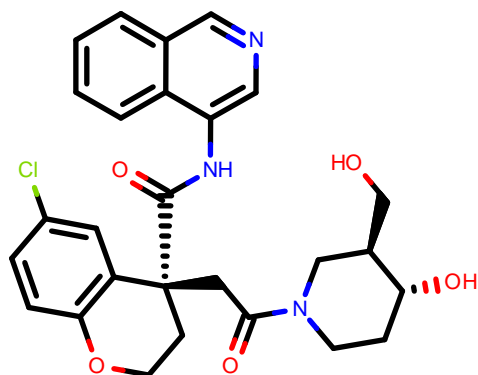
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(oc5)CO

RUN: RUN2832

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.18

EN300-233678_1_4



CID: EN300-233678_1_4

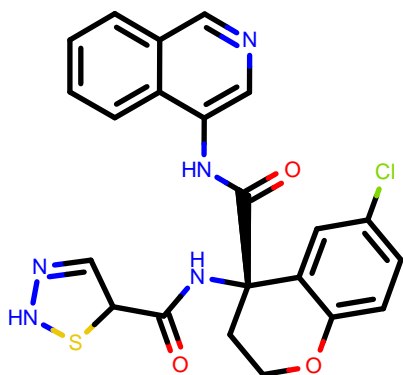
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(O)N5CC[C@H](C3)N5CO

RUN: RUN5117

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.25

EN300-42269_1_1



CID: EN300-42269_1_1

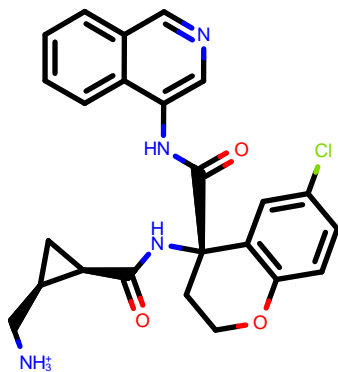
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nnns5

RUN: RUN5694

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.17

EN300-1600363_1_1



CID: EN300-1600363_1_1

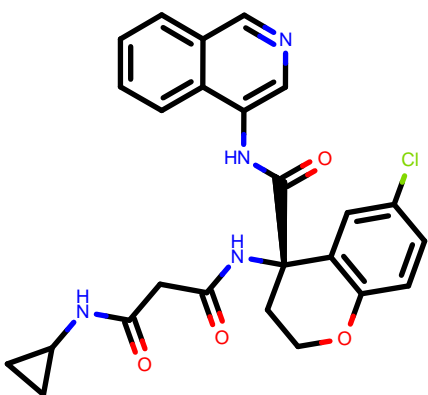
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H5C[C@@]4H5C#N

RUN: RUN7608

DDG (kcal/mol): -2.01

dDDG (kcal/mol): 0.18

EN300-128464_1_1



CID: EN300-128464_1_1

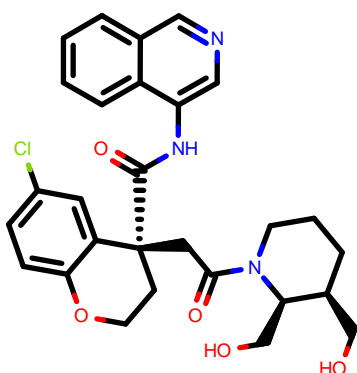
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC(=O)NC5CC5

RUN: RUN7616

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.21

EN300-343562_1_1



CID: EN300-343562_1_1

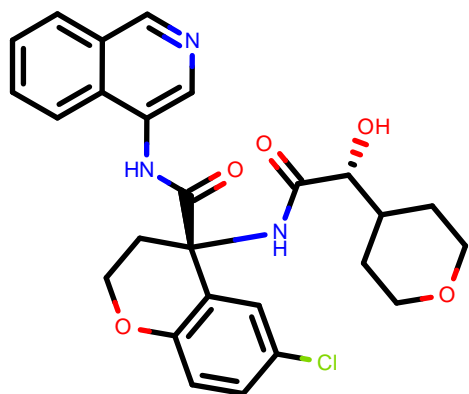
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C)[H]5CO

RUN: RUN9412

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.31

EN300-7443878_1_1



CID: EN300-7443878_1_1

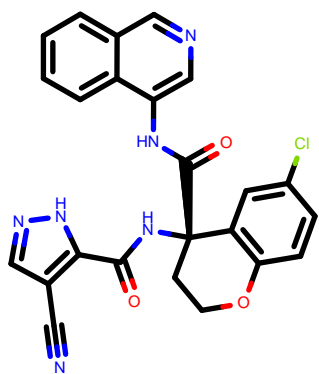
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H[C@H]5COCOC5

RUN: RUN3782

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.23

EN300-1267109_1_1



CID: EN300-1267109_1_1

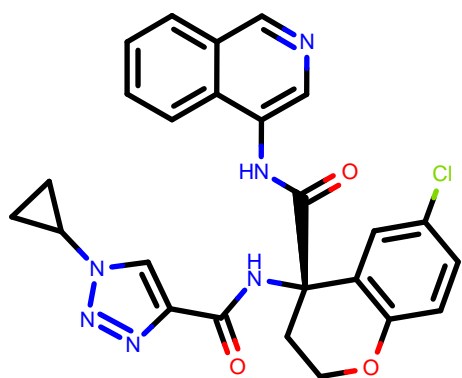
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c(c[nH]5)C#N

RUN: RUN7380

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.19

EN300-210110_1_1



CID: EN300-210110_1_1

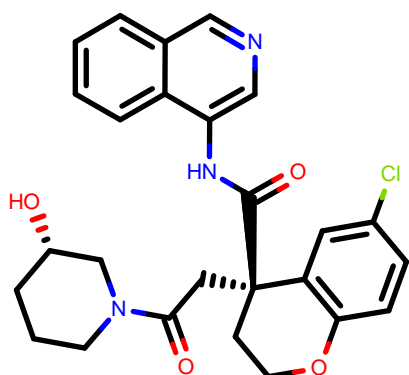
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(n5)C6CC6

RUN: RUN1625

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.19

EN300-188582_1_1



CID: EN300-188582_1_1

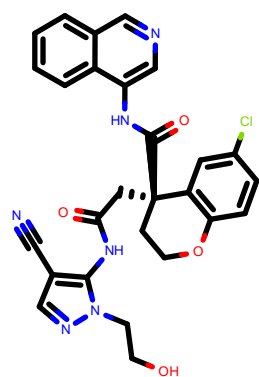
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN9448

DDG (kcal/mol): -2.00

dDDG (kcal/mol): 0.21

EN300-70133_1_1



CID: EN300-70133_1_1

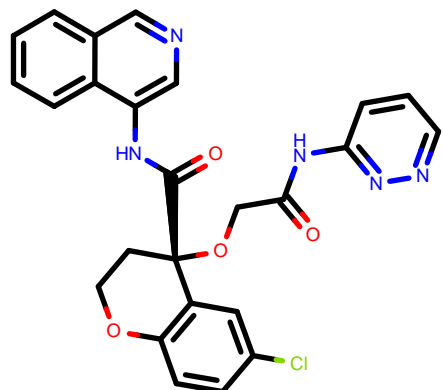
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5cncn5CCO

RUN: RUN12620

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.22

EN300-761618_1_1



CID: EN300-761618_1_1

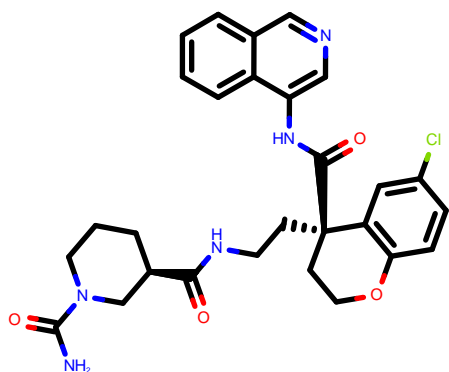
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)Nc5ccnnc5

RUN: RUN1741

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.26

EN300-14767_3_1



CID: EN300-14767_3_1

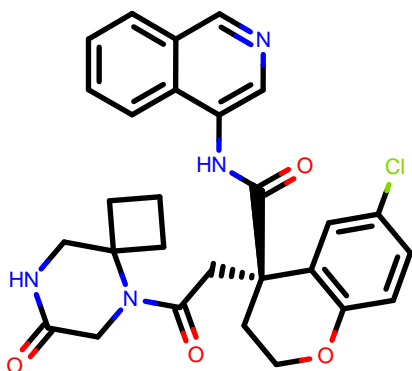
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5H5CCCN(C5)C(=O)N

RUN: RUN681

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.29

EN300-7349829_1_1



CID: EN300-7349829_1_1

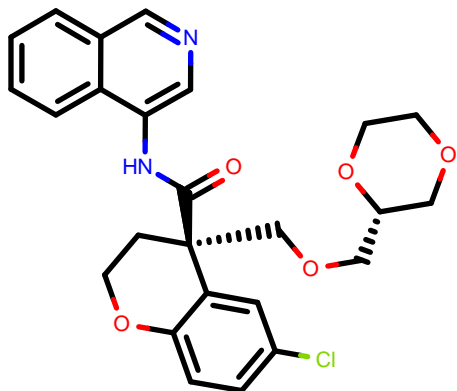
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NCC56CCC6

RUN: RUN11920

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.31

EN300-139167_2_1



CID: EN300-139167_2_1

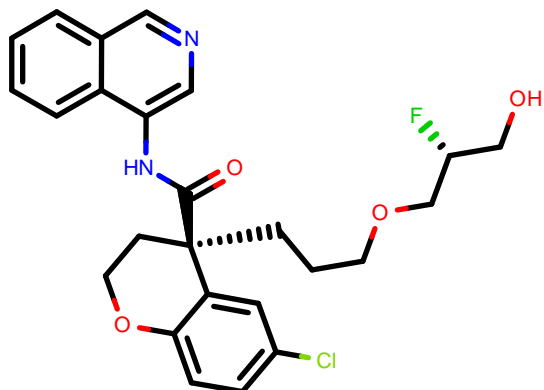
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5H5COCOC5

RUN: RUN1362

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.22

EN300-1600517_4_2



CID: EN300-1600517_4_2

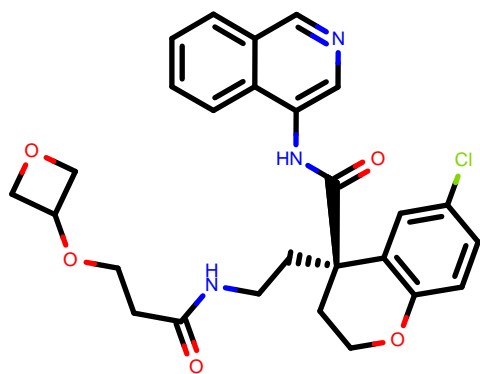
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5H5(CO)F

RUN: RUN389

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.26

EN300-321703_3_1



CID: EN300-321703_3_1

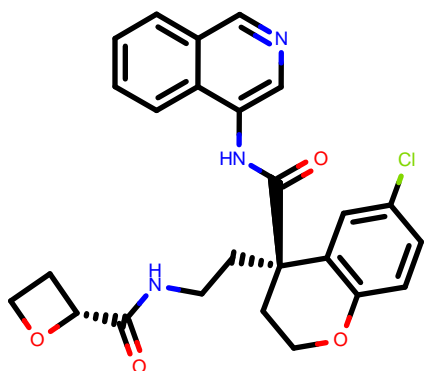
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCOC5COC5

RUN: RUN10998

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.26

EN300-85760_3_2



CID: EN300-85760_3_2

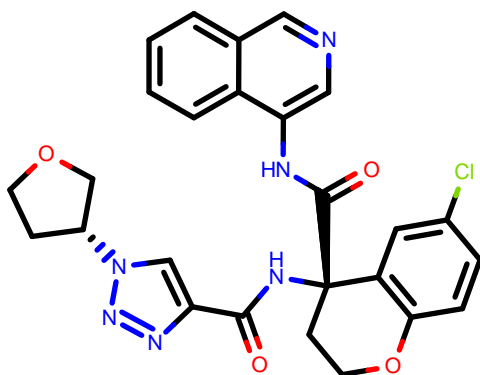
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5COC5

RUN: RUN15023

DDG (kcal/mol): -1.99

dDDG (kcal/mol): 0.18

EN300-151461_1_1



CID: EN300-151461_1_1

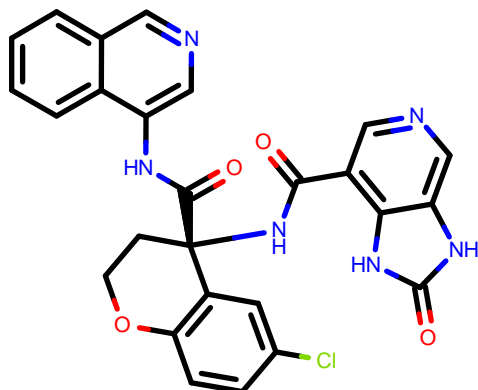
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(n5)[C@@H]6COC6

RUN: RUN4206

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.21

EN300-7434209_1_1



CID: EN300-7434209_1_1

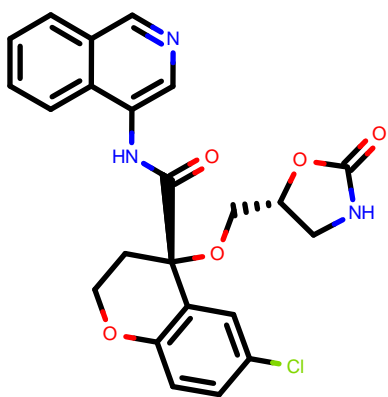
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncnc6c5[nH]c1=O[nH]6

RUN: RUN7652

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.19

EN300-203293_1_1



CID: EN300-203293_1_1

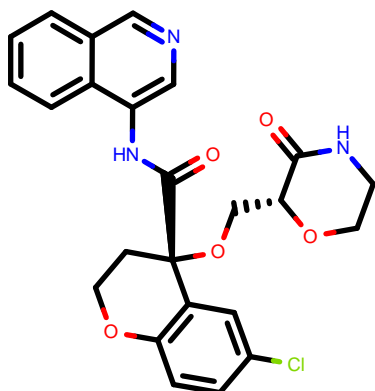
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)OC[C@@H]5CNC(=O)O5

RUN: RUN2754

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.28

EN300-1706036_1_2



CID: EN300-1706036_1_2

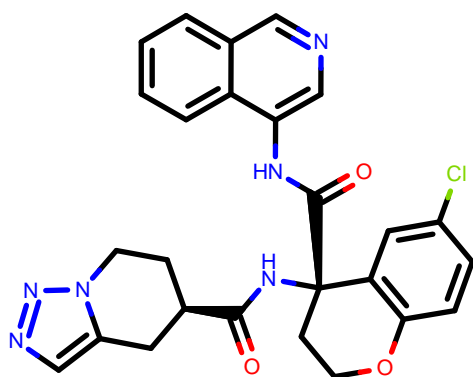
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)OC[C@@H]5C(=O)NCCO5

RUN: RUN1860

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.24

EN300-7430501_1_2



CID: EN300-7430501_1_2

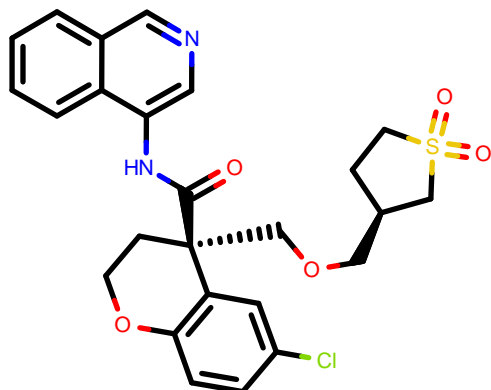
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)NC(=O)[C@@H]5CNC6c(cnn6)C5

RUN: RUN5974

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.20

EN300-1448603_2_2



CID: EN300-1448603_2_2

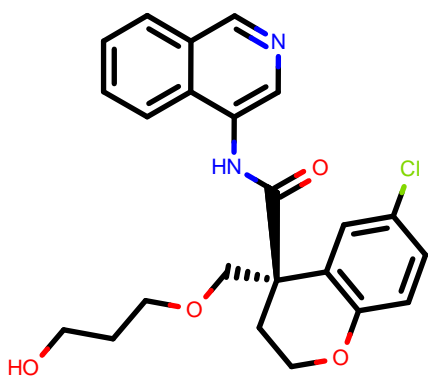
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COCc4c3cc(cc4)Cl)COC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN1146

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.30

EN300-221518_2_1



CID: EN300-221518_2_1

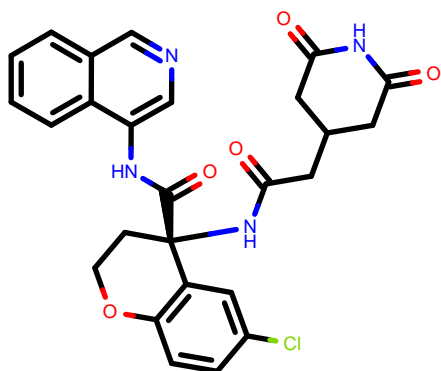
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC

RUN: RUN1937

DDG (kcal/mol): -1.98

dDDG (kcal/mol): 0.19

EN300-225165_1_1



CID: EN300-225165_1_1

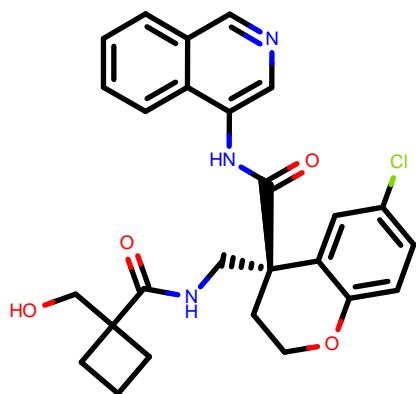
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5CC(=O)NC(=O)C5

RUN: RUN8721

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.25

EN300-149975_2_1



CID: EN300-149975_2_1

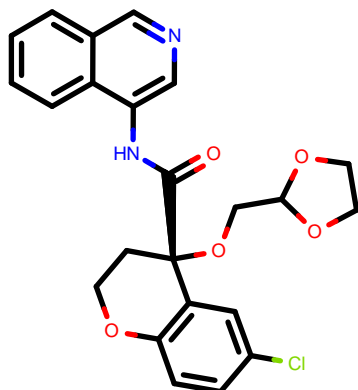
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCC5)CO

RUN: RUN6342

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.24

EN300-77092_1_1



CID: EN300-77092_1_1

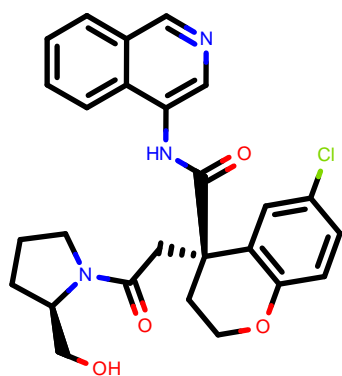
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5OCCO5

RUN: RUN1749

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.25

EN300-54891_1_1



CID: EN300-54891_1_1

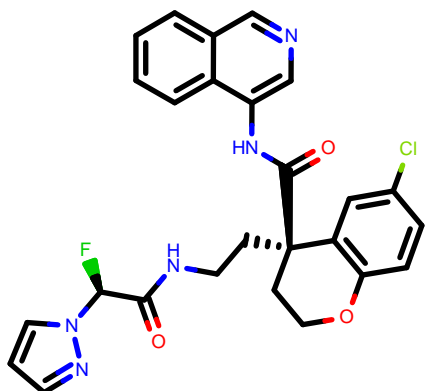
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5CO

RUN: RUN3241

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.22

EN300-1726277_3_1



CID: EN300-1726277_3_1

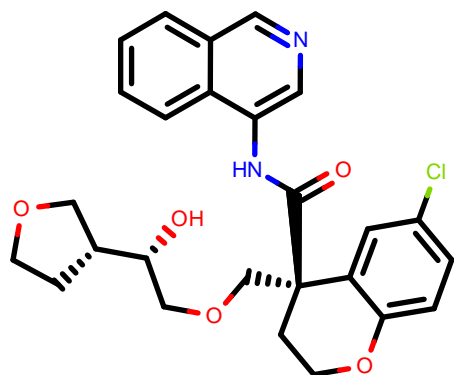
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](n5cccn5)F

RUN: RUN6723

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.22

EN300-1911992_2_1



CID: EN300-1911992_2_1

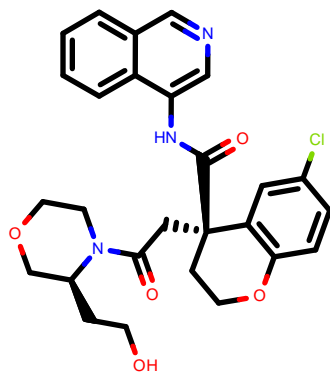
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](C)[C@@H]5CCOC5O

RUN: RUN1786

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.28

EN300-345754_1_1



CID: EN300-345754_1_1

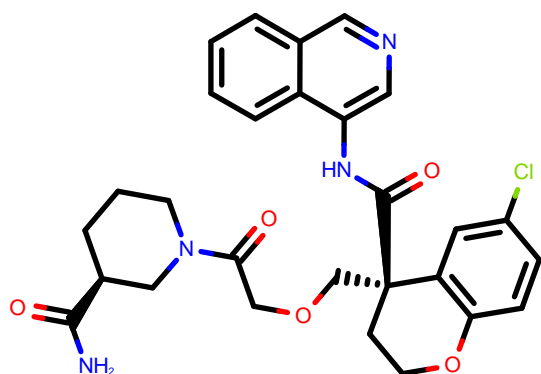
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN11453

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.29

EN300-22880_2_1



CID: EN300-22880_2_1

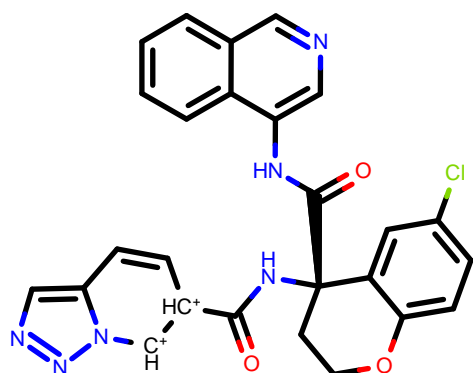
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)C(=O)N5CCOC[C@@H]5C(Cl)=O

RUN: RUN2527

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.28

EN300-6491316_1_1



CID: EN300-6491316_1_1

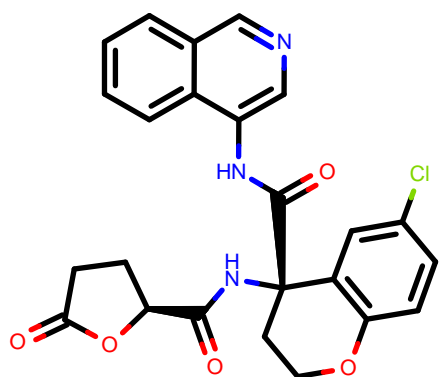
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)NC(=O)c5ccc6cnnn6c5

RUN: RUN4118

DDG (kcal/mol): -1.97

dDDG (kcal/mol): 0.22

EN300-359750_1_1



CID: EN300-359750_1_1

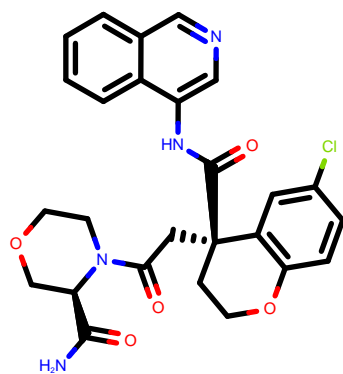
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)NC(=O)[C@@H]5CCCC(=O)O5

RUN: RUN7604

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.21

EN300-124383_1_2



CID: EN300-124383_1_2

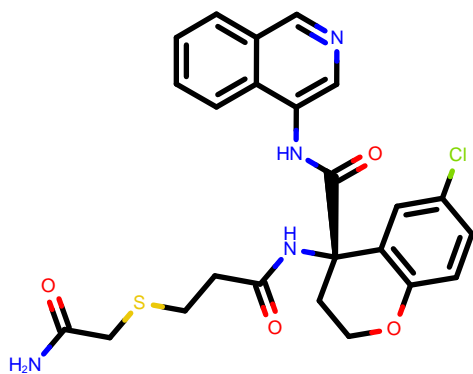
SMILES: c1ccc2c(c1)nccc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CC(=O)N5CCOC[C@@H]5C(Cl)=O

RUN: RUN6256

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.22

EN300-31015_1_1



CID: EN300-31015_1_1

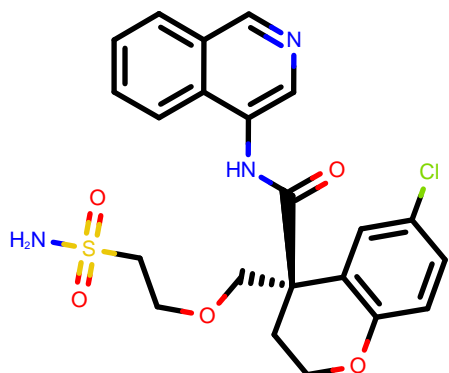
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCSCC(=O)N

RUN: RUN2700

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.23

EN300-270710_2_1



CID: EN300-270710_2_1

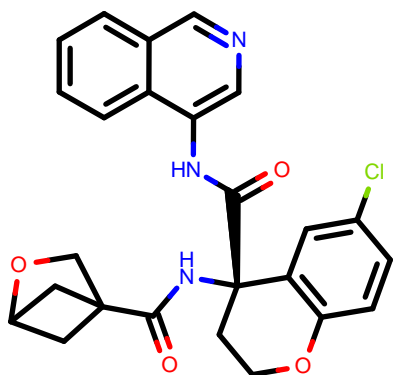
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)S(=O)(=O)N

RUN: RUN684

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.27

EN300-1604607_1_1



CID: EN300-1604607_1_1

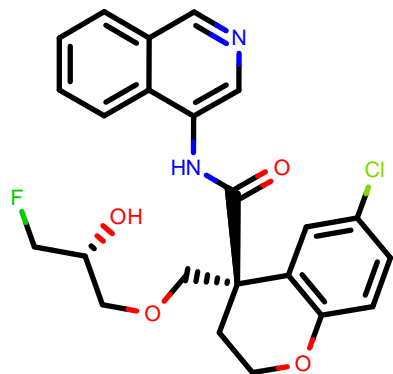
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(C5)O6

RUN: RUN4142

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.22

EN300-1968342_2_2



CID: EN300-1968342_2_2

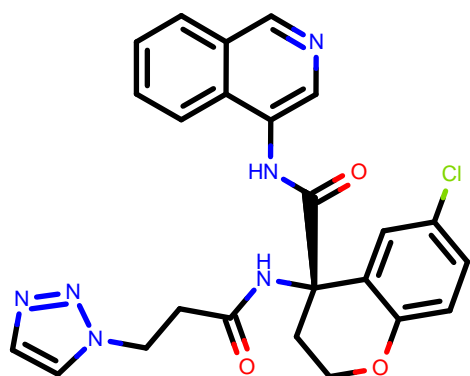
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN1873

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.25

EN300-28871_1_1



CID: EN300-28871_1_1

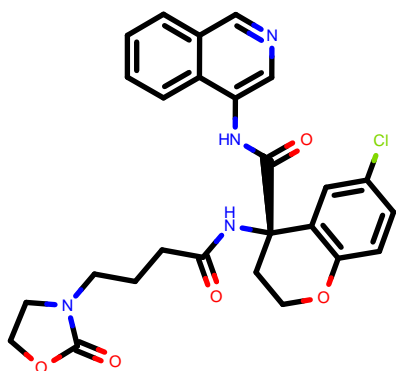
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5

RUN: RUN9101

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.20

EN300-45182_1_1



CID: EN300-45182_1_1

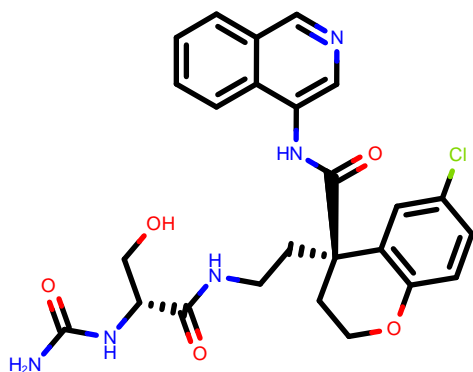
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCN5CCOC5=O

RUN: RUN7284

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.26

EN300-10170_3_1



CID: EN300-10170_3_1

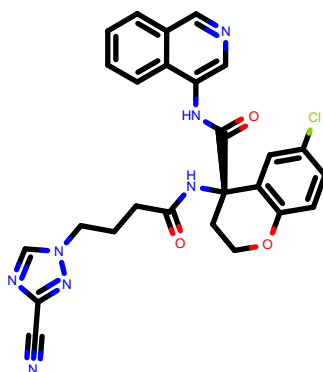
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](CO)NC(=O)N

RUN: RUN3249

DDG (kcal/mol): -1.96

dDDG (kcal/mol): 0.35

EN300-245265_1_1



CID: EN300-245265_1_1

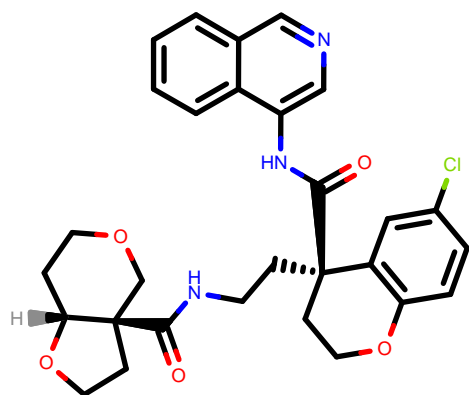
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCN5cnc(n5)C#N

RUN: RUN4994

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.27

EN300-341337_3_2



CID: EN300-341337_3_2

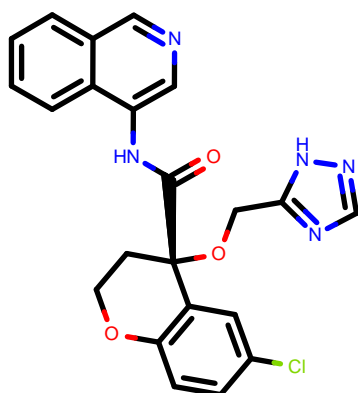
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCNC(=O)[C@@]56CCO[C@@H]5CCO6

RUN: RUN15134

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.25

EN300-306316_1_1



CID: EN300-306316_1_1

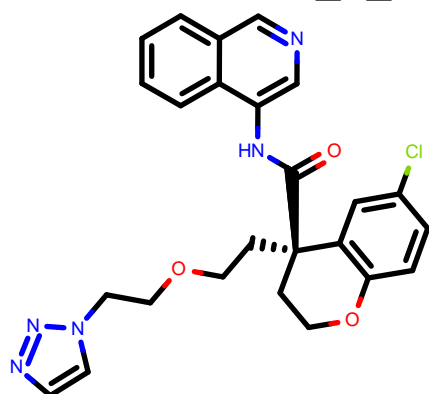
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)OCc5[nH]ncn5

RUN: RUN951

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.14

EN300-1715993_3_1



CID: EN300-1715993_3_1

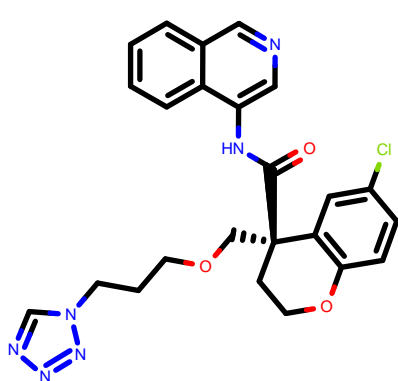
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCOCCn5cnnn5

RUN: RUN1887

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.23

EN300-1696962_2_1



CID: EN300-1696962_2_1

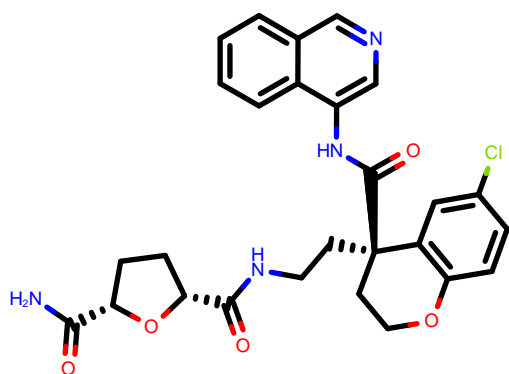
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)COCCCN5cnnn5

RUN: RUN428

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.24

EN300-315238_3_1



CID: EN300-315238_3_1

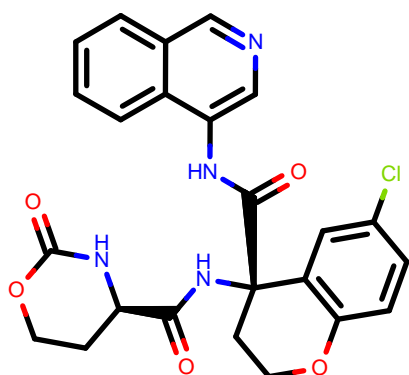
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C1CCNC1=O[C@@H]5CC[C@@H](O5)Cl=O>N

RUN: RUN4621

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.21

EN300-249804_1_2



CID: EN300-249804_1_2

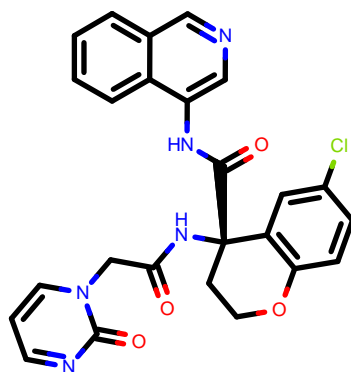
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C1NC(=O)[C@@H]5CCOC(=O)N5

RUN: RUN2167

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.26

EN300-35789_1_1



CID: EN300-35789_1_1

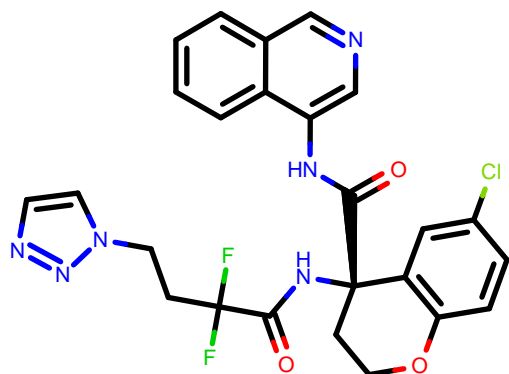
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C1NC(=O)Cn5ccnc5=O

RUN: RUN9703

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.22

EN300-6474220_1_1



CID: EN300-6474220_1_1

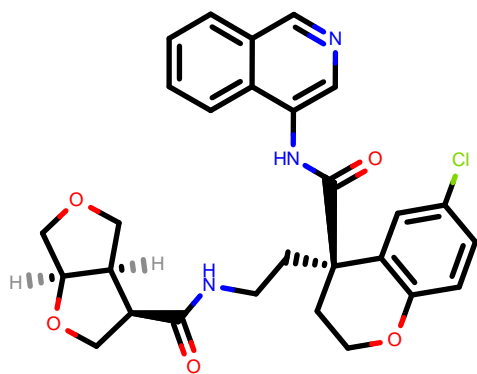
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C1NC(=O)C(Cn5ccnn5)F)F

RUN: RUN3110

DDG (kcal/mol): -1.95

dDDG (kcal/mol): 0.23

EN300-6482296_3_8



CID: EN300-6482296_3_8

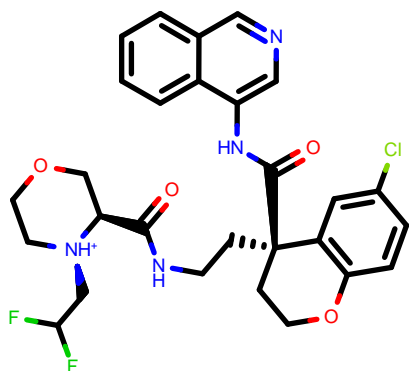
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COC4=CC=CC=C4)C(C)CCNC(=O)C@@H5CO[C@@H]6C@@H5COO6

RUN: RUN15024

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.31

EN300-140582_3_3



CID: EN300-140582_3_3

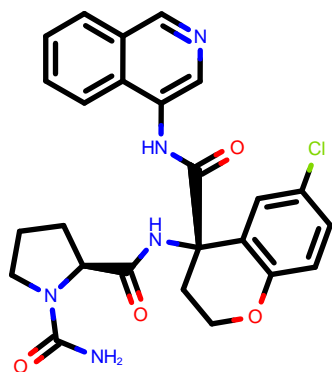
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COC4=CC=CC=C4)C(C)CCNC(=O)C@@H5CO[C@@H]6C@@H5COF6

RUN: RUN13944

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.26

EN300-87536_1_1



CID: EN300-87536_1_1

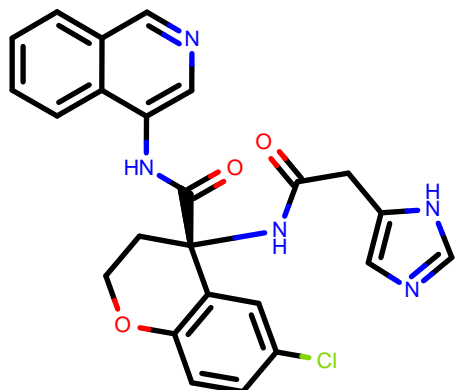
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COC4=CC=CC=C4)C(C)CCNC(=O)C@@H5CCN5C(=O)N

RUN: RUN7344

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.26

EN300-342226_1_1



CID: EN300-342226_1_1

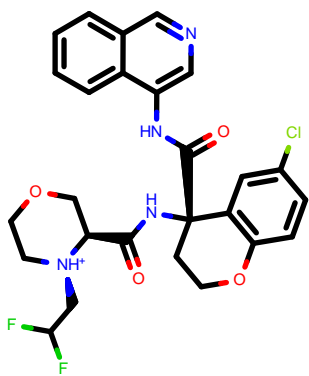
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@H](COC4=CC=CC=C4)C(C)CCNC(=O)C5=CN=C[NH]5

RUN: RUN8180

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.23

EN300-140582_1_1



CID: EN300-140582_1_1

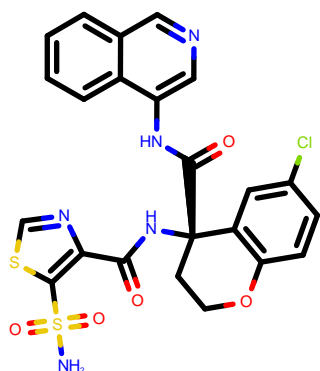
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COCCN5[C@@](F)F

RUN: RUN6760

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.24

EN300-132613_1_1



CID: EN300-132613_1_1

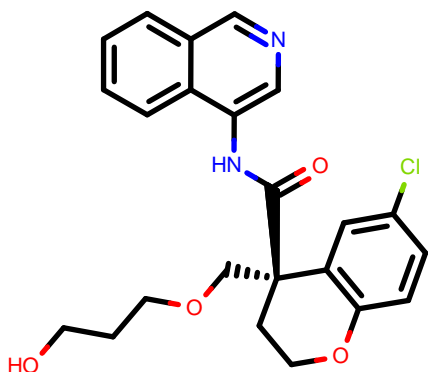
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(scn5)S(=O)(=O)N

RUN: RUN7524

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.23

EN300-221518_2_1



CID: EN300-221518_2_1

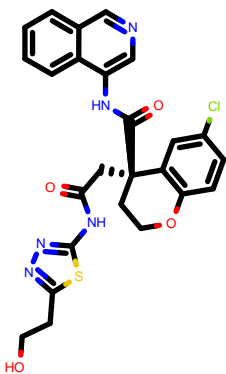
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCO

RUN: RUN1921

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.18

EN300-122590_1_1



CID: EN300-122590_1_1

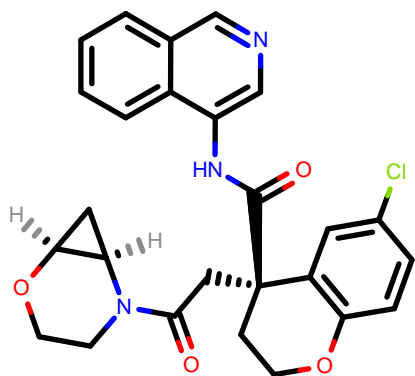
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnc(s5)CCO

RUN: RUN4609

DDG (kcal/mol): -1.94

dDDG (kcal/mol): 0.22

EN300-91609_1_2



CID: EN300-91609_1_2

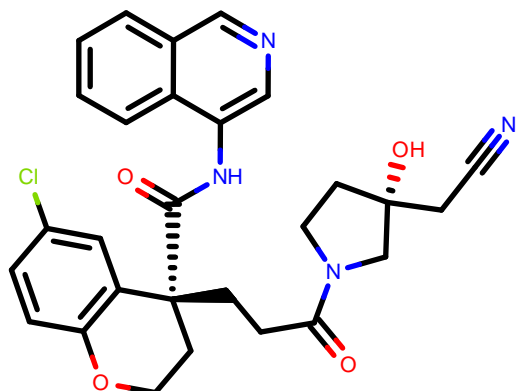
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@@]H[C@@]H5C6

RUN: RUN11671

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.22

EN300-257405_2_2



CID: EN300-257405_2_2

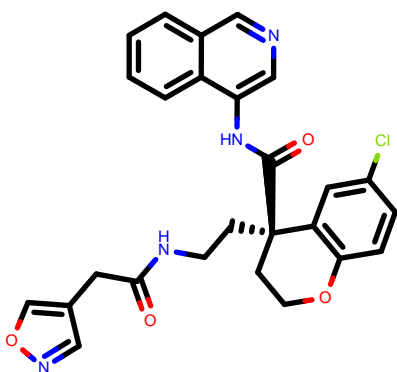
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@]H[C@]5(C)C#N

RUN: RUN8915

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.26

EN300-315963_3_1



CID: EN300-315963_3_1

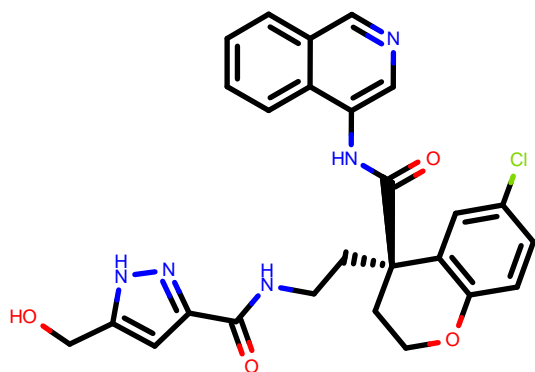
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5cnoc5

RUN: RUN15247

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.21

EN300-658865_3_1



CID: EN300-658865_3_1

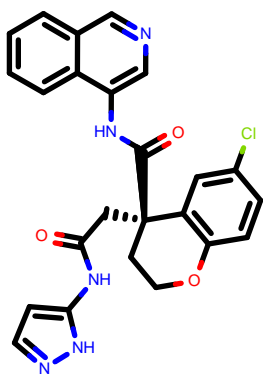
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cc[nH]5CO

RUN: RUN15196

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.23

JAG-UCB-706446eb-6_1



CID: JAG-UCB-706446eb-6_1

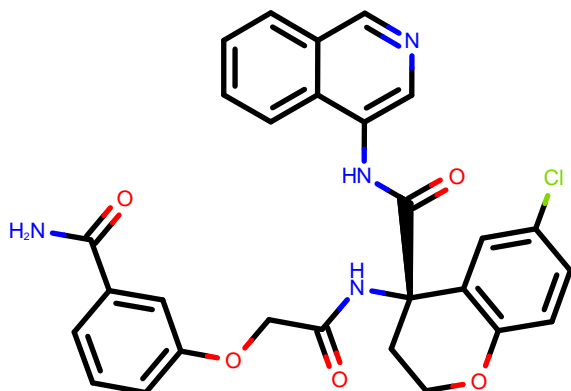
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cc[nH]5

RUN: RUN234

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.16

EN300-51736_1_1



CID: EN300-51736_1_1

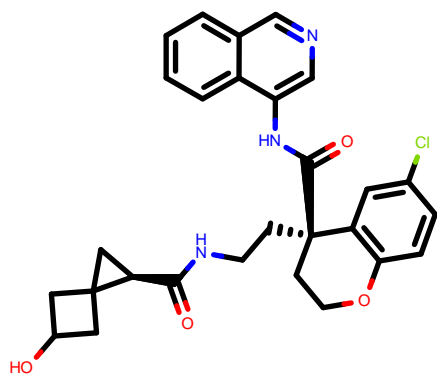
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COc5ccccc5C(=O)N

RUN: RUN9477

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.25

EN300-1717166_3_1



CID: EN300-1717166_3_1

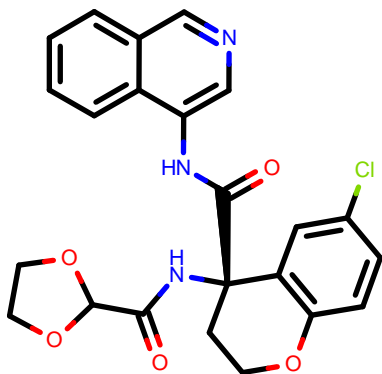
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]3HJ5CC56C(C6)O

RUN: RUN15350

DDG (kcal/mol): -1.93

dDDG (kcal/mol): 0.28

EN300-154942_1_1



CID: EN300-154942_1_1

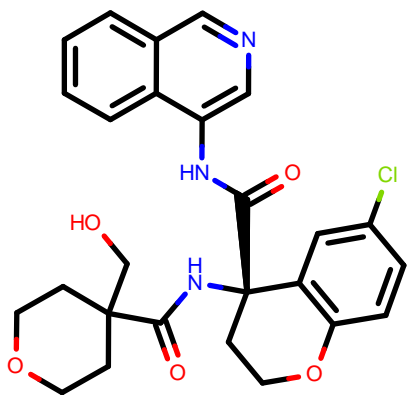
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCO5

RUN: RUN3366

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.19

EN300-244909_1_1



CID: EN300-244909_1_1

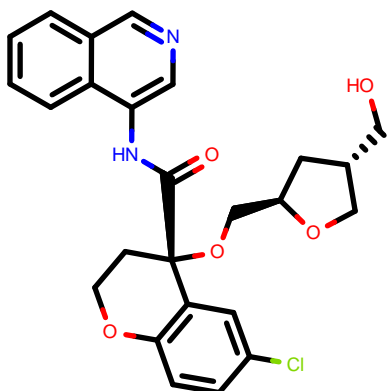
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C5(CCOCC5)CO

RUN: RUN4802

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.27

EN300-6494158_1_1



CID: EN300-6494158_1_1

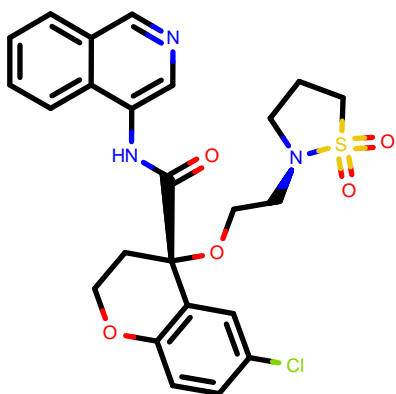
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OC[C@H]5C[C@@H](CO)CO

RUN: RUN2550

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.25

EN300-114134_1_1



CID: EN300-114134_1_1

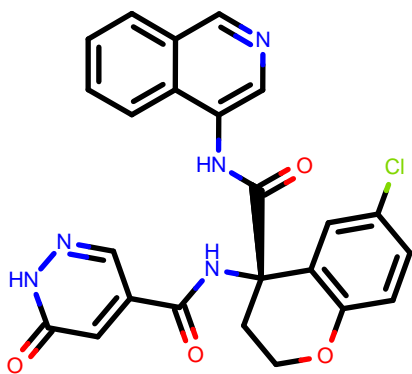
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)OCC[N@]5CCCS5(=O)=O

RUN: RUN1413

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.30

EN300-159634_1_1



CID: EN300-159634_1_1

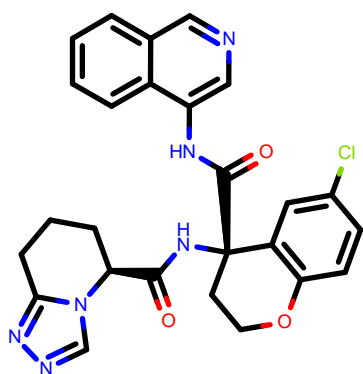
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cc(=O)[nH]ne5

RUN: RUN5594

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.19

EN300-6478631_1_1



CID: EN300-6478631_1_1

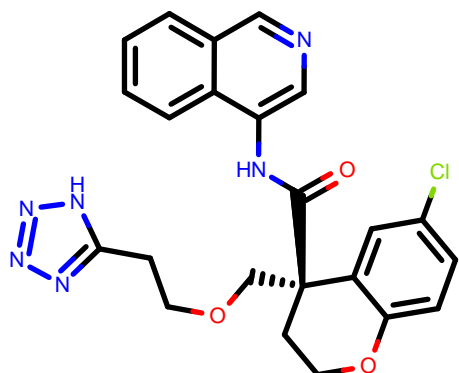
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H5CCc6n5cnn6

RUN: RUN9245

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.27

EN300-183231_2_1



CID: EN300-183231_2_1

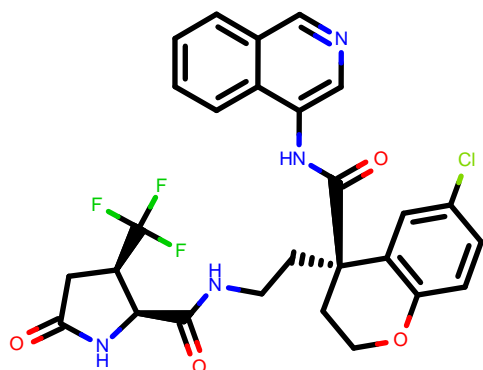
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)COCc5n[n-]nn5

RUN: RUN676

DDG (kcal/mol): -1.92

dDDG (kcal/mol): 0.25

EN300-169955_3_3



CID: EN300-169955_3_3

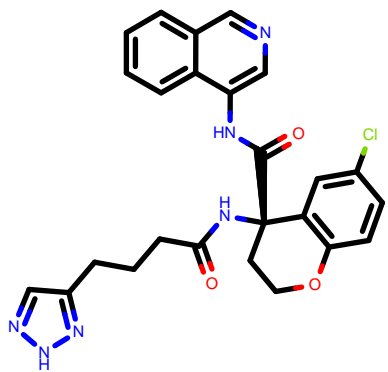
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@@H5C(F)(F)F

RUN: RUN2997

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.26

EN300-156995_1_1



CID: EN300-156995_1_1

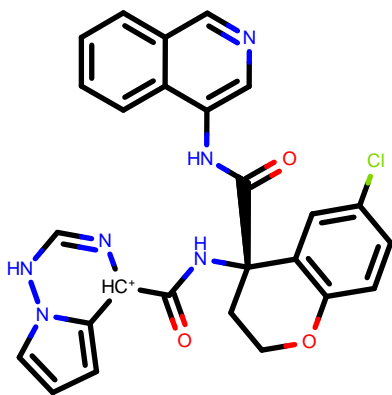
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)CCC5c[nH]n5

RUN: RUN6940

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.23

EN300-7426781_1_1



CID: EN300-7426781_1_1

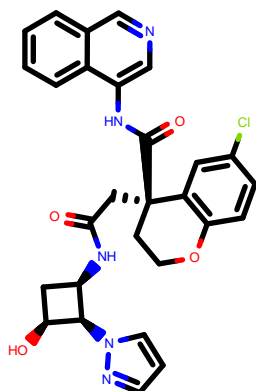
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6cccn6ncn5

RUN: RUN6066

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.17

EN300-260696_1_1



CID: EN300-260696_1_1

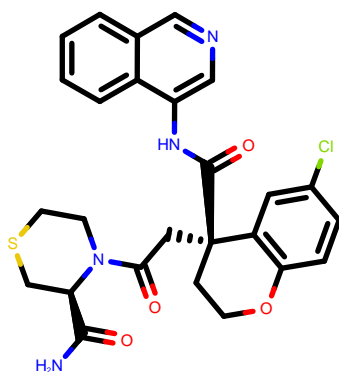
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)C(=O)N[C@@]5H5C[C@@]H[C@@]5H56cccn6O

RUN: RUN6659

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.27

EN300-122866_1_2



CID: EN300-122866_1_2

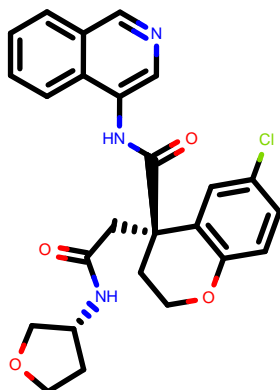
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCSC[C@@]H5C(=O)N

RUN: RUN9480

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.22

EN300-171752_1_1



CID: EN300-171752_1_1

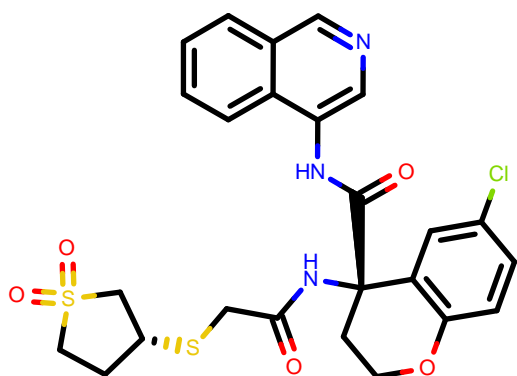
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]H5CCOC5

RUN: RUN5701

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.20

EN300-13890_1_1



CID: EN300-13890_1_1

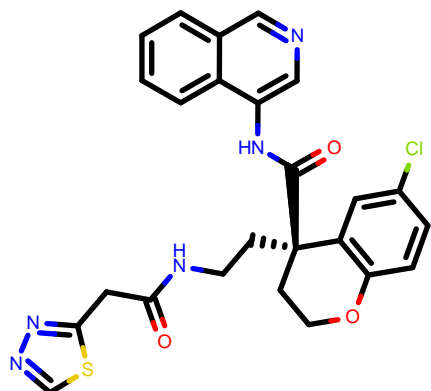
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCO4c3cc(cc4)Cl)NC(=O)CS[C@@H]5CCS(=O)(=O)C5

RUN: RUN4122

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.31

EN300-6488240_3_1



CID: EN300-6488240_3_1

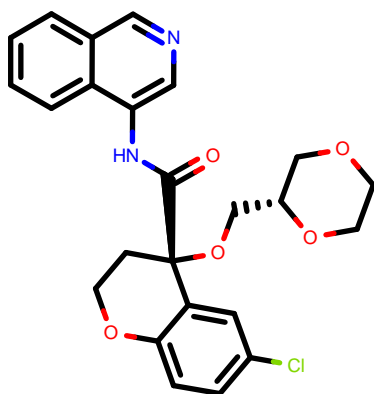
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCO4c3cc(cc4)Cl)CCNC(=O)C5nncs5

RUN: RUN14792

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.23

EN300-139167_1_2



CID: EN300-139167_1_2

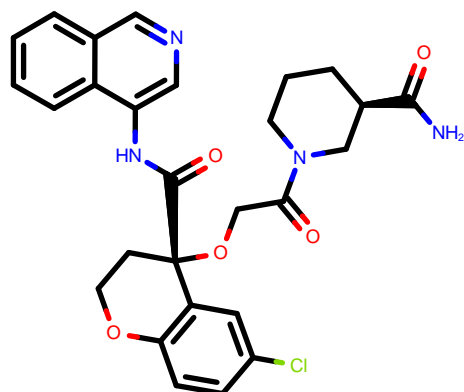
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCO4c3cc(cc4)Cl)OC[C@@H]5COCOC5

RUN: RUN2099

DDG (kcal/mol): -1.91

dDDG (kcal/mol): 0.21

EN300-22880_1_2



CID: EN300-22880_1_2

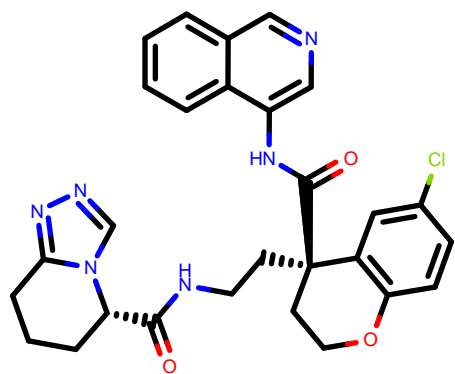
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCO4c3cc(cc4)Cl)OCC(=O)N5CCCC[C@@H](C5)C(=O)N

RUN: RUN511

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.27

EN300-6478631_3_1



CID: EN300-6478631_3_1

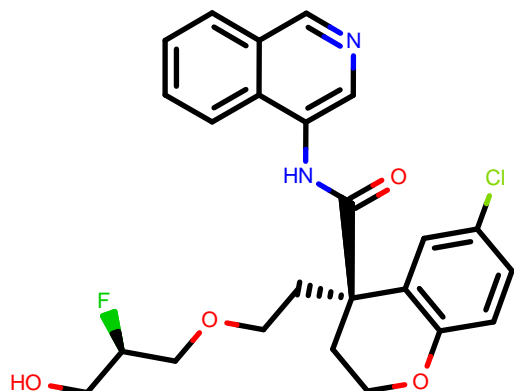
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCC6n5cm6

RUN: RUN15244

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.26

EN300-1600517_3_2



CID: EN300-1600517_3_2

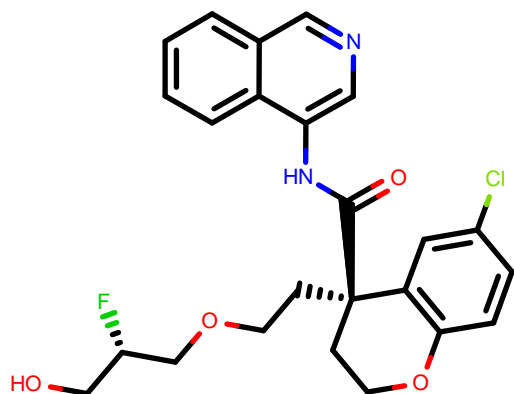
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CO)F

RUN: RUN1048

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.28

EN300-1600517_3_1



CID: EN300-1600517_3_1

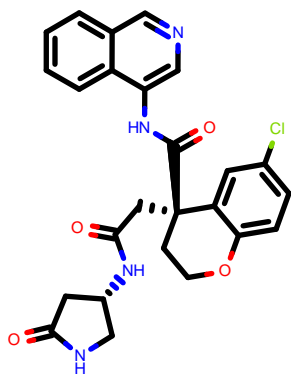
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)F

RUN: RUN1144

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.24

EN300-127487_1_2



CID: EN300-127487_1_2

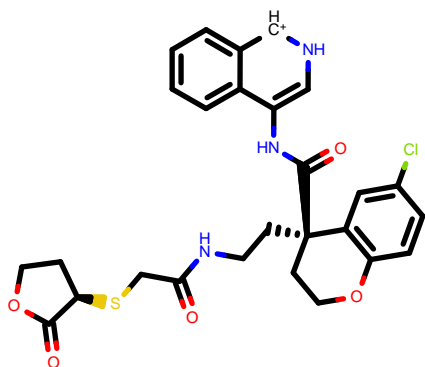
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC(=O)NCS

RUN: RUN10115

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.22

EN300-113218_3_2



CID: EN300-113218_3_2

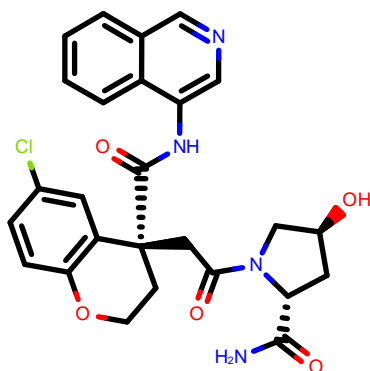
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5CCOC5=O

RUN: RUN14250

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.25

EN300-07752_1_3



CID: EN300-07752_1_3

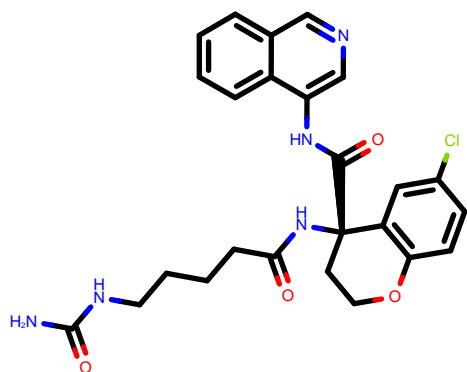
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(Cl)=O)N5C[C@@H](C)[C@@H]5C(=O)N

RUN: RUN7211

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.22

EN300-13499_1_1



CID: EN300-13499_1_1

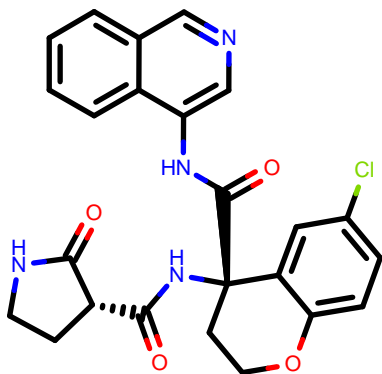
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N(C)C(=O)CCCCNC(=O)N

RUN: RUN6736

DDG (kcal/mol): -1.90

dDDG (kcal/mol): 0.27

EN300-94945_1_1



CID: EN300-94945_1_1

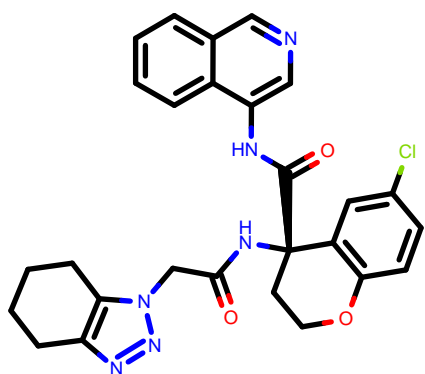
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCNC5=O

RUN: RUN3454

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.21

EN300-223187_1_1



CID: EN300-223187_1_1

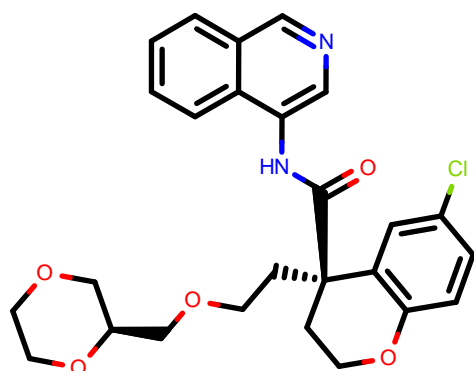
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5c6c(nn5)CCCC6

RUN: RUN9497

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.23

EN300-139167_3_2



CID: EN300-139167_3_2

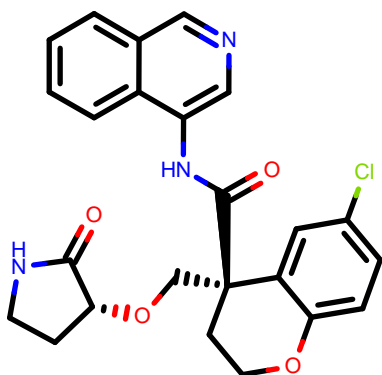
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]H5COC5O5

RUN: RUN1863

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.21

EN300-6736413_2_2



CID: EN300-6736413_2_2

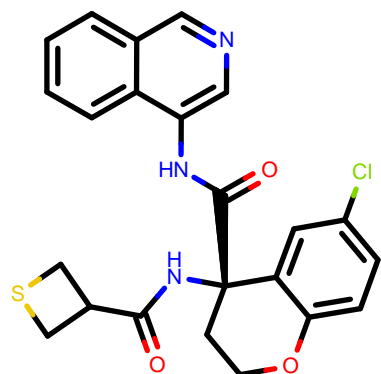
SMILES: c1ccc2c(c1)encc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]H5CNC5=O

RUN: RUN1466

DDG (kcal/mol): -1.89

dDDG (kcal/mol): 0.18

EN300-95094_1_1



CID: EN300-95094_1_1

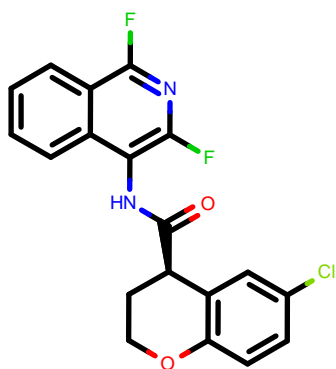
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CSC5

RUN: RUN5674

DDG (kcal/mol): -1.89

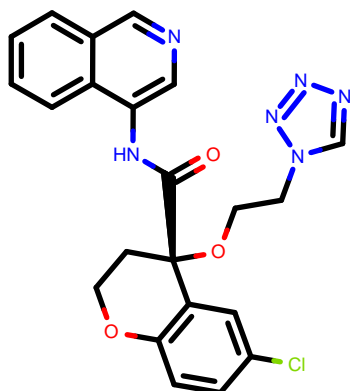
dDDG (kcal/mol): 0.19

JOH-SUS-a69c159d-6_1



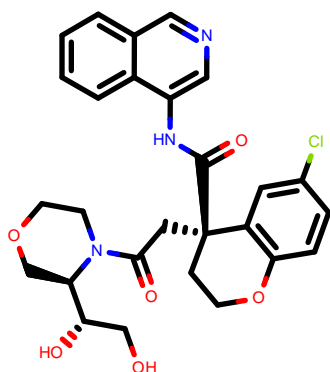
CID:	JOH-SUS-a69c159d-6_1
SMILES:	<chem>c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN1
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.07

EN300-364679_1_1



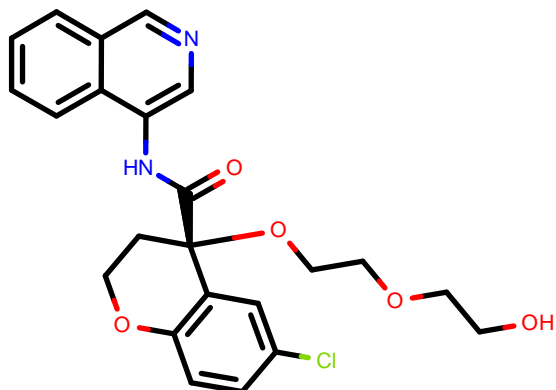
CID:	EN300-364679_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5nnn5</chem>
RUN:	RUN1245
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.20

EN300-1428769_1_1



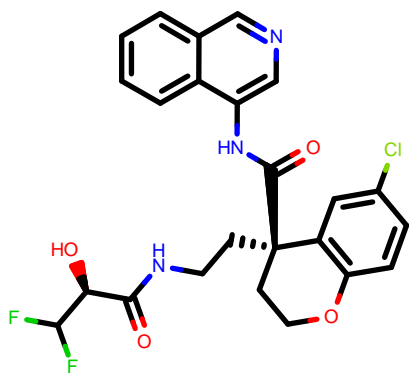
CID:	EN300-1428769_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CCOCC5C(O)CO</chem>
RUN:	RUN9388
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.42

EN300-52467_1_1



CID:	EN300-52467_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO</chem>
RUN:	RUN1221
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.19

EN300-1932780_3_1



CID: EN300-1932780_3_1

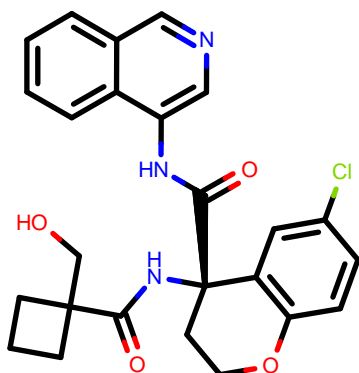
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C(F)F)O

RUN: RUN14094

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.25

EN300-149975_1_1



CID: EN300-149975_1_1

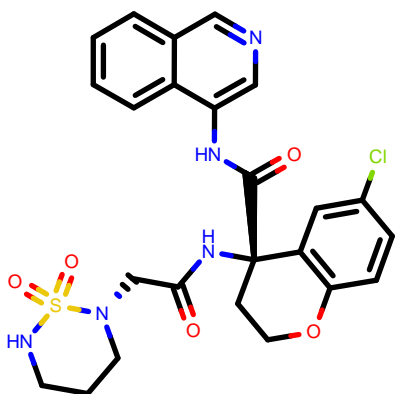
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)NC(=O)C5(CCC5)CO

RUN: RUN3006

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.23

EN300-4726186_1_2



CID: EN300-4726186_1_2

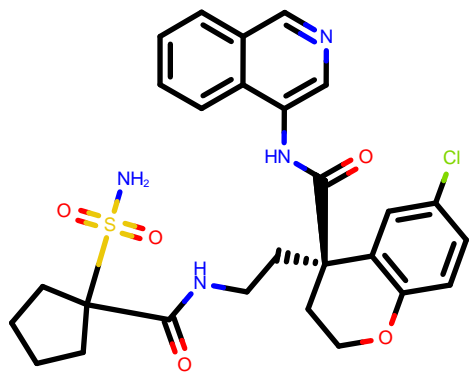
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[N@@]5CCCCNS5(=O)=O

RUN: RUN2561

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.33

EN300-6486793_3_1



CID: EN300-6486793_3_1

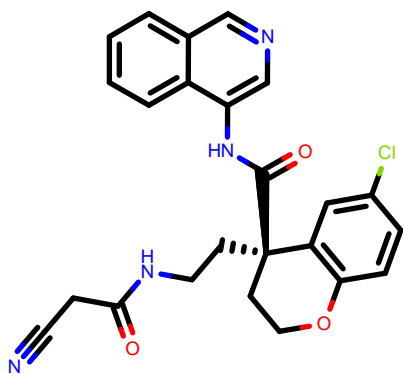
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCC5)S(=O)(=O)N

RUN: RUN4849

DDG (kcal/mol): -1.88

dDDG (kcal/mol): 0.29

EN300-19926_3_1



CID: EN300-19926_3_1

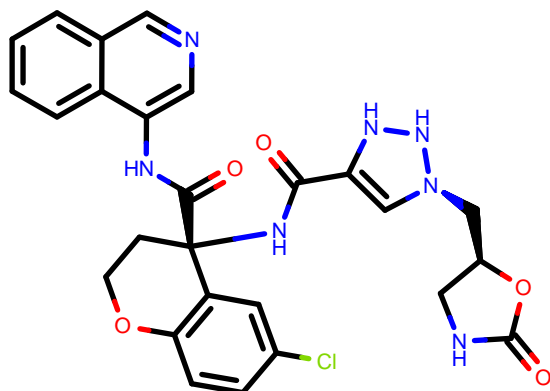
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC#N

RUN: RUN14778

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.17

EN300-379219_1_2



CID: EN300-379219_1_2

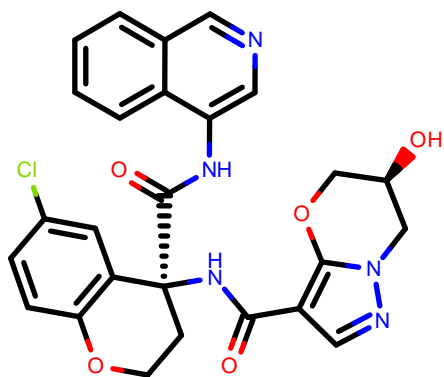
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5n[nH]5[C@@]6H8CN[C@@]6O

RUN: RUN3134

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.24

EN300-6497444_1_1



CID: EN300-6497444_1_1

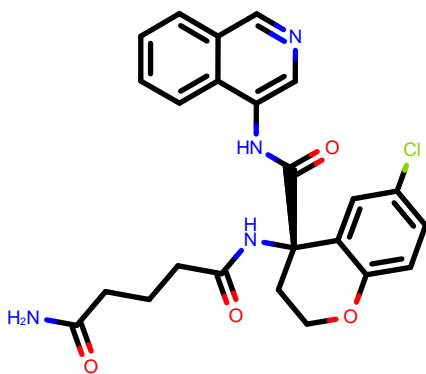
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]6c5O[C@@]6H[C@H](O)O

RUN: RUN8084

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.24

EN300-59478_1_1



CID: EN300-59478_1_1

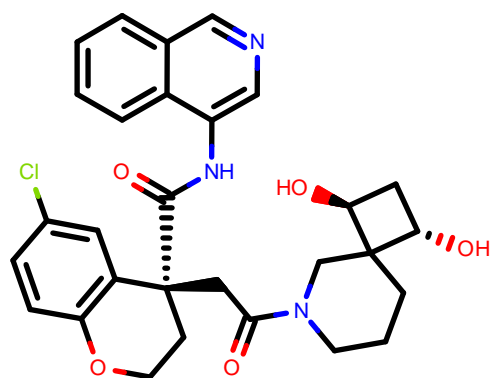
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN2946

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.28

EN300-7445890_1_3



CID: EN300-7445890_1_3

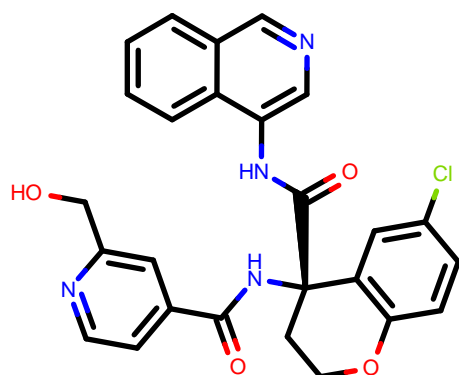
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CC(=O)N5CCCC6(C5)C@H)C[C@@]H6)O

RUN: RUN11629

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.26

EN300-396748_1_1



CID: EN300-396748_1_1

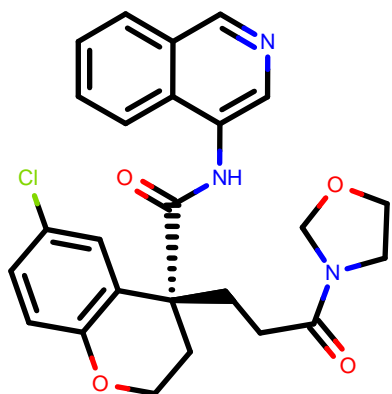
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)NC(=O)c5cccnc5)CO

RUN: RUN5370

DDG (kcal/mol): -1.87

dDDG (kcal/mol): 0.20

EN300-211422_2_1



CID: EN300-211422_2_1

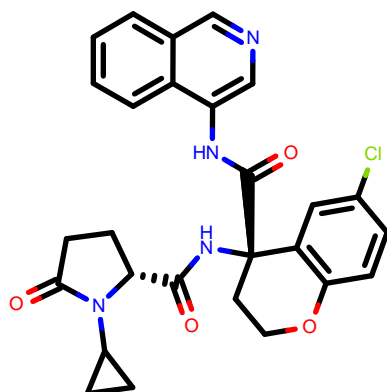
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CCC(=O)N5CCOC5

RUN: RUN14053

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.21

EN300-3044054_1_2



CID: EN300-3044054_1_2

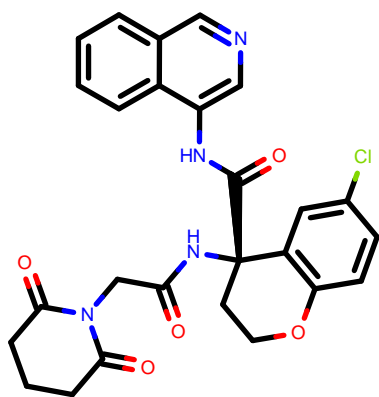
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)NC(=O)[C@@]H5CCC(=O)N5C6CC6

RUN: RUN7928

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.23

EN300-54837_1_1



CID: EN300-54837_1_1

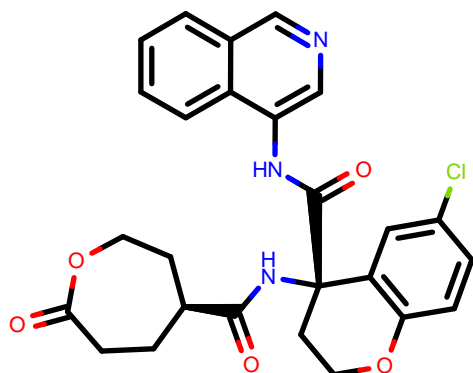
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5C(=O)CCCC5=O

RUN: RUN9273

DDG (kcal/mol): -1.86

dDDG (kcal/mol): 0.24

EN300-2011083_1_2



CID: EN300-2011083_1_2

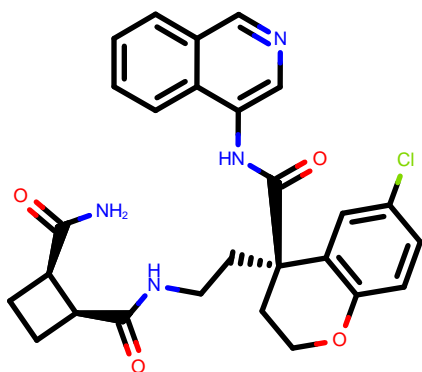
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCCC(=O)OCC5

RUN: RUN4822

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.21

EN300-217107_3_2



CID: EN300-217107_3_2

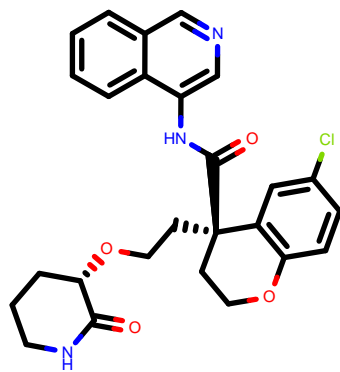
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CC[C@H]5C(=O)N

RUN: RUN8027

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.23

EN300-107267_3_1



CID: EN300-107267_3_1

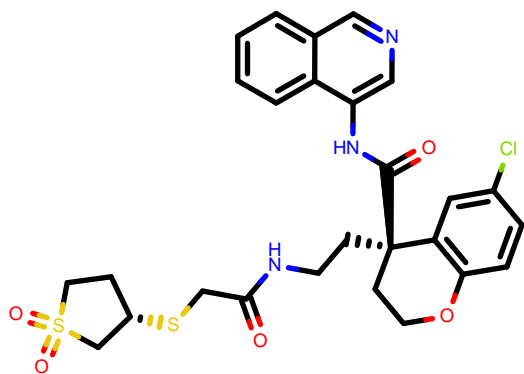
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@H]5CCNCN5=O

RUN: RUN1784

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.24

EN300-13890_3_2



CID: EN300-13890_3_2

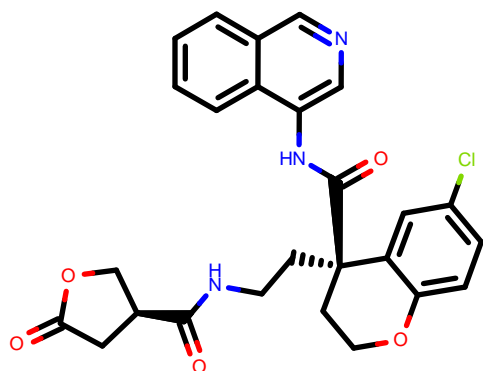
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CS[C@H]5CCS(=O)(=O)C5

RUN: RUN4709

DDG (kcal/mol): -1.85

dDDG (kcal/mol): 0.33

EN300-113234_3_2



CID: EN300-113234_3_2

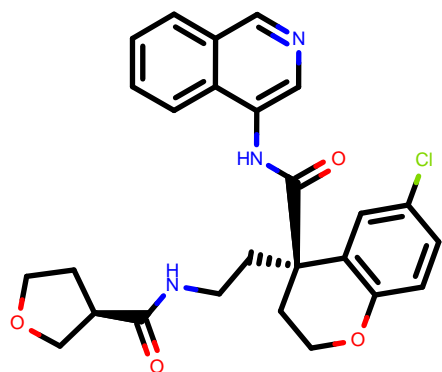
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CC(=O)OC5

RUN: RUN14834

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.22

EN300-697519_3_1



CID: EN300-697519_3_1

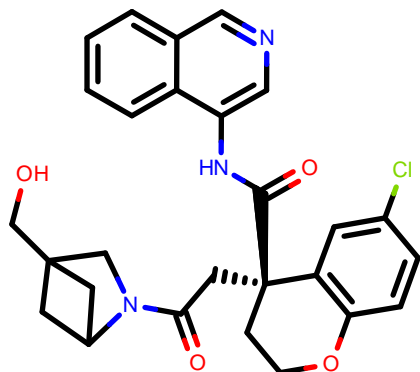
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CCOC5

RUN: RUN4781

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.22

EN300-7439985_1_1



CID: EN300-7439985_1_1

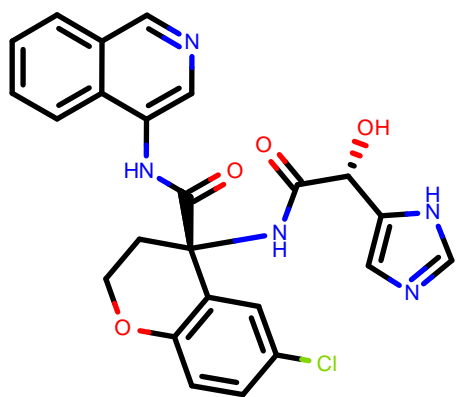
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6(CC5C6)CO

RUN: RUN6803

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.22

EN300-254121_1_2



CID: EN300-254121_1_2

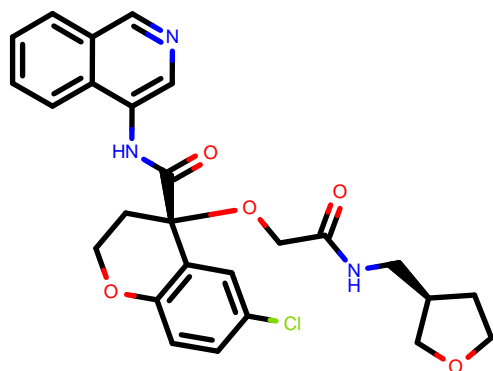
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H(c5nc[nH]5)O

RUN: RUN7552

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.29

EN300-46832_1_2



CID: EN300-46832_1_2

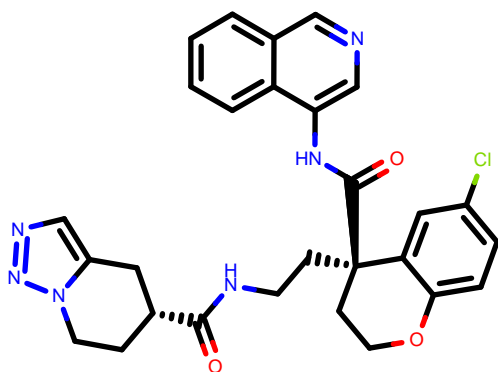
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCOC5

RUN: RUN479

DDG (kcal/mol): -1.84

dDDG (kcal/mol): 0.25

EN300-7430501_3_2



CID: EN300-7430501_3_2

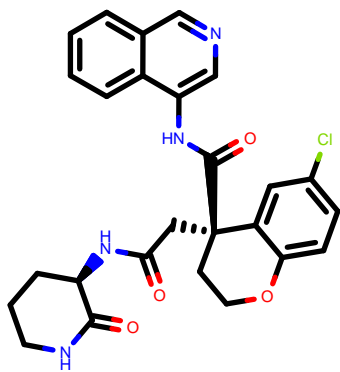
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5Cn6cnc6)C5

RUN: RUN15222

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.28

EN300-60035_1_2



CID: EN300-60035_1_2

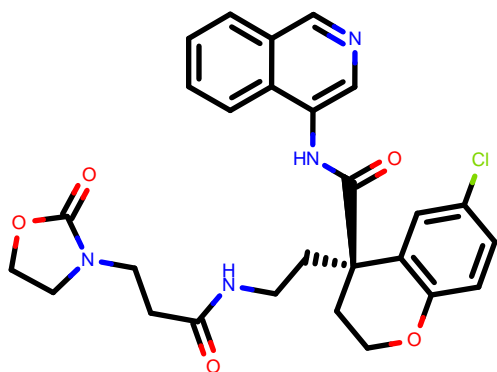
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5Cn6cnc6)O

RUN: RUN12024

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.21

EN300-53918_3_1



CID: EN300-53918_3_1

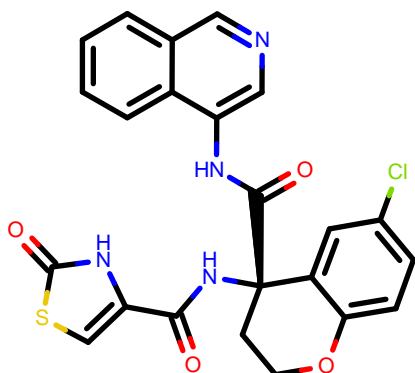
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCN5CCOC5=O

RUN: RUN8832

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.32

EN300-133915_1_1



CID: EN300-133915_1_1

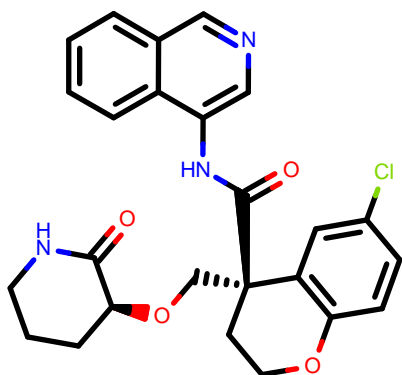
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5scsc(=O)[nH]5

RUN: RUN5222

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.20

EN300-107267_2_1



CID: EN300-107267_2_1

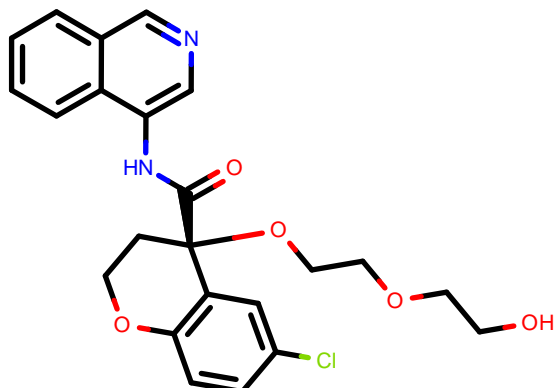
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCNC5=O

RUN: RUN2617

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.20

EN300-52467_1_1



CID: EN300-52467_1_1

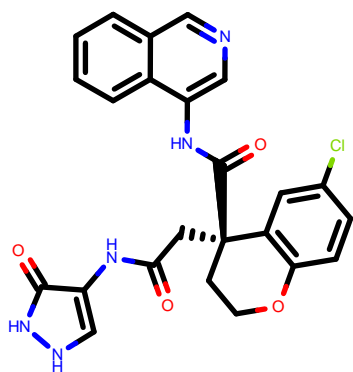
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN1237

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.20

EN300-223284_1_1



CID: EN300-223284_1_1

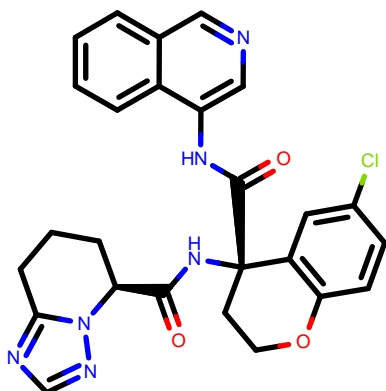
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5[nH][nH]c5=O

RUN: RUN2468

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.20

EN300-1273016_1_1



CID: EN300-1273016_1_1

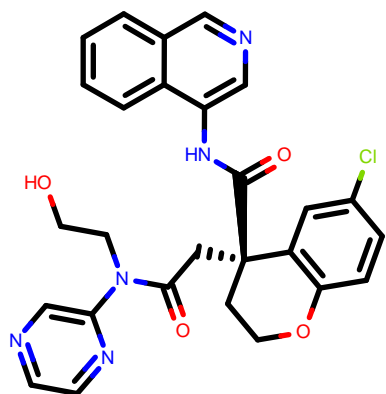
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CNCc6[nH]n6

RUN: RUN8965

DDG (kcal/mol): -1.83

dDDG (kcal/mol): 0.25

EN300-370792_1_1



CID: EN300-370792_1_1

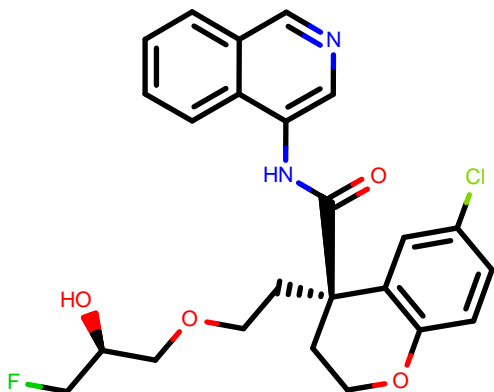
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5nccn5

RUN: RUN4145

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.34

EN300-1968342_3_1



CID: EN300-1968342_3_1

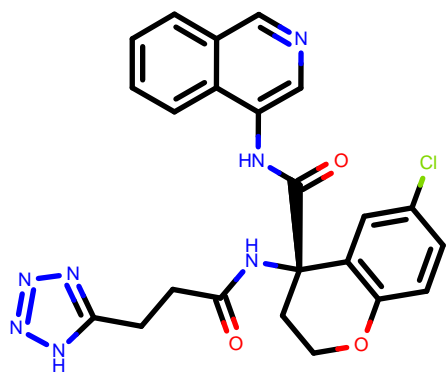
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5N(CF)CO

RUN: RUN1192

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.22

EN300-251851_1_1



CID: EN300-251851_1_1

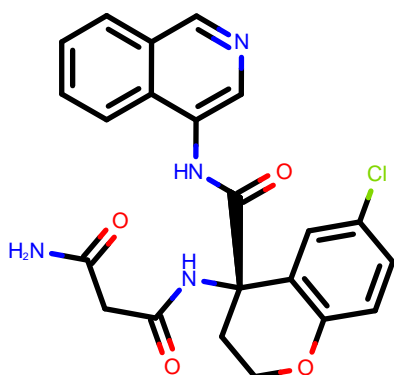
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCc5n[nH]n5

RUN: RUN7172

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.29

EN300-82179_1_1



CID: EN300-82179_1_1

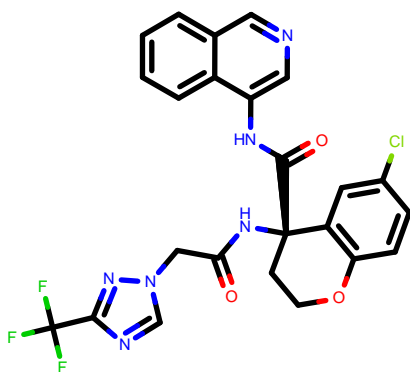
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC(=O)N

RUN: RUN1273

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.18

EN300-7385389_1_1



CID: EN300-7385389_1_1

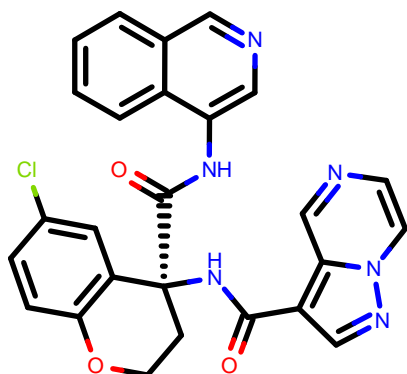
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5nc(n5)C(F)(F)F

RUN: RUN9724

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-131572_1_1



CID: EN300-131572_1_1

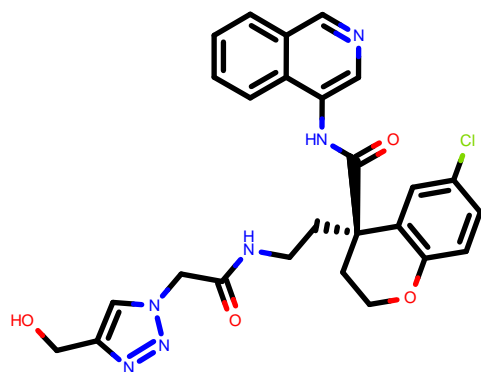
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnn6c5ncn6

RUN: RUN3346

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.19

EN300-108236_3_1



CID: EN300-108236_3_1

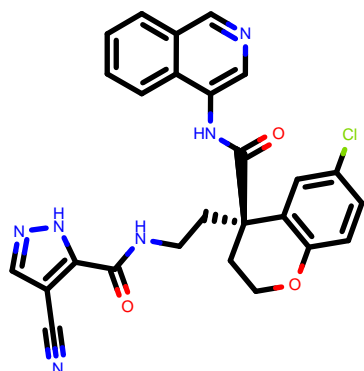
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cc(nn5)CO

RUN: RUN6177

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.26

EN300-1267109_3_1



CID: EN300-1267109_3_1

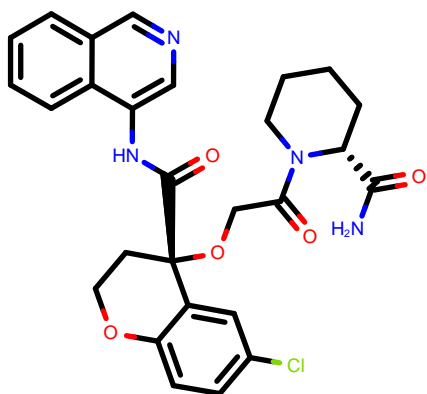
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5c[nH]5C#N

RUN: RUN15379

DDG (kcal/mol): -1.82

dDDG (kcal/mol): 0.21

EN300-22879_1_2



CID: EN300-22879_1_2

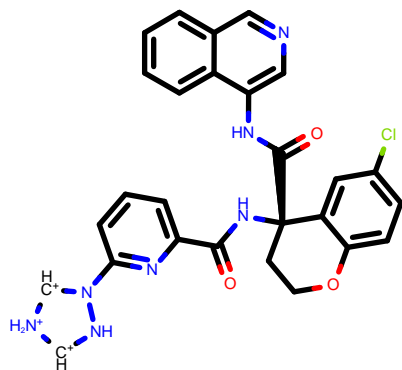
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCCC[C@@]3(H)5C(=O)N

RUN: RUN2431

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.27

EN300-123712_1_1



CID: EN300-123712_1_1

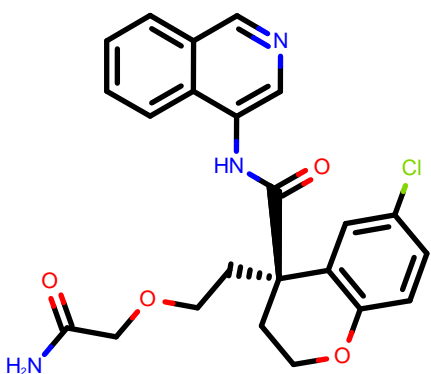
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(nc5)n6cncn6

RUN: RUN1409

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.22

EN300-18249_3_1



CID: EN300-18249_3_1

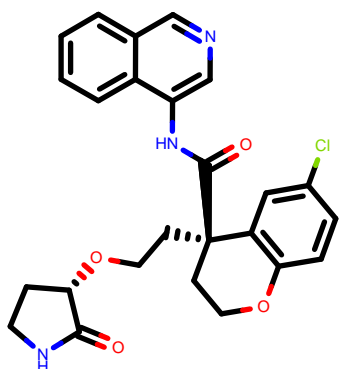
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N

RUN: RUN1088

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.19

EN300-6736413_3_1



CID: EN300-6736413_3_1

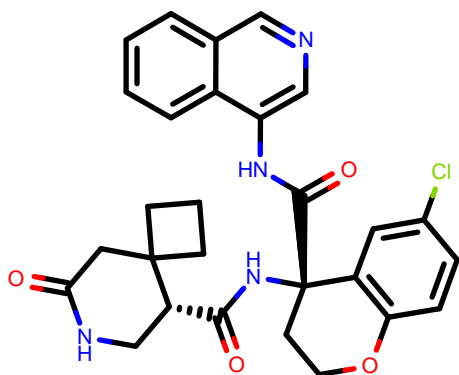
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCNC5=O

RUN: RUN1568

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.21

EN300-1704404_1_1



CID: EN300-1704404_1_1

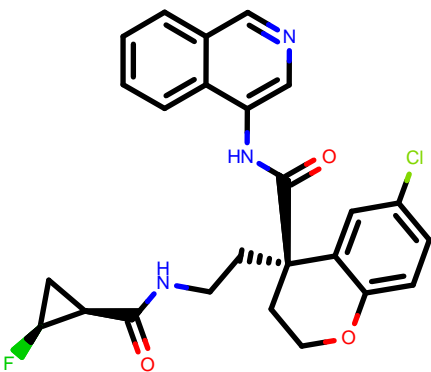
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]3[C@@]3(CCN(C=O)CC56CCC6

RUN: RUN9775

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.26

EN300-4698402_3_1



CID: EN300-4698402_3_1

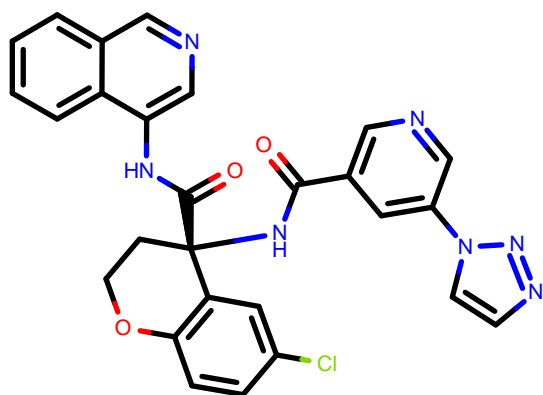
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]3[C@@]3(CCN(C=O)C@F)F

RUN: RUN9004

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.18

EN300-151298_1_1



CID: EN300-151298_1_1

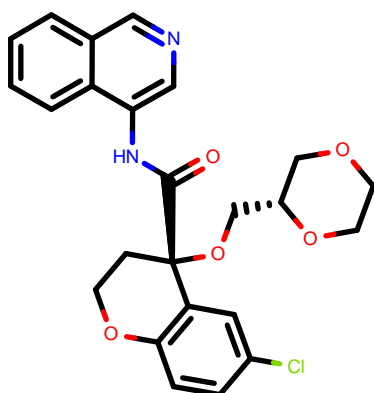
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn(cnc5)n6ccnn6

RUN: RUN4486

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.22

EN300-139167_1_2



CID: EN300-139167_1_2

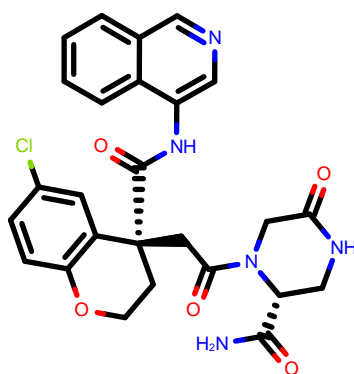
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@]5H5COCOC5

RUN: RUN2083

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.23

EN300-2009745_1_2



CID: EN300-2009745_1_2

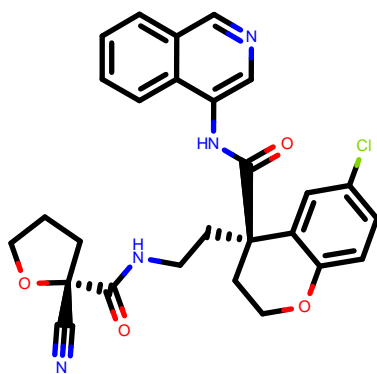
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(=O)NC[C@@]5H5C(=O)N

RUN: RUN5905

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.24

EN300-3710141_3_1



CID: EN300-3710141_3_1

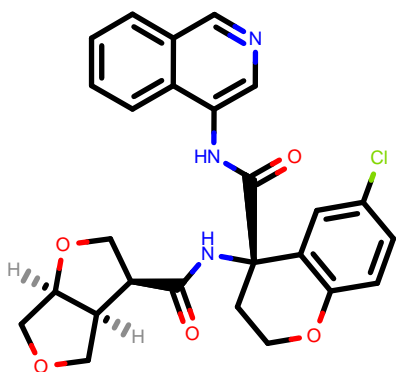
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN8672

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.24

EN300-6482296_1_1



CID: EN300-6482296_1_1

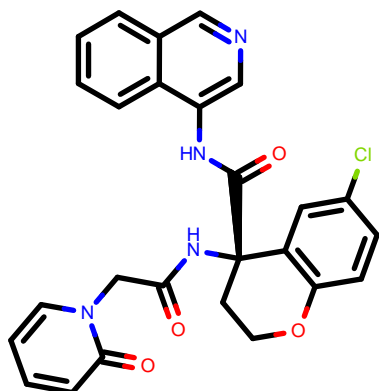
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)N(C=O)C@H5CO[C@@H]6C@H5COO6

RUN: RUN8785

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.26

EN300-11714_1_1



CID: EN300-11714_1_1

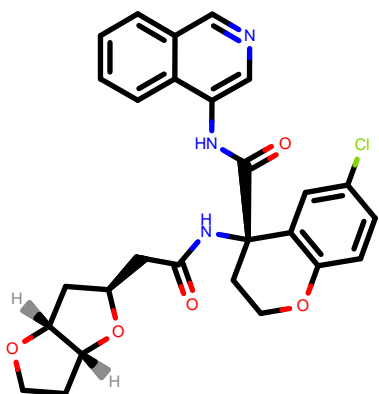
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)N(C=O)Cn5cccc5=O

RUN: RUN9469

DDG (kcal/mol): -1.81

dDDG (kcal/mol): 0.23

EN300-7355519_1_6



CID: EN300-7355519_1_6

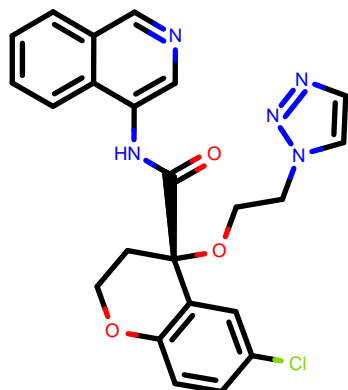
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)N(C=O)C@H5C[C@@H]6[C@@H]5O5CCO6

RUN: RUN411

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.21

EN300-1715993_1_1



CID: EN300-1715993_1_1

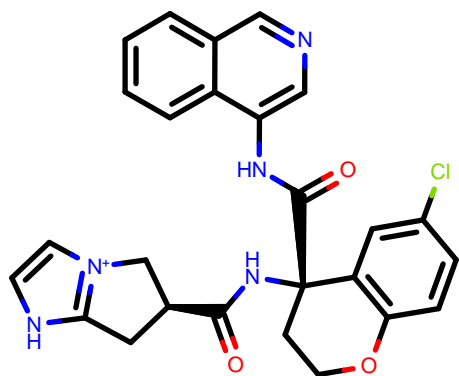
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)OCCn5ccnn5

RUN: RUN2004

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.21

EN300-7385329_1_2



CID: EN300-7385329_1_2

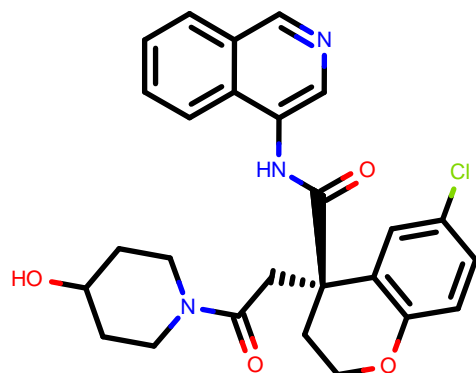
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C6[nH+]cnc6C5

RUN: RUN8861

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.23

EN300-379533_1_1



CID: EN300-379533_1_1

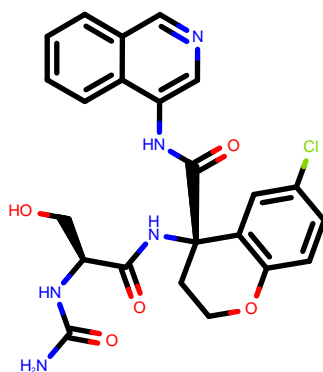
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(C5)O

RUN: RUN5137

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.21

EN300-10170_1_2



CID: EN300-10170_1_2

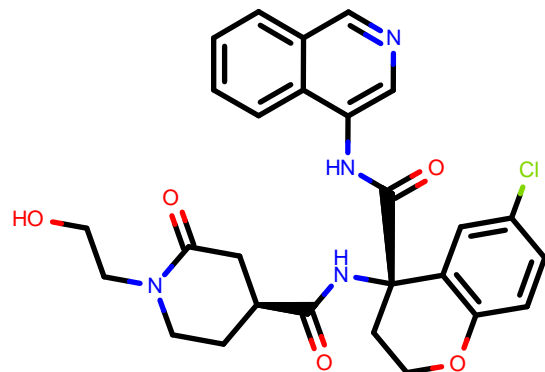
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](CO)NC(=O)N

RUN: RUN1457

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.33

EN300-1723663_1_1



CID: EN300-1723663_1_1

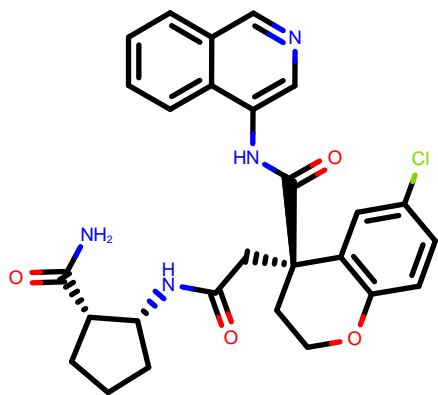
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCN(C(=O)C5)CCO

RUN: RUN8116

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.33

EN300-90531_1_3



CID: EN300-90531_1_3

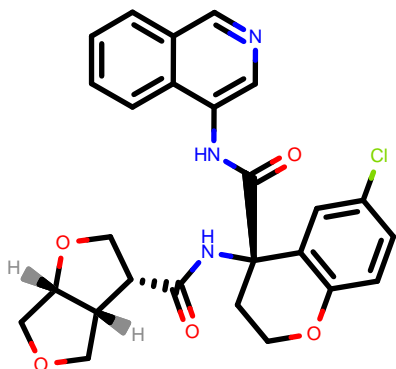
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](CCOc4cc3cc4)CNC(=O)C@@H5C[C@@H]5Cl=O

RUN: RUN12364

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.27

EN300-6482296_1_8



CID: EN300-6482296_1_8

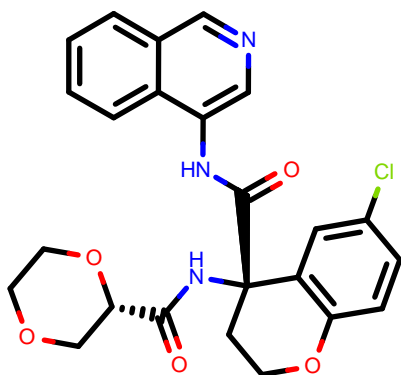
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](CCOc4cc3cc4)CNC(=O)C@@H5C[C@@H]5COC6

RUN: RUN2309

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.27

EN300-36158_1_1



CID: EN300-36158_1_1

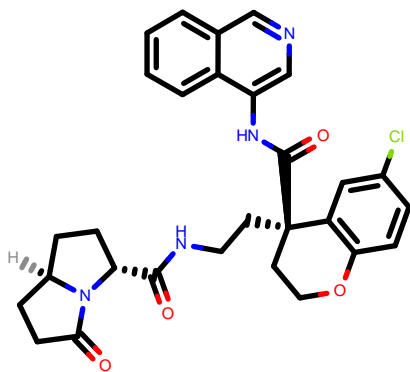
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](CCOc4cc3cc4)CNC(=O)C@@H5C[C@@H]5COC6

RUN: RUN7308

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.23

EN300-6479181_3_4



CID: EN300-6479181_3_4

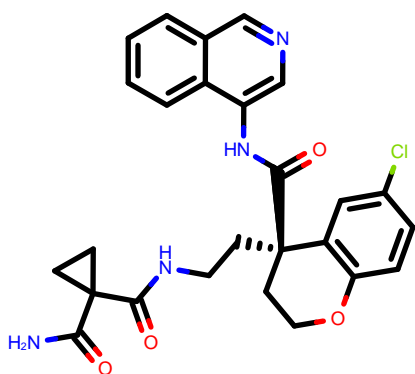
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@3[C@@H](CCOc4cc3cc4)CNC(=O)C@@H5C[C@@H]5N6C=O

RUN: RUN13790

DDG (kcal/mol): -1.80

dDDG (kcal/mol): 0.29

EN300-69070_3_1



CID: EN300-69070_3_1

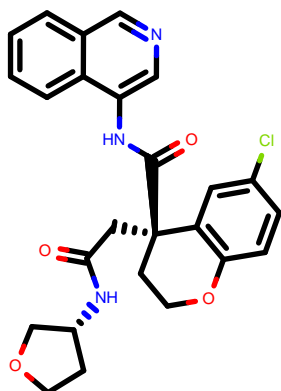
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5(C)=O

RUN: RUN11128

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.24

EN300-171752_1_1



CID: EN300-171752_1_1

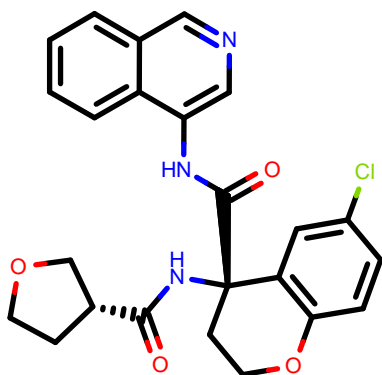
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCOC5

RUN: RUN5697

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.21

EN300-53423_1_1



CID: EN300-53423_1_1

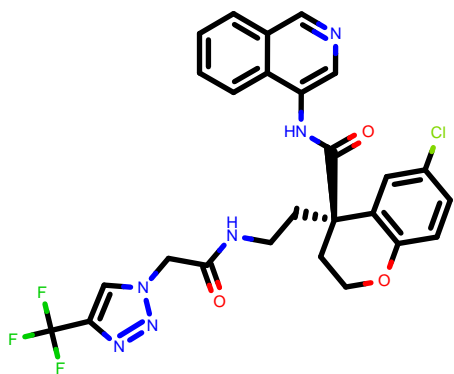
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCOC5

RUN: RUN4914

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.22

EN300-2910941_3_1



CID: EN300-2910941_3_1

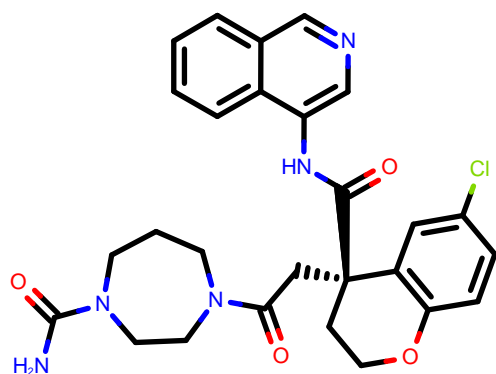
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ccn(n5)C(F)(F)F

RUN: RUN15316

DDG (kcal/mol): -1.79

dDDG (kcal/mol): 0.26

EN300-65063_1_1



CID: EN300-65063_1_1

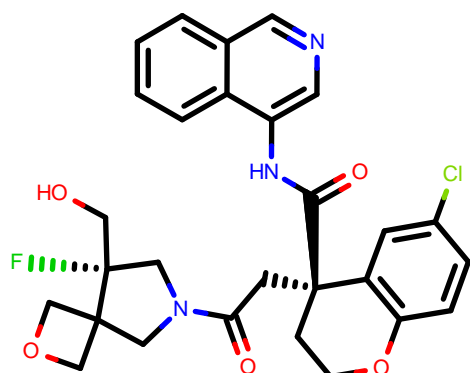
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN(CC5)C(=O)N

RUN: RUN3061

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.25

EN300-1719075_1_1



CID: EN300-1719075_1_1

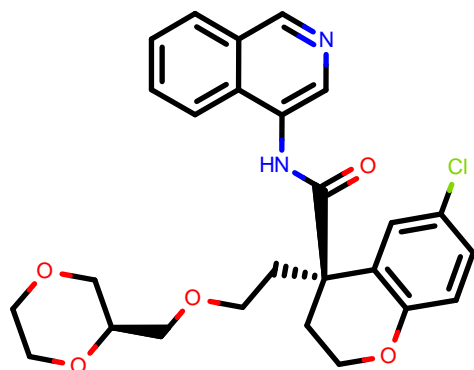
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]6(C6)COC6(CO)F

RUN: RUN5613

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.32

EN300-139167_3_2



CID: EN300-139167_3_2

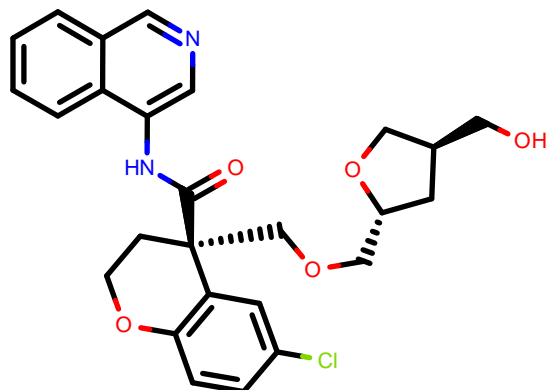
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(H)COC5CO5

RUN: RUN1847

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.24

EN300-6494158_2_1



CID: EN300-6494158_2_1

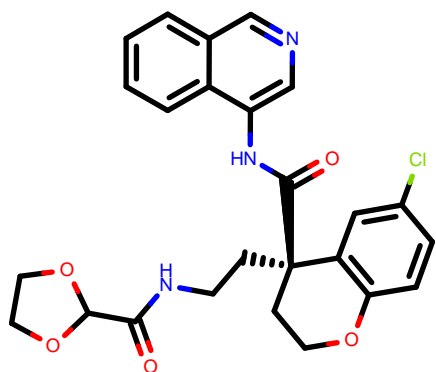
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(H)C[C@@]6(H)CO5)CO

RUN: RUN420

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.21

EN300-154942_3_1



CID: EN300-154942_3_1

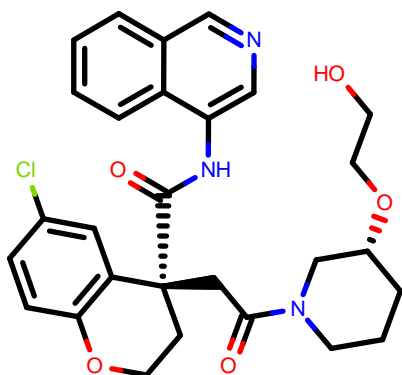
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5OCCO5

RUN: RUN8792

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.18

EN300-157830_1_2



CID: EN300-157830_1_2

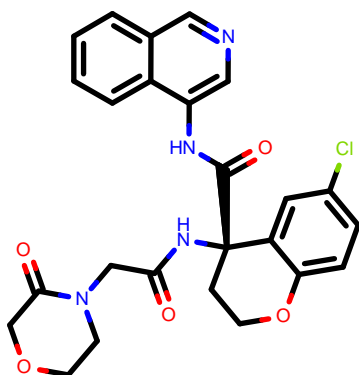
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H](C5)OCCO

RUN: RUN9380

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.25

EN300-186943_1_1



CID: EN300-186943_1_1

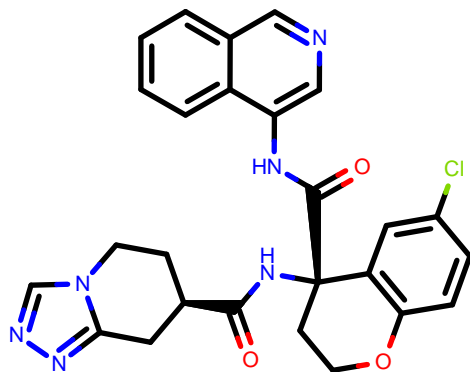
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5COCC5=O

RUN: RUN9533

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.25

EN300-6474341_1_2



CID: EN300-6474341_1_2

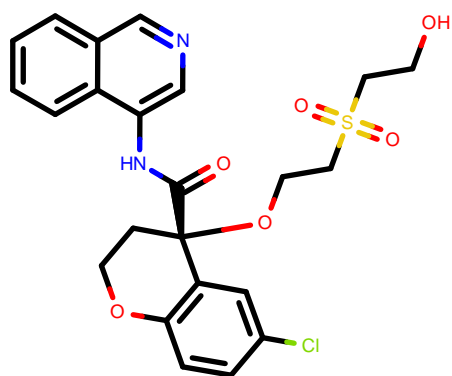
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4H5CCN6enn6C5

RUN: RUN9353

DDG (kcal/mol): -1.78

dDDG (kcal/mol): 0.25

EN300-7463171_1_1



CID: EN300-7463171_1_1

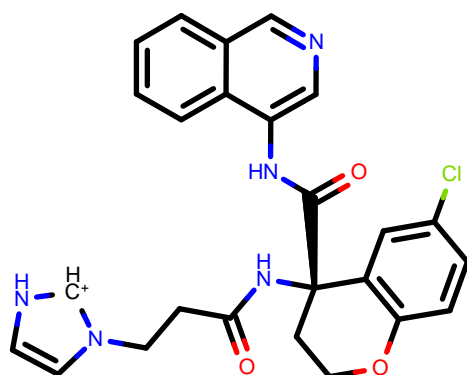
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCO

RUN: RUN919

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.43

EN300-75342_1_1



CID: EN300-75342_1_1

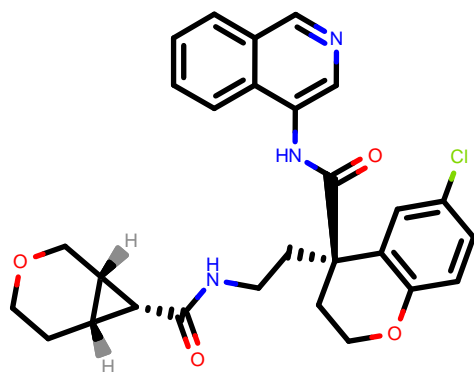
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5cnc5

RUN: RUN8917

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.23

EN300-1644723_3_3



CID: EN300-1644723_3_3

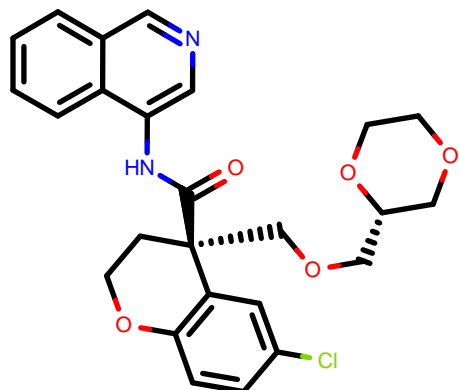
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(C@)5C6C7C8C6C7C8

RUN: RUN14204

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.24

EN300-139167_2_1



CID: EN300-139167_2_1

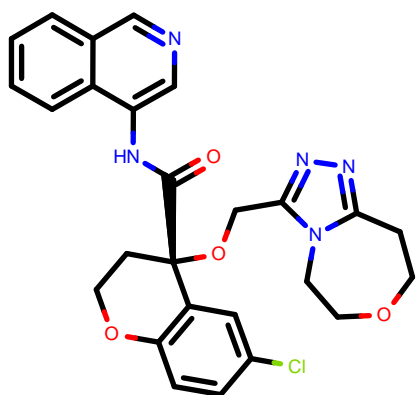
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5COC5

RUN: RUN1370

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.22

EN300-310888_1_1



CID: EN300-310888_1_1

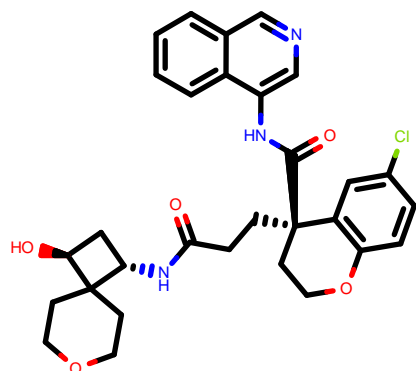
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nn6n5CCOC6

RUN: RUN407

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.22

EN300-704039_2_2



CID: EN300-704039_2_2

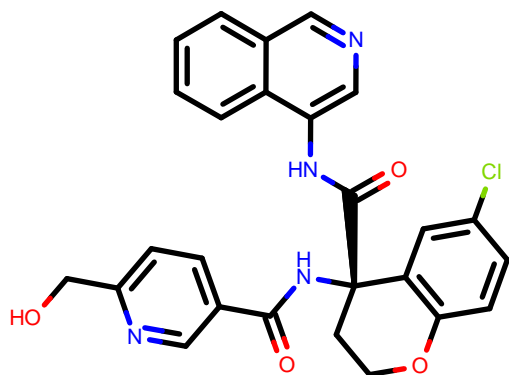
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5[C@@H](C6OCOC6)O

RUN: RUN480

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.29

EN300-146051_1_1



CID: EN300-146051_1_1

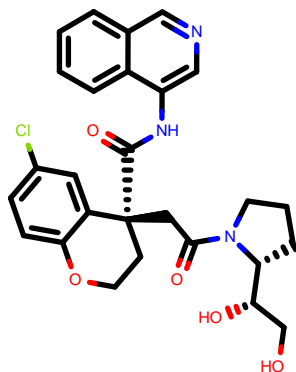
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(nc5)CO

RUN: RUN1217

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.21

EN300-7459540_1_3



CID: EN300-7459540_1_3

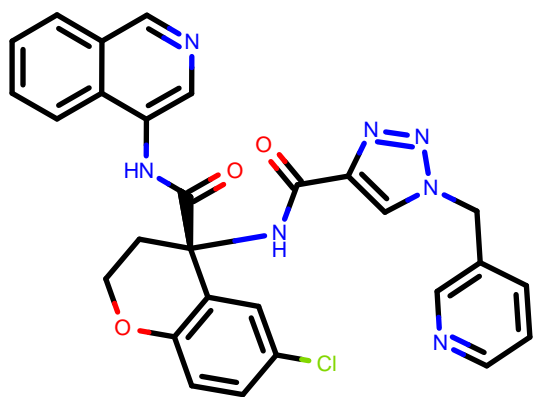
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5[C@@H](CO)O

RUN: RUN3093

DDG (kcal/mol): -1.77

dDDG (kcal/mol): 0.37

EN300-91314_1_1



CID: EN300-91314_1_1

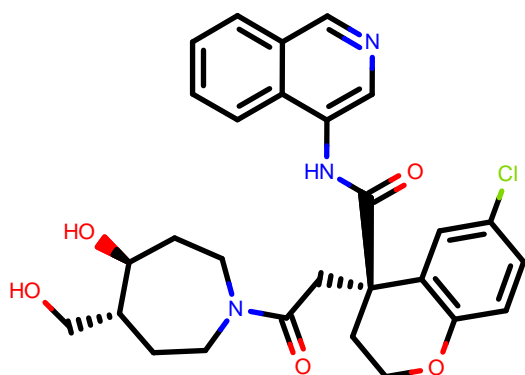
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(n5)Cc6ccncc6

RUN: RUN3062

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.23

EN300-7353672_1_1



CID: EN300-7353672_1_1

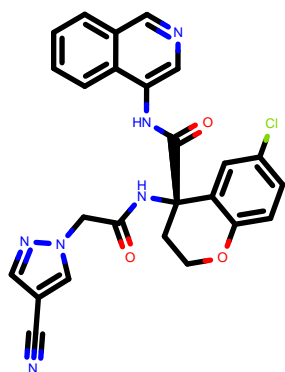
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C1(=O)N5CC[C@@H](C5)O)CO

RUN: RUN1167

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.29

EN300-1590388_1_1



CID: EN300-1590388_1_1

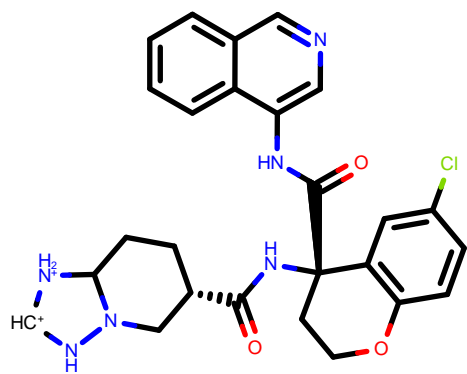
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5cc(n5)C#N

RUN: RUN9365

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.23

EN300-1662365_1_2



CID: EN300-1662365_1_2

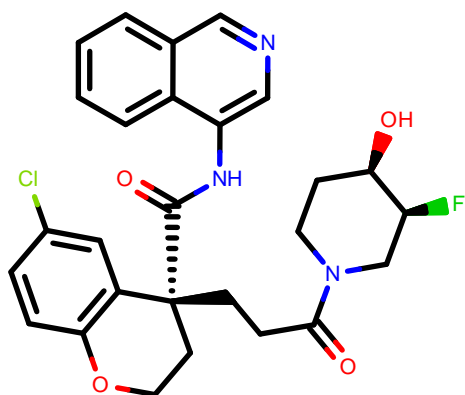
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCc6nncn6C5

RUN: RUN5082

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.20

EN300-741926_2_2



CID: EN300-741926_2_2

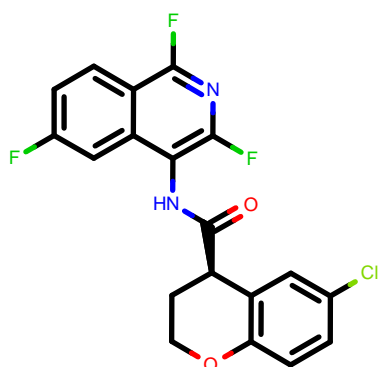
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCC@H(C5)F)O

RUN: RUN13543

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.25

JOH-SUS-a69c159d-7_1



CID: JOH-SUS-a69c159d-7_1

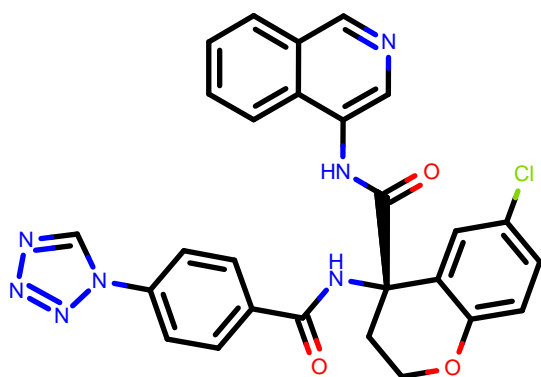
SMILES: c1cc2c(cc1F)c(nc2F)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl

RUN: RUN3

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.07

EN300-06030_1_1



CID: EN300-06030_1_1

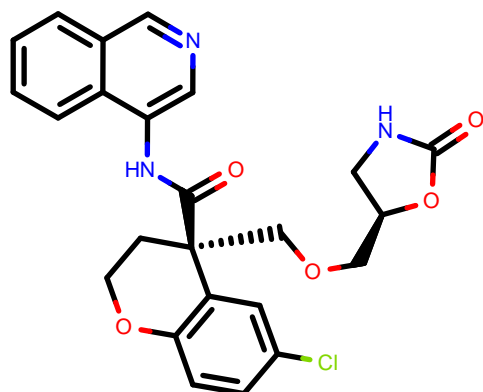
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(c5)n6cnnn6

RUN: RUN9877

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.21

EN300-203293_2_1



CID: EN300-203293_2_1

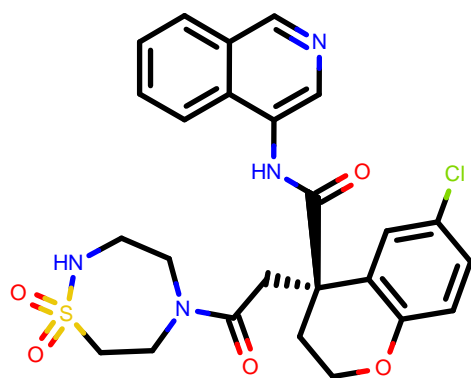
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@H]5CNC(=O)O5

RUN: RUN1754

DDG (kcal/mol): -1.76

dDDG (kcal/mol): 0.20

EN300-6489145_1_1



CID: EN300-6489145_1_1

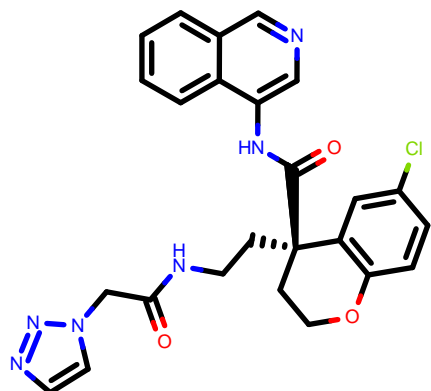
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNS(=O)(=O)CC5

RUN: RUN7399

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.34

EN300-100467_3_1



CID: EN300-100467_3_1

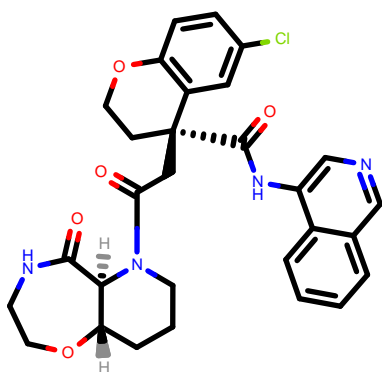
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnn5

RUN: RUN11417

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.21

EN300-364612_1_2



CID: EN300-364612_1_2

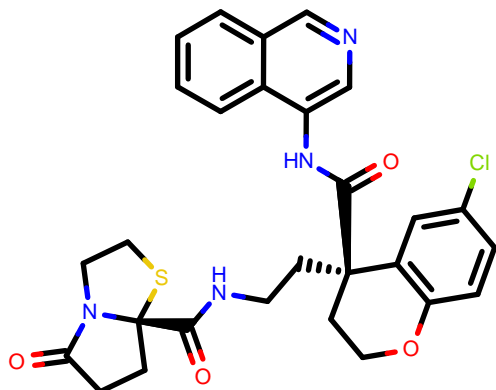
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]6(C)NCC[C@]6H5[C@]7(O)NCCO7

RUN: RUN4209

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.30

EN300-10334_3_1



CID: EN300-10334_3_1

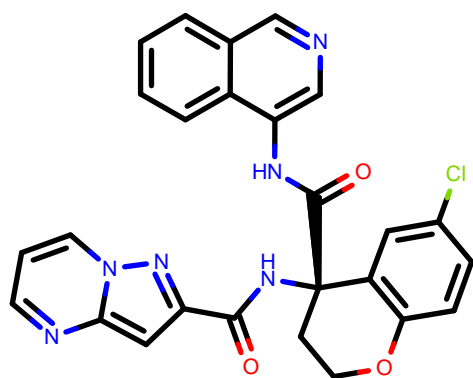
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]56CCCC(=O)N5CCS6

RUN: RUN14572

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.24

EN300-83527_1_1



CID: EN300-83527_1_1

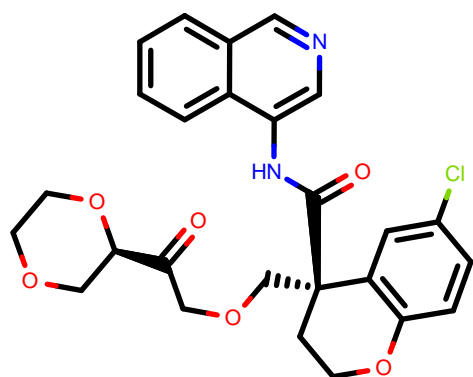
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnccn6n5

RUN: RUN603

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.18

EN300-6238494_2_2



CID: EN300-6238494_2_2

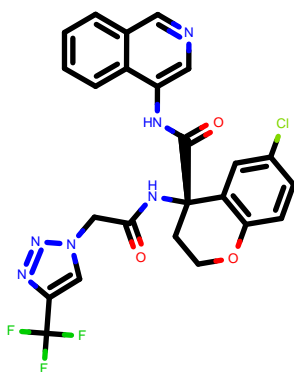
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)[C@H]5COCCO5

RUN: RUN2080

DDG (kcal/mol): -1.75

dDDG (kcal/mol): 0.22

EN300-2910941_1_1



CID: EN300-2910941_1_1

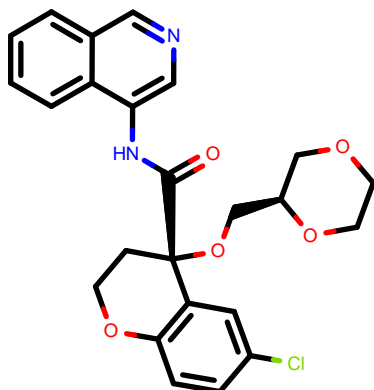
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ccn(n5)C(F)(F)F

RUN: RUN9637

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.23

EN300-139167_1_1



CID: EN300-139167_1_1

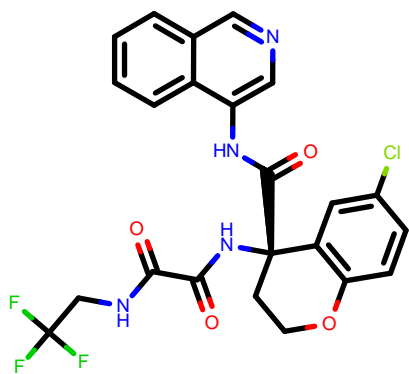
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5COCCO5

RUN: RUN2709

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.24

EN300-139268_1_1



CID: EN300-139268_1_1

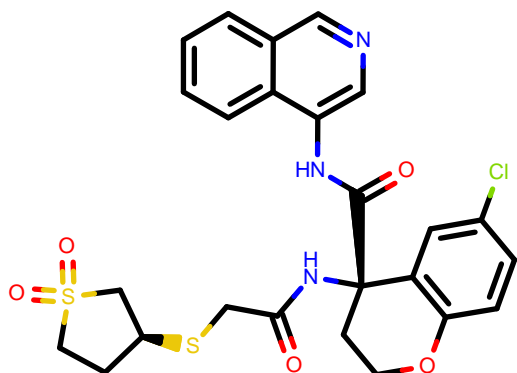
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NC(F)(F)F

RUN: RUN1097

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.17

EN300-13890_1_2



CID: EN300-13890_1_2

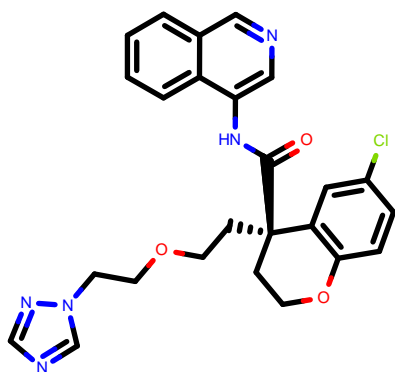
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@@H]5CCS(=O)(=O)C5

RUN: RUN6209

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-6255179_3_1



CID: EN300-6255179_3_1

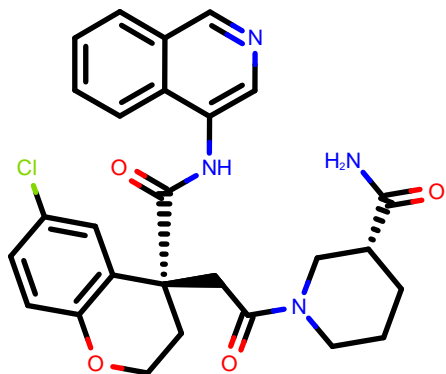
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5ncn5

RUN: RUN1648

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.21

EN300-18610_1_2



CID: EN300-18610_1_2

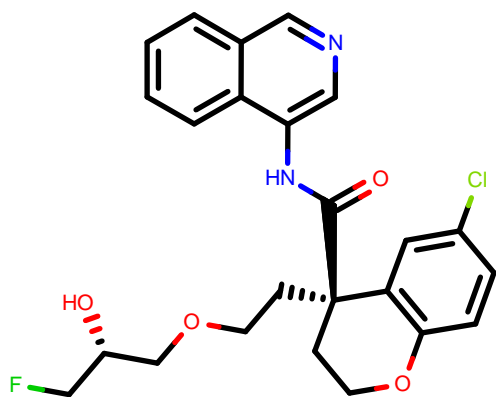
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)C(=O)N

RUN: RUN5645

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.25

EN300-1968342_3_2



CID: EN300-1968342_3_2

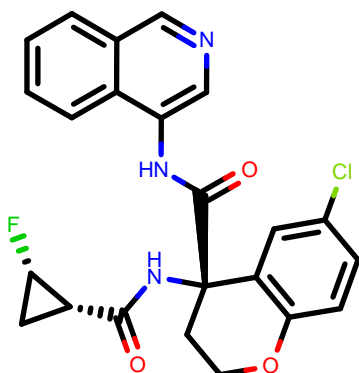
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN1160

DDG (kcal/mol): -1.74

dDDG (kcal/mol): 0.29

EN300-97300_1_3



CID: EN300-97300_1_3

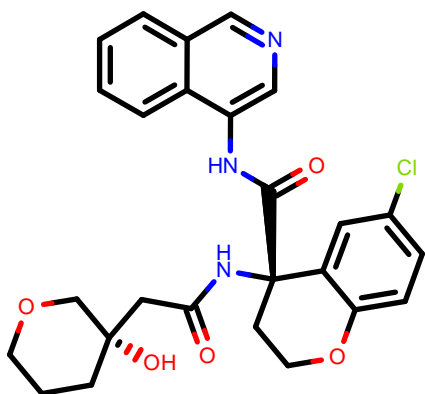
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C[C@]([H])F

RUN: RUN6321

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.17

EN300-1071940_1_2



CID: EN300-1071940_1_2

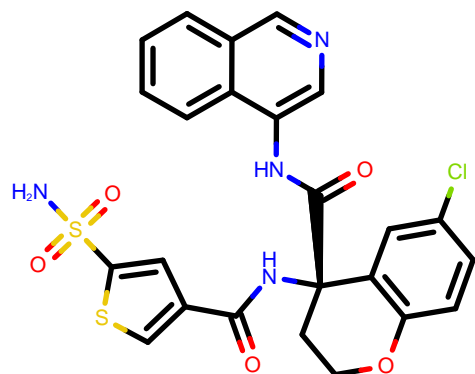
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@]5(CCCOC5)O

RUN: RUN7932

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.25

EN300-23792_1_1



CID: EN300-23792_1_1

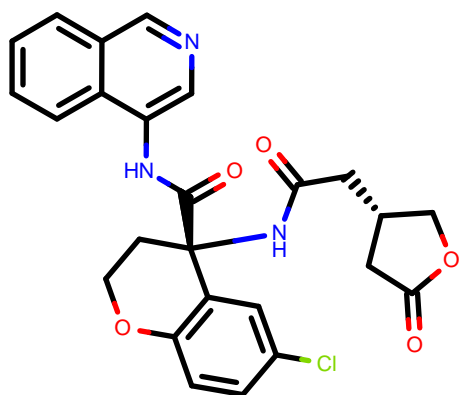
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(s5)S(=O)(=O)N

RUN: RUN4310

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.28

EN300-109535_1_2



CID: EN300-109535_1_2

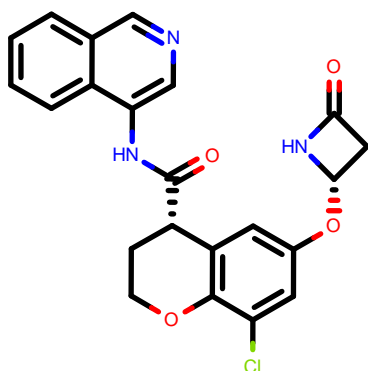
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)OC5

RUN: RUN5362

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

FRA-DIA-b66f7109-3_2



CID: FRA-DIA-b66f7109-3_2

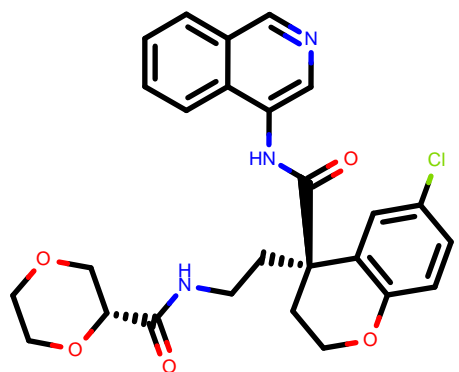
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)O[C@H]5CC(=O)N5

RUN: RUN164

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-36158_3_2



CID: EN300-36158_3_2

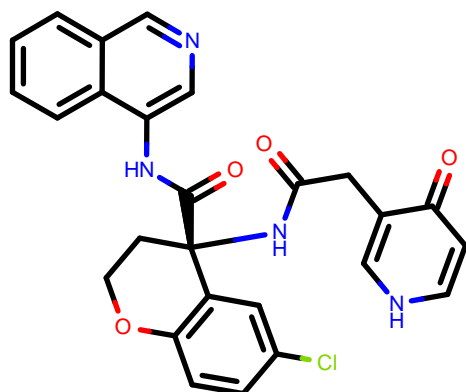
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5COCOC5

RUN: RUN8788

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.22

EN300-205486_1_1



CID: EN300-205486_1_1

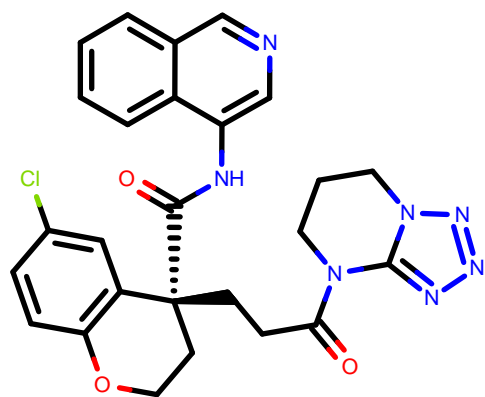
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]c5=O

RUN: RUN5170

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.29

EN300-217416_2_1



CID: EN300-217416_2_1

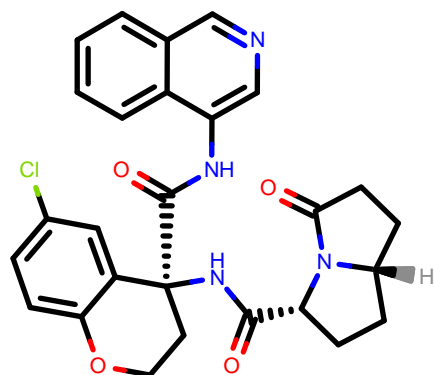
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4Cl)CCC(=O)N5CCc6c5nnn6

RUN: RUN8907

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.30

EN300-6479181_1_2



CID: EN300-6479181_1_2

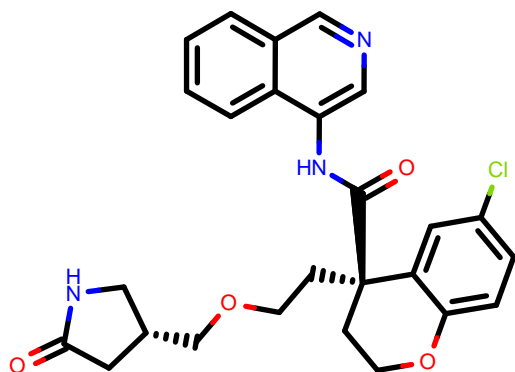
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4Cl)NC(=O)[C@H]5CC[C@@H]6NSC[C@]6O5

RUN: RUN9589

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-246747_3_1



CID: EN300-246747_3_1

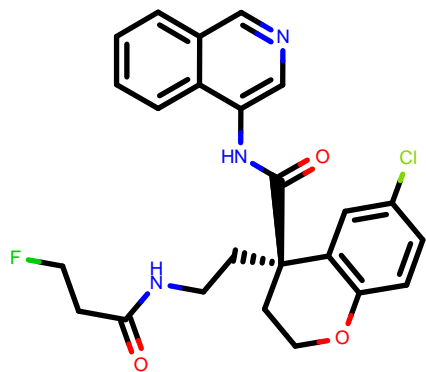
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4Cl)CCOC[C@@]5H5CC(=O)N5

RUN: RUN1935

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.23

EN300-97758_3_1



CID: EN300-97758_3_1

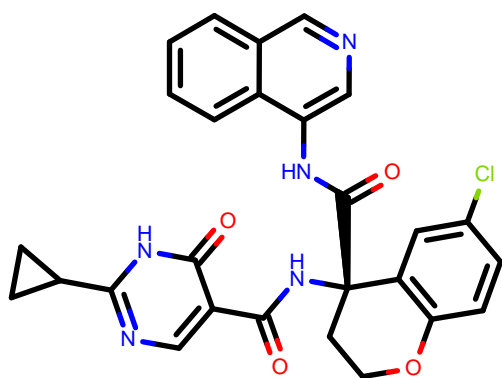
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4Cl)CCNC(=O)CCF

RUN: RUN14780

DDG (kcal/mol): -1.73

dDDG (kcal/mol): 0.20

EN300-118045_1_1



CID: EN300-118045_1_1

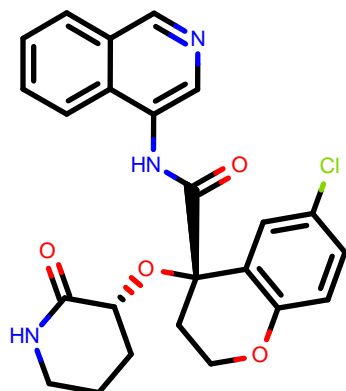
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ncn([nH]c5=O)C6CC6

RUN: RUN7808

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.26

EN300-107267_1_2



CID: EN300-107267_1_2

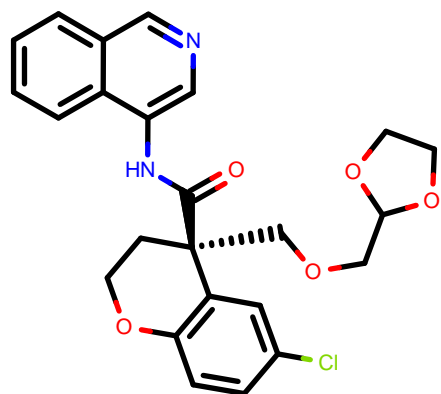
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)O[C@@]4H5CCCCN5=O

RUN: RUN2195

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.20

EN300-77092_2_1



CID: EN300-77092_2_1

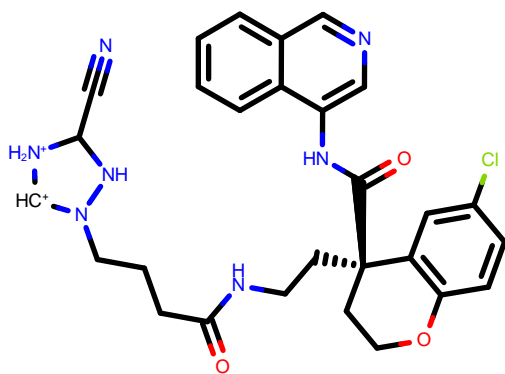
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC5OCCC5

RUN: RUN2064

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.20

EN300-245265_3_1



CID: EN300-245265_3_1

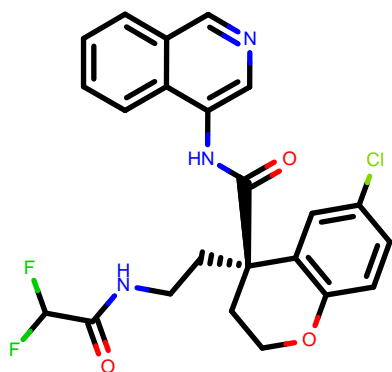
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCc5ncn([nH]c5=O)C6=O

RUN: RUN9228

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.29

EN300-19507_3_1



CID: EN300-19507_3_1

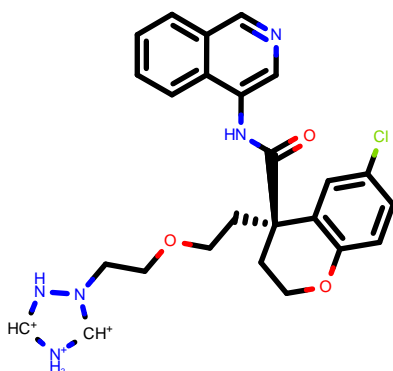
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(F)F

RUN: RUN14722

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.17

EN300-6255179_3_1



CID: EN300-6255179_3_1

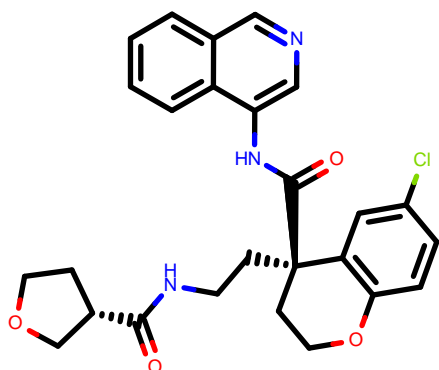
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cncn5

RUN: RUN1656

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.22

EN300-170463_3_1



CID: EN300-170463_3_1

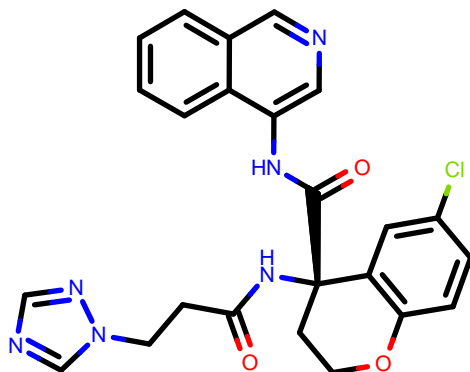
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOCS5

RUN: RUN8319

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.19

EN300-26147_1_1



CID: EN300-26147_1_1

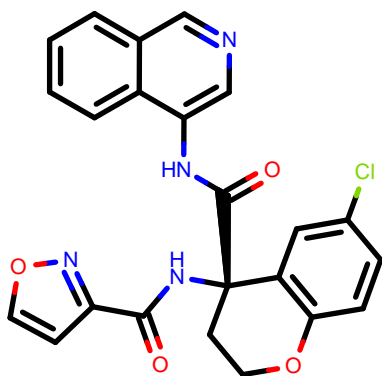
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5

RUN: RUN8757

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.22

EN300-22245_1_1



CID: EN300-22245_1_1

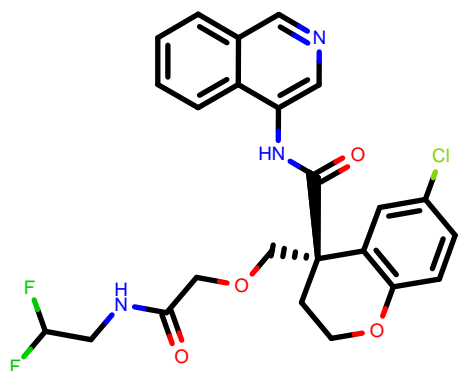
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccon5

RUN: RUN2870

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.17

EN300-120586_2_1



CID: EN300-120586_2_1

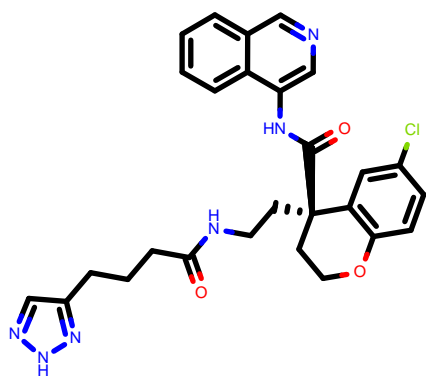
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NCC(F)F

RUN: RUN2048

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.19

EN300-156995_3_1



CID: EN300-156995_3_1

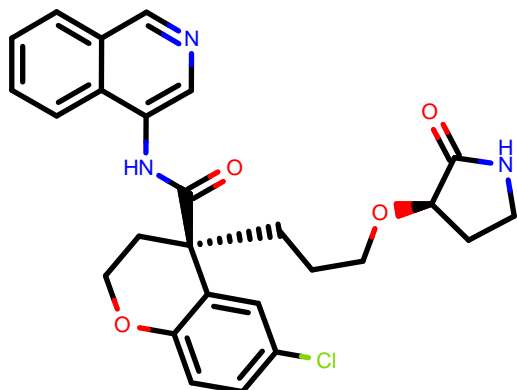
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCc5cn[nH]5

RUN: RUN8175

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.26

EN300-6736413_4_2



CID: EN300-6736413_4_2

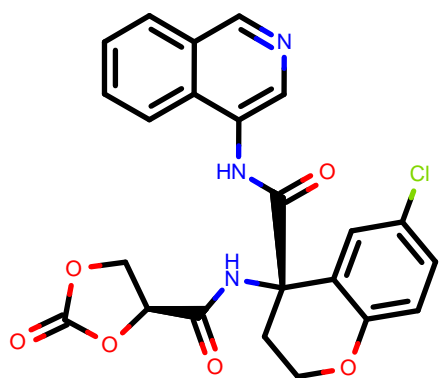
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN669

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.21

EN300-5253939_1_1



CID: EN300-5253939_1_1

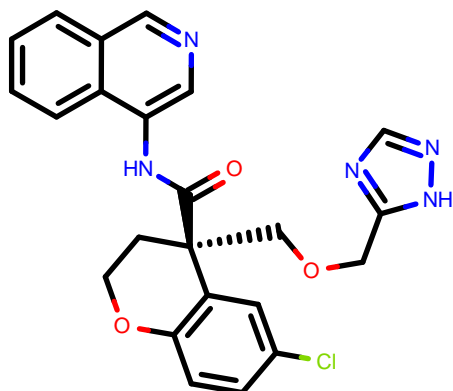
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5COC(=O)O5

RUN: RUN1880

DDG (kcal/mol): -1.72

dDDG (kcal/mol): 0.19

EN300-306316_2_1



CID: EN300-306316_2_1

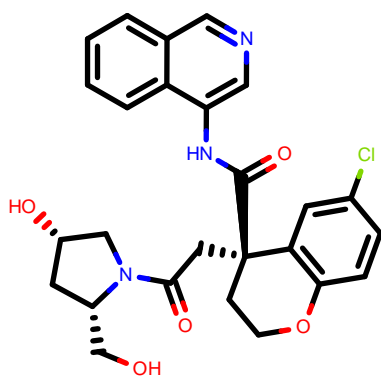
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCc5[nH]ncn5

RUN: RUN1298

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.19

EN300-153245_1_1



CID: EN300-153245_1_1

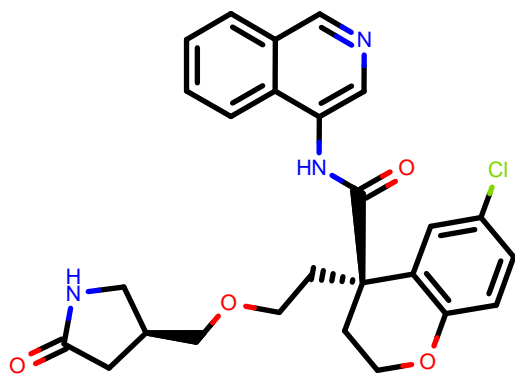
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C[C@@H]5CO)O

RUN: RUN1407

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.27

EN300-246747_3_2



CID: EN300-246747_3_2

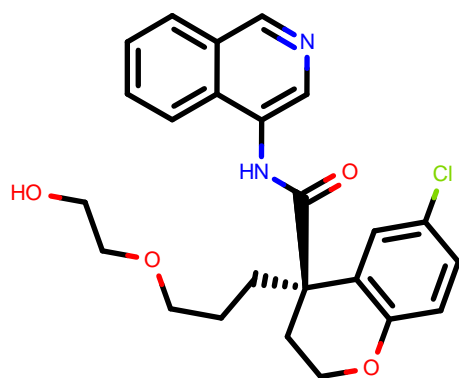
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5CC(=O)NCS

RUN: RUN1392

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.24

EN300-21258_4_1



CID: EN300-21258_4_1

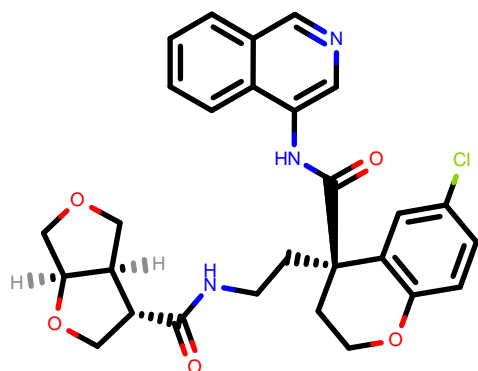
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCO

RUN: RUN1795

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.19

EN300-6482296_3_7



CID: EN300-6482296_3_7

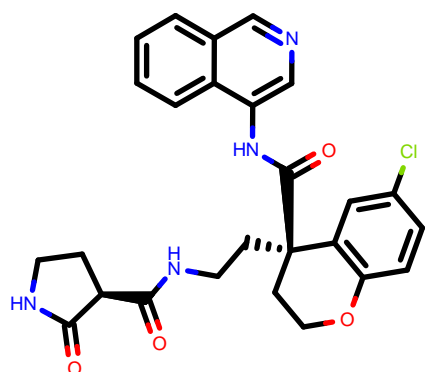
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5[C@@]5COC6=C[C@@]5COC6

RUN: RUN15012

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.26

EN300-94945_3_1



CID: EN300-94945_3_1

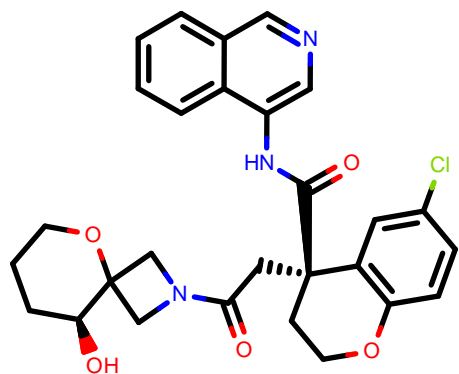
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5[C@@]5CNC6=O

RUN: RUN2945

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.24

EN300-7434114_1_1



CID: EN300-7434114_1_1

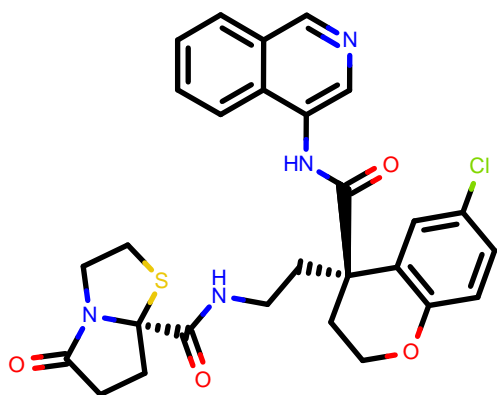
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)[C@@H](C6CO)O

RUN: RUN12354

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.21

EN300-10334_3_2



CID: EN300-10334_3_2

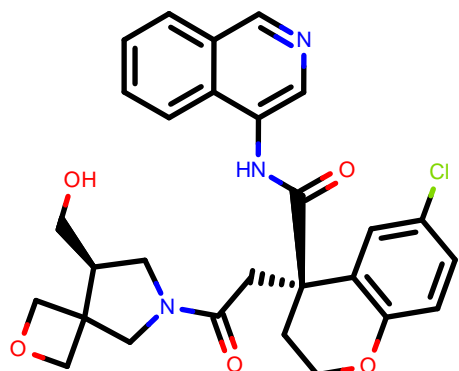
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@56CCC(=O)N5CCS6

RUN: RUN15048

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.27

EN300-395654_1_1



CID: EN300-395654_1_1

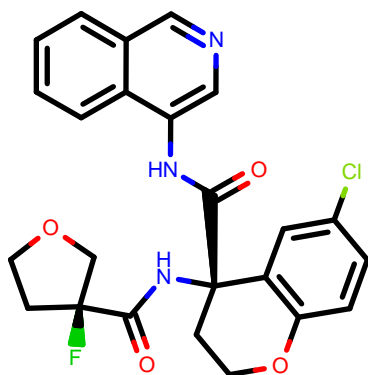
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C6(C5)COO6)CO

RUN: RUN6161

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.25

EN300-188356_1_1



CID: EN300-188356_1_1

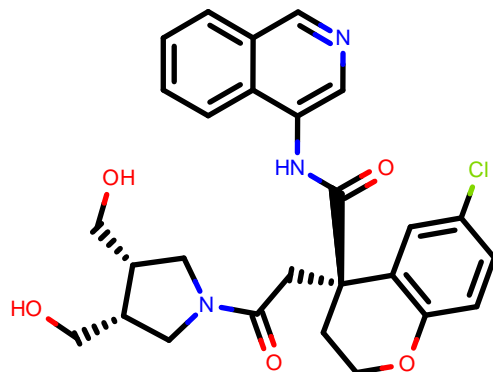
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)NC(=O)C@5(CCOO5)F

RUN: RUN4382

DDG (kcal/mol): -1.71

dDDG (kcal/mol): 0.20

EN300-314088_1_1



CID: EN300-314088_1_1

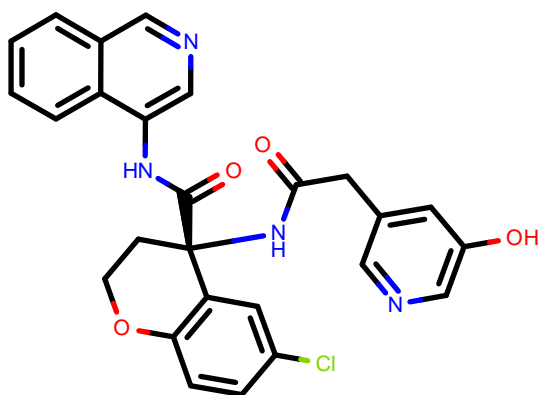
SMILES: c1ccc2c(c1)ncoc2NC(=O)C@@3(CCOc4c3cc(cc4)Cl)CC(O)N5C[C@@H](C6(C5)CO)CO

RUN: RUN1215

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.25

EN300-222620_1_1



CID: EN300-222620_1_1

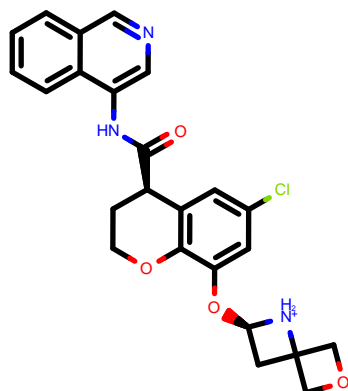
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cc(ncs5)O

RUN: RUN9269

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.24

DAR-DIA-23e5a6a0-3_1



CID: DAR-DIA-23e5a6a0-3_1

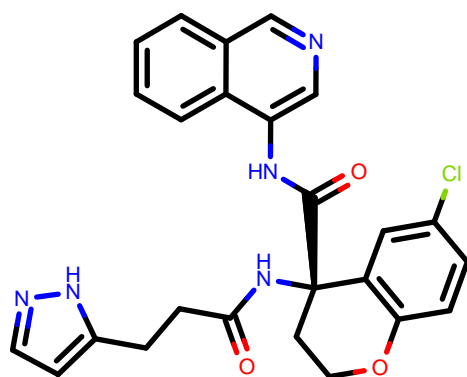
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)C@@H)5CC6([NH2+])COC6)Cl

RUN: RUN14

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.42

EN300-1664603_1_1



CID: EN300-1664603_1_1

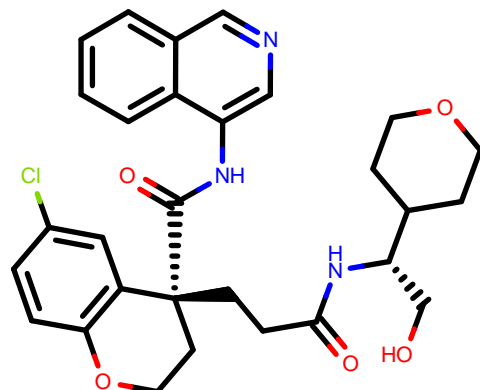
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5cn[nH]5

RUN: RUN1665

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.20

EN300-97746_2_2



CID: EN300-97746_2_2

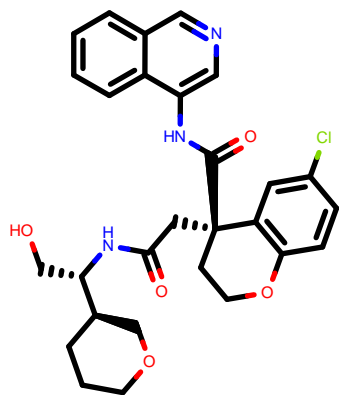
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CO)C5COC5

RUN: RUN1294

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.33

EN300-254105_1_2



CID: EN300-254105_1_2

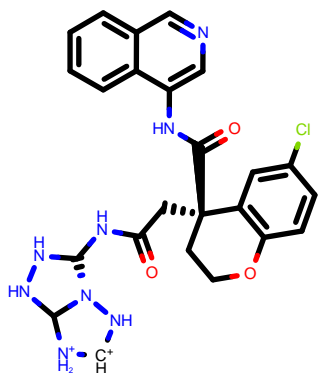
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4Cl)CC(=O)N[C@@H](CO)C@H5COCOC5

RUN: RUN13434

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.31

EN300-214849_1_1



CID: EN300-214849_1_1

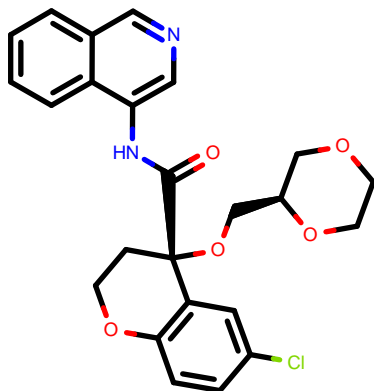
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4Cl)CC(=O)Nc5nc6n5[nH]cn6

RUN: RUN11335

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.19

EN300-139167_1_1



CID: EN300-139167_1_1

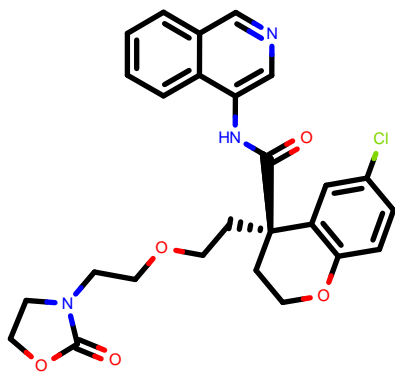
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4Cl)OC[C@@H]5COCOC5

RUN: RUN2697

DDG (kcal/mol): -1.70

dDDG (kcal/mol): 0.24

EN300-370967_3_1



CID: EN300-370967_3_1

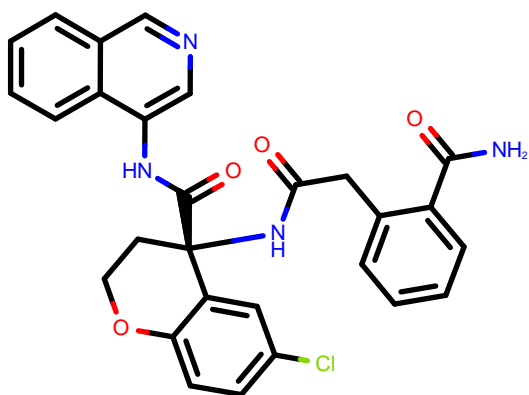
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4Cl)CCOCNC5COC5=O

RUN: RUN2150

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.29

EN300-121144_1_1



CID: EN300-121144_1_1

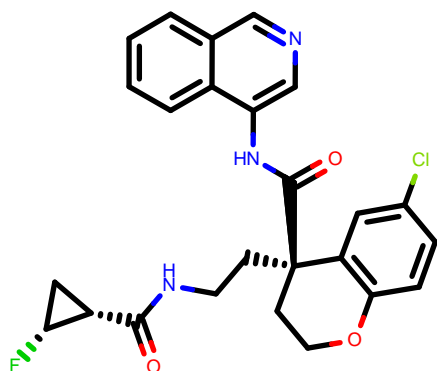
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cc5ccc5C(=O)N

RUN: RUN3706

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-97300_3_2



CID: EN300-97300_3_2

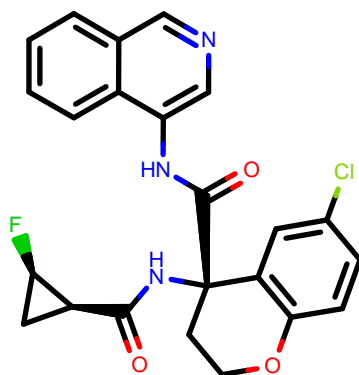
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C[C@H]5F

RUN: RUN15000

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.19

EN300-97300_1_2



CID: EN300-97300_1_2

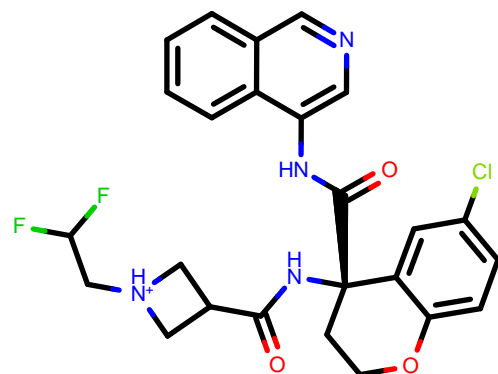
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C[C@H]5F

RUN: RUN2039

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.17

EN300-182579_1_1



CID: EN300-182579_1_1

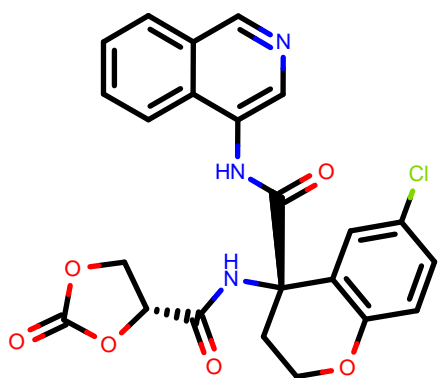
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CN(C5)CC(F)F

RUN: RUN6337

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.23

EN300-5253939_1_2



CID: EN300-5253939_1_2

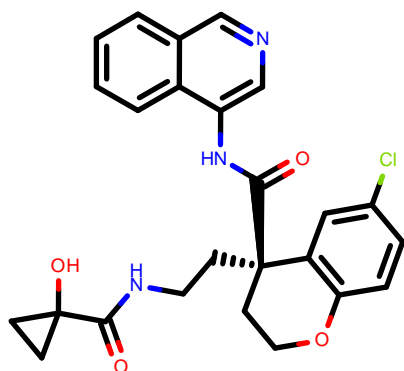
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5COC(=O)O5

RUN: RUN4954

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.22

EN300-25702_3_1



CID: EN300-25702_3_1

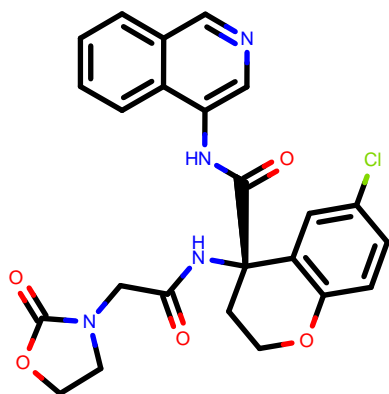
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)C5(C)C5O

RUN: RUN14874

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.22

EN300-172179_1_1



CID: EN300-172179_1_1

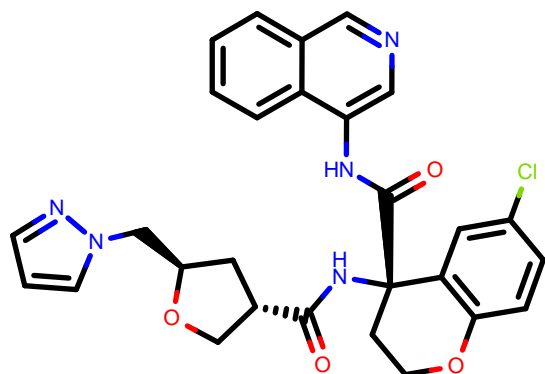
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5COCOC5=O

RUN: RUN9137

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.24

EN300-6494859_1_4



CID: EN300-6494859_1_4

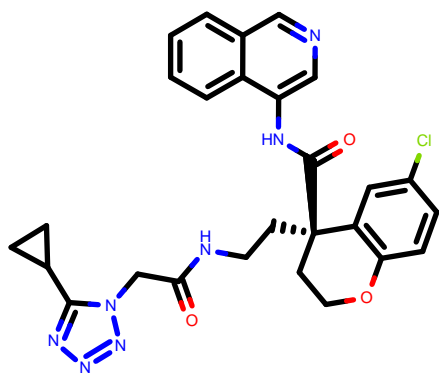
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5C(C@H)OC5C6CCN6

RUN: RUN4862

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.27

EN300-872798_3_1



CID: EN300-872798_3_1

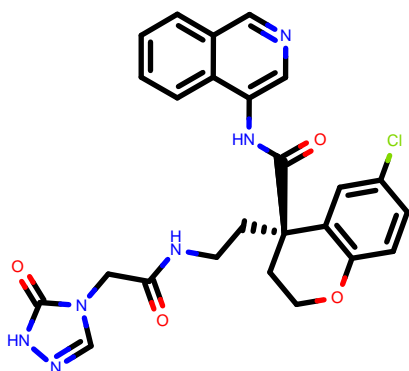
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5c(nnn5)C6CC6

RUN: RUN10595

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.27

EN300-120820_3_1



CID: EN300-120820_3_1

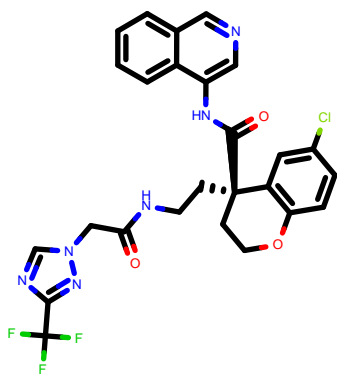
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5c[nH]5=O

RUN: RUN13598

DDG (kcal/mol): -1.69

dDDG (kcal/mol): 0.23

EN300-7385389_3_1



CID: EN300-7385389_3_1

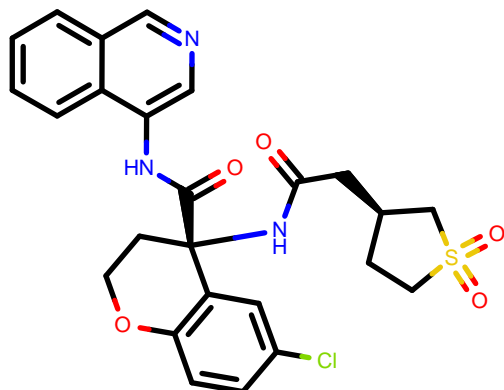
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cnc(n5)C(F)(F)F

RUN: RUN15323

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.32

EN300-14006_1_1



CID: EN300-14006_1_1

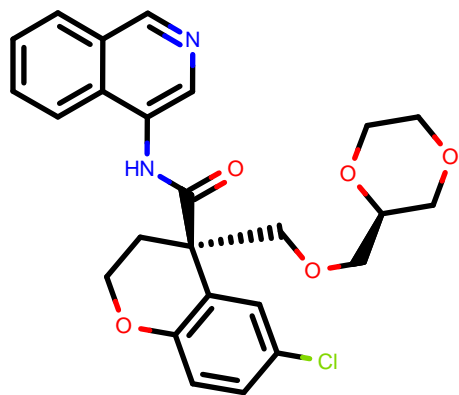
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]4H5SCCS(=O)(=O)C5

RUN: RUN8464

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.31

EN300-139167_2_2



CID: EN300-139167_2_2

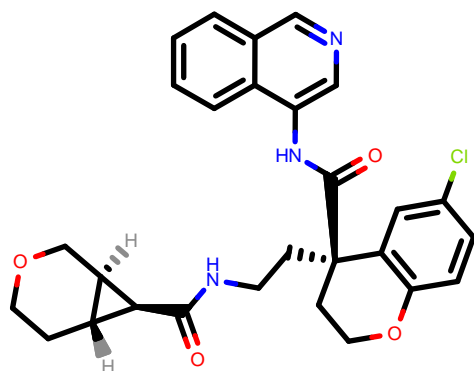
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5COCOC5

RUN: RUN908

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.21

EN300-1644723_3_8



CID: EN300-1644723_3_8

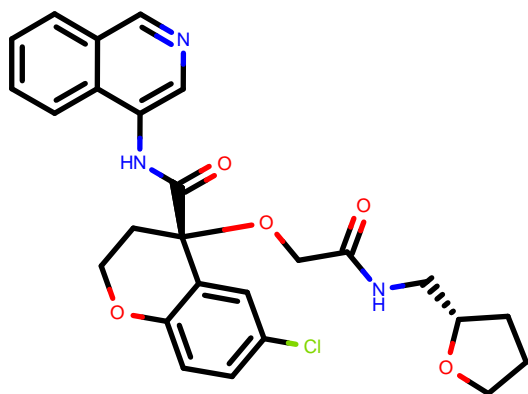
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5COCOC5

RUN: RUN15327

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.21

EN300-01527_1_2



CID: EN300-01527_1_2

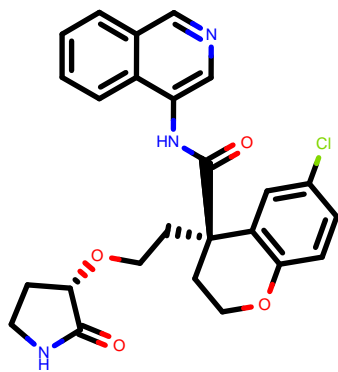
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5COCOC5

RUN: RUN615

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-6736413_3_1



CID: EN300-6736413_3_1

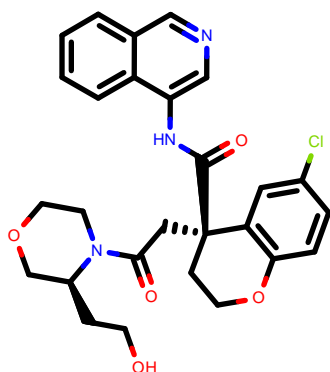
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CNCNS=O

RUN: RUN1576

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.22

EN300-345754_1_1



CID: EN300-345754_1_1

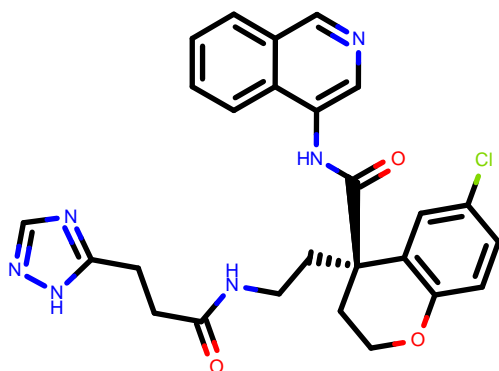
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CCO

RUN: RUN11451

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-101197_3_1



CID: EN300-101197_3_1

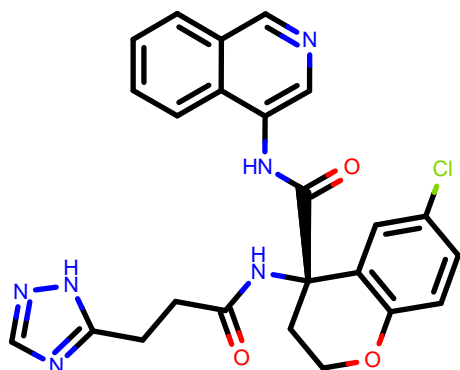
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5[nH]n5

RUN: RUN1862

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.26

EN300-101197_1_1



CID: EN300-101197_1_1

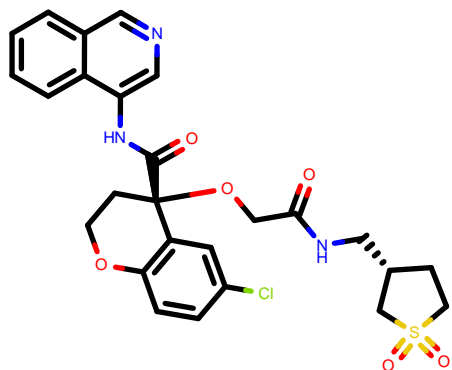
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NCC(=O)CCc5[nH]n5

RUN: RUN9089

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.22

EN300-47606_1_1



CID: EN300-47606_1_1

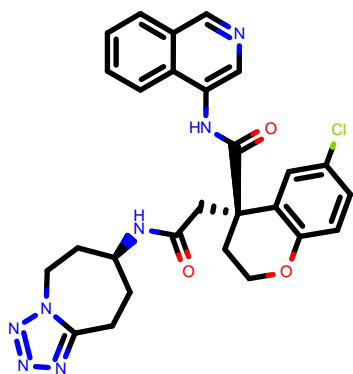
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5SCCS(=O)(=O)C5

RUN: RUN631

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.30

EN300-256798_1_2



CID: EN300-256798_1_2

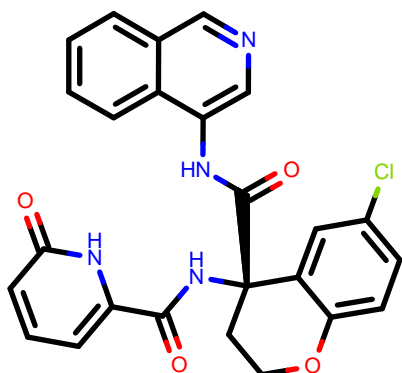
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCc6nnn6CC5

RUN: RUN15335

DDG (kcal/mol): -1.68

dDDG (kcal/mol): 0.22

EN300-34636_1_1



CID: EN300-34636_1_1

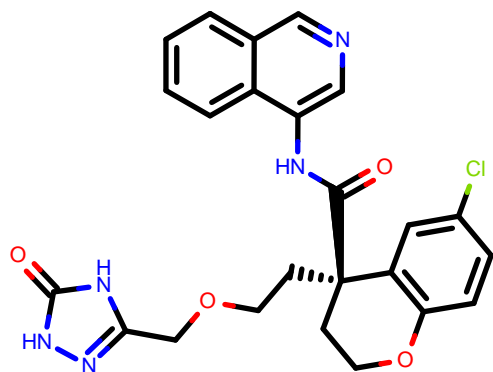
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccc(=O)[nH]5

RUN: RUN3834

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.21

EN300-73772_3_1



CID: EN300-73772_3_1

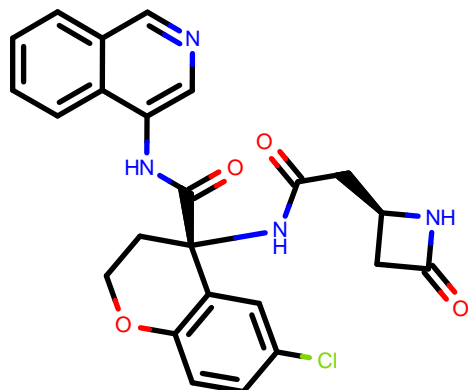
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]5

RUN: RUN1839

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.21

EN300-250593_1_2



CID: EN300-250593_1_2

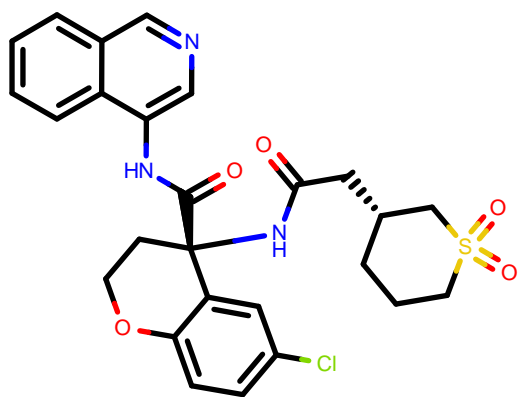
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(=O)N5

RUN: RUN379

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.28

EN300-220676_1_2



CID: EN300-220676_1_2

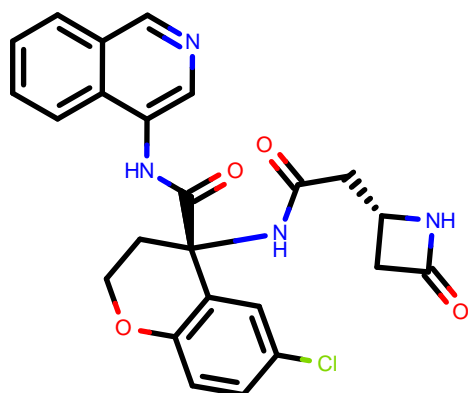
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCS(=O)(=O)C5

RUN: RUN6389

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.44

EN300-250593_1_1



CID: EN300-250593_1_1

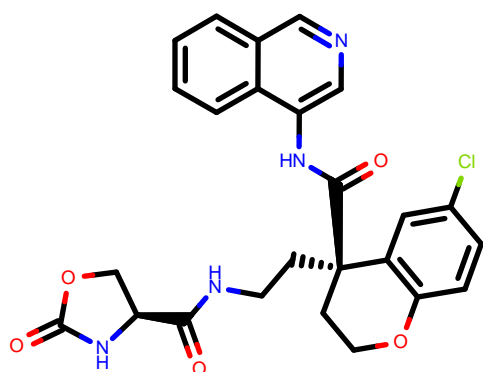
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)N5

RUN: RUN867

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.32

EN300-201346_3_1



CID: EN300-201346_3_1

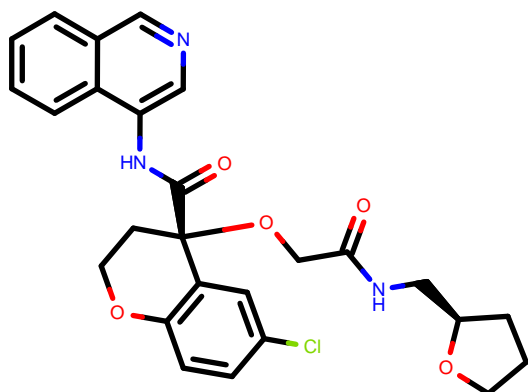
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5HJ5COC(=O)N5

RUN: RUN15338

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.21

EN300-01527_1_1



CID: EN300-01527_1_1

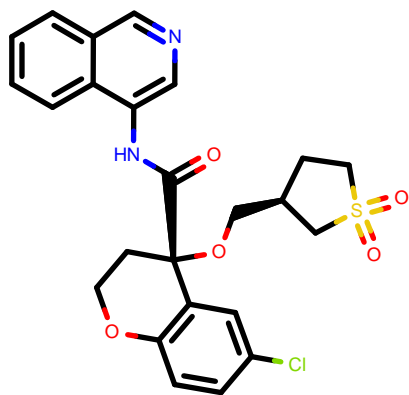
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5CCOC5

RUN: RUN1397

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.31

EN300-1448603_1_2



CID: EN300-1448603_1_2

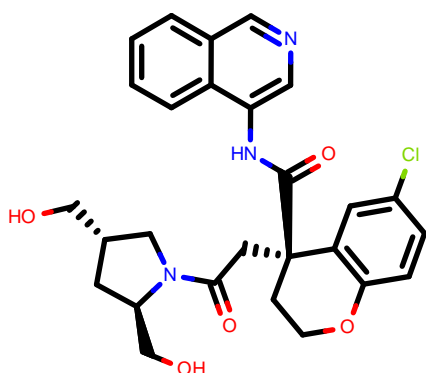
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCS(=O)(=O)O5

RUN: RUN1006

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.31

EN300-1212400_1_1



CID: EN300-1212400_1_1

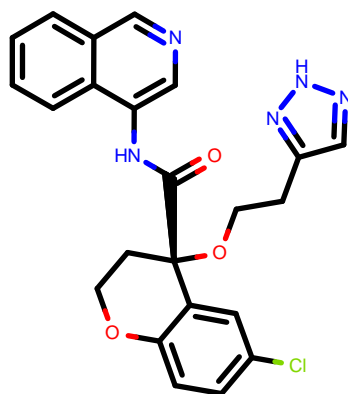
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C)[C@@H]5CO

RUN: RUN3033

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.27

EN300-222357_1_1



CID: EN300-222357_1_1

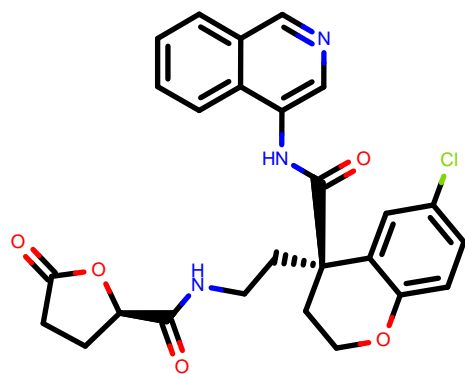
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cn[nH]n5

RUN: RUN1109

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.19

EN300-332606_3_1



CID: EN300-332606_3_1

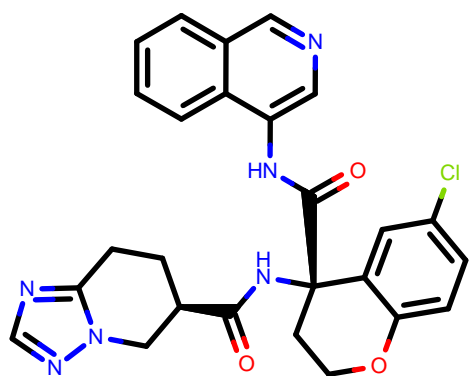
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)O5

RUN: RUN2889

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.20

EN300-1662365_1_1



CID: EN300-1662365_1_1

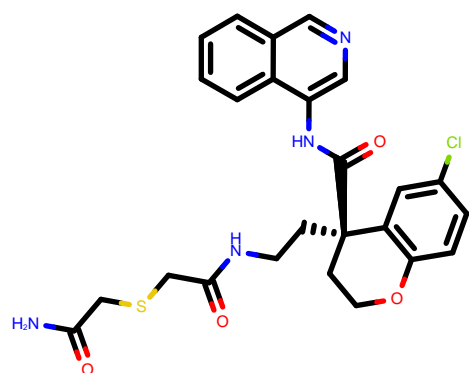
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CCc6nncn6C5

RUN: RUN9361

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.20

EN300-33513_3_1



CID: EN300-33513_3_1

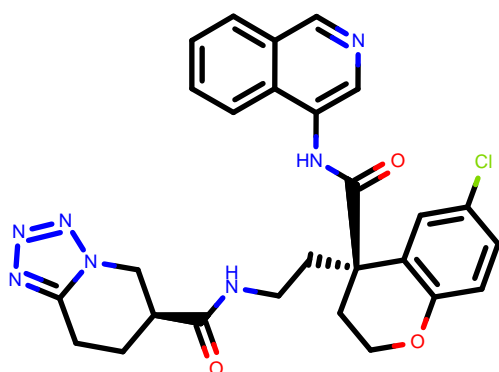
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CSCC(=O)N

RUN: RUN8543

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.25

EN300-269453_3_2



CID: EN300-269453_3_2

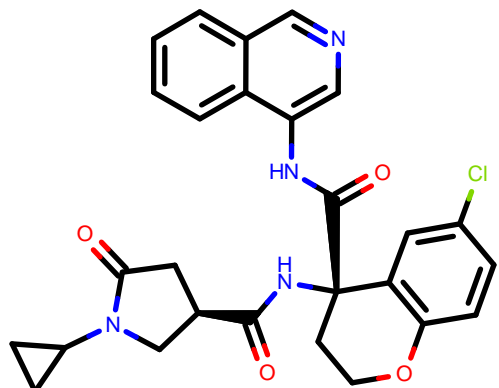
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5H5CCc6nncn6C5

RUN: RUN15397

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.30

EN300-12440_1_1



CID: EN300-12440_1_1

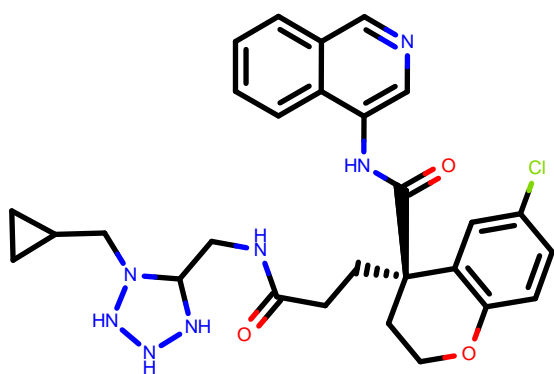
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5CC(=O)N(C5)C6CC6

RUN: RUN7236

DDG (kcal/mol): -1.67

dDDG (kcal/mol): 0.23

EN300-140751_2_1



CID: EN300-140751_2_1

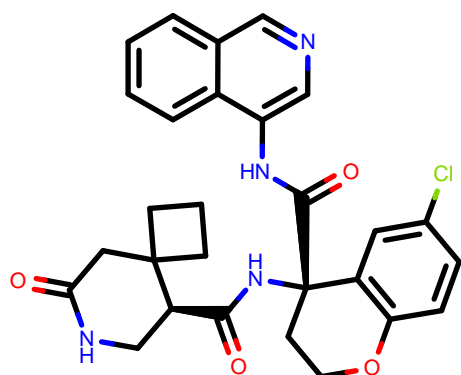
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5nnn5COC6C6

RUN: RUN10142

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.33

EN300-1704404_1_2



CID: EN300-1704404_1_2

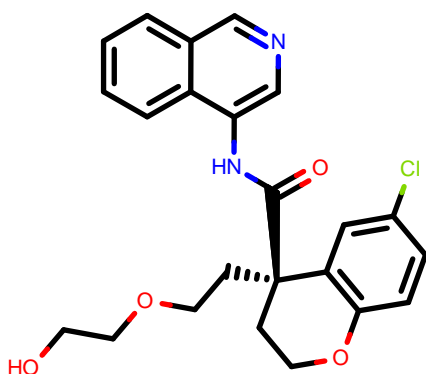
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)CC56C6C6

RUN: RUN8729

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.20

EN300-21258_3_1



CID: EN300-21258_3_1

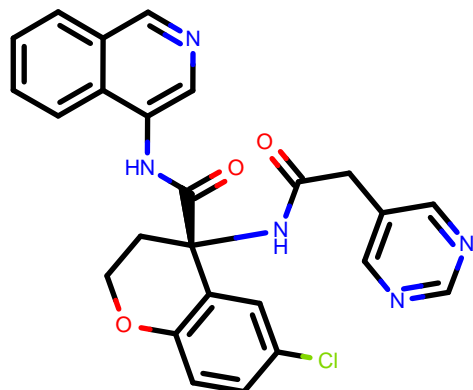
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC6C6

RUN: RUN1033

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.19

EN300-185751_1_1



CID: EN300-185751_1_1

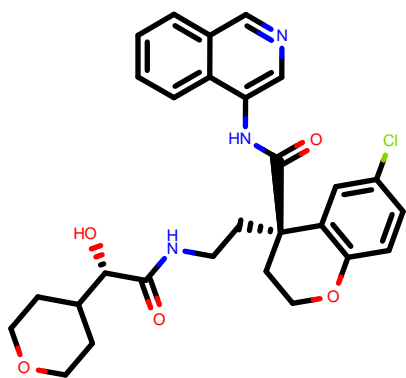
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nncn5

RUN: RUN9325

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.22

EN300-79180_3_2



CID: EN300-79180_3_2

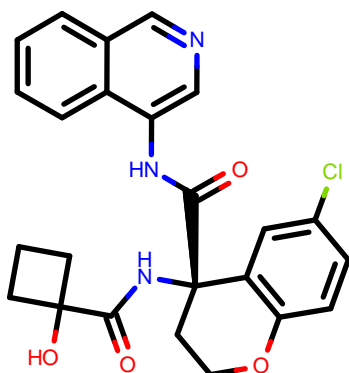
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CCOCC5)O

RUN: RUN4677

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.29

EN300-52009_1_1



CID: EN300-52009_1_1

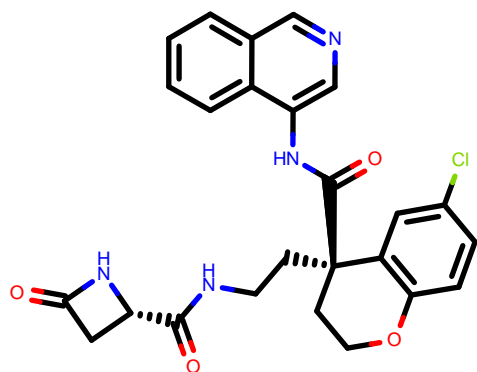
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)O

RUN: RUN2724

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.21

EN300-101505_3_1



CID: EN300-101505_3_1

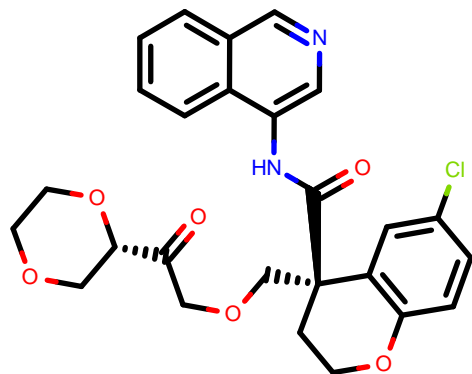
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)N5

RUN: RUN15205

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.23

EN300-6238494_2_1



CID: EN300-6238494_2_1

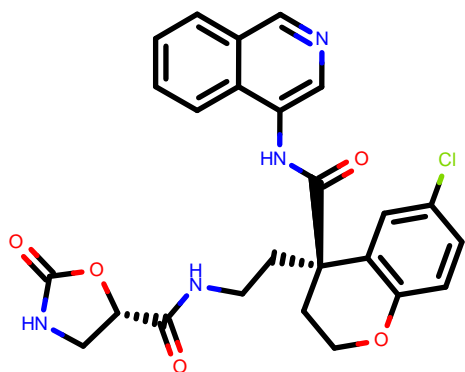
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)[C@H]5COC(CO)5

RUN: RUN1682

DDG (kcal/mol): -1.66

dDDG (kcal/mol): 0.27

EN300-244403_3_1



CID: EN300-244403_3_1

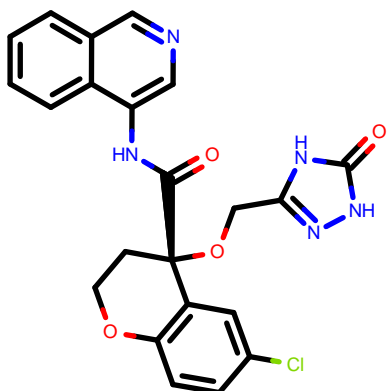
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5H5NC(=O)O5

RUN: RUN5089

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.20

EN300-73772_1_1



CID: EN300-73772_1_1

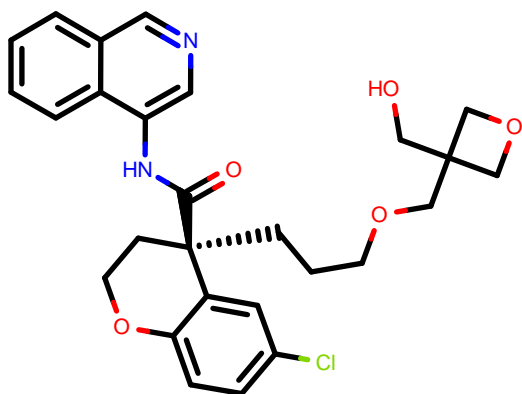
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5[nH]c(=O)[nH]n5

RUN: RUN1797

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.18

EN300-102347_4_1



CID: EN300-102347_4_1

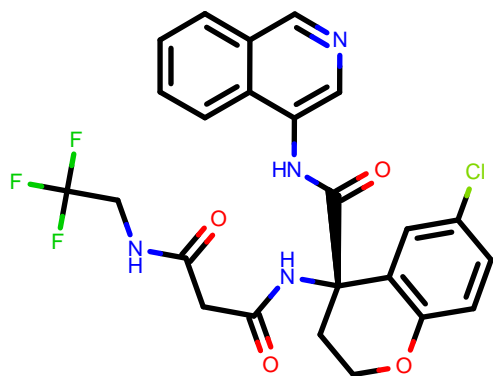
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC5(COC5)CO

RUN: RUN1299

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.21

EN300-128715_1_1



CID: EN300-128715_1_1

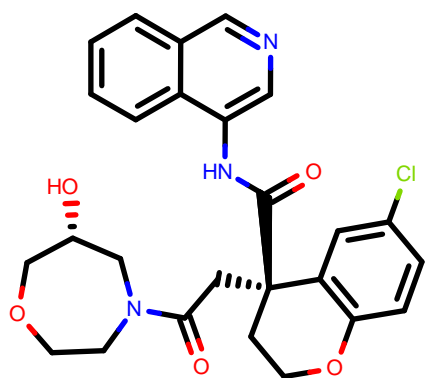
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC(=O)N(C(F)F)F

RUN: RUN8260

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.22

EN300-233951_1_2



CID: EN300-233951_1_2

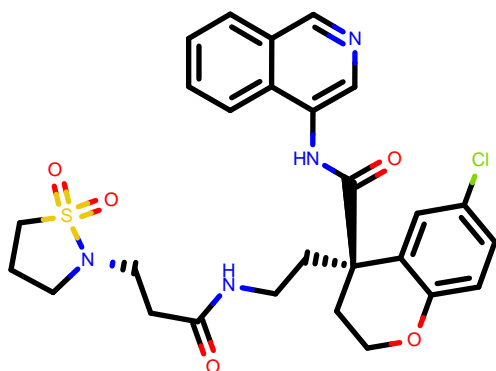
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)O

RUN: RUN1367

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.30

EN300-44873_3_2



CID: EN300-44873_3_2

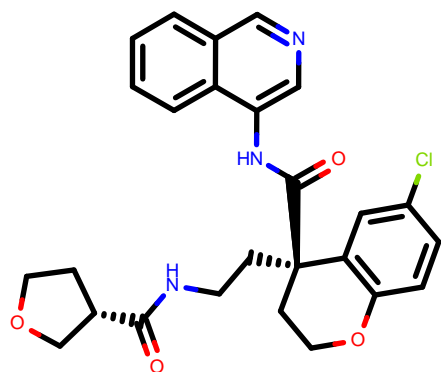
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[N@@]5CCCS5(=O)=O

RUN: RUN13464

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.64

EN300-170463_3_1



CID: EN300-170463_3_1

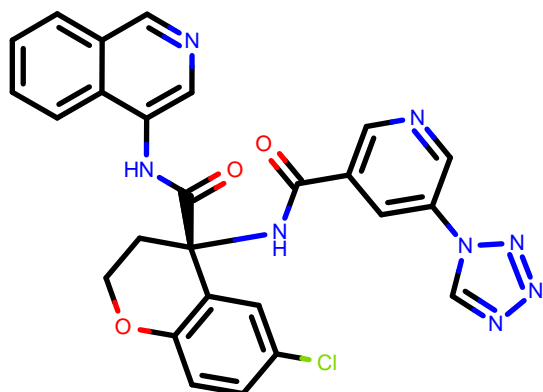
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCOC5

RUN: RUN8315

DDG (kcal/mol): -1.65

dDDG (kcal/mol): 0.23

EN300-2690393_1_1



CID: EN300-2690393_1_1

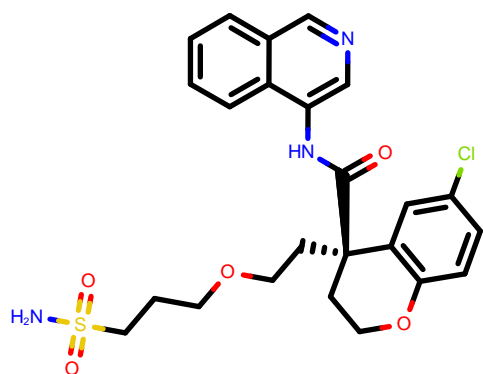
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(nc5)n6nnn6

RUN: RUN4442

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.27

EN300-79588_3_1



CID: EN300-79588_3_1

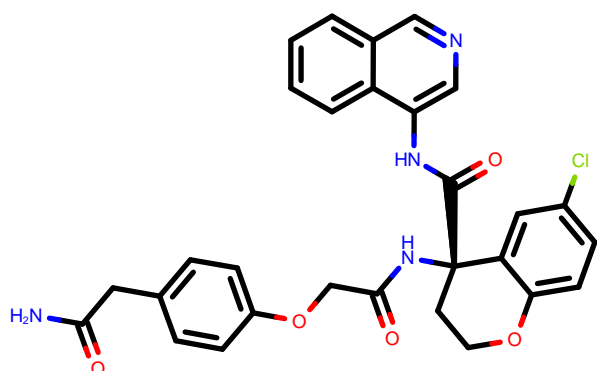
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CCOc4cc3cc(cc4)C)CCOCCCS(=O)(=O)N

RUN: RUN1504

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.27

EN300-50514_1_1



CID: EN300-50514_1_1

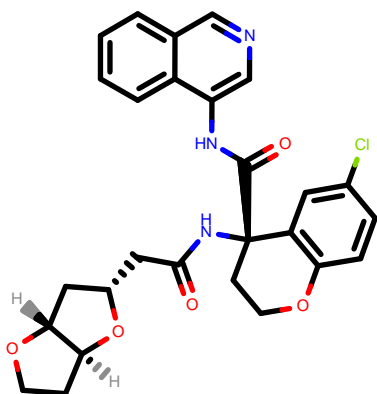
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CCOc4ccc(cc4)C)COC(=O)CC(=O)N

RUN: RUN7568

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-7355519_1_1



CID: EN300-7355519_1_1

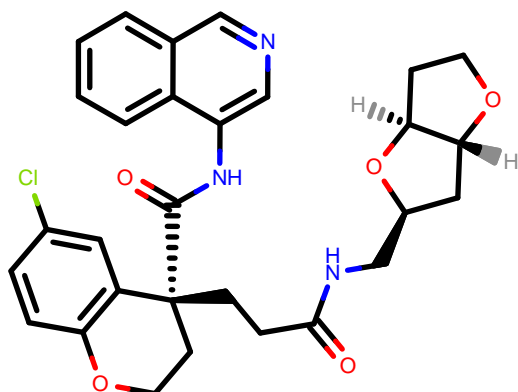
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CCOc4cc3cc(cc4)C)C(=O)NCC1C2C1C1OC1

RUN: RUN9157

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.25

EN300-6760278_2_2



CID: EN300-6760278_2_2

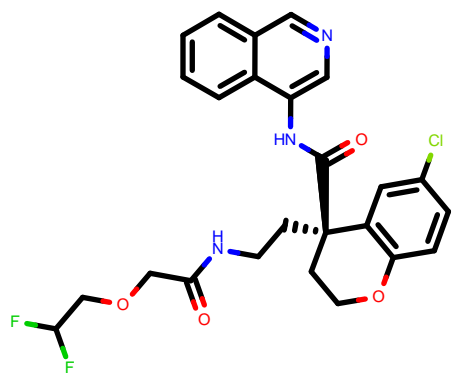
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CCOc4cc3cc(cc4)C)C(=O)NCC1C2C1C1OC1

RUN: RUN9809

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.28

EN300-315792_3_1



CID: EN300-315792_3_1

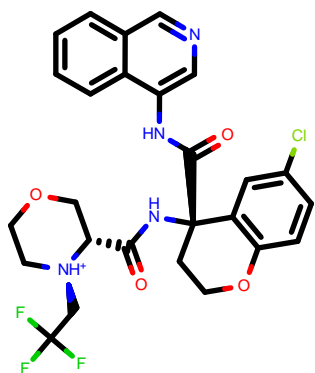
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COCC(F)F

RUN: RUN11950

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.24

EN300-201551_1_4



CID: EN300-201551_1_4

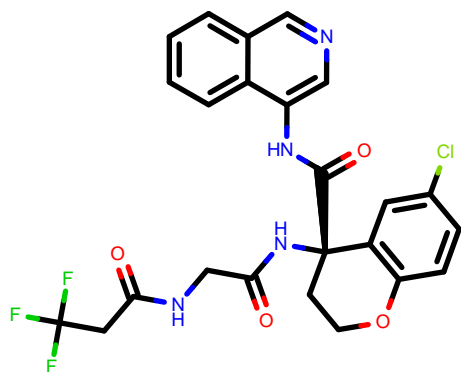
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H5COCCN@5JCC(F)F

RUN: RUN7128

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.28

EN300-43939_1_1



CID: EN300-43939_1_1

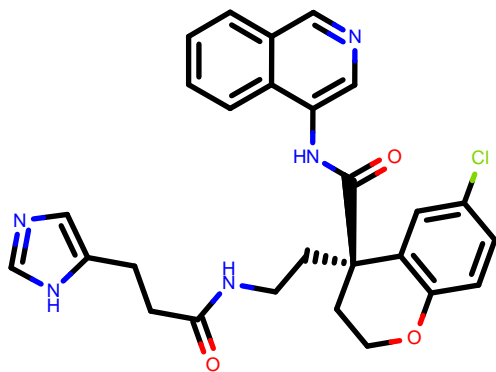
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)CC(F)F

RUN: RUN6984

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.23

EN300-145616_3_1



CID: EN300-145616_3_1

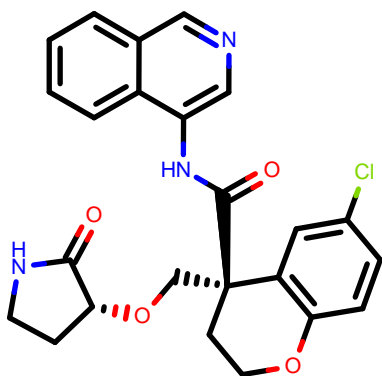
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5nc[nH]5

RUN: RUN15357

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.26

EN300-6736413_2_2



CID: EN300-6736413_2_2

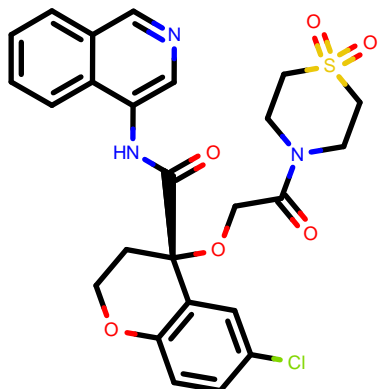
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCNC5=O

RUN: RUN1474

DDG (kcal/mol): -1.64

dDDG (kcal/mol): 0.19

EN300-1265948_1_1



CID: EN300-1265948_1_1

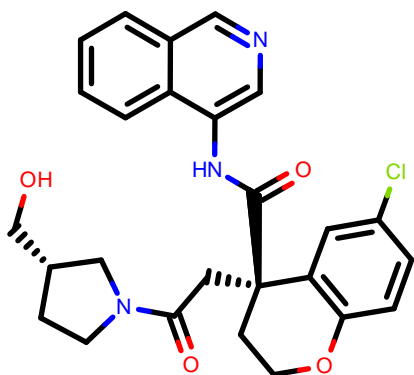
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN2438

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.30

EN300-88131_1_1



CID: EN300-88131_1_1

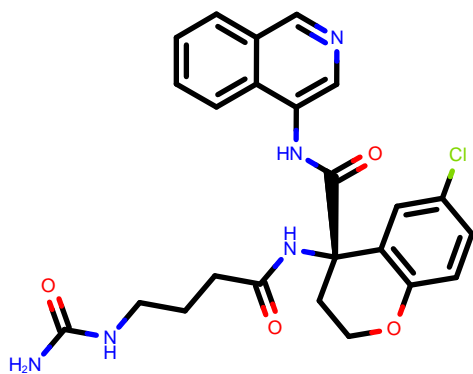
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN5585

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.21

EN300-05620_1_1



CID: EN300-05620_1_1

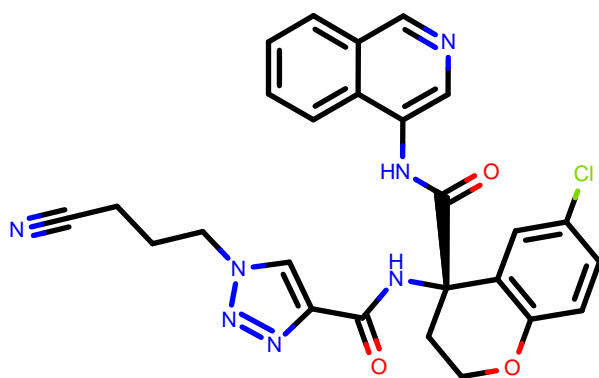
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCC(=O)N

RUN: RUN5418

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.21

EN300-120569_1_1



CID: EN300-120569_1_1

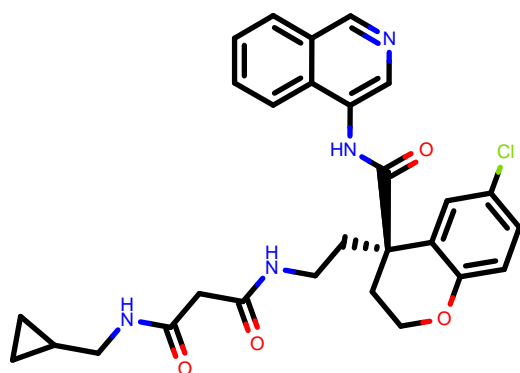
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)CCCC#N

RUN: RUN2942

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.23

EN300-178829_3_1



CID: EN300-178829_3_1

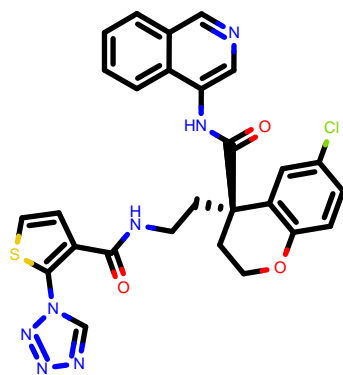
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CC(=O)NCC5CC5

RUN: RUN6013

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.25

EN300-6744029_3_1



CID: EN300-6744029_3_1

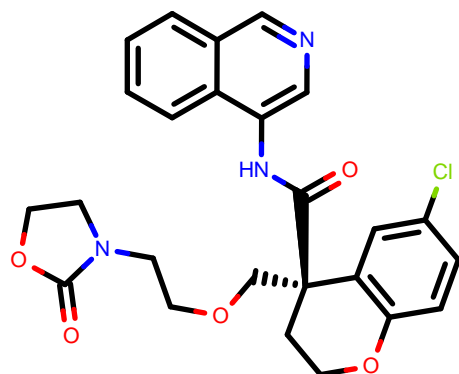
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccsc5n6cnm6

RUN: RUN13994

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.31

EN300-370967_2_1



CID: EN300-370967_2_1

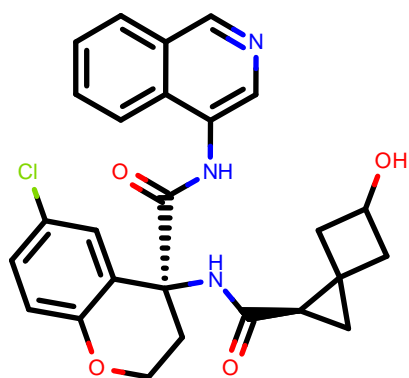
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COCN5CCOC5=O

RUN: RUN1090

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.26

EN300-1717166_1_1



CID: EN300-1717166_1_1

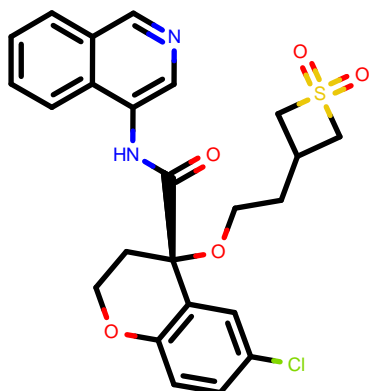
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CC56C(C)C6O

RUN: RUN7780

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.24

EN300-189563_1_1



CID: EN300-189563_1_1

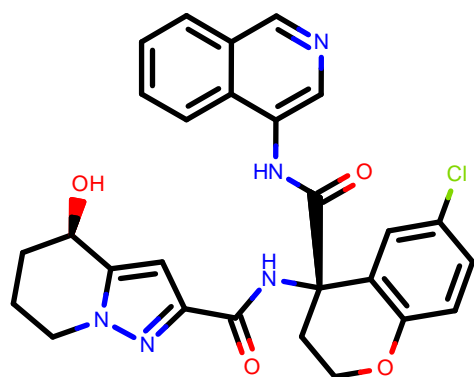
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCS(=O)(=O)CS

RUN: RUN439

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.23

EN300-399606_1_2



CID: EN300-399606_1_2

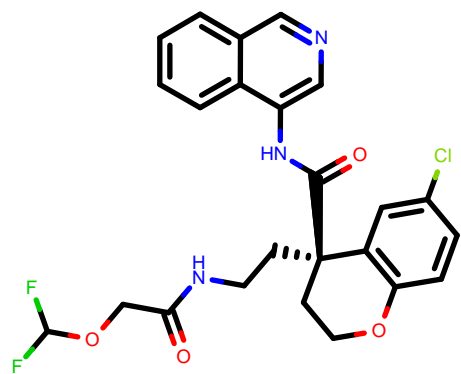
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c6n(n5)CCC[C@@H]6O

RUN: RUN347

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.19

EN300-179091_3_1



CID: EN300-179091_3_1

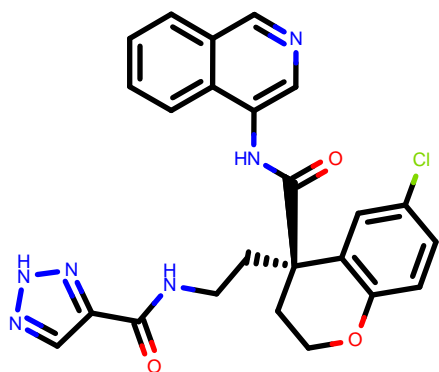
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC(F)F

RUN: RUN11893

DDG (kcal/mol): -1.63

dDDG (kcal/mol): 0.19

EN300-31998_3_1



CID: EN300-31998_3_1

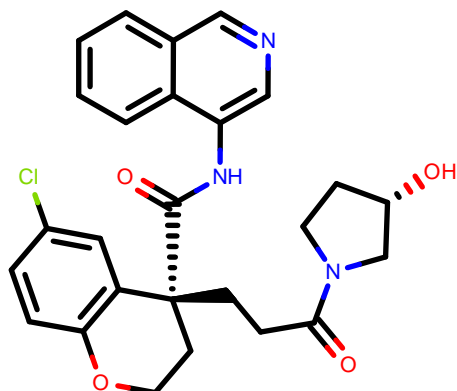
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cn[nH]n5

RUN: RUN15347

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.18

EN300-69312_2_1



CID: EN300-69312_2_1

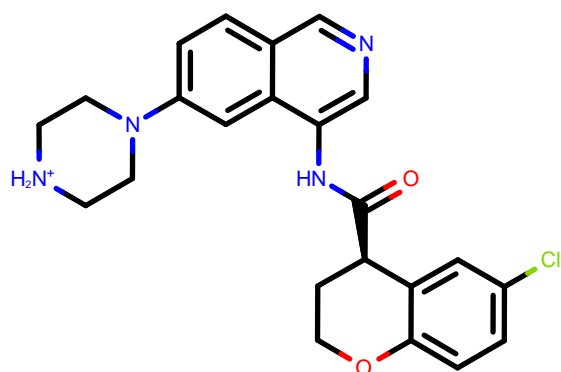
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)O

RUN: RUN14307

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.25

MAK-UNK-8be7dca9-4_1



CID: MAK-UNK-8be7dca9-4_1

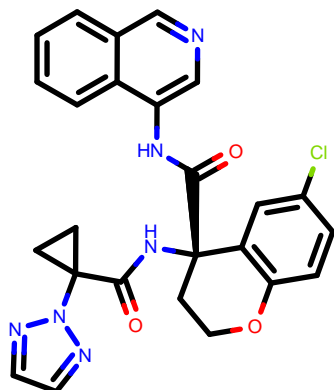
SMILES: c1cc2ncnc(c2cc1N3CC[NH2+][CC3])NC(=O)[C@@]4(CCOc5c4cc(cc5)Cl

RUN: RUN100

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.11

EN300-1722017_1_1



CID: EN300-1722017_1_1

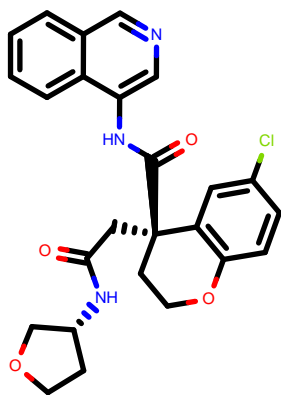
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5n6ncn6

RUN: RUN7580

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.19

EN300-171752_1_1



CID: EN300-171752_1_1

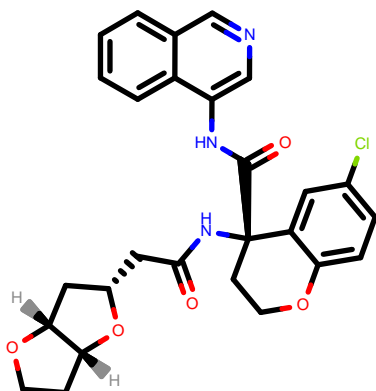
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCOC5

RUN: RUN5705

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.22

EN300-7355519_1_5



CID: EN300-7355519_1_5

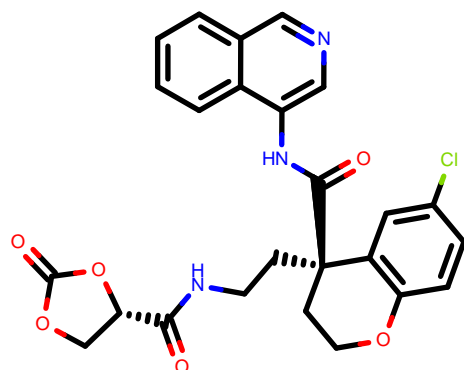
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]6[C@@H]7OC6

RUN: RUN9393

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.25

EN300-5253939_3_1



CID: EN300-5253939_3_1

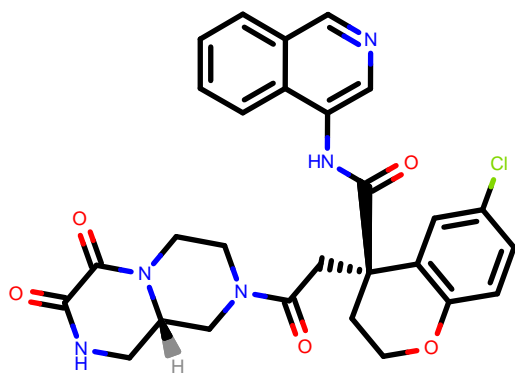
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5COC(=O)O5

RUN: RUN15249

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.21

EN300-100768_1_1



CID: EN300-100768_1_1

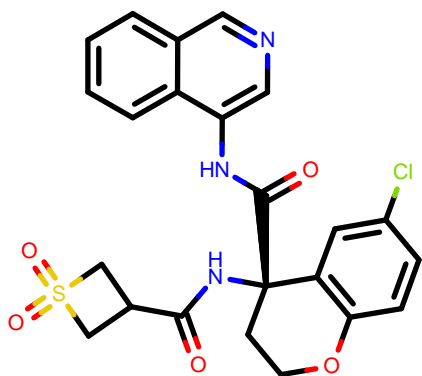
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN(C@H)5C(=O)OC6=O

RUN: RUN9408

DDG (kcal/mol): -1.62

dDDG (kcal/mol): 0.24

EN300-261365_1_1



CID: EN300-261365_1_1

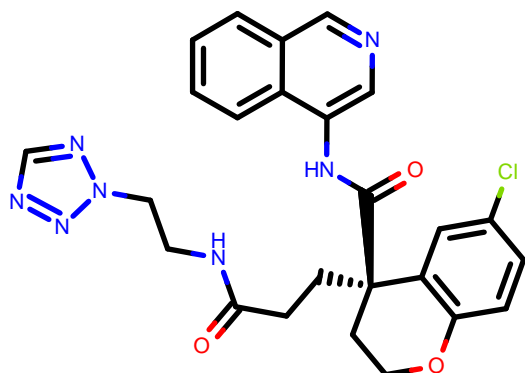
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CS(=O)=O

RUN: RUN7508

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.21

EN300-107823_2_1



CID: EN300-107823_2_1

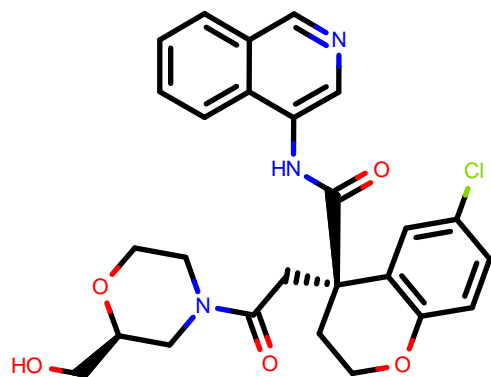
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCn5nncn5

RUN: RUN12715

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.28

EN300-175487_1_1



CID: EN300-175487_1_1

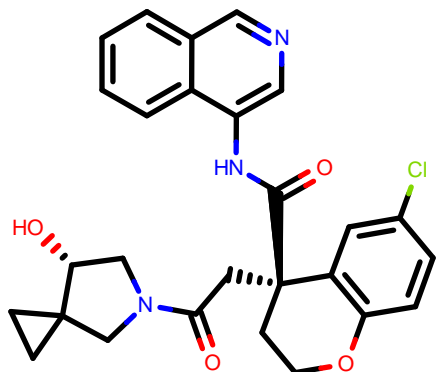
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)CO

RUN: RUN5201

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.27

EN300-142333_1_2



CID: EN300-142333_1_2

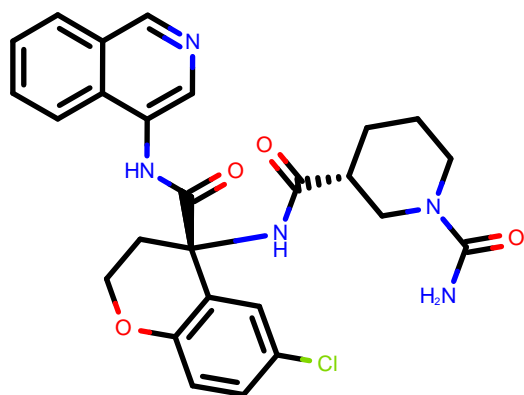
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C6(C5)CC6)O

RUN: RUN11501

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.23

EN300-14767_1_1



CID: EN300-14767_1_1

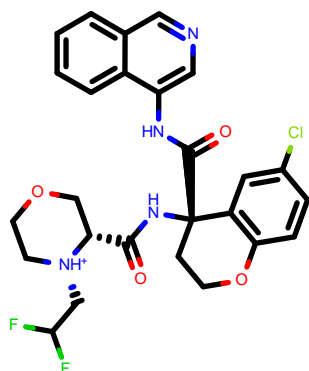
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5H5CCCN(C5)C(=O)N

RUN: RUN4450

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.20

EN300-140582_1_4



CID: EN300-140582_1_4

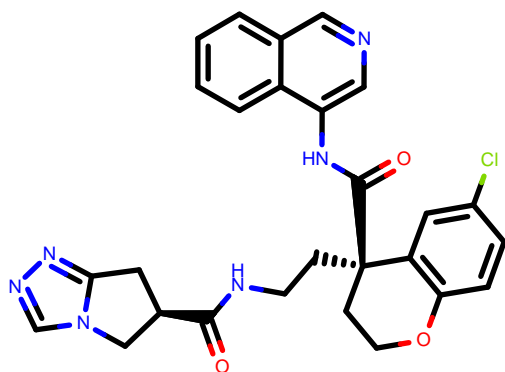
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5H5COC[N@@]5C(F)F

RUN: RUN2747

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.26

EN300-6745453_3_1



CID: EN300-6745453_3_1

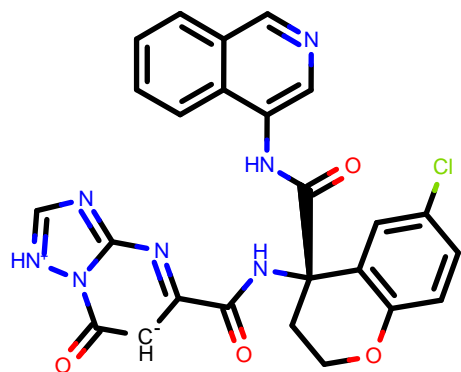
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5H5Cc6nnn6C5

RUN: RUN15414

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.28

EN300-135182_1_1



CID: EN300-135182_1_1

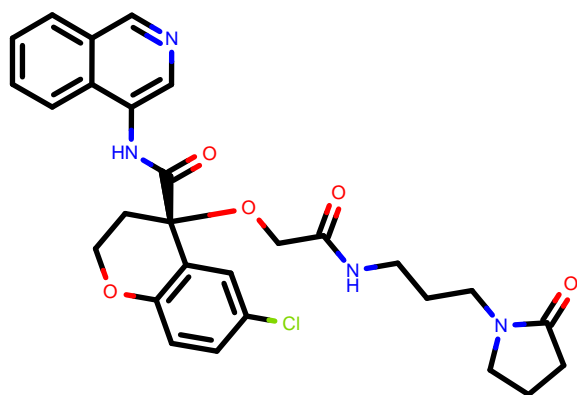
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(O)n6c(n5)nc[nH]6

RUN: RUN3222

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.21

EN300-08259_1_1



CID: EN300-08259_1_1

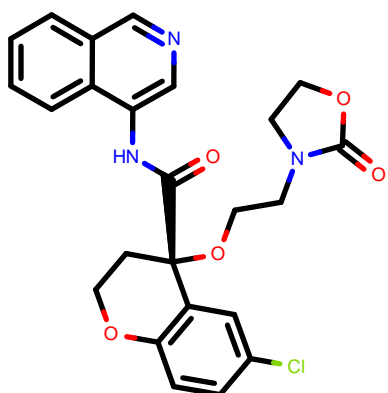
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCN5CCCC5=O

RUN: RUN799

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.31

EN300-370967_1_1



CID: EN300-370967_1_1

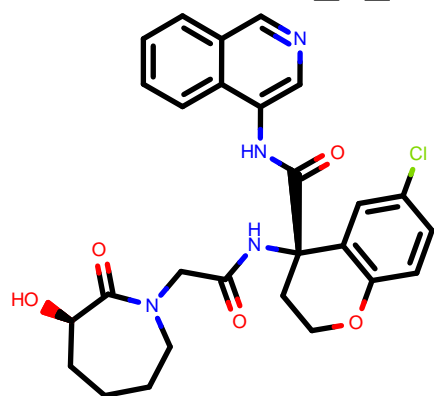
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O

RUN: RUN2028

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.26

EN300-259849_1_1



CID: EN300-259849_1_1

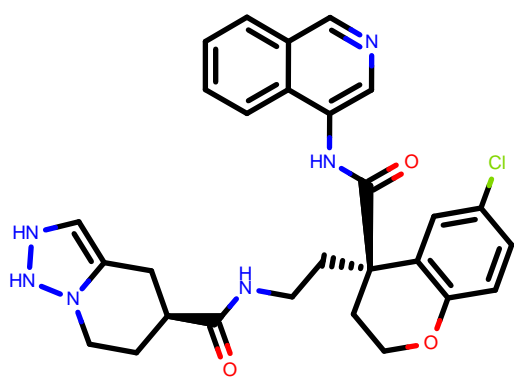
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC[C@H](C5=O)O

RUN: RUN9622

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.24

EN300-7430501_3_1



CID: EN300-7430501_3_1

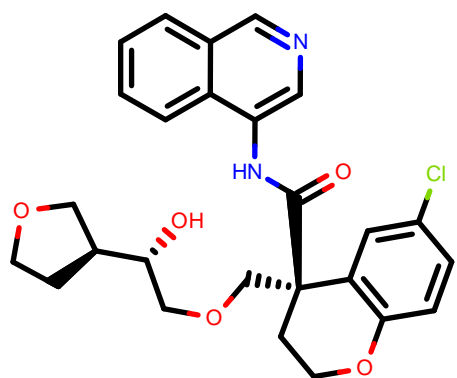
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCN6c(cnn6)C5

RUN: RUN15380

DDG (kcal/mol): -1.61

dDDG (kcal/mol): 0.27

EN300-1911992_2_3



CID: EN300-1911992_2_3

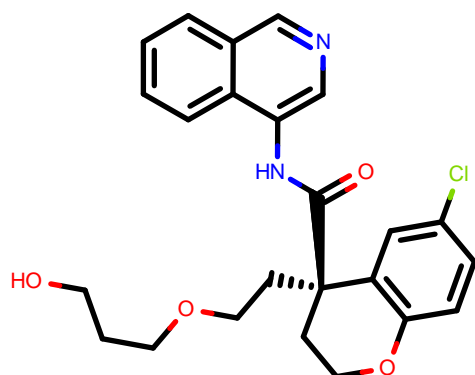
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]3[C@H]5CCOC5O

RUN: RUN276

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.30

EN300-221518_3_1



CID: EN300-221518_3_1

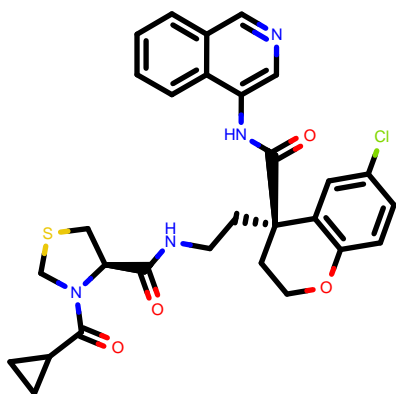
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO

RUN: RUN1064

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.19

EN300-18928_3_1



CID: EN300-18928_3_1

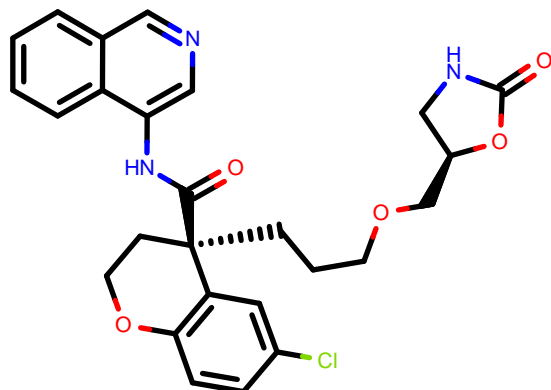
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNCN[C@H]3[C@H]5CSCN6C(=O)O6C0C0

RUN: RUN11976

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.27

EN300-203293_4_1



CID: EN300-203293_4_1

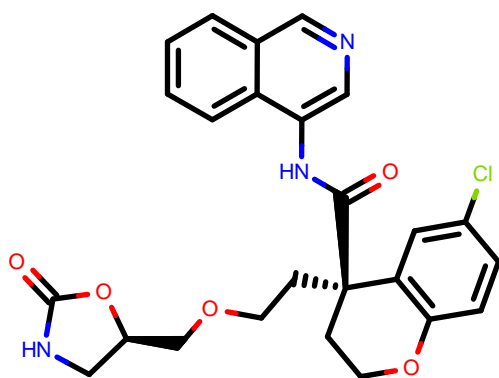
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]3CNC(=O)O5

RUN: RUN1898

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.24

EN300-203293_3_1



CID: EN300-203293_3_1

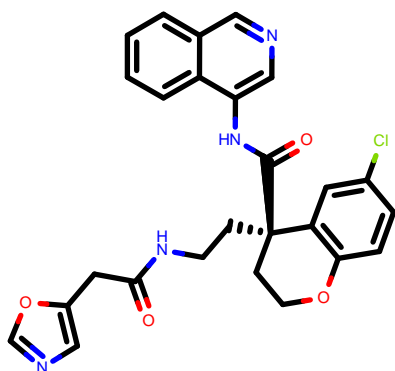
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5CNC(=O)O5

RUN: RUN1744

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.25

EN300-6491117_3_1



CID: EN300-6491117_3_1

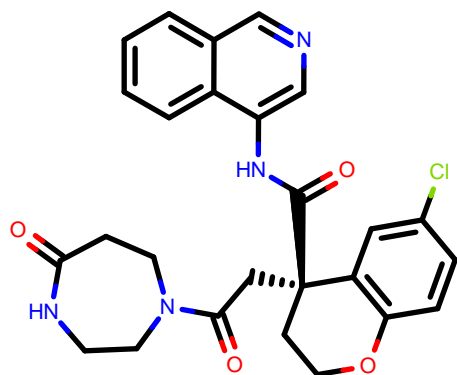
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5cnoc5

RUN: RUN15262

DDG (kcal/mol): -1.60

dDDG (kcal/mol): 0.24

EN300-69107_1_1



CID: EN300-69107_1_1

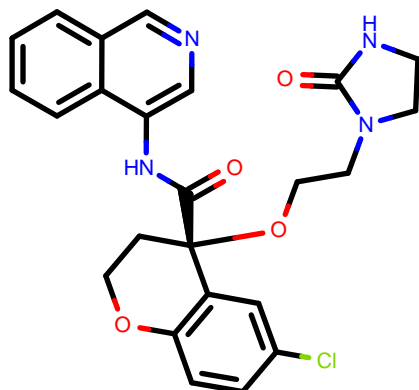
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(=O)NCC5

RUN: RUN9556

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.26

EN300-214800_1_1



CID: EN300-214800_1_1

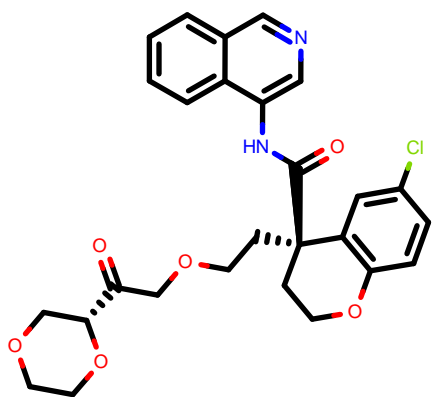
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCN5CCNC5=O

RUN: RUN911

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.27

EN300-6238494_3_2



CID: EN300-6238494_3_2

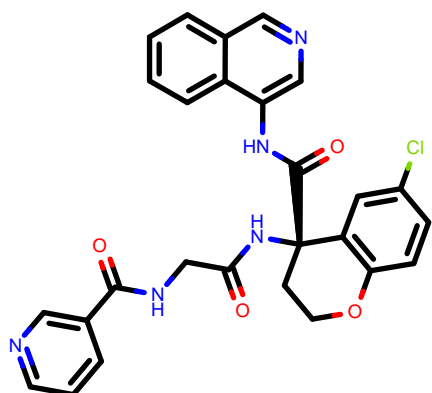
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@H]5COCCO5

RUN: RUN562

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.26

EN300-107990_1_1



CID: EN300-107990_1_1

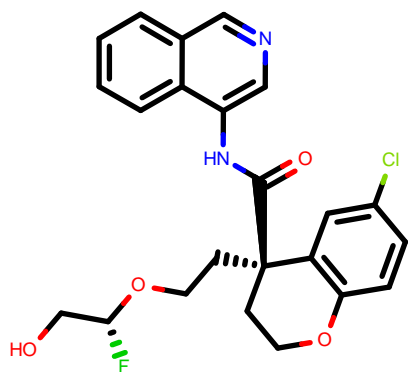
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5ccncc5

RUN: RUN9569

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

EN300-861925_3_2



CID: EN300-861925_3_2

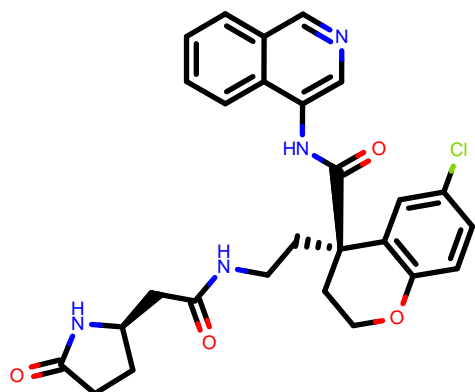
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H](CO)F

RUN: RUN1056

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.23

EN300-68203_3_1



CID: EN300-68203_3_1

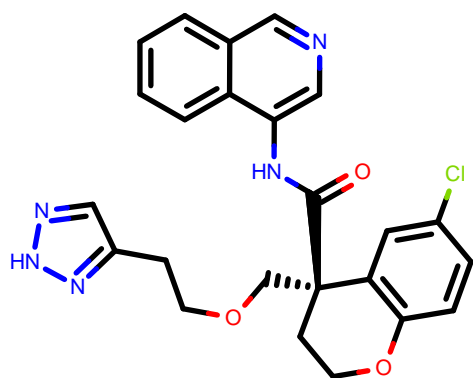
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCC(=O)N5

RUN: RUN8608

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

EN300-222357_2_1



CID: EN300-222357_2_1

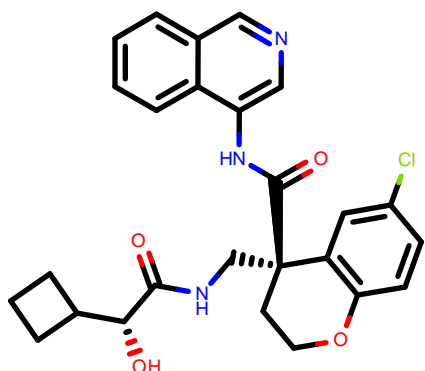
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCc5cn[nH]n5

RUN: RUN628

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.19

EN300-249764_2_1



CID: EN300-249764_2_1

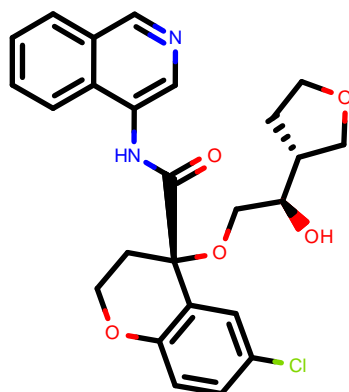
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]H(C5CCCC5)O

RUN: RUN3571

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.26

EN300-1911992_1_2



CID: EN300-1911992_1_2

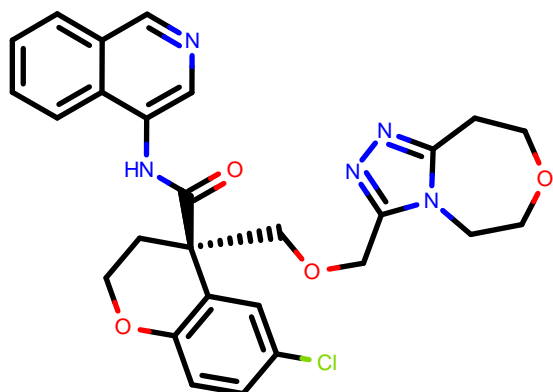
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]H(C5CCOC5)O

RUN: RUN599

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.26

EN300-310888_2_1



CID: EN300-310888_2_1

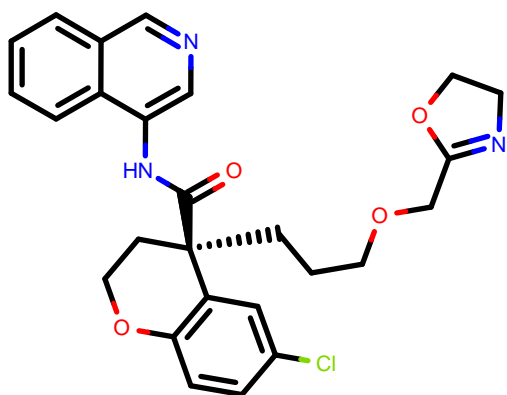
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nn6n5CCOC6

RUN: RUN828

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.24

EN300-317555_4_1



CID: EN300-317555_4_1

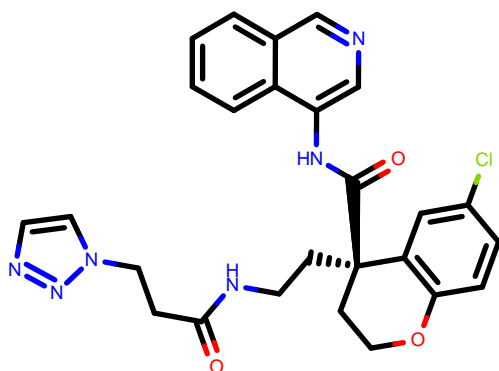
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5

RUN: RUN1962

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.18

EN300-28871_3_1



CID: EN300-28871_3_1

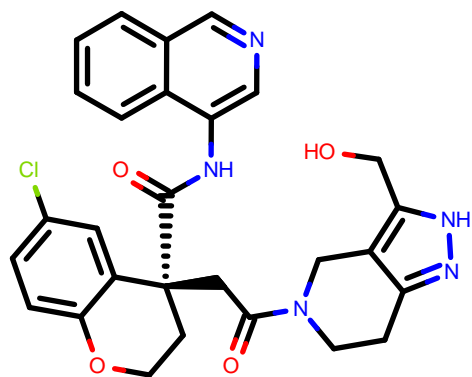
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5C=CN5

RUN: RUN3941

DDG (kcal/mol): -1.59

dDDG (kcal/mol): 0.25

EN300-6732784_1_1



CID: EN300-6732784_1_1

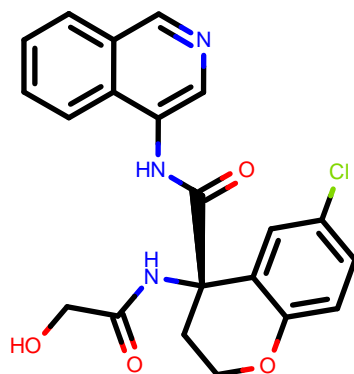
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6c(c([nH]6)CO)C5

RUN: RUN4477

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.24

EN300-19242_1_1



CID: EN300-19242_1_1

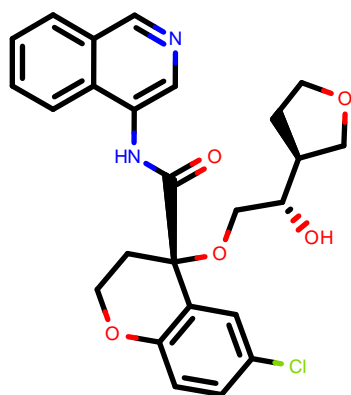
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO

RUN: RUN3894

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.15

EN300-1911992_1_3



CID: EN300-1911992_1_3

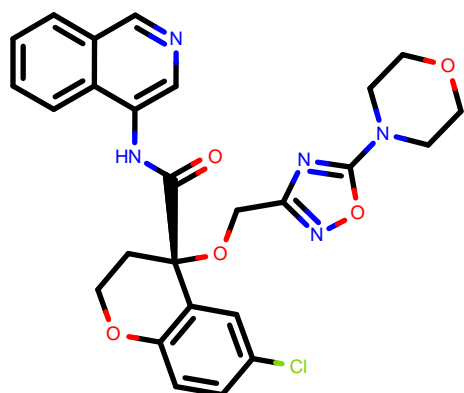
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCOC5O

RUN: RUN1980

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.25

EN300-1608590_1_1



CID: EN300-1608590_1_1

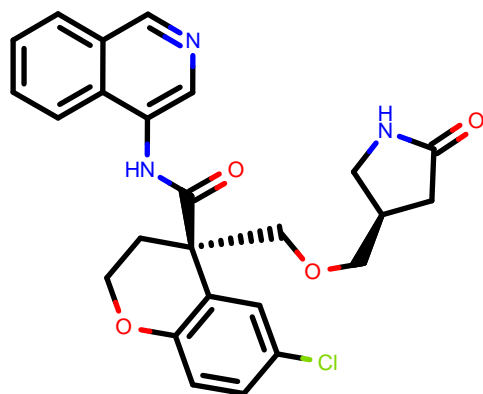
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(on5)N6COCOC6

RUN: RUN975

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.26

EN300-246747_2_1



CID: EN300-246747_2_1

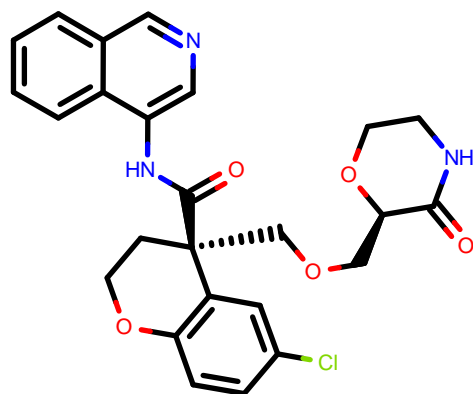
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C(=O)NC5

RUN: RUN1849

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.23

EN300-1706036_2_2



CID: EN300-1706036_2_2

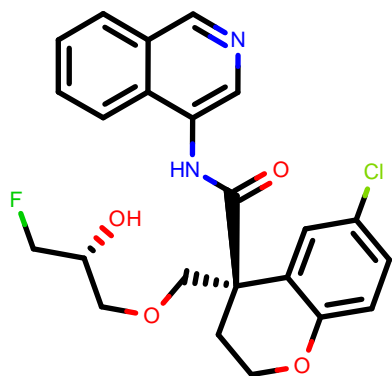
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C(=O)NCCO5

RUN: RUN780

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.21

EN300-1968342_2_2



CID: EN300-1968342_2_2

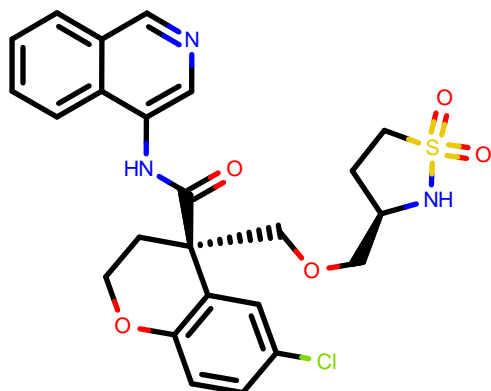
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O

RUN: RUN1865

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.25

EN300-1699871_2_1



CID: EN300-1699871_2_1

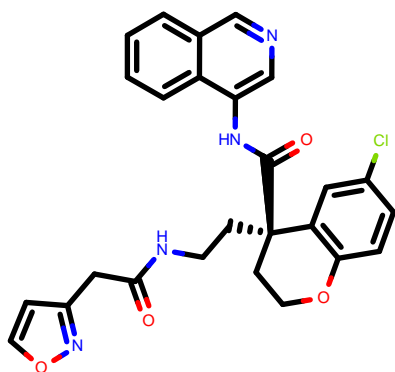
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCS(=O)(=O)N5

RUN: RUN2387

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.28

EN300-82037_3_1



CID: EN300-82037_3_1

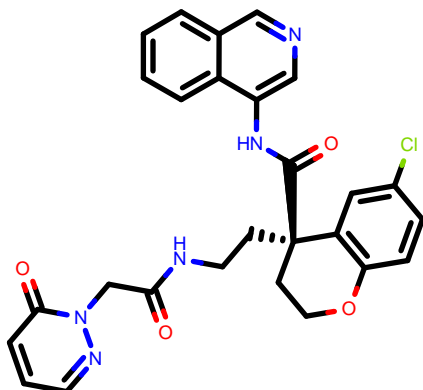
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5=CN=CN5

RUN: RUN14824

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.24

EN300-237561_3_1



CID: EN300-237561_3_1

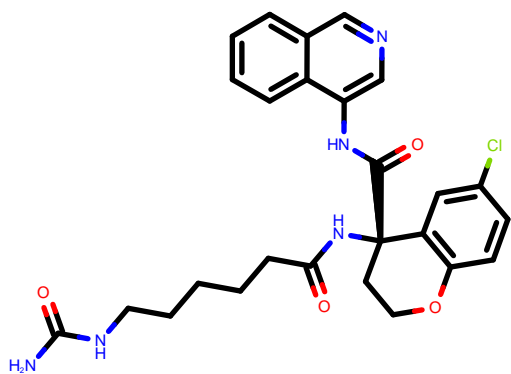
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5c(=O)ccn5

RUN: RUN11449

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.28

EN300-13252_1_1



CID: EN300-13252_1_1

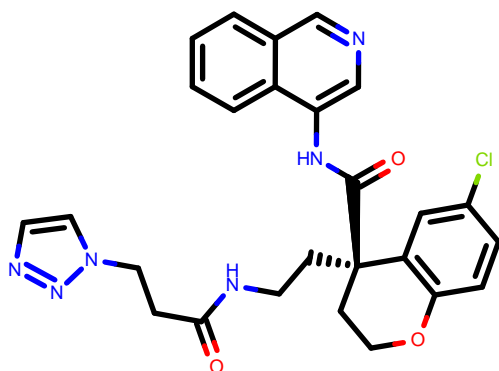
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCCNC(=O)N

RUN: RUN4306

DDG (kcal/mol): -1.58

dDDG (kcal/mol): 0.30

EN300-28871_3_1



CID: EN300-28871_3_1

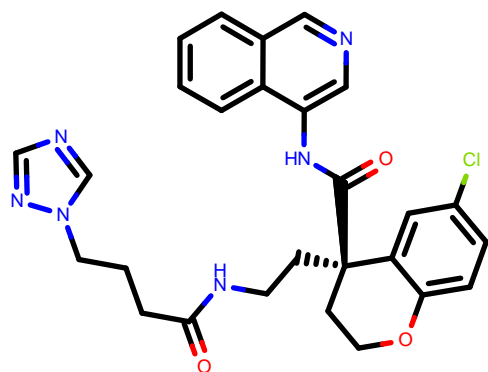
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5ccn5

RUN: RUN3937

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.25

EN300-316216_3_1



CID: EN300-316216_3_1

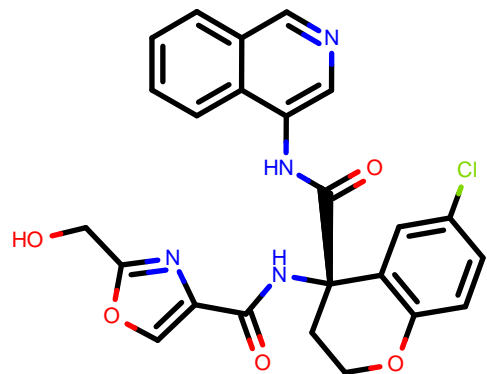
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCCn5ccn5

RUN: RUN11214

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.29

EN300-7549555_1_1



CID: EN300-7549555_1_1

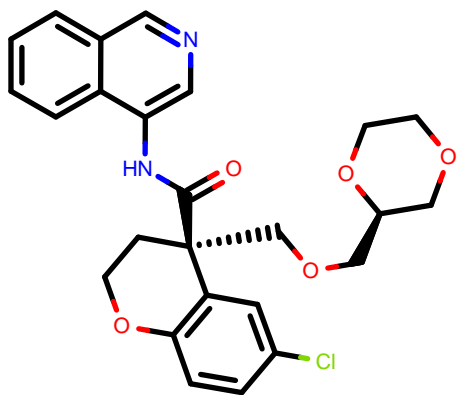
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccn5CO

RUN: RUN1537

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.19

EN300-139167_2_2



CID: EN300-139167_2_2

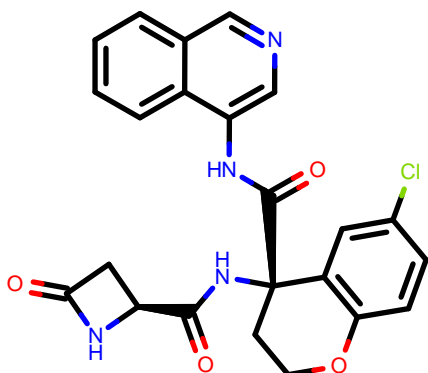
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@H]5COC(=O)5

RUN: RUN924

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.20

EN300-101505_1_1



CID: EN300-101505_1_1

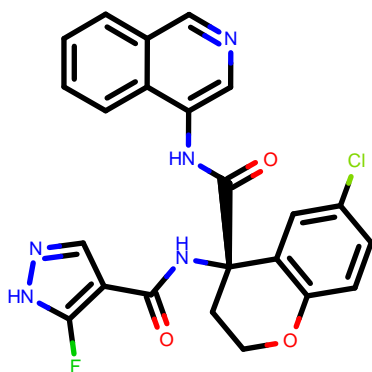
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CC(=O)N5

RUN: RUN1169

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.19

EN300-7121836_1_1



CID: EN300-7121836_1_1

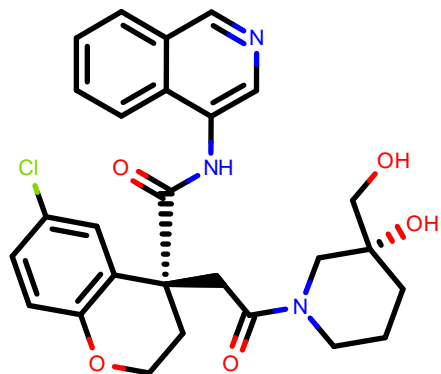
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn[nH]c5F

RUN: RUN3338

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.18

EN300-251396_1_1



CID: EN300-251396_1_1

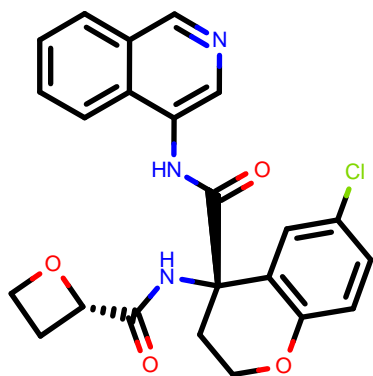
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@]3(C5)C(O)O

RUN: RUN6911

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.28

EN300-85760_1_1



CID: EN300-85760_1_1

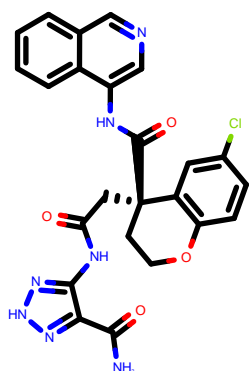
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]HJ5CCO5

RUN: RUN2938

DDG (kcal/mol): -1.57

dDDG (kcal/mol): 0.20

EN300-116238_1_1



CID: EN300-116238_1_1

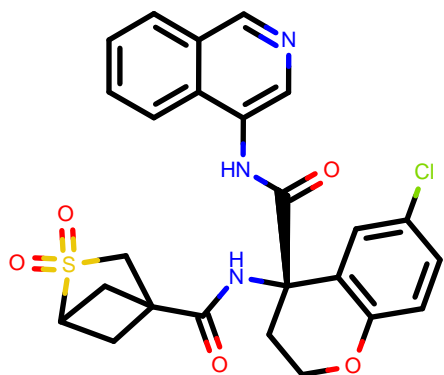
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5c(n[nH]n5)C(=O)N

RUN: RUN14134

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.22

EN300-7354033_1_1



CID: EN300-7354033_1_1

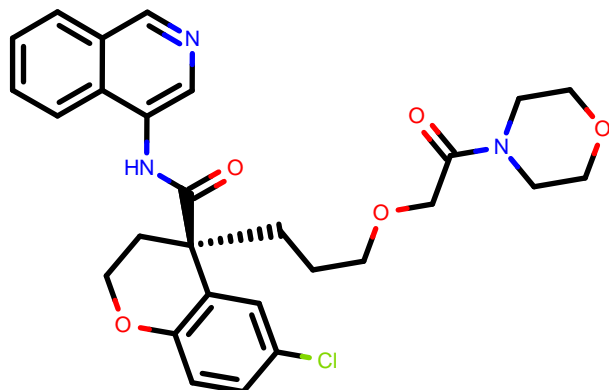
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C56CC(C5)S(=O)(=O)C6

RUN: RUN3890

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.23

EN300-1241327_4_1



CID: EN300-1241327_4_1

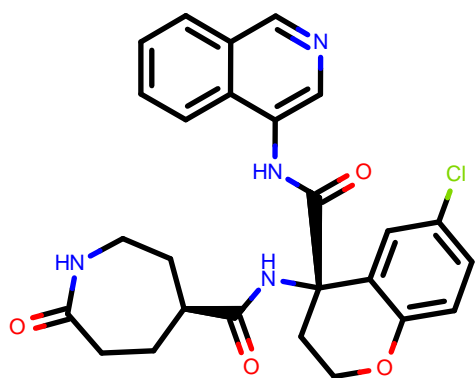
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)N5CCOCC5

RUN: RUN1291

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.26

EN300-152337_1_2



CID: EN300-152337_1_2

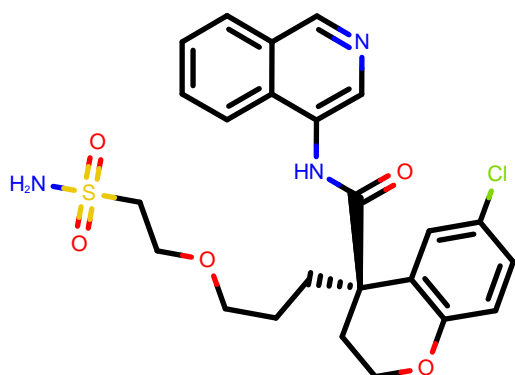
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCC(=O)NCC5

RUN: RUN3402

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.21

EN300-270710_4_1



CID: EN300-270710_4_1

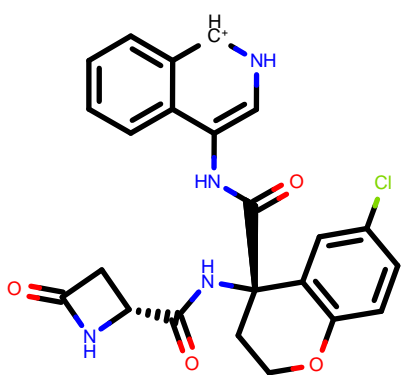
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)N

RUN: RUN1906

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.27

EN300-101505_1_2



CID: EN300-101505_1_2

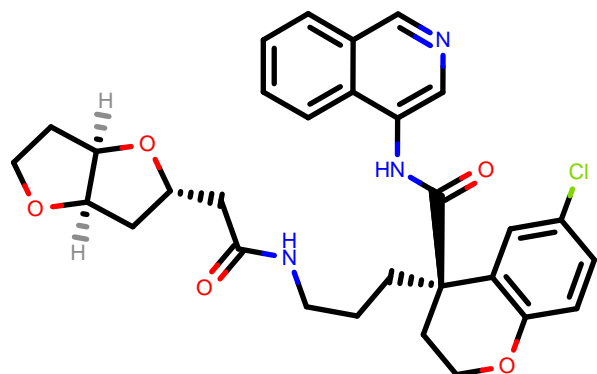
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5

RUN: RUN3578

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.20

EN300-7355519_4_6



CID: EN300-7355519_4_6

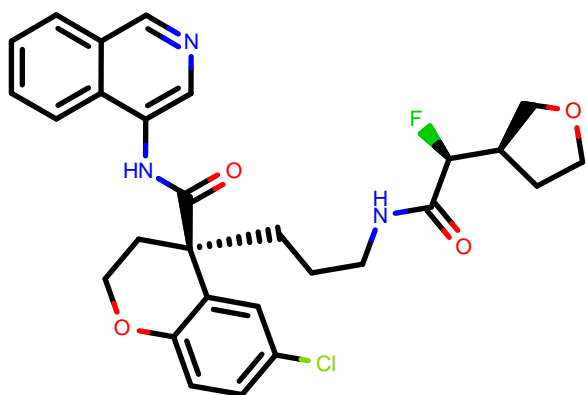
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@@H]5OCOC5

RUN: RUN11516

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.29

EN300-783124_4_2



CID: EN300-783124_4_2

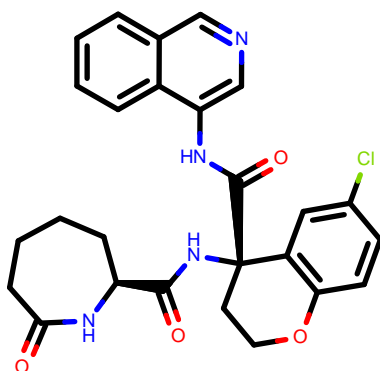
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@@H5CCOC5F

RUN: RUN10784

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.24

EN300-80083_1_1



CID: EN300-80083_1_1

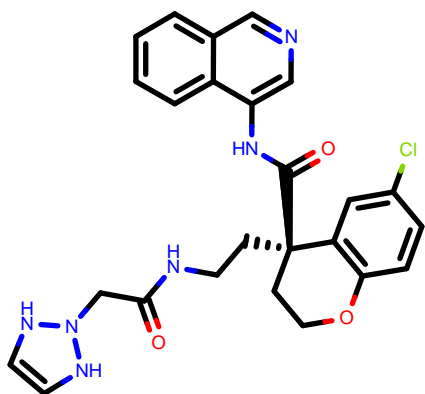
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN251

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.21

EN300-100916_3_1



CID: EN300-100916_3_1

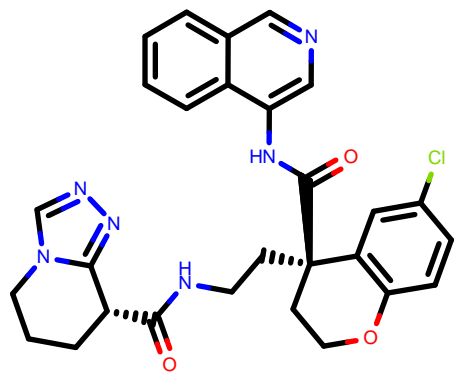
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5nccn5

RUN: RUN11431

DDG (kcal/mol): -1.56

dDDG (kcal/mol): 0.21

EN300-748981_3_1



CID: EN300-748981_3_1

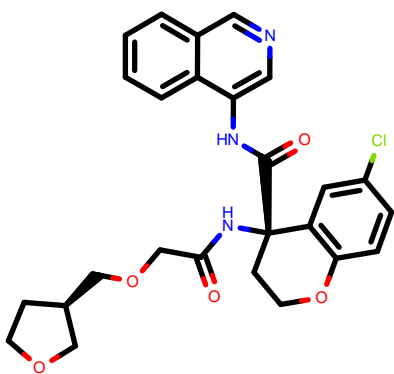
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCN6c5nnc6

RUN: RUN9252

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.31

EN300-80522_1_1



CID: EN300-80522_1_1

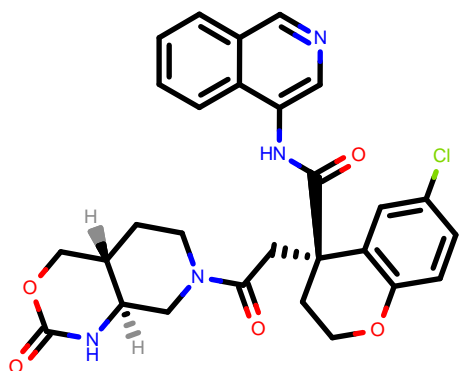
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@]5CCOC5

RUN: RUN7400

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.23

EN300-262599_1_1



CID: EN300-262599_1_1

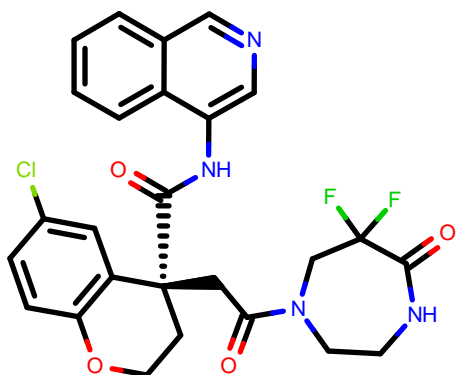
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6COC(=O)N[C@@]6C5

RUN: RUN6105

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.25

EN300-1083988_1_1



CID: EN300-1083988_1_1

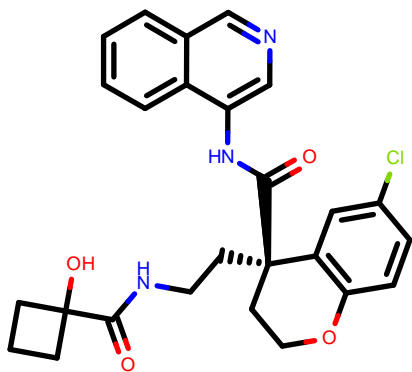
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)C(C5)(F)F

RUN: RUN10347

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.25

EN300-52009_3_1



CID: EN300-52009_3_1

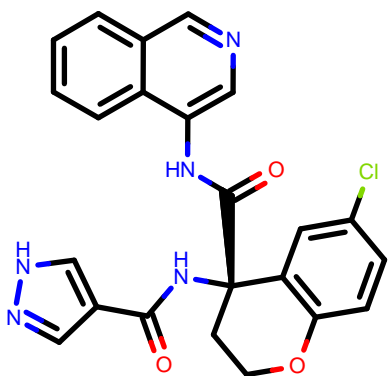
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)O

RUN: RUN4229

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.24

EN300-41863_1_1



CID: EN300-41863_1_1

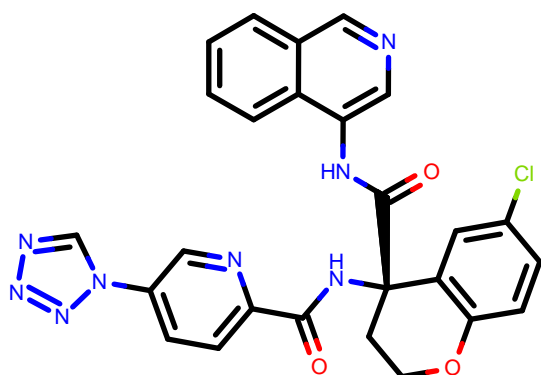
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]nc5

RUN: RUN5726

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.17

EN300-262409_1_1



CID: EN300-262409_1_1

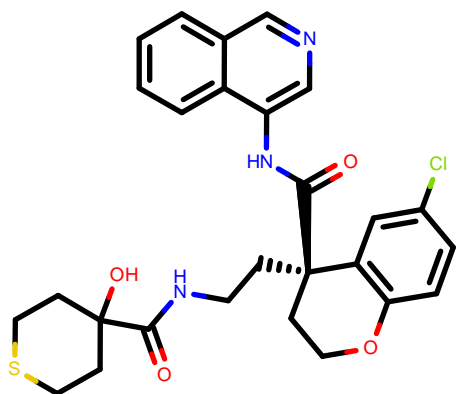
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(cn5)n6cnm6

RUN: RUN9901

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.16

EN300-122340_3_1



CID: EN300-122340_3_1

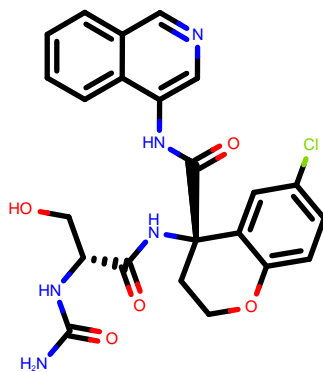
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCSCC5)O

RUN: RUN9036

DDG (kcal/mol): -1.55

dDDG (kcal/mol): 0.28

EN300-10170_1_1



CID: EN300-10170_1_1

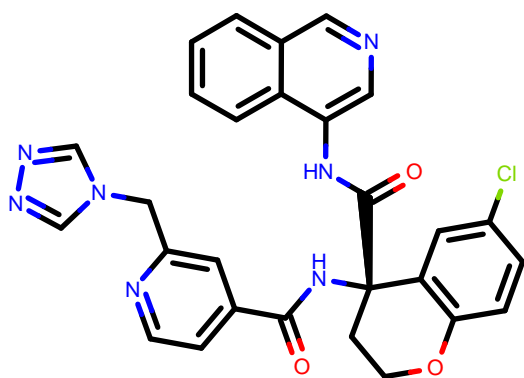
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4(CO)NC(=O)N

RUN: RUN643

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.33

EN300-5309123_1_1



CID: EN300-5309123_1_1

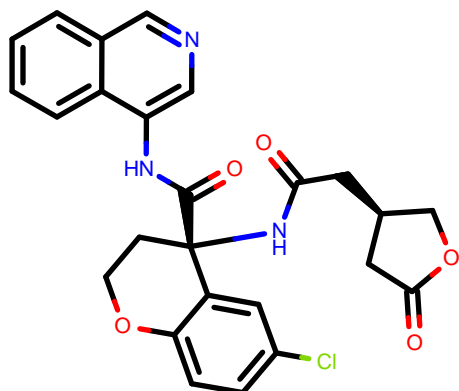
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnc(c5)Cn6cnnc6

RUN: RUN5510

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.28

EN300-109535_1_1



CID: EN300-109535_1_1

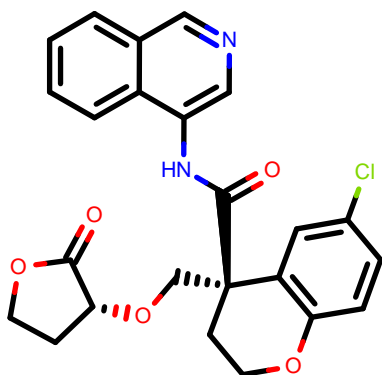
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]4H5CC(=O)OC5

RUN: RUN5190

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.23

EN300-20496_2_2



CID: EN300-20496_2_2

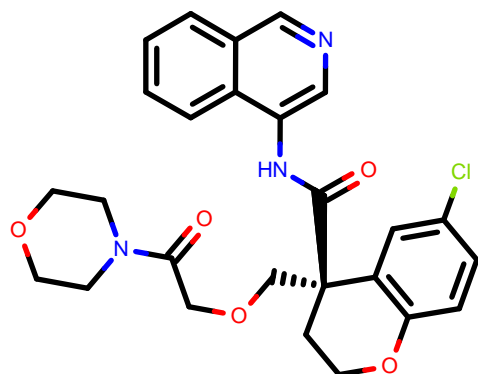
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]4H5CCOC5=O

RUN: RUN484

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.17

EN300-1241327_2_1



CID: EN300-1241327_2_1

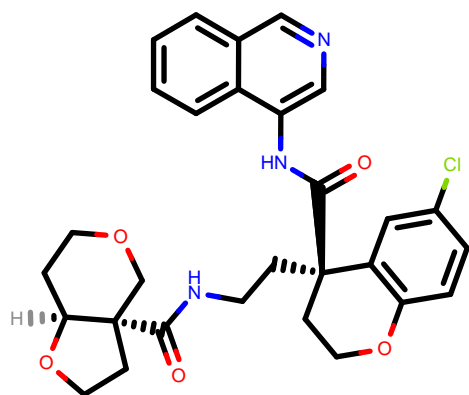
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC(=O)N5CCOC5

RUN: RUN844

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.21

EN300-341337_3_3



CID: EN300-341337_3_3

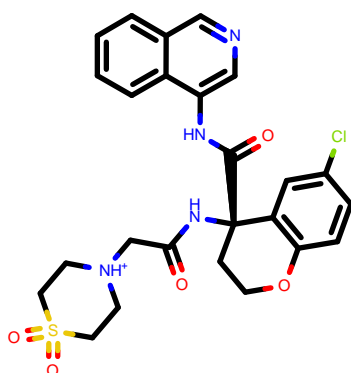
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CCNC(=O)[C@@]56CCO[C@@H]5COO6

RUN: RUN14788

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.26

EN300-39305_1_1



CID: EN300-39305_1_1

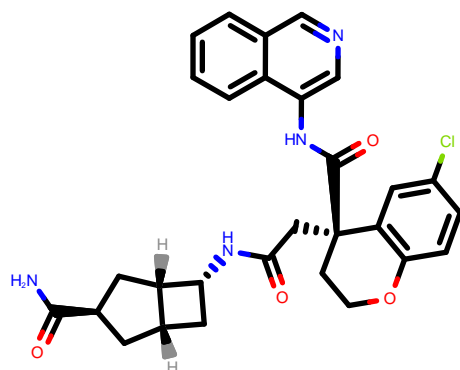
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)NC(=O)N5SCCS(=O)(=O)C5S

RUN: RUN9121

DDG (kcal/mol): -1.54

dDDG (kcal/mol): 0.29

EN300-1268016_1_15



CID: EN300-1268016_1_15

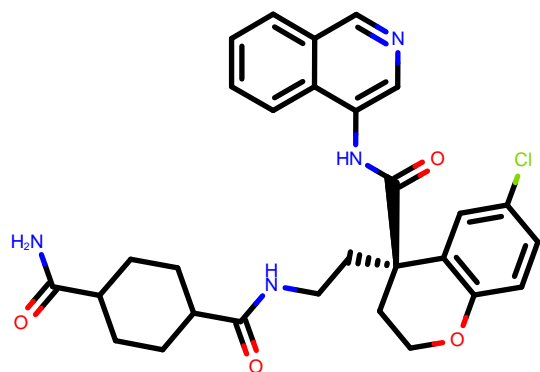
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)C(C)=O)N[C@@]5H5C[C@@H]6[C@@H]5C[C@@]7H[C@@]6)C1=O)N

RUN: RUN5877

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.31

EN300-35778_3_1



CID: EN300-35778_3_1

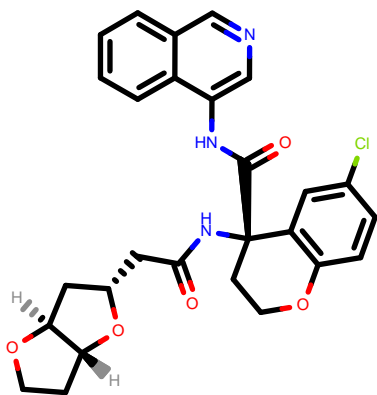
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CCNC(=O)C5CCCC(C5)C(=O)N

RUN: RUN13506

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.30

EN300-735519_1_7



CID: EN300-735519_1_7

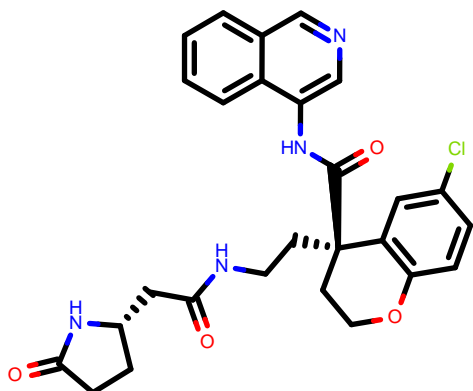
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CNC(=O)C[C@@H]5C[C@@H]5OCCO6

RUN: RUN9679

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.22

EN300-68203_3_2



CID: EN300-68203_3_2

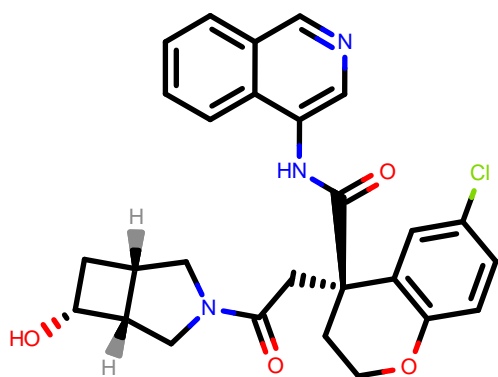
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CNC(=O)C[C@@H]5C[C@@H]5O

RUN: RUN8728

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.27

EN300-305294_1_7



CID: EN300-305294_1_7

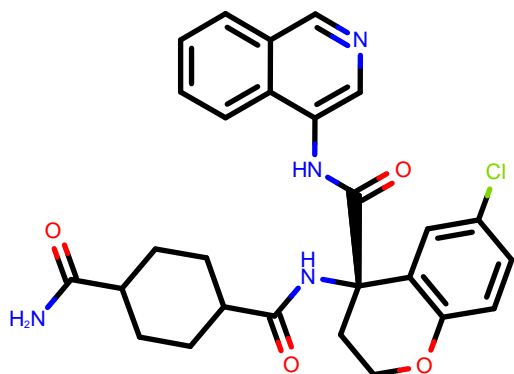
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CNC(=O)C[C@@H]5C[C@@H]5O

RUN: RUN11922

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.22

EN300-35778_1_1



CID: EN300-35778_1_1

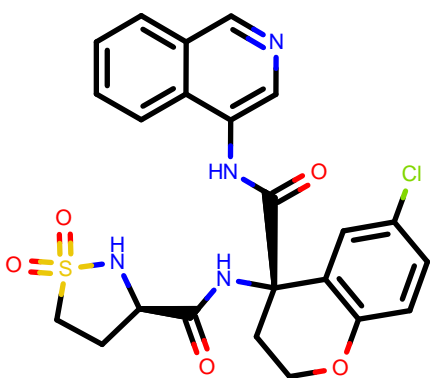
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CNC(=O)C5CCCC(C5)N

RUN: RUN3502

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-45049_1_2



CID: EN300-45049_1_2

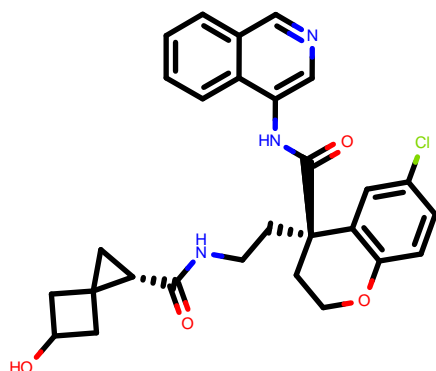
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCS(=O)(=O)N5

RUN: RUN6796

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.32

EN300-1717166_3_2



CID: EN300-1717166_3_2

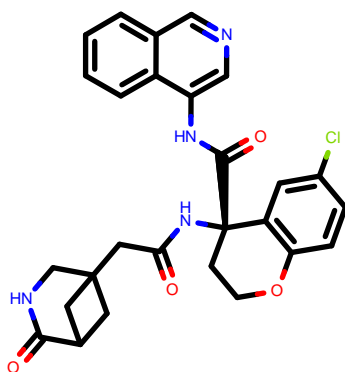
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CC56C(C)C6O

RUN: RUN15348

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-6487134_1_1



CID: EN300-6487134_1_1

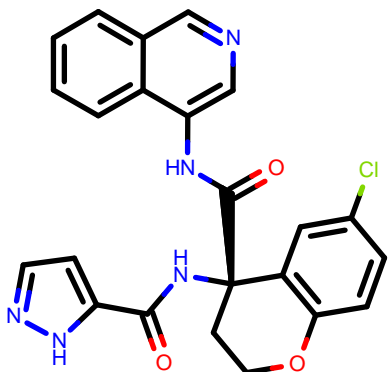
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC56CC(C5)C(=O)NC6

RUN: RUN9793

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.23

EN300-37077_1_1



CID: EN300-37077_1_1

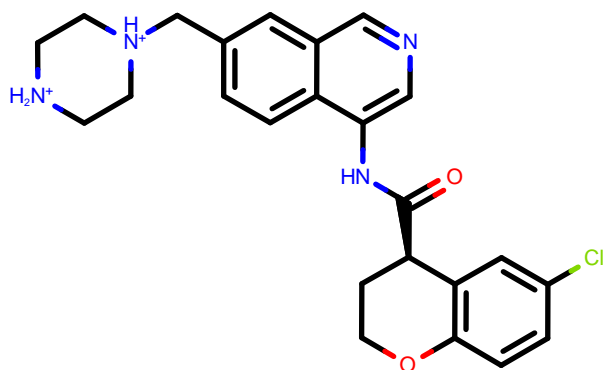
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc[nH]5

RUN: RUN4138

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.19

MAK-UNK-8be7dca9-1_1



CID: MAK-UNK-8be7dca9-1_1

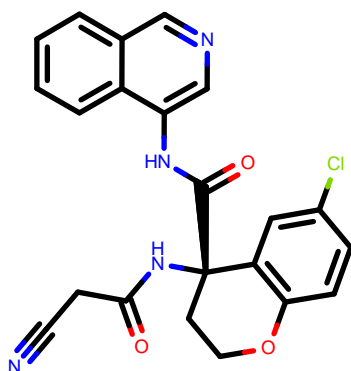
SMILES: c1ccc2c(cc1CN3CC[NH2+][CC3])ncc2NC(=O)[C@@H]4CCOC5c4cc(cc5)Cl

RUN: RUN40

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.13

EN300-19926_1_1



CID: EN300-19926_1_1

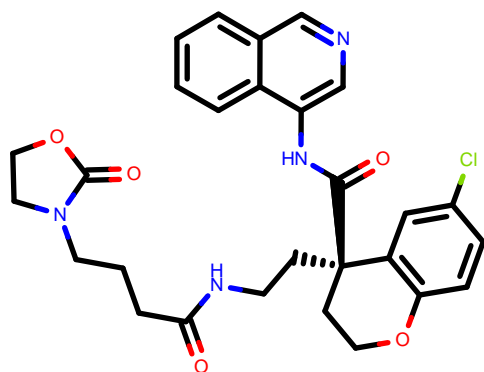
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC#N

RUN: RUN5698

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.16

EN300-45182_3_1



CID: EN300-45182_3_1

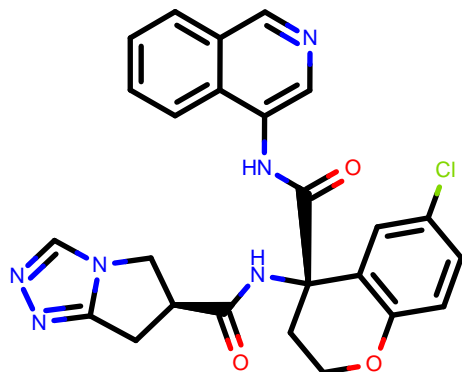
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCN5CCOC5=O

RUN: RUN11164

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.28

EN300-6745453_1_2



CID: EN300-6745453_1_2

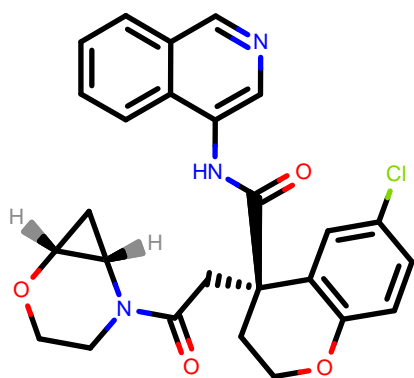
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C6nncn6C5

RUN: RUN8436

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.24

EN300-91609_1_3



CID: EN300-91609_1_3

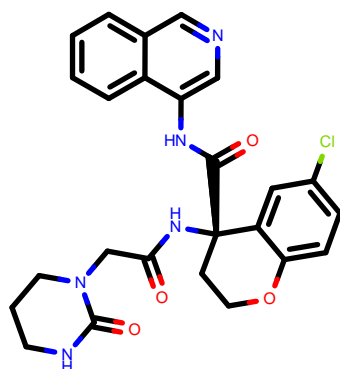
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@H]6[C@@H]5C6

RUN: RUN11563

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.20

EN300-36096_1_1



CID: EN300-36096_1_1

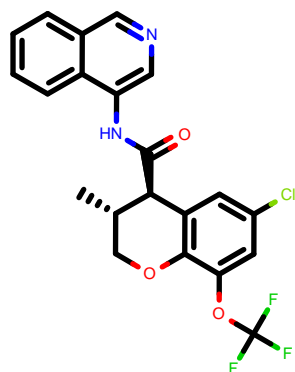
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CN5CCNC5=O

RUN: RUN9577

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.26

DAR-DIA-0d514e7d-18_1



CID: DAR-DIA-0d514e7d-18_1

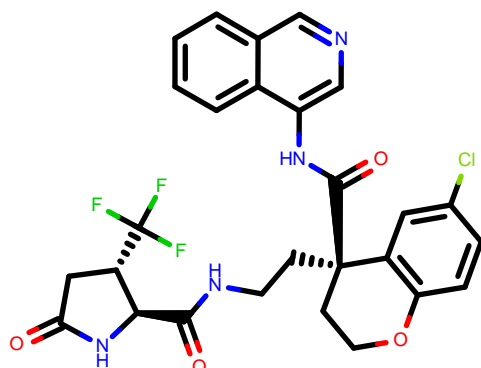
SMILES: C[C@H]1COc2c(cc(cc2OC(F)(F)F)C)I[C@@H]1C(=O)Nc3cncc4c3cccc4

RUN: RUN159

DDG (kcal/mol): -1.53

dDDG (kcal/mol): 0.13

EN300-169955_3_1



CID: EN300-169955_3_1

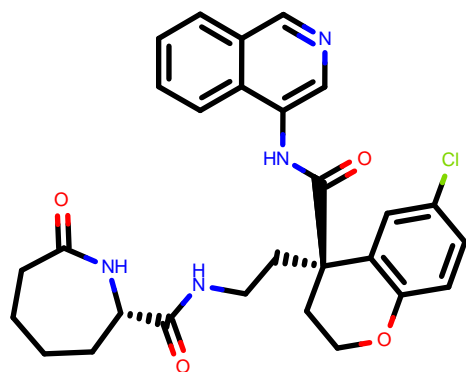
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5[C@H](CC(=O)N5)C(F)F

RUN: RUN15055

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.27

EN300-80083_3_1



CID: EN300-80083_3_1

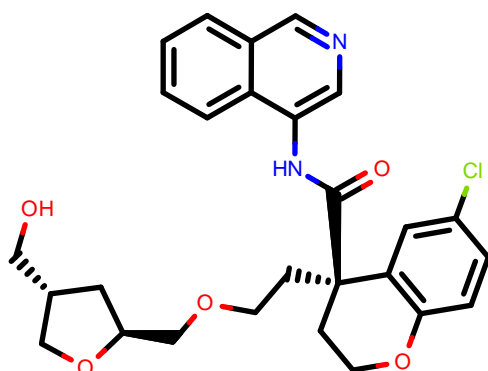
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5CCCCC(=O)N5

RUN: RUN14376

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.28

EN300-6494158_3_4



CID: EN300-6494158_3_4

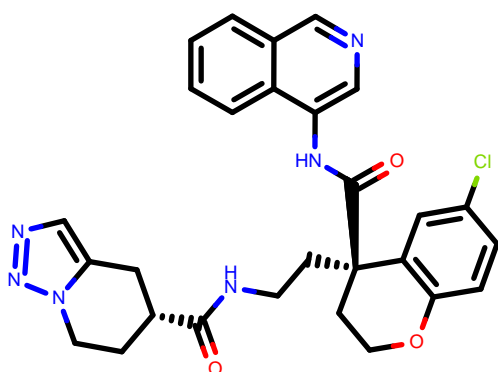
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]H5C[C@H](CO)5CO

RUN: RUN2126

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

EN300-7430501_3_2



CID: EN300-7430501_3_2

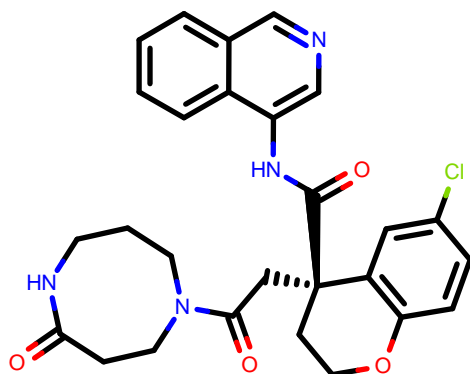
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5C[C@H](c6nnc6)C5

RUN: RUN15223

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.27

EN300-1072874_1_1



CID: EN300-1072874_1_1

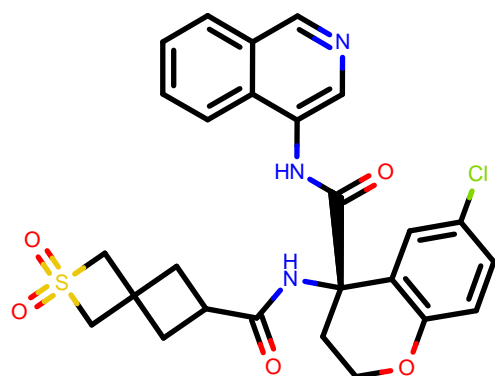
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCCNC(=O)CC5

RUN: RUN11713

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.27

EN300-318305_1_1



CID: EN300-318305_1_1

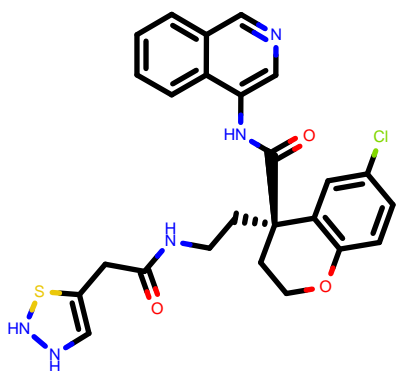
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CC6(C5)CS(=O)(=O)C6

RUN: RUN8496

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.23

EN300-260152_3_1



CID: EN300-260152_3_1

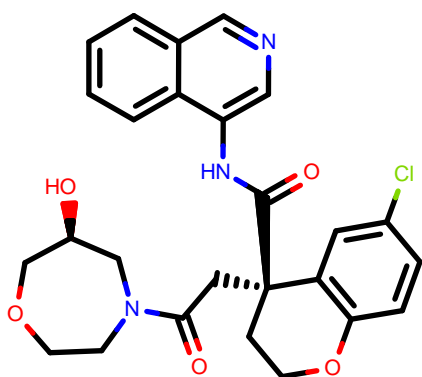
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5enns5

RUN: RUN14664

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.22

EN300-233951_1_1



CID: EN300-233951_1_1

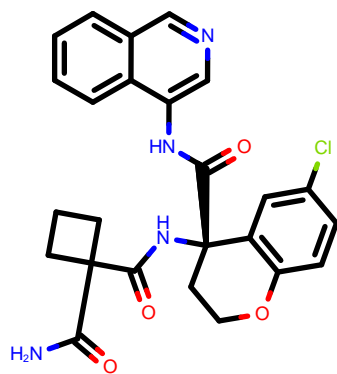
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCOC[C@H](C5)O

RUN: RUN9777

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.29

EN300-68747_1_1



CID: EN300-68747_1_1

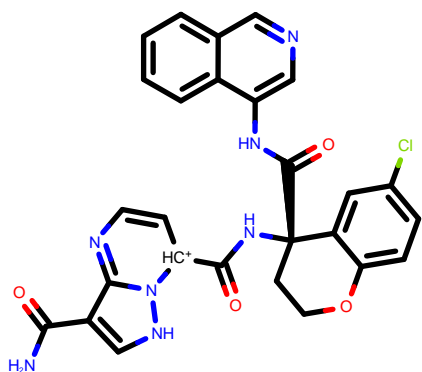
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCC5)C(=O)N

RUN: RUN6688

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

EN300-113564_1_1



CID: EN300-113564_1_1

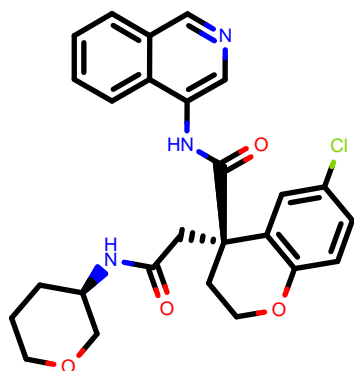
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6n5ncc6C(=O)N

RUN: RUN6956

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.25

JAG-UCB-706446eb-7_1



CID: JAG-UCB-706446eb-7_1

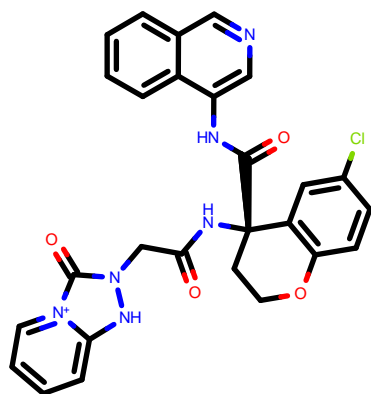
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4H5CCCCO45

RUN: RUN238

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.21

EN300-27476_1_1



CID: EN300-27476_1_1

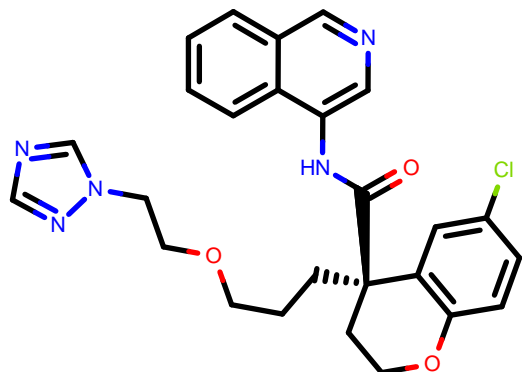
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6ccccc6n5

RUN: RUN9808

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.31

EN300-6255179_4_1



CID: EN300-6255179_4_1

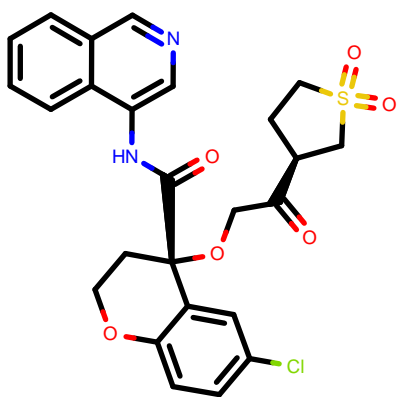
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCn5cnc5

RUN: RUN1379

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.23

EN300-226314_1_2



CID: EN300-226314_1_2

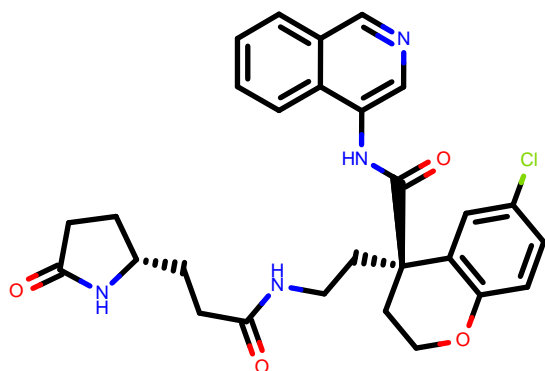
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5CCS(=O)(=O)C5

RUN: RUN351

DDG (kcal/mol): -1.52

dDDG (kcal/mol): 0.34

EN300-104592_3_1



CID: EN300-104592_3_1

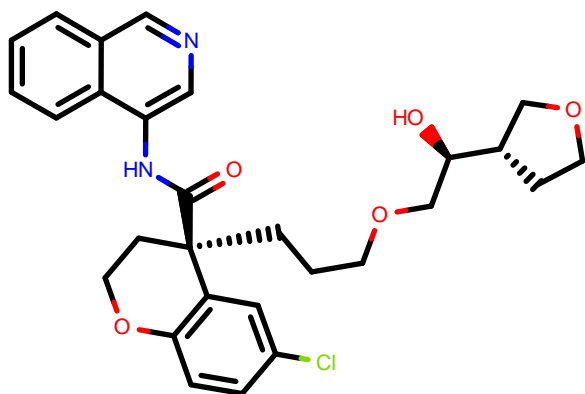
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[C@H]5CCCC(=O)N5

RUN: RUN6360

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.29

EN300-1911992_4_3



CID: EN300-1911992_4_3

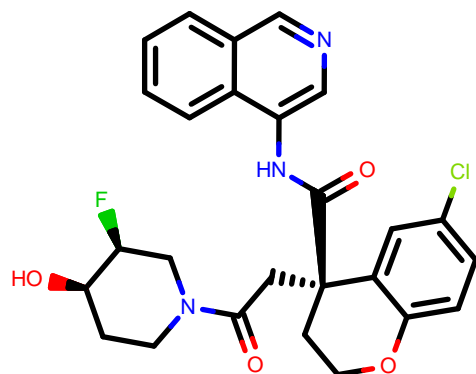
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]([C@H]5CCOC5)O

RUN: RUN957

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.29

EN300-741926_1_2



CID: EN300-741926_1_2

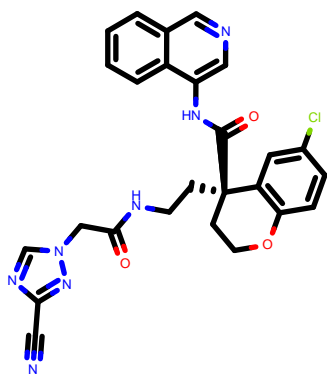
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@H](C5)F)O

RUN: RUN10655

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.17

EN300-111863_3_1



CID: EN300-111863_3_1

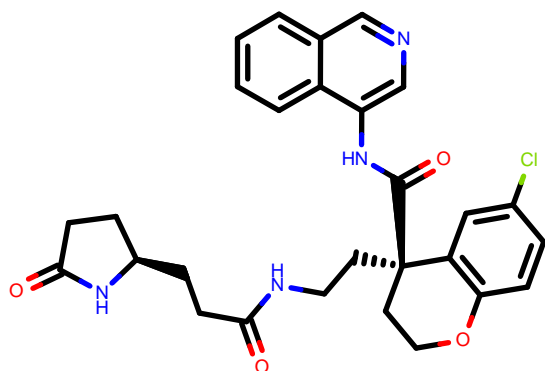
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ncnc5#N

RUN: RUN15345

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.28

EN300-104592_3_2



CID: EN300-104592_3_2

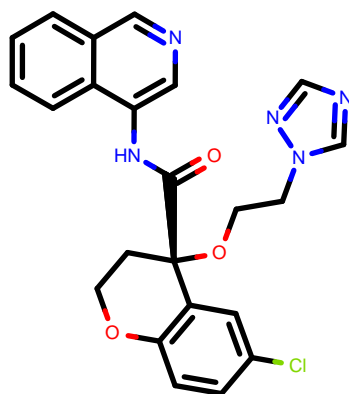
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC[C@@]4H5CCCC(=O)N5

RUN: RUN13718

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.31

EN300-6255179_1_1



CID: EN300-6255179_1_1

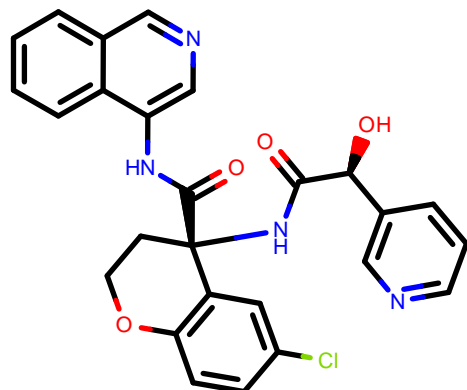
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCn5ncnc5

RUN: RUN1141

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.21

EN300-134855_1_1



CID: EN300-134855_1_1

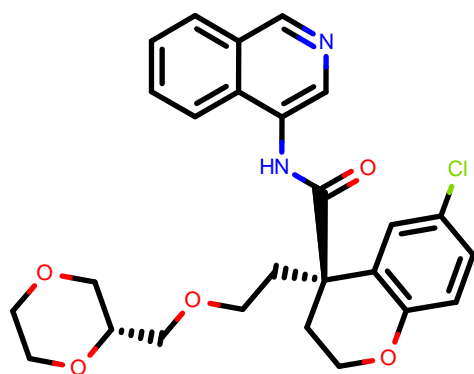
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H](c5ccncc5)O

RUN: RUN8548

DDG (kcal/mol): -1.51

dDDG (kcal/mol): 0.23

EN300-139167_3_1



CID: EN300-139167_3_1

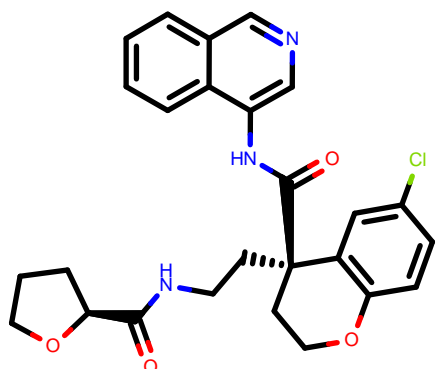
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN1959

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.21

EN300-104395_3_1



CID: EN300-104395_3_1

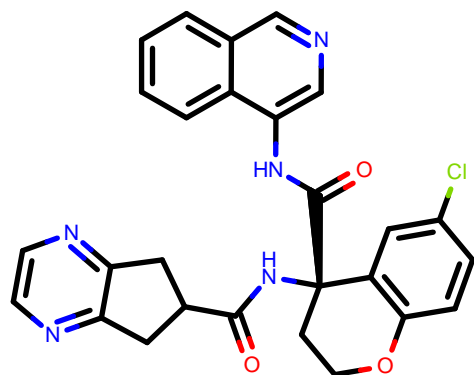
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COCOC5

RUN: RUN14622

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.20

EN300-2011576_1_1



CID: EN300-2011576_1_1

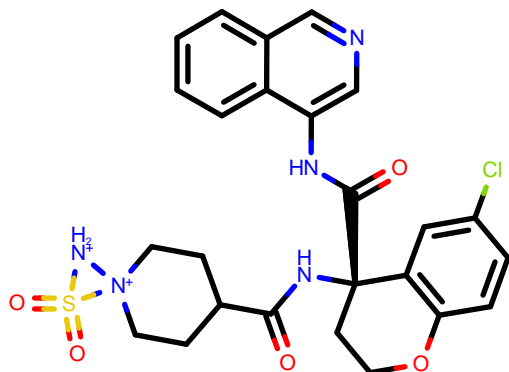
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5C6B(ncn6)C5

RUN: RUN9417

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.24

EN300-31102_1_1



CID: EN300-31102_1_1

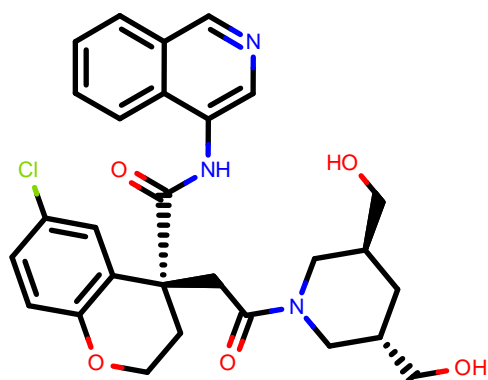
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCN(C5)S(=O)(=O)N

RUN: RUN3586

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.37

EN300-2007627_1_1



CID: EN300-2007627_1_1

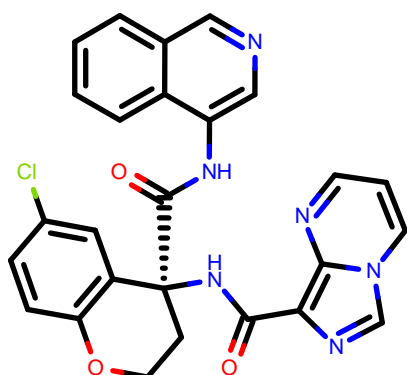
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C1CC1=O)NSC(C@H)(C)C(=O)CO

RUN: RUN9690

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.27

EN300-249899_1_1



CID: EN300-249899_1_1

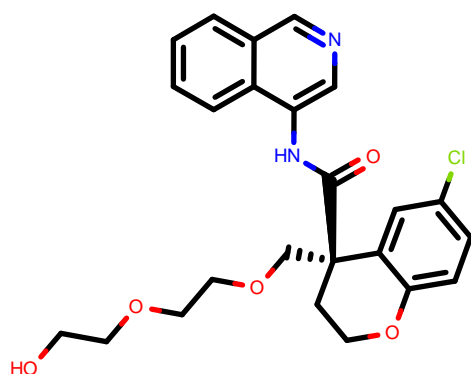
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C1CC1=O)NC(=O)c5c6ncccn6c5

RUN: RUN2095

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.21

EN300-52467_2_1



CID: EN300-52467_2_1

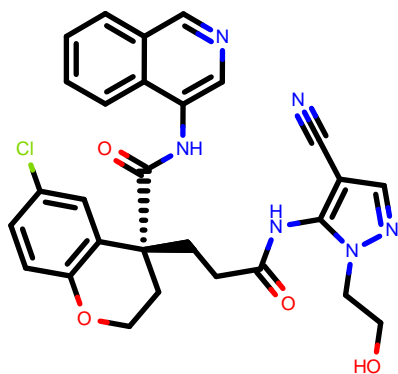
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C1CC1=O)COCOC(=O)C

RUN: RUN748

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.20

EN300-70133_2_1



CID: EN300-70133_2_1

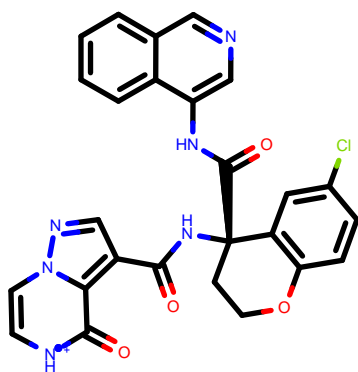
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)C1CC1=O)CCC(=O)Nc5c(cnn5C(=O)C)C#N

RUN: RUN12935

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.26

EN300-7463176_1_1



CID: EN300-7463176_1_1

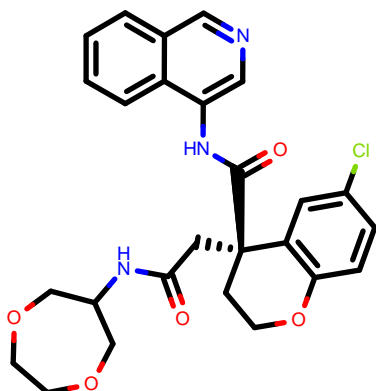
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]c5=O

RUN: RUN8941

DDG (kcal/mol): -1.50

dDDG (kcal/mol): 0.25

EN300-108171_1_1



CID: EN300-108171_1_1

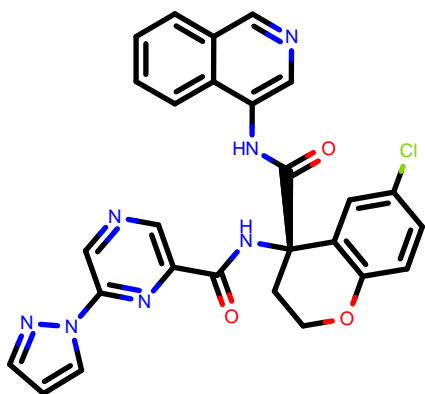
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5OCCOC5

RUN: RUN10693

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.25

EN300-2666483_1_1



CID: EN300-2666483_1_1

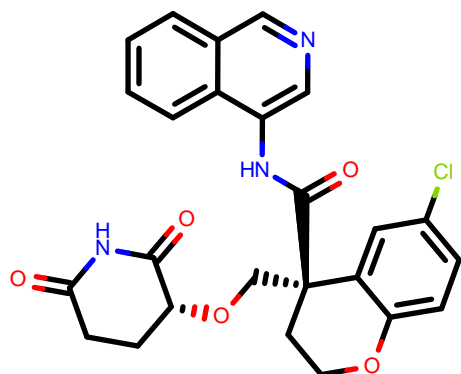
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c5n6cc[nH]6

RUN: RUN8572

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.23

EN300-120920_2_2



CID: EN300-120920_2_2

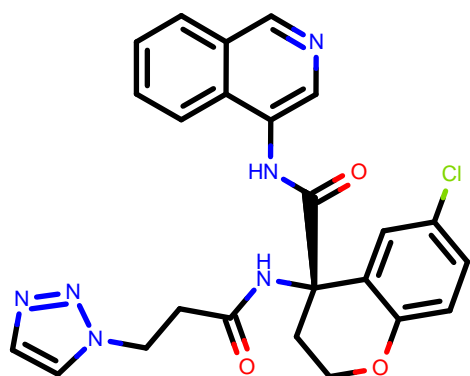
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCCC(=O)NC5=O

RUN: RUN1578

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.21

EN300-28871_1_1



CID: EN300-28871_1_1

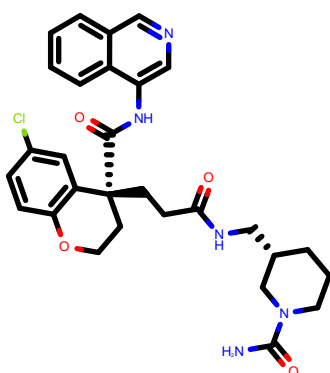
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5

RUN: RUN9105

DDG (kcal/mol): -1.49

dDDG (kcal/mol): 0.22

EN300-212381_2_1



CID: EN300-212381_2_1

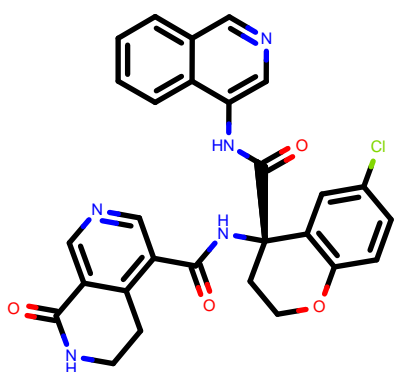
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(C)CCN(C)C5

RUN: RUN5604

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.27

EN300-314274_1_1



CID: EN300-314274_1_1

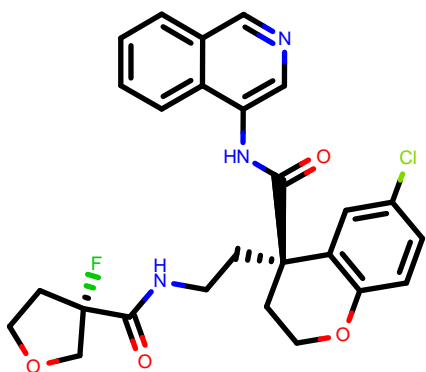
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6c5CCNC6=O

RUN: RUN8849

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.26

EN300-188356_3_1



CID: EN300-188356_3_1

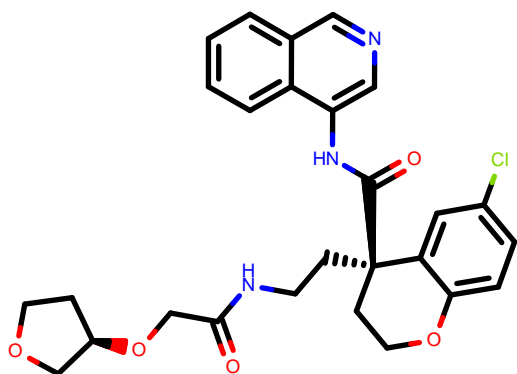
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(C)COC(F)F5

RUN: RUN4981

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.23

EN300-99391_3_1



CID: EN300-99391_3_1

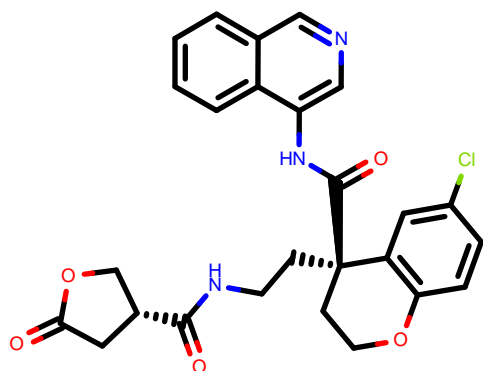
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN8227

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.24

EN300-113234_3_1



CID: EN300-113234_3_1

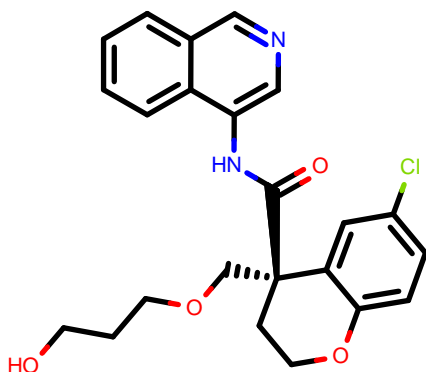
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5OC(=O)OC5

RUN: RUN9200

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.21

EN300-221518_2_1



CID: EN300-221518_2_1

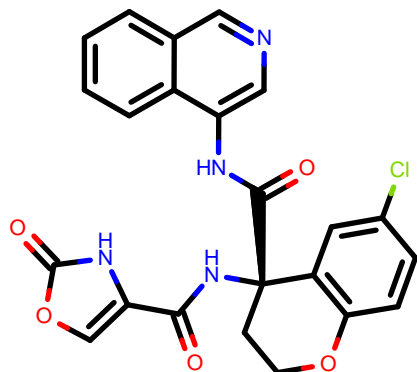
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(CCO)O

RUN: RUN1929

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.18

EN300-246486_1_1



CID: EN300-246486_1_1

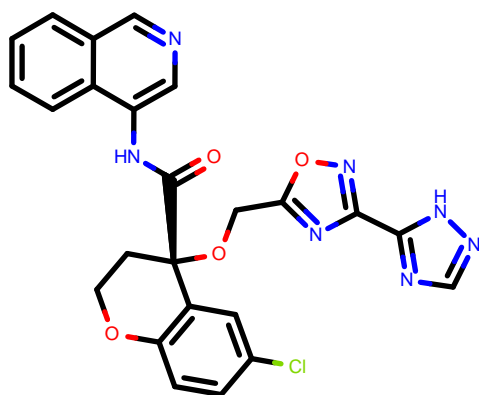
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(=O)[nH]5

RUN: RUN4386

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.19

EN300-92031_1_1



CID: EN300-92031_1_1

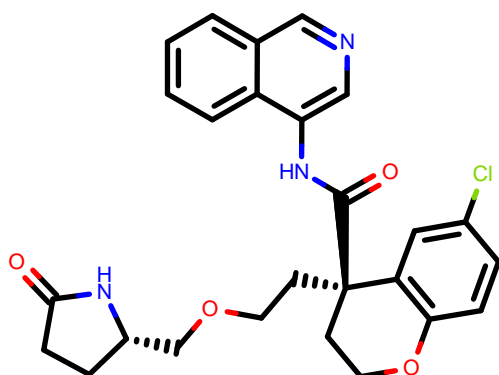
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5nc(no5)c6[nH]nc6

RUN: RUN1269

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.22

EN300-195756_3_2



CID: EN300-195756_3_2

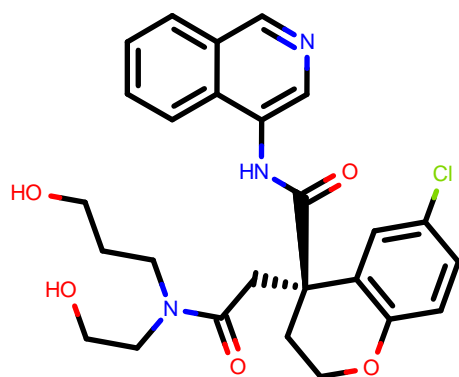
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@]5H5CCC(=O)N5

RUN: RUN1919

DDG (kcal/mol): -1.48

dDDG (kcal/mol): 0.25

EN300-74200_1_1



CID: EN300-74200_1_1

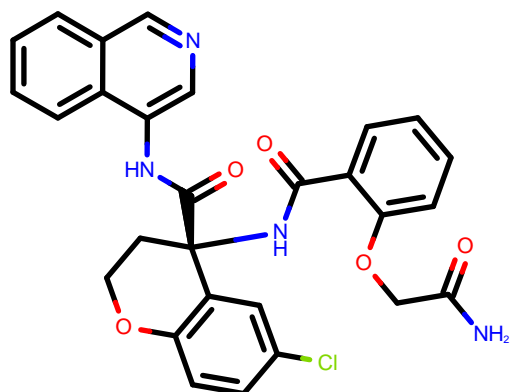
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(CCCO)CCO

RUN: RUN5381

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.34

EN300-15368_1_1



CID: EN300-15368_1_1

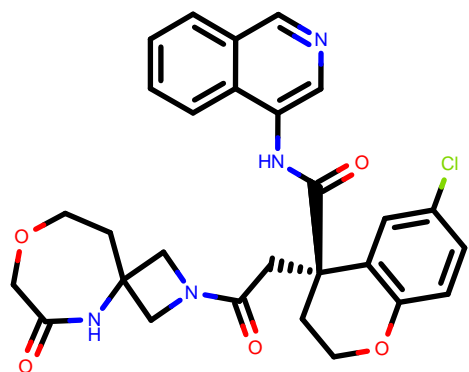
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccccc5OCC(=O)N

RUN: RUN2554

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.25

EN300-7425362_1_1



CID: EN300-7425362_1_1

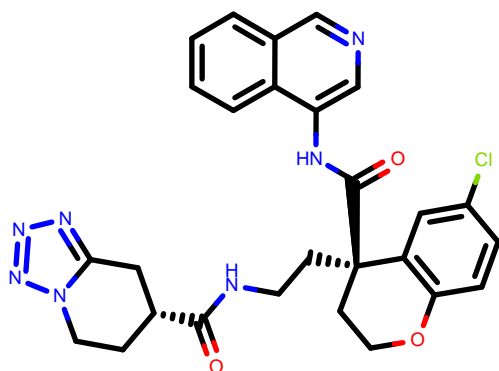
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)COCOC(=O)N6

RUN: RUN14486

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.24

EN300-1653482_3_2



CID: EN300-1653482_3_2

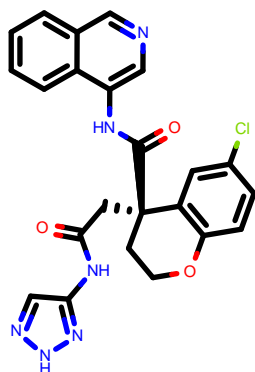
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5Cn6c(nnn6)C5

RUN: RUN15365

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.27

EN300-131132_1_1



CID: EN300-131132_1_1

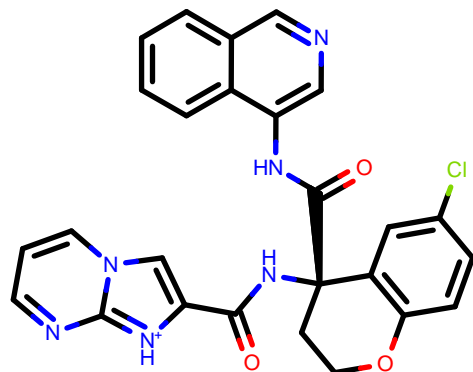
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cn[nH]n5

RUN: RUN15273

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.19

EN300-42252_1_1



CID: EN300-42252_1_1

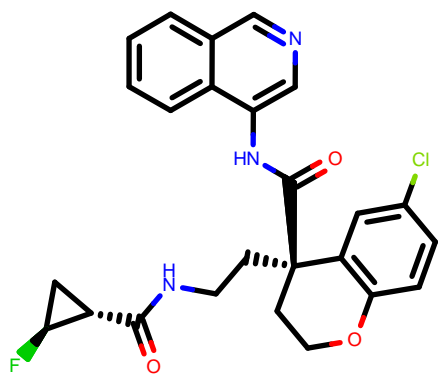
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn6ccnc6[nH]n5

RUN: RUN4998

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.23

EN300-6953121_3_1



CID: EN300-6953121_3_1

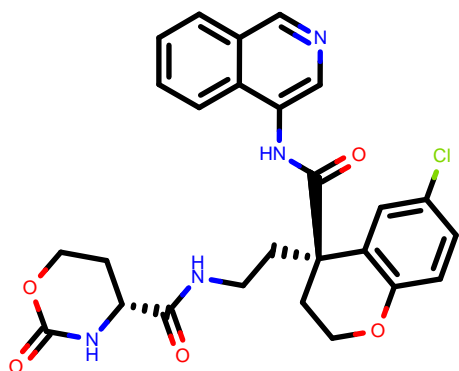
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@@H]5F

RUN: RUN15027

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.19

EN300-249804_3_2



CID: EN300-249804_3_2

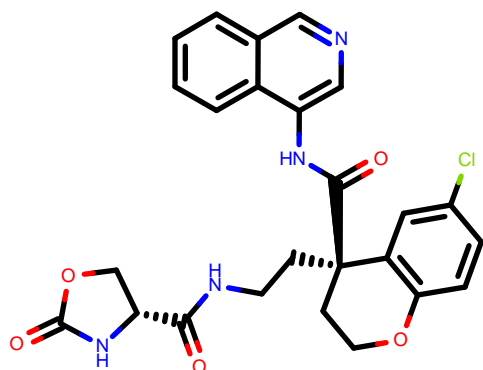
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5COC(=O)N5

RUN: RUN15361

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.28

EN300-201346_3_2



CID: EN300-201346_3_2

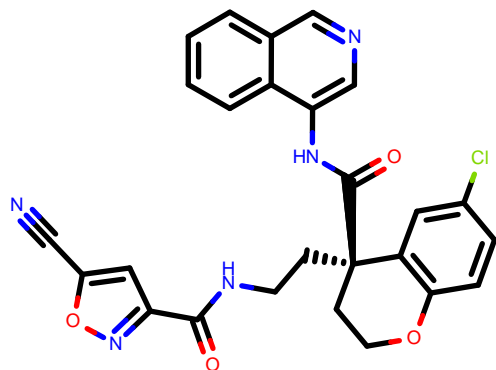
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5COC(=O)N5

RUN: RUN15264

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.21

EN300-1178005_3_1



CID: EN300-1178005_3_1

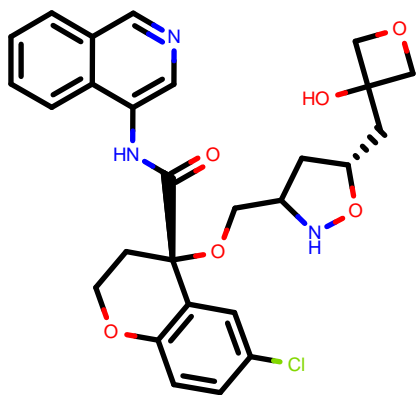
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc(on5)C#N

RUN: RUN15507

DDG (kcal/mol): -1.47

dDDG (kcal/mol): 0.24

EN300-7457160_1_2



CID: EN300-7457160_1_2

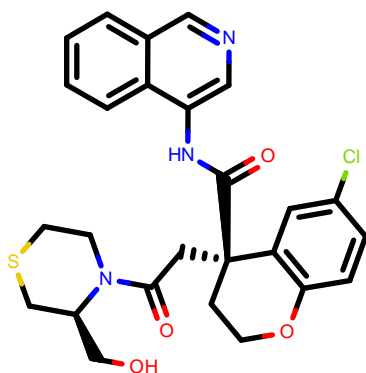
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NO[C@H](C5)CC6(COC6)O

RUN: RUN399

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.29

EN300-122579_1_1



CID: EN300-122579_1_1

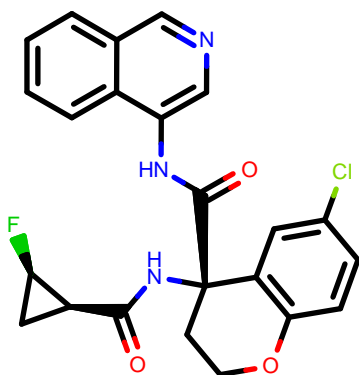
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCSC[C@@]H5CO

RUN: RUN9636

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.30

EN300-97300_1_2



CID: EN300-97300_1_2

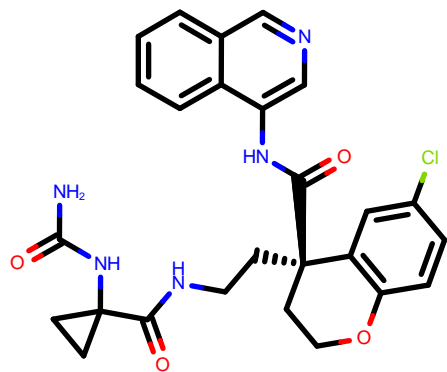
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5F

RUN: RUN2032

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.19

EN300-123614_3_1



CID: EN300-123614_3_1

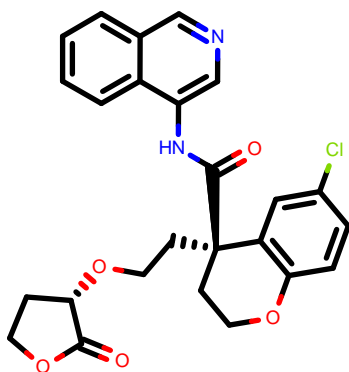
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CS)NC(=O)N

RUN: RUN609

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.26

EN300-20496_3_1



CID: EN300-20496_3_1

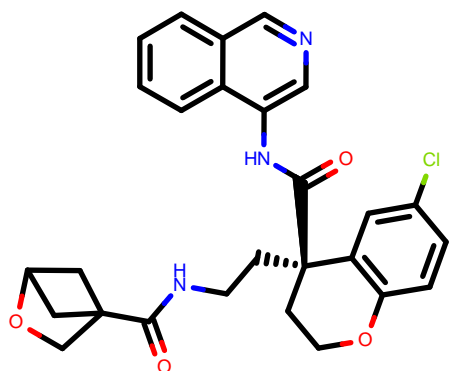
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@H]5CCOC5=O

RUN: RUN1424

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.21

EN300-1604607_3_1



CID: EN300-1604607_3_1

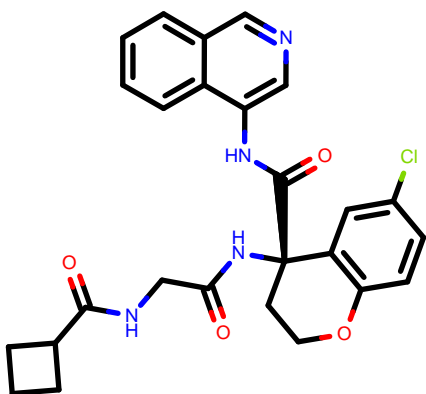
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C56CC(C5)OC6

RUN: RUN2801

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.19

EN300-62448_1_1



CID: EN300-62448_1_1

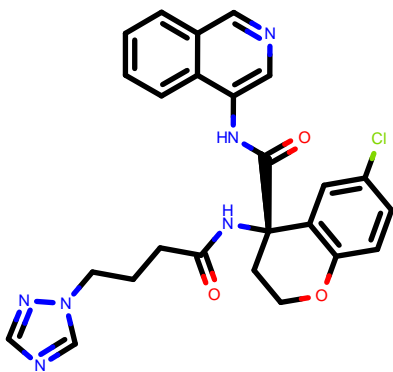
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)C5CC5

RUN: RUN8168

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EN300-316216_1_1



CID: EN300-316216_1_1

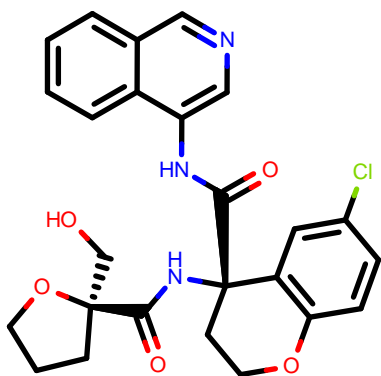
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5cn5

RUN: RUN6684

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.25

EN300-1425677_1_1



CID: EN300-1425677_1_1

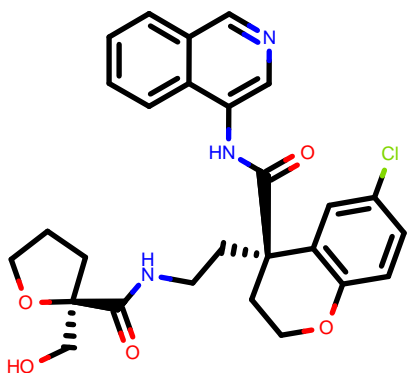
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5(CCCO5)CO

RUN: RUN6824

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.27

EN300-1425677_3_2



CID: EN300-1425677_3_2

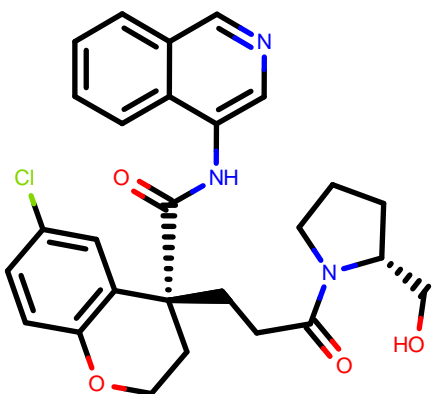
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCCO5)CO

RUN: RUN10837

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.32

EN300-55109_2_1



CID: EN300-55109_2_1

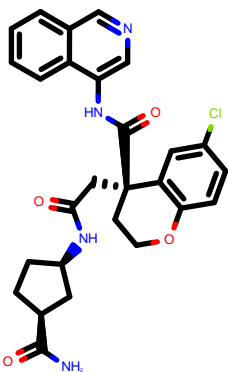
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC[C@@]5CO

RUN: RUN6666

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EN300-249086_1_1



CID: EN300-249086_1_1

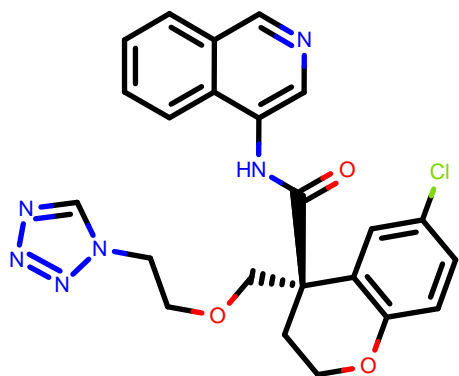
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5(C)C[C@@]5N

RUN: RUN7315

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.23

EN300-364679_2_1



CID: EN300-364679_2_1

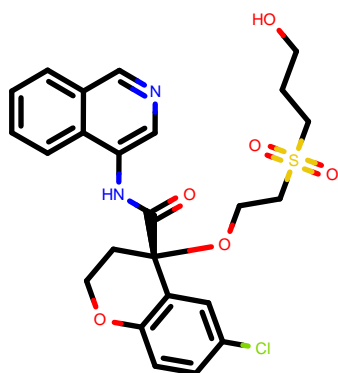
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5n5

RUN: RUN668

DDG (kcal/mol): -1.46

dDDG (kcal/mol): 0.20

EN300-7456499_1_1



CID: EN300-7456499_1_1

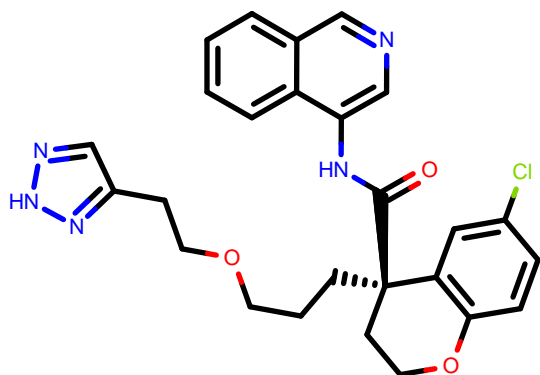
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCO

RUN: RUN343

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.35

EN300-222357_4_1



CID: EN300-222357_4_1

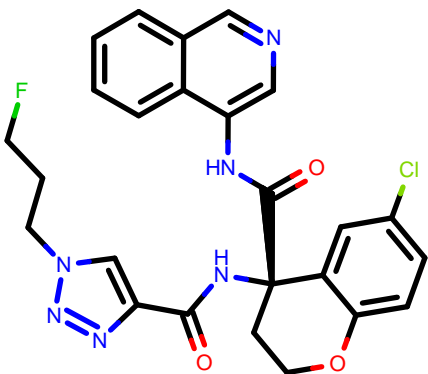
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOCc5cn[nH]5

RUN: RUN349

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.21

EN300-1704723_1_1



CID: EN300-1704723_1_1

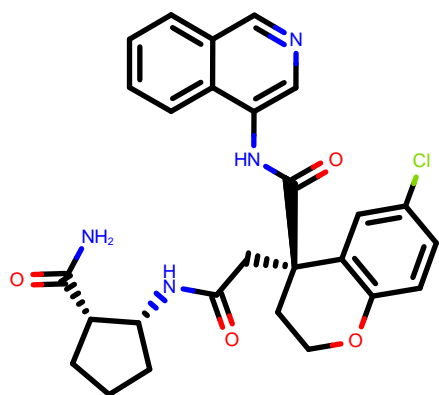
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]5COCF

RUN: RUN4434

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.19

EN300-90531_1_3



CID: EN300-90531_1_3

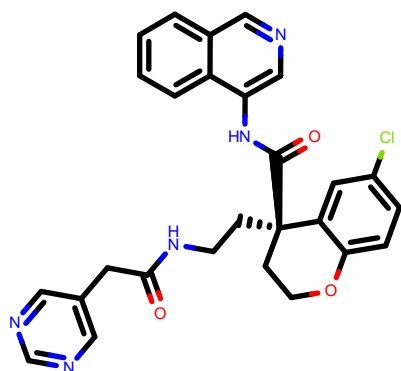
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5H5CCC[C@@]5H5Cl=O

RUN: RUN12366

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.34

EN300-185751_3_1



CID: EN300-185751_3_1

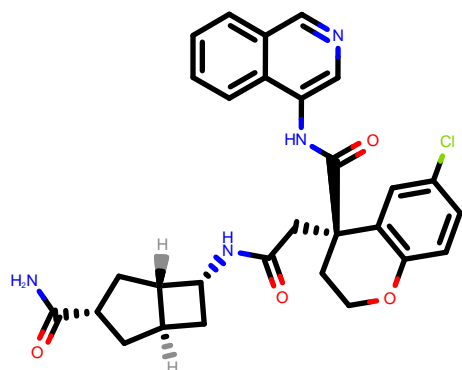
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5cnccc5

RUN: RUN9256

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.21

EN300-1268016_1_5



CID: EN300-1268016_1_5

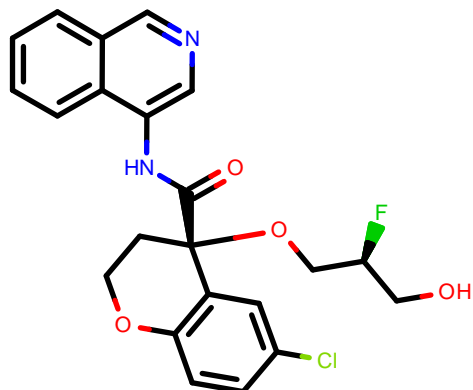
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C[C@@]5H5[C@@]6H5[C@@]6H5[C@@]6H5Cl=O

RUN: RUN10145

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.23

EN300-1600517_1_1



CID: EN300-1600517_1_1

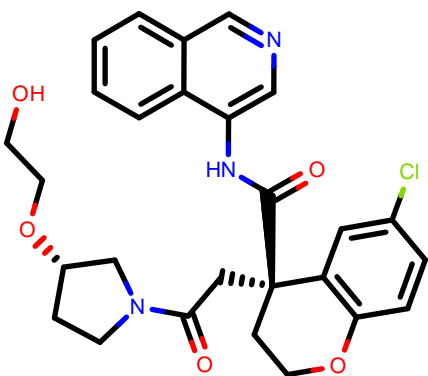
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H](CO)F

RUN: RUN2012

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.22

EN300-6764893_1_1



CID: EN300-6764893_1_1

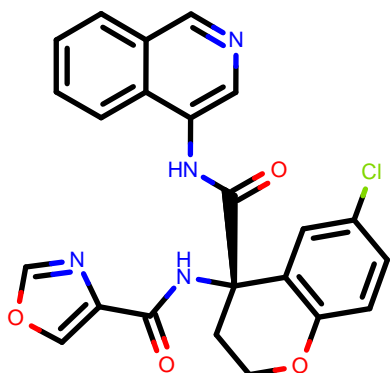
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)OCCO

RUN: RUN601

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.22

EN300-68618_1_1



CID: EN300-68618_1_1

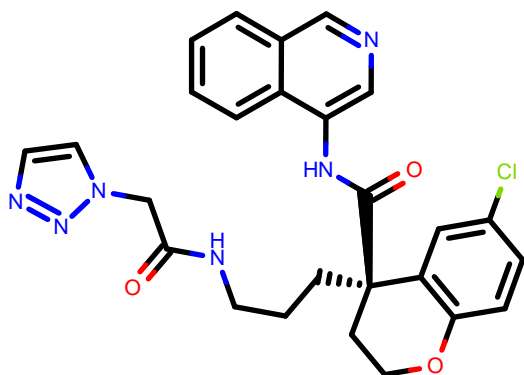
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ocn5

RUN: RUN2797

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.16

EN300-100467_4_1



CID: EN300-100467_4_1

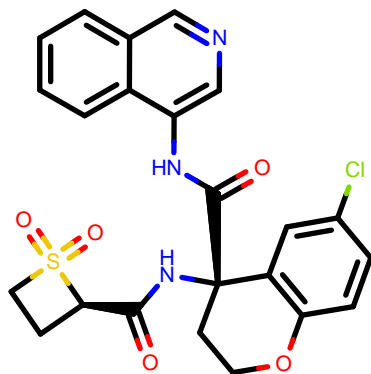
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn5

RUN: RUN7478

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.21

EN300-1387104_1_2



CID: EN300-1387104_1_2

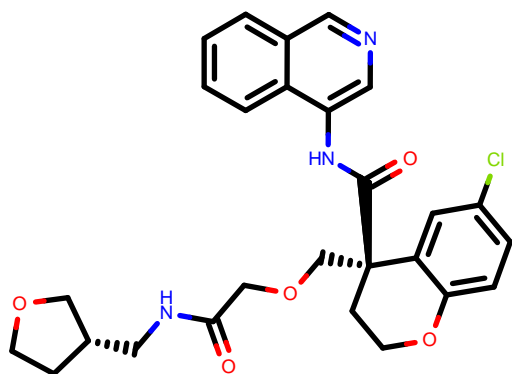
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C(=O)S(=O)(=O)C5

RUN: RUN6952

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.25

EN300-46832_2_1



CID: EN300-46832_2_1

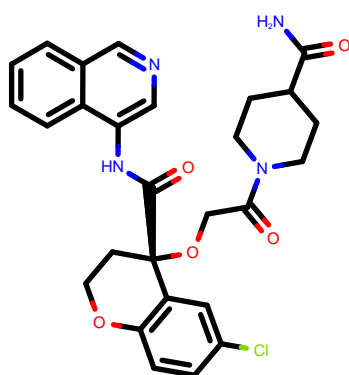
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@@H]5CCOC5

RUN: RUN364

DDG (kcal/mol): -1.45

dDDG (kcal/mol): 0.26

EN300-08063_1_1



CID: EN300-08063_1_1

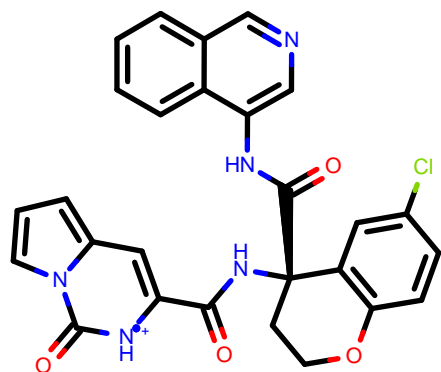
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCCC(C5)C(=O)N

RUN: RUN2480

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.26

EN300-7441080_1_1



CID: EN300-7441080_1_1

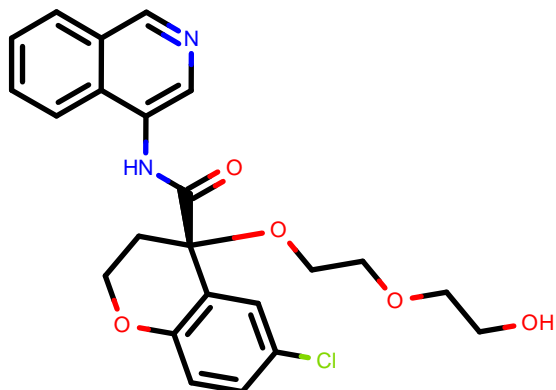
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6ccn6c(=O)[nH]5

RUN: RUN3046

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.20

EN300-52467_1_1



CID: EN300-52467_1_1

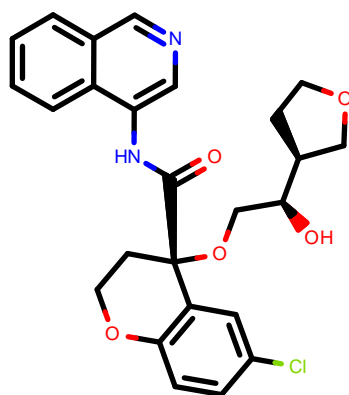
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO

RUN: RUN1229

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.20

EN300-1911992_1_4



CID: EN300-1911992_1_4

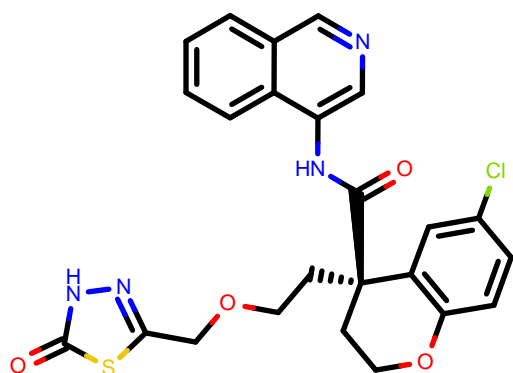
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C@H)5CCOC5O

RUN: RUN2445

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.29

EN300-171766_3_1



CID: EN300-171766_3_1

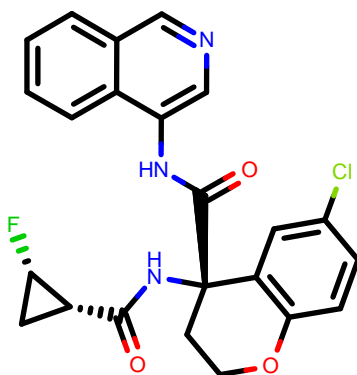
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5N[nH]c(=O)s5

RUN: RUN1544

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.22

EN300-97300_1_3



CID: EN300-97300_1_3

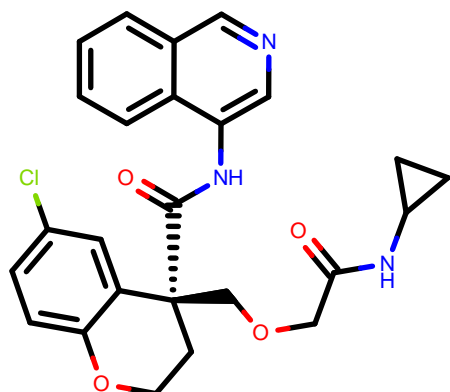
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H]5F

RUN: RUN6313

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.18

EN300-1253178_2_1



CID: EN300-1253178_2_1

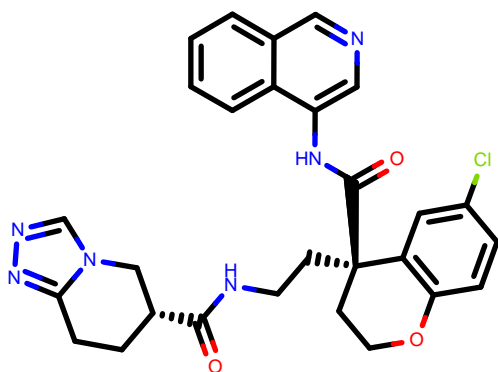
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CC5

RUN: RUN860

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.18

EN300-51350_3_1



CID: EN300-51350_3_1

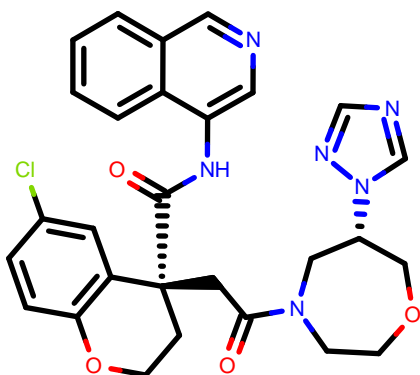
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCc6nncn6C5

RUN: RUN15204

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.31

EN300-6504498_1_1



CID: EN300-6504498_1_1

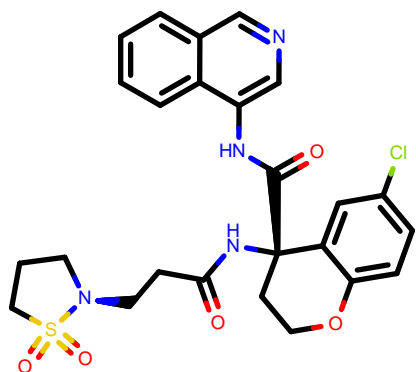
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)n6cncn6

RUN: RUN5589

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.33

EN300-44873_1_1



CID: EN300-44873_1_1

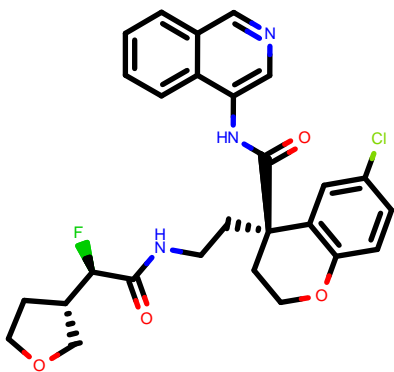
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[N@]5CCS(=O)=O

RUN: RUN3942

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.32

EN300-783124_3_3



CID: EN300-783124_3_3

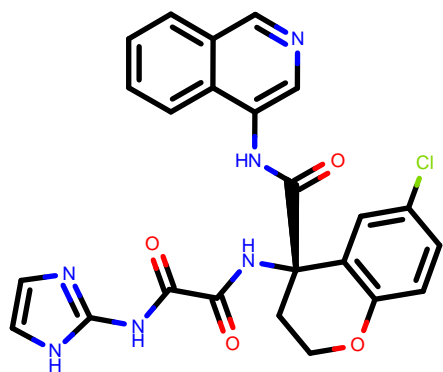
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C@H)5CCOC(=O)F

RUN: RUN4685

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.23

EN300-1703015_1_1



CID: EN300-1703015_1_1

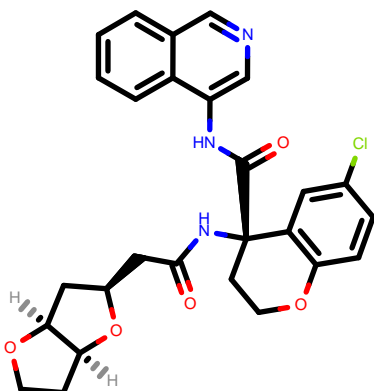
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@O]c4c3cc(cc4)C)NC(=O)C(=O)Nc5[nH]cn5

RUN: RUN4942

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.19

EN300-7355519_1_4



CID: EN300-7355519_1_4

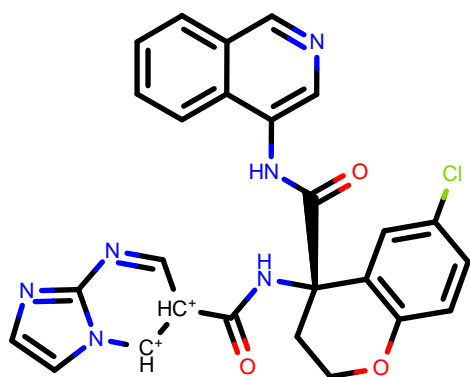
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@O]c4c3cc(cc4)C)NC(=O)C@@@H5C[C@@H]6[C@@H]O5CCO6

RUN: RUN7068

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.25

EN300-147397_1_1



CID: EN300-147397_1_1

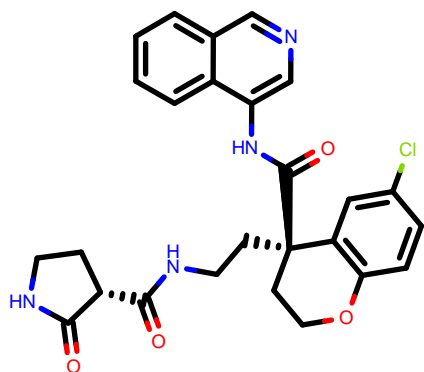
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@O]c4c3cc(cc4)C)NC(=O)c5cnc6nncn6

RUN: RUN5798

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.19

EN300-94945_3_2



CID: EN300-94945_3_2

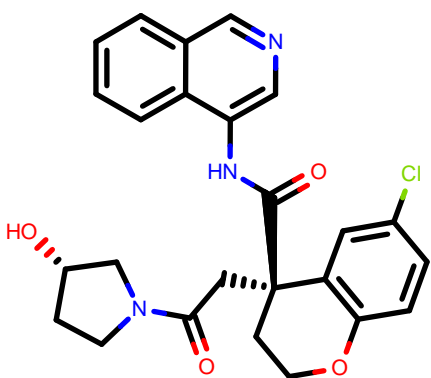
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@@3[C@@O]c4c3cc(cc4)C)CCNC(=O)C@H5CNCN5=O

RUN: RUN5005

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.22

EN300-69312_1_1



CID: EN300-69312_1_1

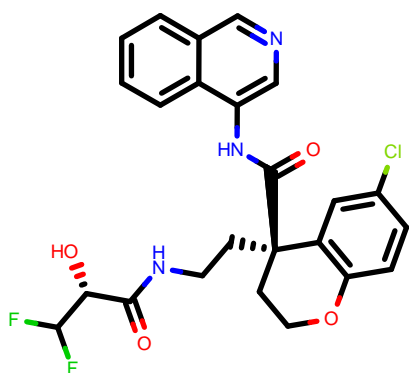
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O

RUN: RUN3353

DDG (kcal/mol): -1.44

dDDG (kcal/mol): 0.18

EN300-1932780_3_2



CID: EN300-1932780_3_2

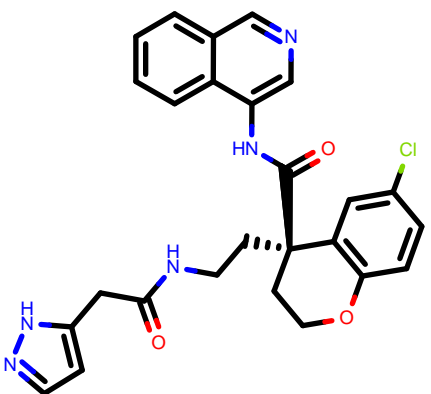
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C(F)F)O

RUN: RUN4217

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.24

EN300-71405_3_1



CID: EN300-71405_3_1

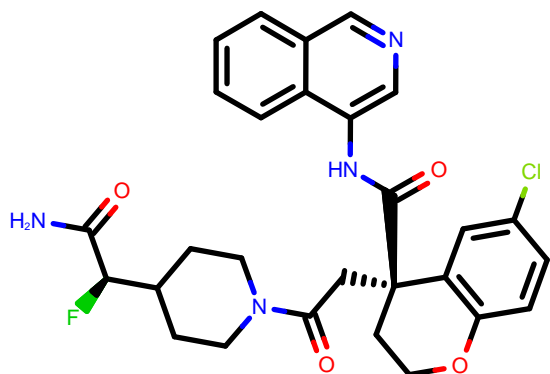
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5ccn[nH]5

RUN: RUN1079

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.22

EN300-318110_1_1



CID: EN300-318110_1_1

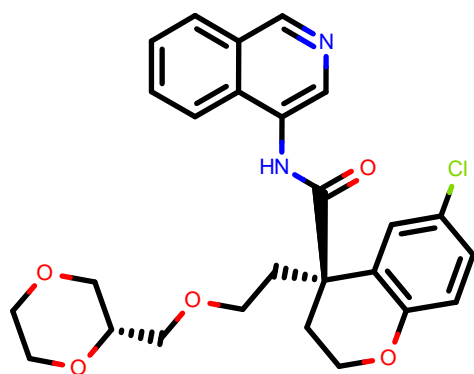
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)[C@H](C(=O)N)F

RUN: RUN12652

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.28

EN300-139167_3_1



CID: EN300-139167_3_1

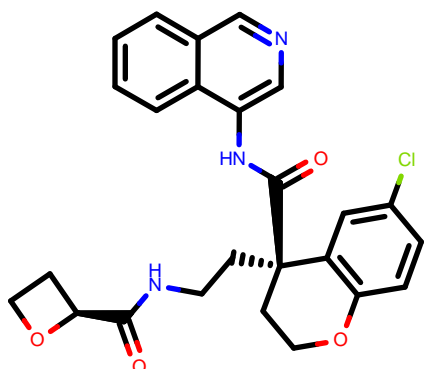
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN1951

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.29

EN300-85760_3_1



CID: EN300-85760_3_1

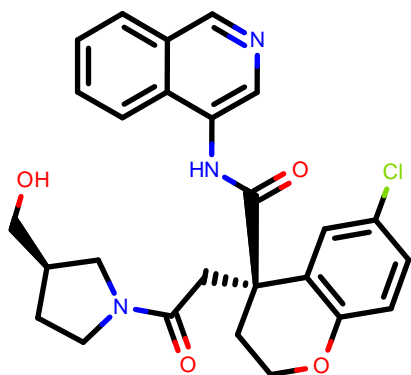
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COCOC5

RUN: RUN8992

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.19

EN300-144970_1_1



CID: EN300-144970_1_1

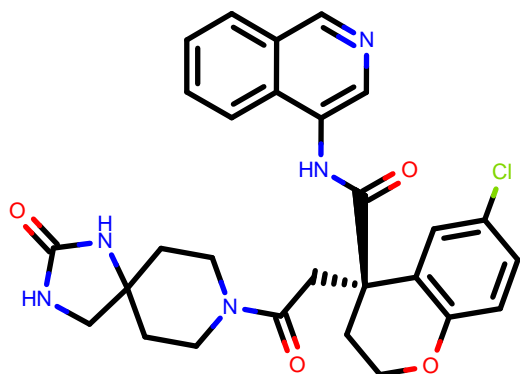
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO

RUN: RUN5825

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.20

EN300-6745712_1_1



CID: EN300-6745712_1_1

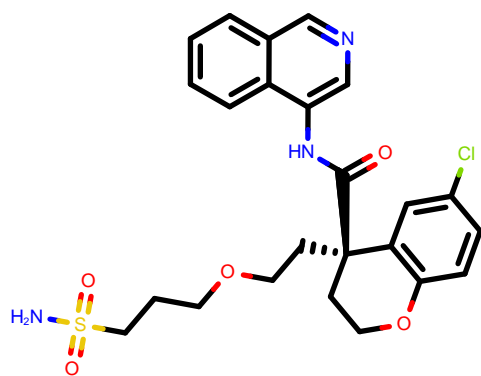
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC6(C5)CNC(=O)N6

RUN: RUN13378

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.25

EN300-79588_3_1



CID: EN300-79588_3_1

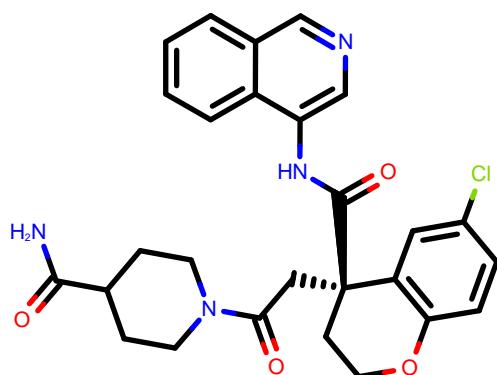
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCCS(=O)(=O)N

RUN: RUN1496

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.29

EN300-1265946_1_1



CID: EN300-1265946_1_1

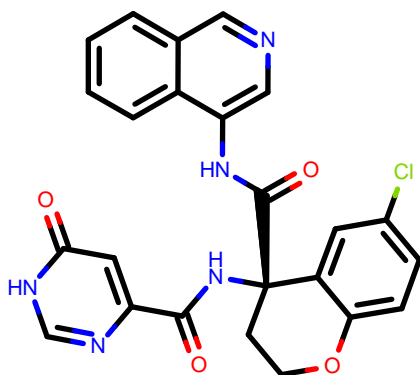
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(C5)C(=O)N

RUN: RUN5333

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.25

EN300-817811_1_1



CID: EN300-817811_1_1

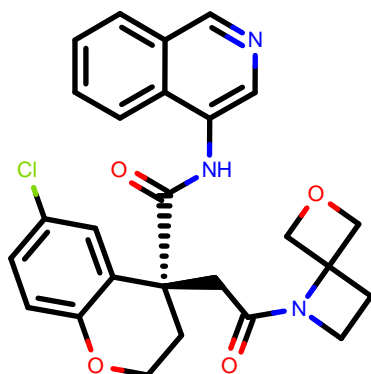
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(=O)[nH]jcn5

RUN: RUN4838

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.20

EN300-247468_1_1



CID: EN300-247468_1_1

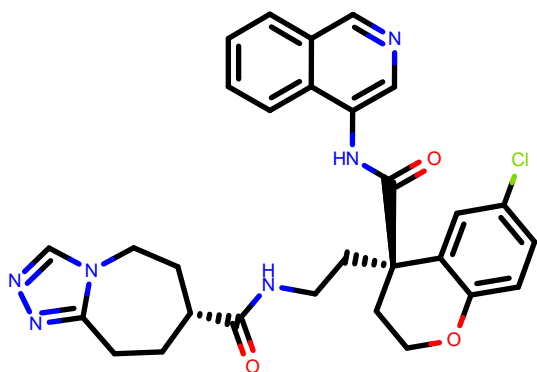
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC56COC6

RUN: RUN10677

DDG (kcal/mol): -1.43

dDDG (kcal/mol): 0.19

EN300-366687_3_1



CID: EN300-366687_3_1

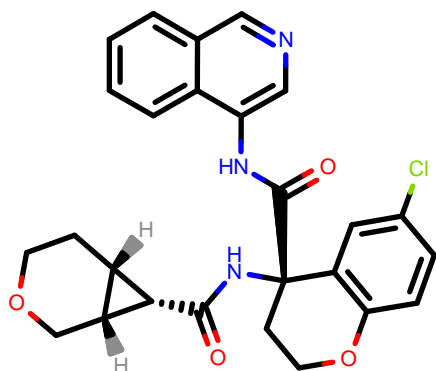
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCc6nncn6CC5

RUN: RUN15302

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.30

EN300-1644723_1_6



CID: EN300-1644723_1_6

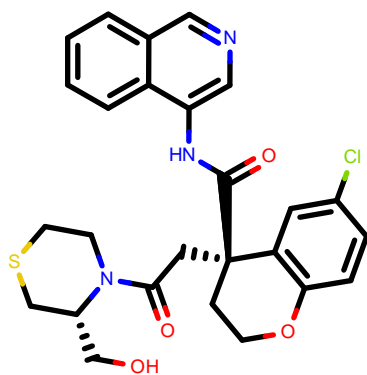
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5[C@@H]6[C@@H]5COC6

RUN: RUN3730

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.22

EN300-122579_1_2



CID: EN300-122579_1_2

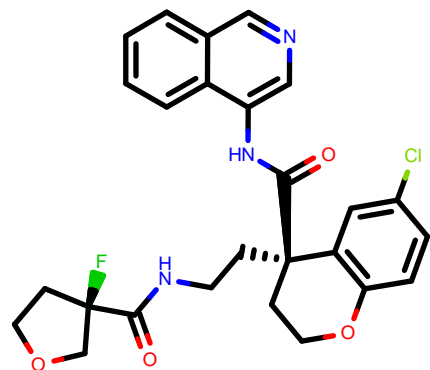
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCSC[C@@H]5CO

RUN: RUN12156

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.27

EN300-188356_3_2



CID: EN300-188356_3_2

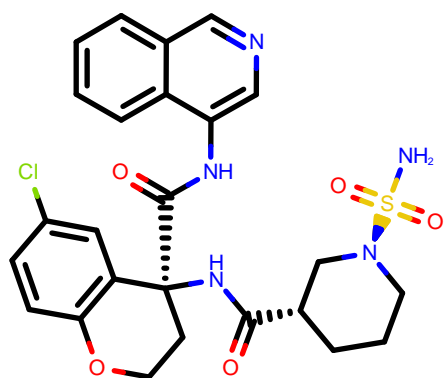
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(CCOCC5)F

RUN: RUN9084

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.21

EN300-219496_1_2



CID: EN300-219496_1_2

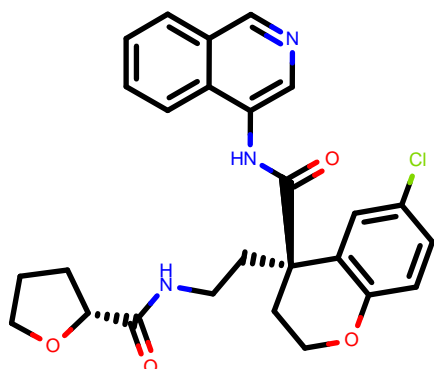
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCCN@@]C5(S(=O)(=O)N

RUN: RUN9541

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.50

EN300-116234_3_1



CID: EN300-116234_3_1

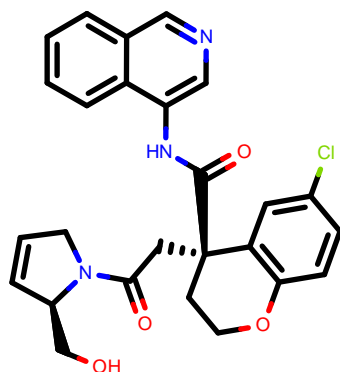
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CCCO5

RUN: RUN4909

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.19

EN300-378343_1_1



CID: EN300-378343_1_1

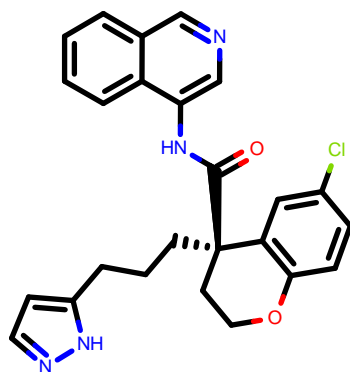
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC=C[C@H]5CO

RUN: RUN1647

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.22

VLA-UCB-34f3ed0c-10_1



CID: VLA-UCB-34f3ed0c-10_1

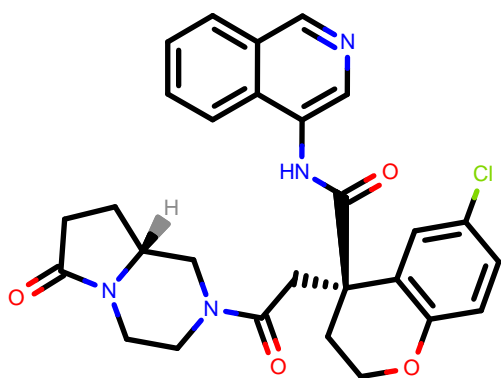
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC5cc[nH]5

RUN: RUN47

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.18

EN300-60330_1_2



CID: EN300-60330_1_2

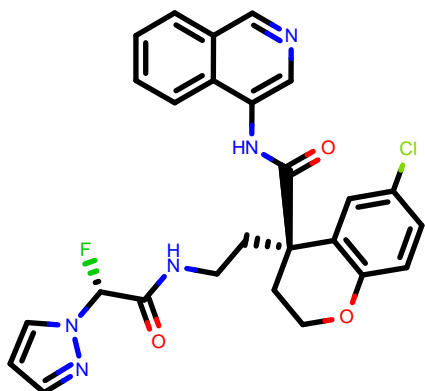
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@H](C5)CCC6=O

RUN: RUN10365

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.22

EN300-1726277_3_2



CID: EN300-1726277_3_2

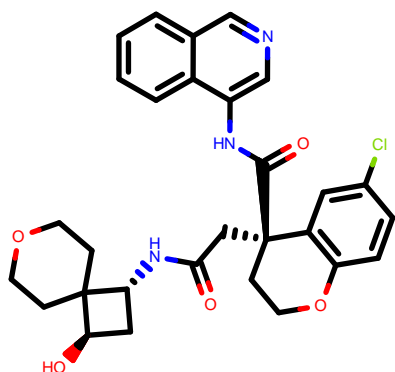
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(=O)[C@@H](n5cccn5)F

RUN: RUN8255

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.24

EN300-640503_1_1



CID: EN300-640503_1_1

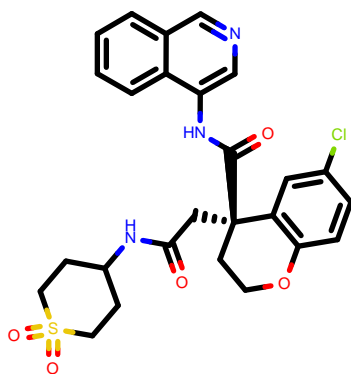
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4(O)CCO[C@H]4

RUN: RUN13842

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.31

EN300-39278_1_1



CID: EN300-39278_1_1

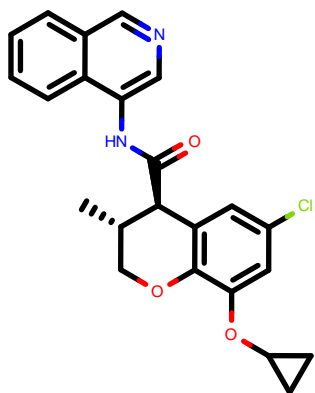
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CCS(=O)(=O)CC5

RUN: RUN4481

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.17

DAR-DIA-0d514e7d-6_1



CID: DAR-DIA-0d514e7d-6_1

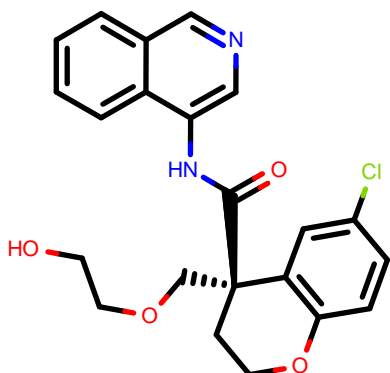
SMILES: C[C@H]1COc2c(cc2OC3CC3)Cl[C@@H]1C(=O)Nc4cncc5c4cccc5

RUN: RUN26

DDG (kcal/mol): -1.42

dDDG (kcal/mol): 0.16

EN300-21258_2_1



CID: EN300-21258_2_1

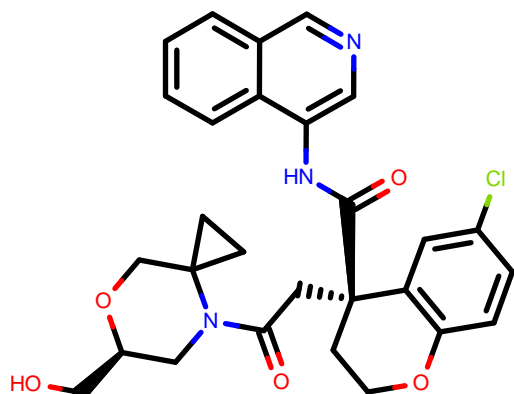
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCO

RUN: RUN1993

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.16

EN300-7493255_1_1



CID: EN300-7493255_1_1

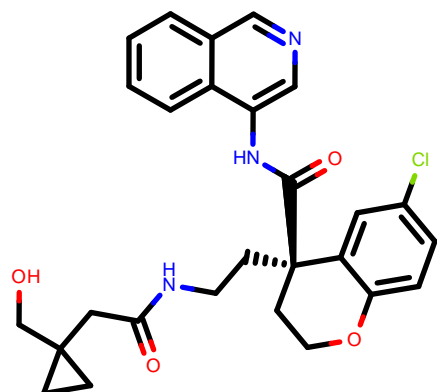
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](OCC56CC6)CO

RUN: RUN10003

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.33

EN300-107048_3_1



CID: EN300-107048_3_1

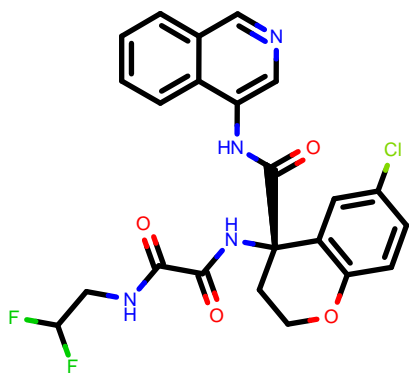
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(C)CO

RUN: RUN6141

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.27

EN300-128277_1_1



CID: EN300-128277_1_1

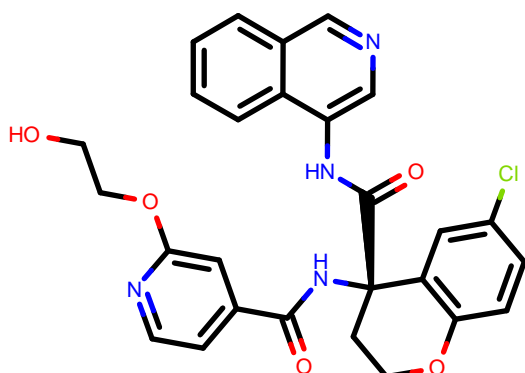
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C(=O)NCC(F)F

RUN: RUN1057

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.18

EN300-101796_1_1



CID: EN300-101796_1_1

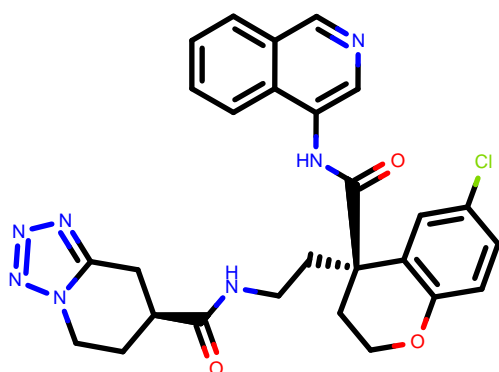
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccncc5OCCO

RUN: RUN4210

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.28

EN300-1653482_3_1



CID: EN300-1653482_3_1

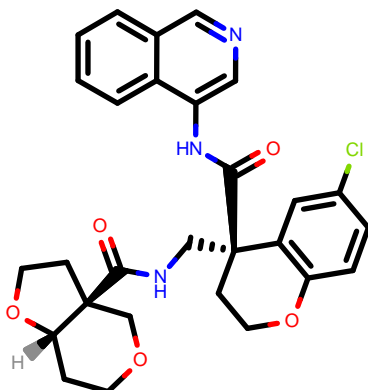
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C6Cn6c(nnn6)C5

RUN: RUN15398

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.24

EN300-341337_2_3



CID: EN300-341337_2_3

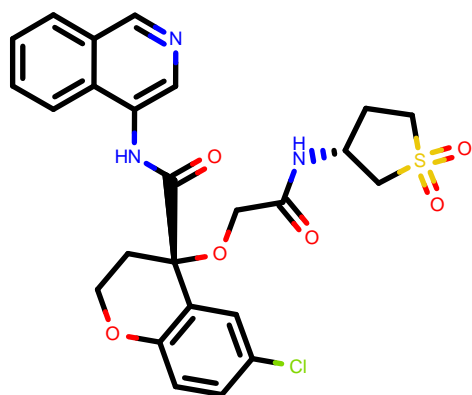
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@]56CCO[C@H]5CCOC6

RUN: RUN7945

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.32

EN300-05512_1_1



CID: EN300-05512_1_1

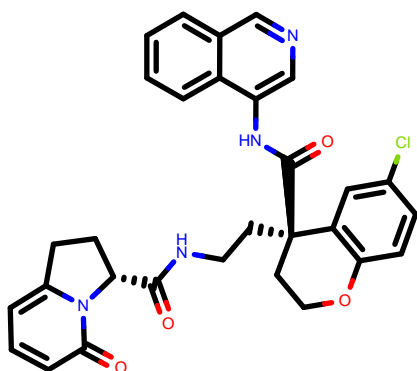
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@[3](CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCCS(=O)(=O)C5

RUN: RUN815

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.41

EN300-332002_3_2



CID: EN300-332002_3_2

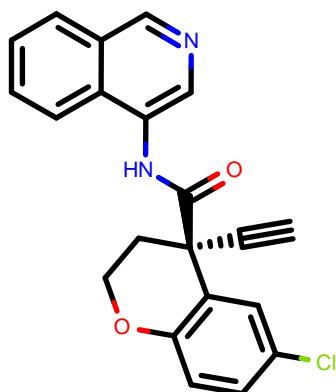
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@[3](CCOc4c3cc(cc4)Cl)CCNC(=O)Nc5cnc6c5c(=O)ccc6

RUN: RUN2973

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.28

PET-UNK-29afea89-1_1



CID: PET-UNK-29afea89-1_1

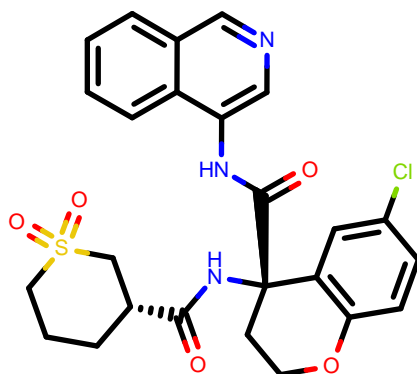
SMILES: C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN64

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.09

EN300-77778_1_1



CID: EN300-77778_1_1

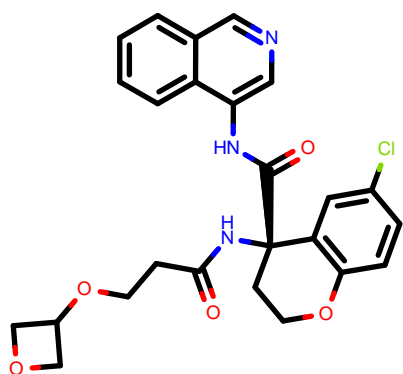
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@[3](CCOc4c3cc(cc4)Cl)NC(=O)N[C@@H]5CCCS(=O)(=O)C5

RUN: RUN1401

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.24

EN300-321703_1_1



CID: EN300-321703_1_1

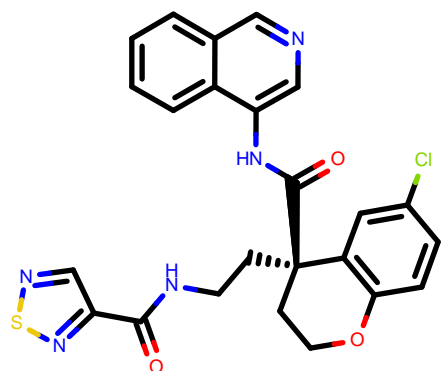
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCOC5COCS

RUN: RUN8773

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.23

EN300-42270_3_1



CID: EN300-42270_3_1

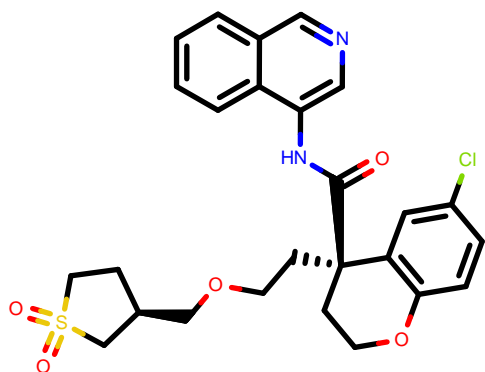
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cnsn5

RUN: RUN15284

DDG (kcal/mol): -1.41

dDDG (kcal/mol): 0.20

EN300-1448603_3_1



CID: EN300-1448603_3_1

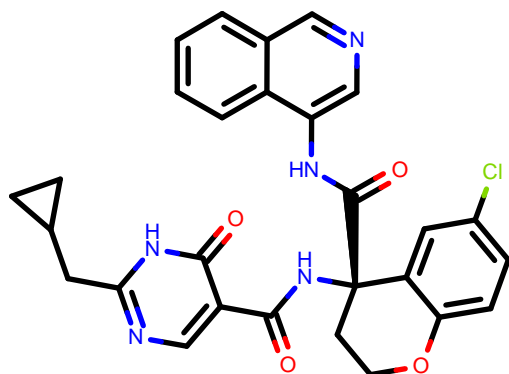
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5SCCS(=O)=O)C5

RUN: RUN2198

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.25

EN300-363154_1_1



CID: EN300-363154_1_1

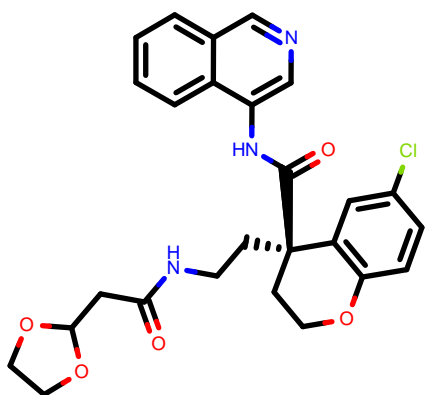
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cnc([nH]c5=O)CC6CC6

RUN: RUN9907

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.28

EN300-154944_3_1



CID: EN300-154944_3_1

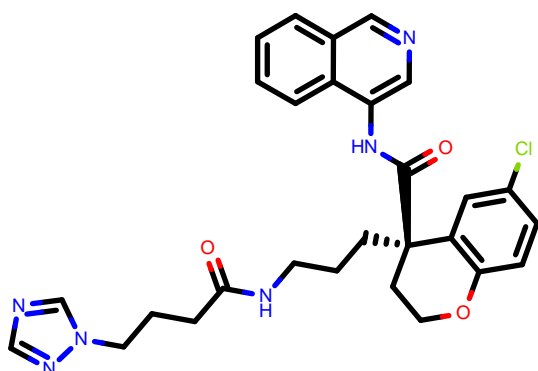
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5OCCO5

RUN: RUN14718

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.27

EN300-316216_4_1



CID: EN300-316216_4_1

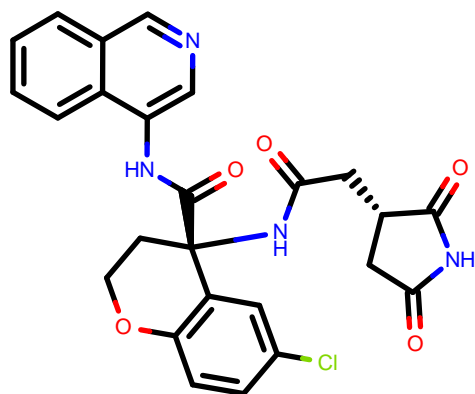
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCC5=CN=C5

RUN: RUN11548

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.26

EN300-227055_1_1



CID: EN300-227055_1_1

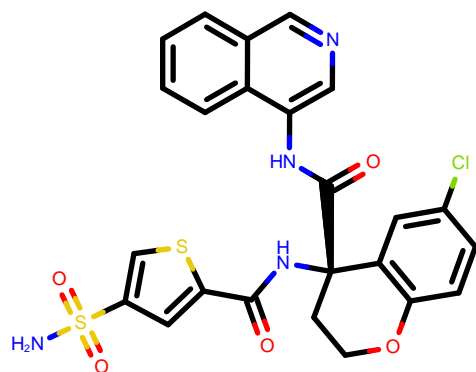
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)NC5=O

RUN: RUN2540

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-98099_1_1



CID: EN300-98099_1_1

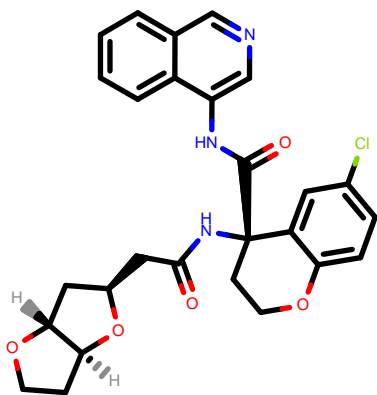
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)S(=O)(=O)N

RUN: RUN6170

DDG (kcal/mol): -1.40

dDDG (kcal/mol): 0.24

EN300-7355519_1_2



CID: EN300-7355519_1_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(coc4)C)NC(=O)C[C@@H]3C[C@@H]3(O)COC6

RUN:

RUN8637

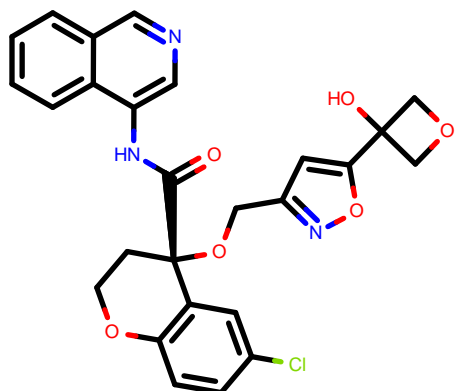
DDG (kcal/mol):

-1.40

dDDG (kcal/mol):

0.24

EN300-7457159_1_1



CID: EN300-7457159_1_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(coc4)C)OCc5cc(oc5)C6(COC6)O

RUN:

RUN359

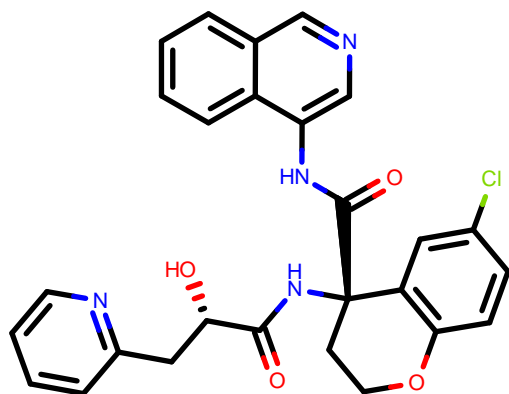
DDG (kcal/mol):

-1.40

dDDG (kcal/mol):

0.23

EN300-6762327_1_2



CID: EN300-6762327_1_2

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(coc4)C)NC(=O)[C@@H](C)c5ccccc5O

RUN:

RUN2842

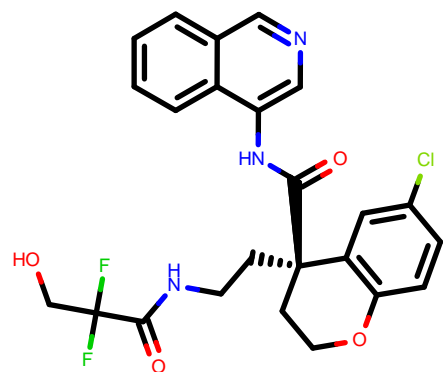
DDG (kcal/mol):

-1.40

dDDG (kcal/mol):

0.29

EN300-123489_3_1



CID: EN300-123489_3_1

SMILES:

c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(coc4)C)CCNC(=O)C(CO)(F)F

RUN:

RUN13622

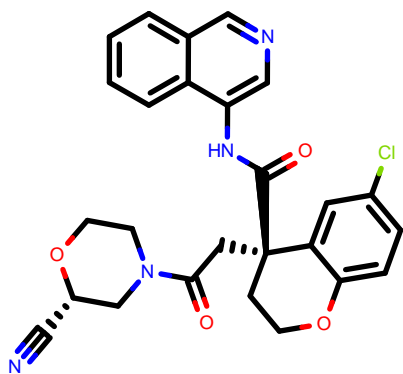
DDG (kcal/mol):

-1.39

dDDG (kcal/mol):

0.31

EN300-70489_1_1



CID: EN300-70489_1_1

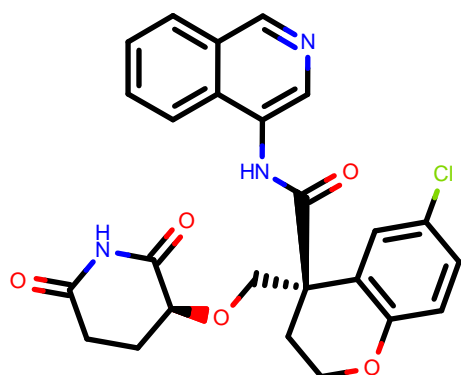
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)C#N

RUN: RUN10733

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.22

EN300-120920_2_1



CID: EN300-120920_2_1

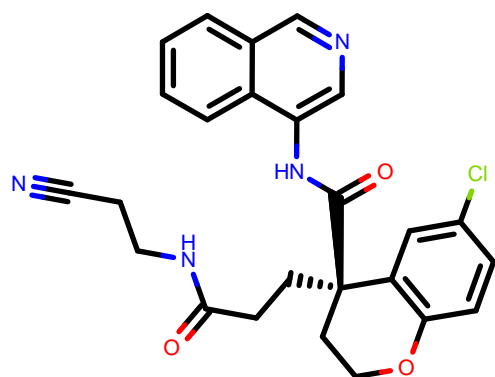
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NCS=O

RUN: RUN2596

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.19

EN300-183001_2_1



CID: EN300-183001_2_1

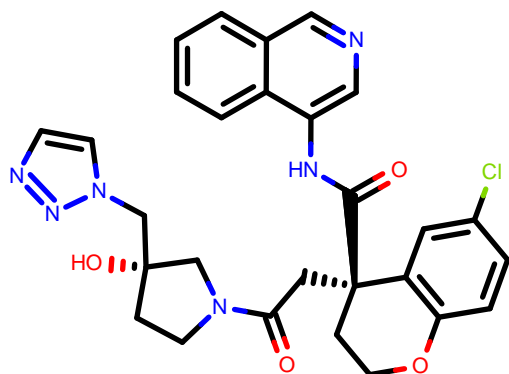
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCC#N

RUN: RUN11410

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.23

EN300-269627_1_2



CID: EN300-269627_1_2

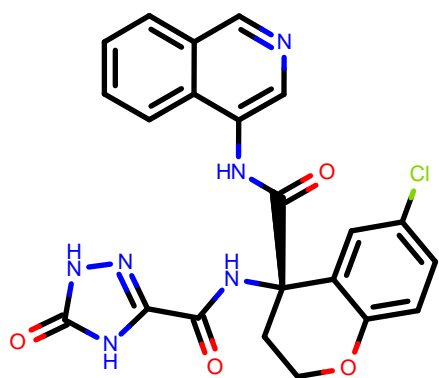
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@](C)(C5)Cn6ccnn6O

RUN: RUN1950

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.32

EN300-35843_1_1



CID: EN300-35843_1_1

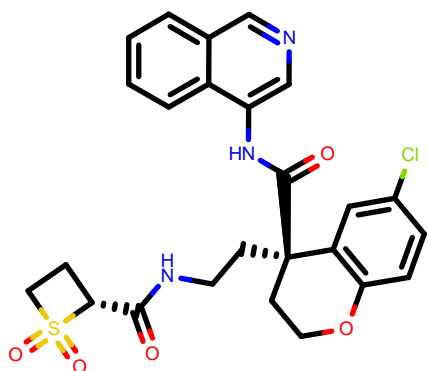
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]c(=O)[nH]n5

RUN: RUN4598

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.20

EN300-1387104_3_2



CID: EN300-1387104_3_2

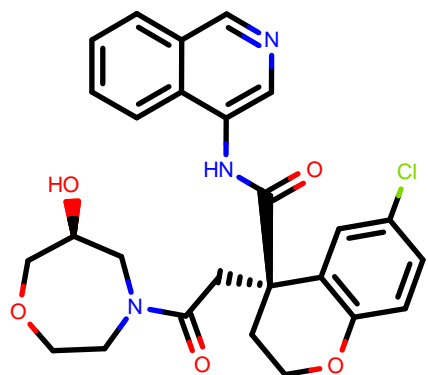
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5SCCS5(=O)=O

RUN: RUN2786

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.21

EN300-233951_1_1



CID: EN300-233951_1_1

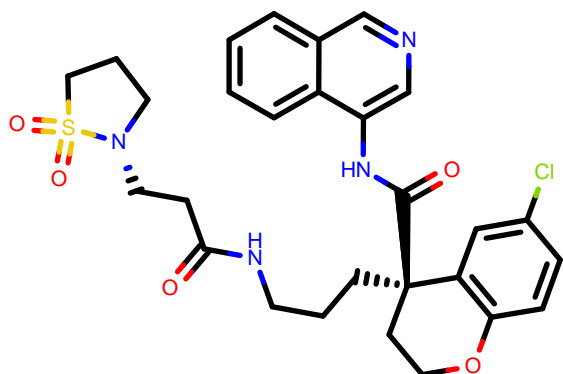
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5COC[C@H](C5)O

RUN: RUN9774

DDG (kcal/mol): -1.39

dDDG (kcal/mol): 0.30

EN300-44873_4_2



CID: EN300-44873_4_2

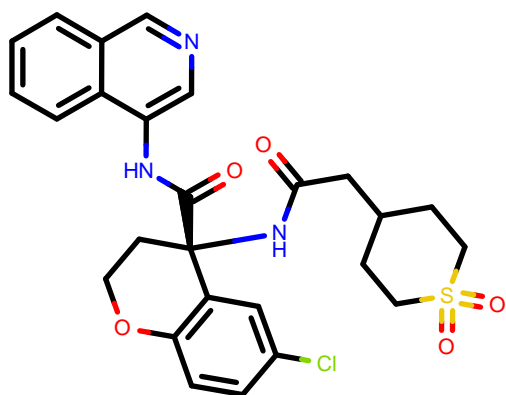
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(N@@)5CCCS5(=O)=O

RUN: RUN11502

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.48

EN300-250120_1_1



CID: EN300-250120_1_1

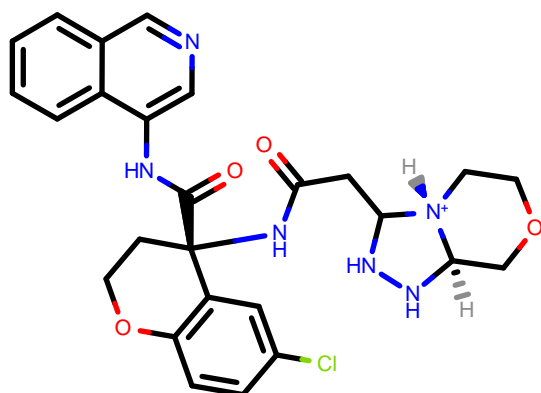
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5CCS(=O)(=O)CC5

RUN: RUN9097

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.25

EN300-1718836_1_1



CID: EN300-1718836_1_1

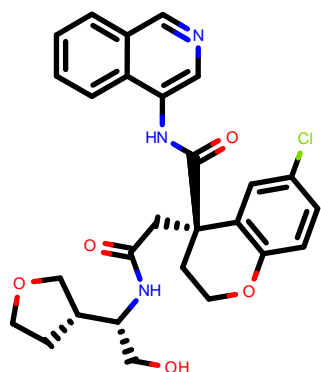
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5nnc6n5CCOC6

RUN: RUN6142

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.24

EN300-104493_1_1



CID: EN300-104493_1_1

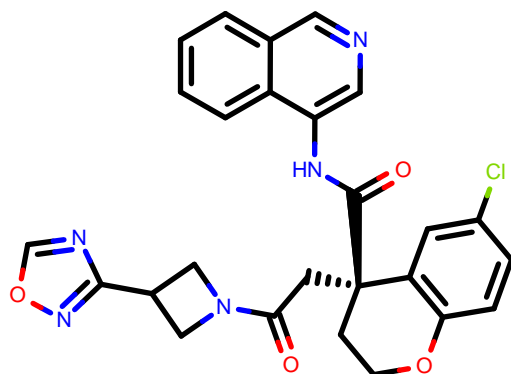
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)[C@@H]5CCOC5

RUN: RUN13168

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.38

EN300-1700143_1_1



CID: EN300-1700143_1_1

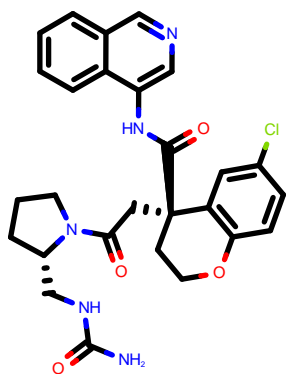
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)c6ncon6

RUN: RUN3569

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.20

EN300-212795_1_2



CID: EN300-212795_1_2

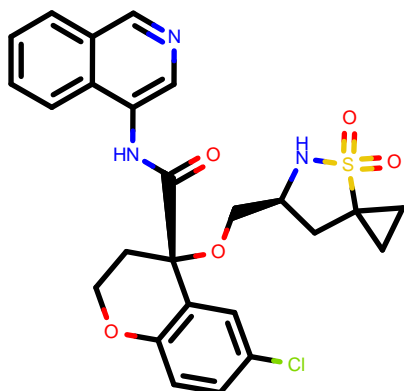
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5CNC(=O)N

RUN: RUN5717

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.26

EN300-6504697_1_2



CID: EN300-6504697_1_2

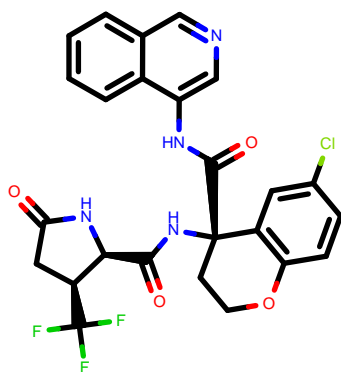
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@]5(C)SC(=O)N5

RUN: RUN823

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.29

EN300-169955_1_2



CID: EN300-169955_1_2

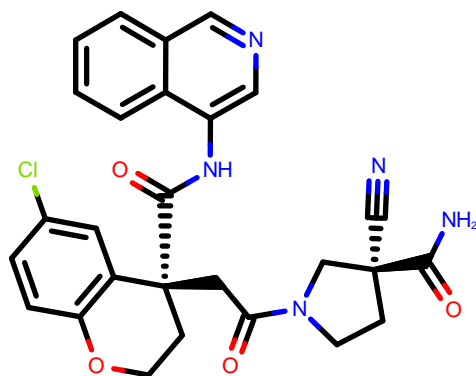
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H](C(F)(F)F)N5

RUN: RUN3854

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.21

EN300-1608992_1_2



CID: EN300-1608992_1_2

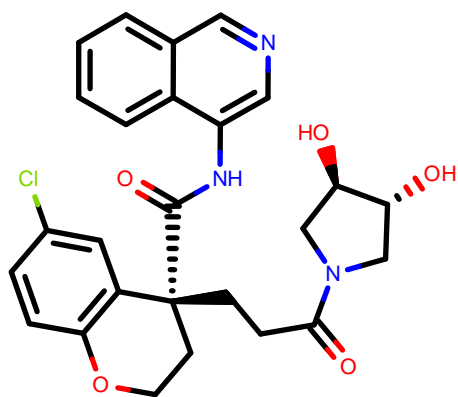
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]5(C)C#N

RUN: RUN7723

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.30

EN300-97938_2_1



CID: EN300-97938_2_1

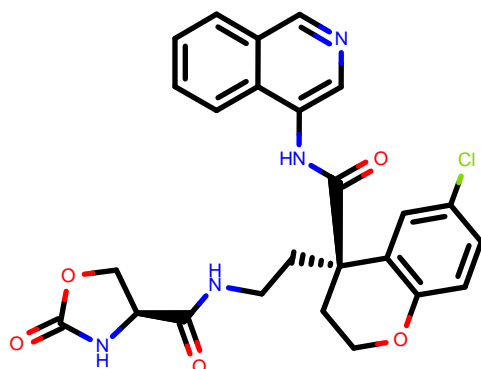
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C[C@H]([C@@H](C5)O)O

RUN: RUN9966

DDG (kcal/mol): -1.38

dDDG (kcal/mol): 0.24

EN300-201346_3_1



CID: EN300-201346_3_1

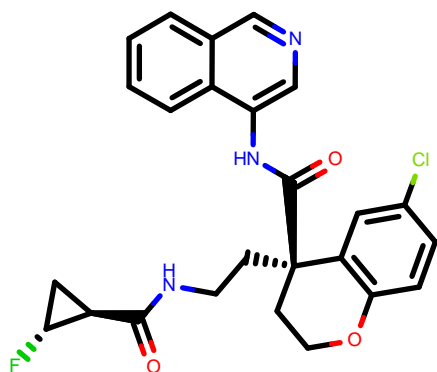
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]4H5COC(=O)N5

RUN: RUN15337

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.22

EN300-1654606_3_1



CID: EN300-1654606_3_1

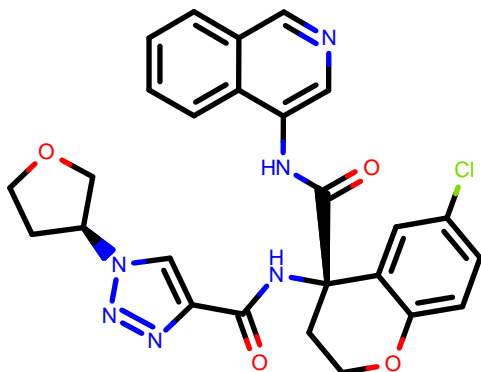
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]4H5C[C@H]5F

RUN: RUN15060

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.21

EN300-151461_1_2



CID: EN300-151461_1_2

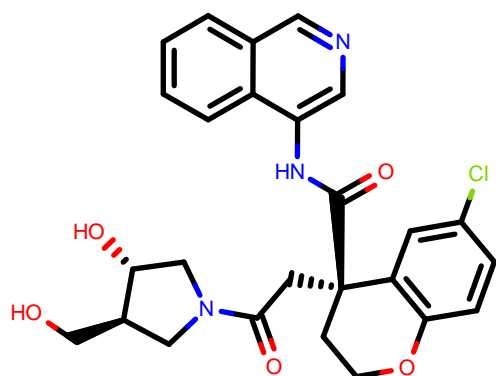
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(n5)[C@H]6CCOC6

RUN: RUN1345

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.19

EN300-248521_1_4



CID: EN300-248521_1_4

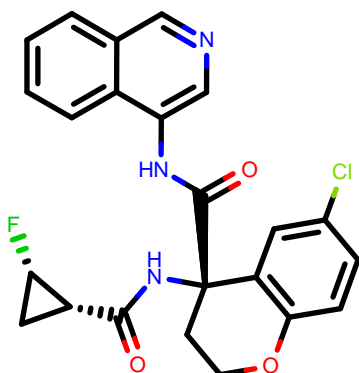
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)O)CO

RUN: RUN3017

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.22

EN300-97300_1_3



CID: EN300-97300_1_3

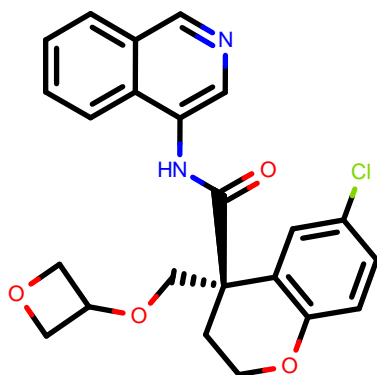
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H5C[C@@]H5F

RUN: RUN6317

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.16

EN300-317082_2_1



CID: EN300-317082_2_1

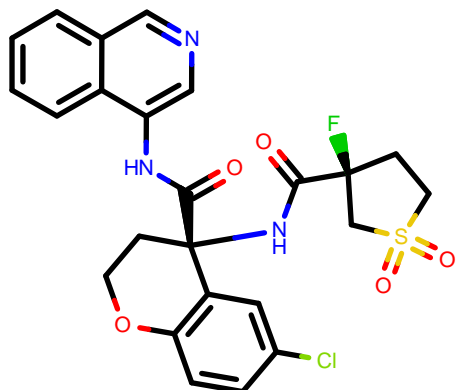
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC5COC5

RUN: RUN2072

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.15

EN300-311920_1_1



CID: EN300-311920_1_1

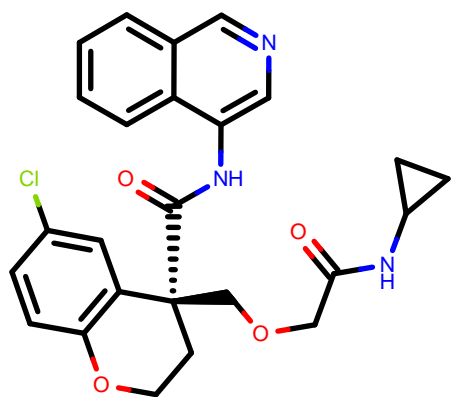
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCS(=O)(=O)C5)F

RUN: RUN4218

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.26

EN300-1253178_2_1



CID: EN300-1253178_2_1

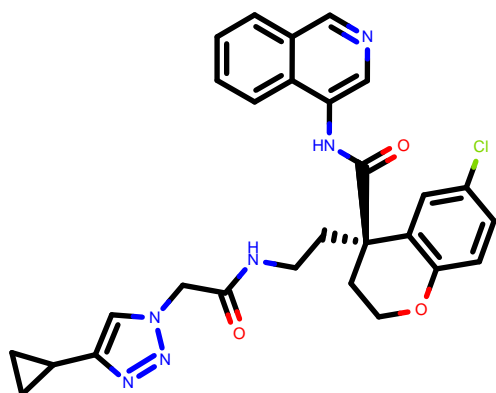
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CC5

RUN: RUN868

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.18

EN300-107892_3_1



CID: EN300-107892_3_1

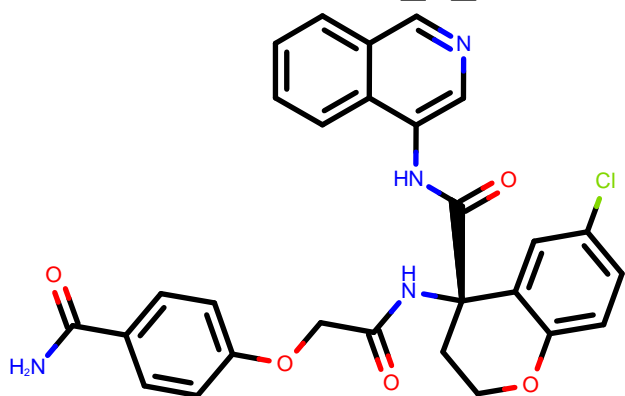
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(n5)O6CC6

RUN: RUN11783

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.29

EN300-55498_1_1



CID: EN300-55498_1_1

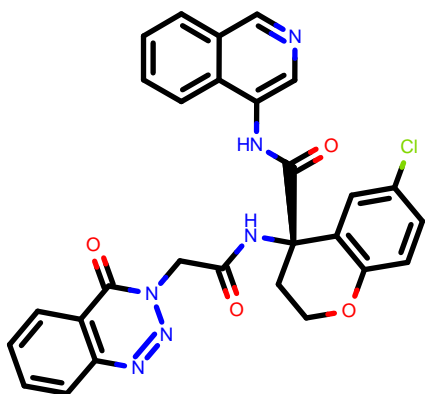
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COc5ccc(cc5)C(=O)N

RUN: RUN9802

DDG (kcal/mol): -1.37

dDDG (kcal/mol): 0.24

EN300-21813_1_1



CID: EN300-21813_1_1

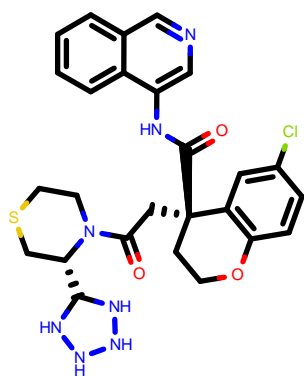
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)c6ccccc6n5

RUN: RUN9847

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.25

EN300-141254_1_1



CID: EN300-141254_1_1

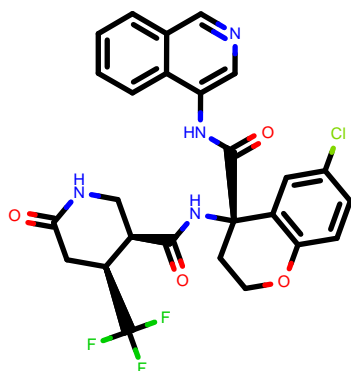
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CC(=O)N5CCSC[C@H]5c6n(n-j)nn6

RUN: RUN9985

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.28

EN300-208959_1_3



CID: EN300-208959_1_3

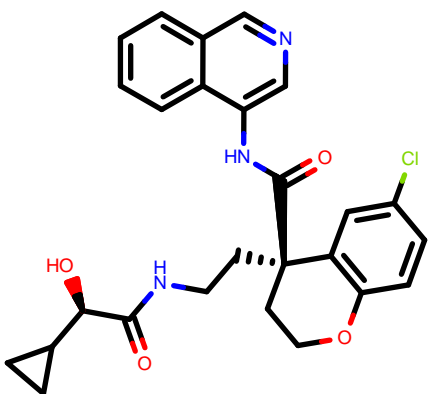
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)NC(=O)[C@@]5[C@@]NCCN5C(F)(F)F

RUN: RUN6568

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.30

EN300-72211_3_1



CID: EN300-72211_3_1

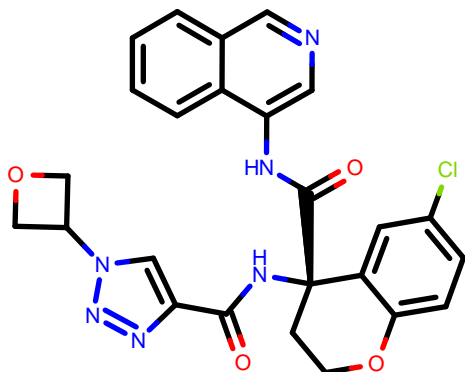
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CCNC(=O)[C@@]5[C@@]NCC5O

RUN: RUN8988

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-1696043_1_1



CID: EN300-1696043_1_1

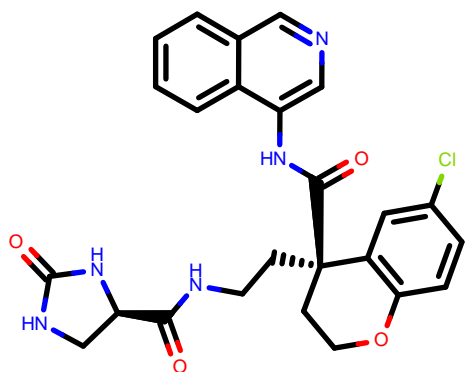
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C6COC6

RUN: RUN3094

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.18

EN300-222145_3_1



CID: EN300-222145_3_1

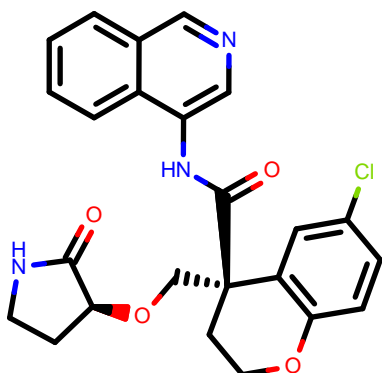
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CNC(=O)N5

RUN: RUN5101

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.22

EN300-6736413_2_1



CID: EN300-6736413_2_1

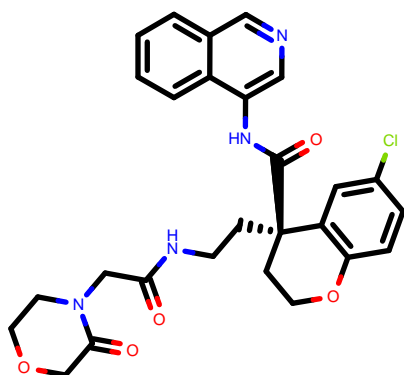
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CNC5=O

RUN: RUN2513

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.18

EN300-186943_3_1



CID: EN300-186943_3_1

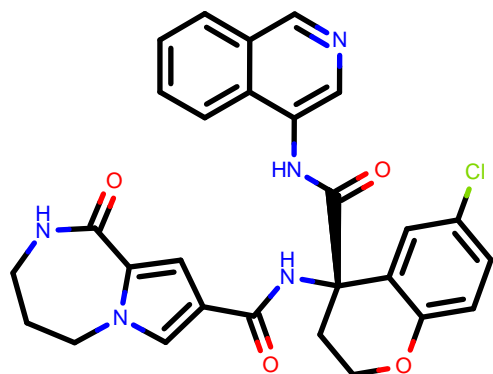
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5COCOC5=O

RUN: RUN13390

DDG (kcal/mol): -1.36

dDDG (kcal/mol): 0.26

EN300-7431365_1_1



CID: EN300-7431365_1_1

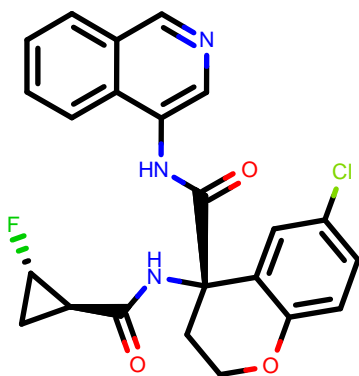
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(c5)CCNC6=O

RUN: RUN6544

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-97300_1_4



CID: EN300-97300_1_4

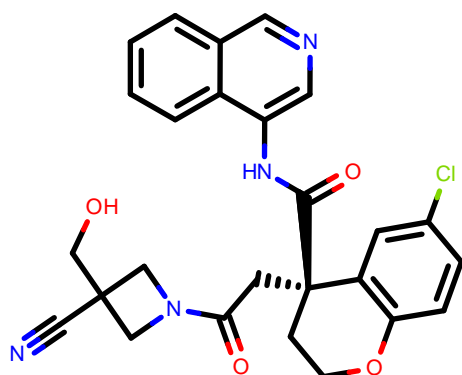
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5[C@@H]5F

RUN: RUN3278

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.17

EN300-227044_1_1



CID: EN300-227044_1_1

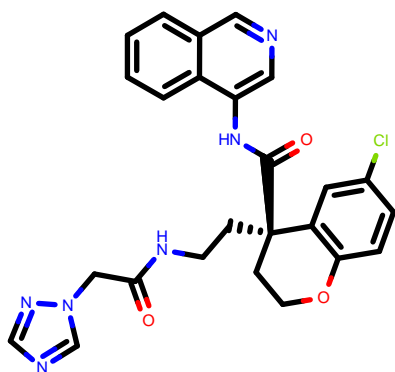
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)C#N

RUN: RUN12244

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.22

EN300-06654_3_1



CID: EN300-06654_3_1

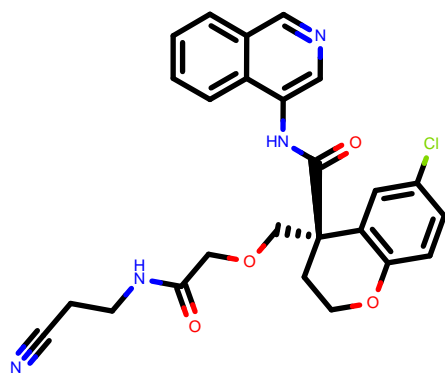
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cn5

RUN: RUN15157

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.24

EN300-10895_2_1



CID: EN300-10895_2_1

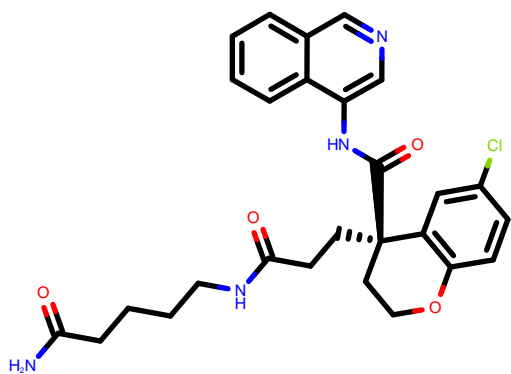
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)NCCC#N

RUN: RUN2040

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-125143_2_1



CID: EN300-125143_2_1

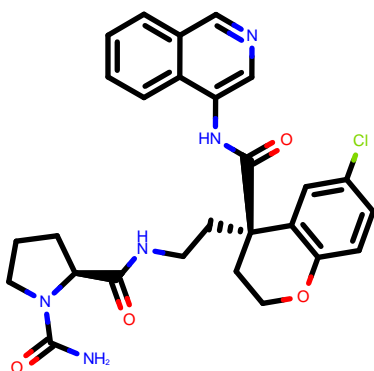
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCCCC(=O)N

RUN: RUN5112

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-87536_3_1



CID: EN300-87536_3_1

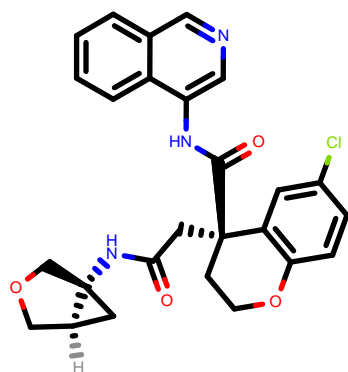
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5CCCN5C(=O)N

RUN: RUN4557

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.22

EN300-367383_1_1



CID: EN300-367383_1_1

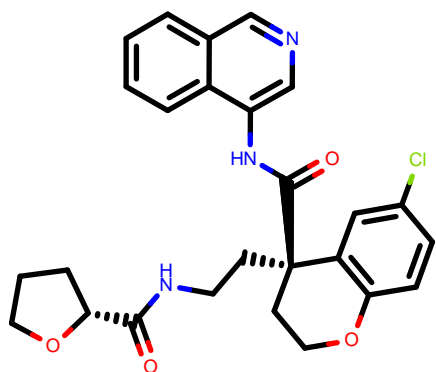
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]56C[C@H]5CCOC6

RUN: RUN4377

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-116234_3_1



CID: EN300-116234_3_1

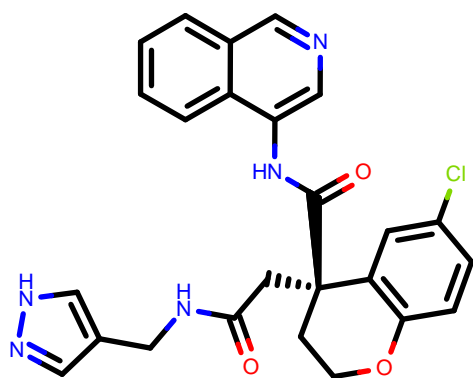
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5CCOC5

RUN: RUN4905

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.22

EN300-31562_1_1



CID: EN300-31562_1_1

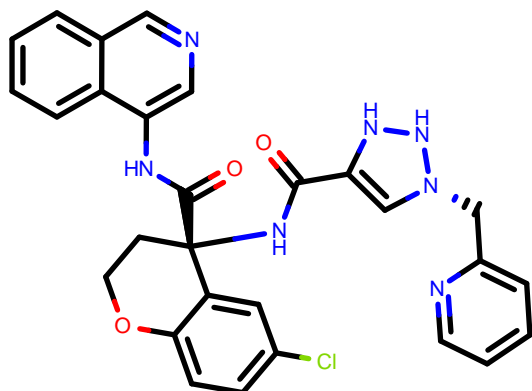
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5c[nH]j5

RUN: RUN3817

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.23

EN300-91315_1_1



CID: EN300-91315_1_1

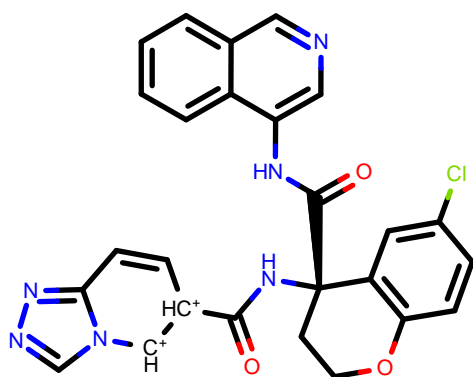
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5en[nH]5Cc6ccccc6

RUN: RUN3050

DDG (kcal/mol): -1.35

dDDG (kcal/mol): 0.22

EN300-60837_1_1



CID: EN300-60837_1_1

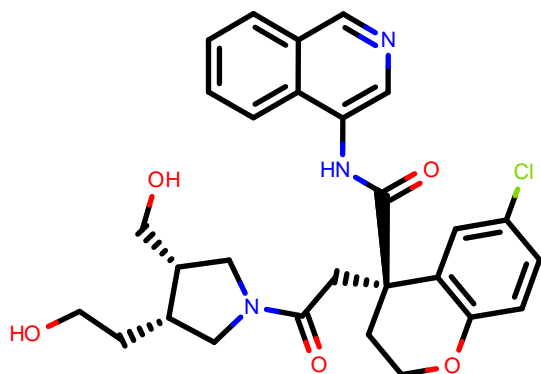
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc[nH]n5

RUN: RUN4330

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.19

EN300-1425608_1_3



CID: EN300-1425608_1_3

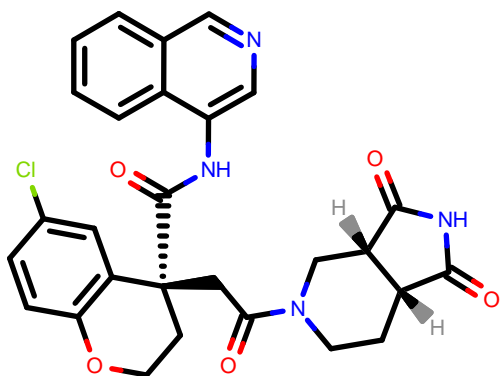
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H](CO)CO

RUN: RUN1263

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.28

EN300-104029_1_1



CID: EN300-104029_1_1

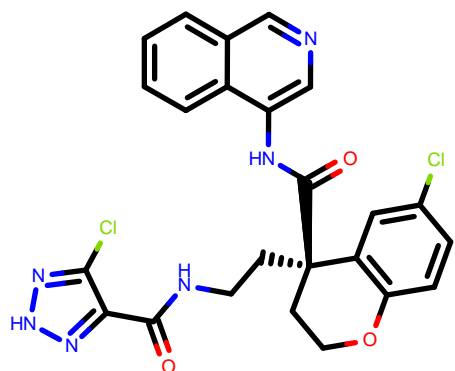
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N5CC[C@H]3[C@@H](C5)C1=O

RUN: RUN2061

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.26

EN300-149013_3_1



CID: EN300-149013_3_1

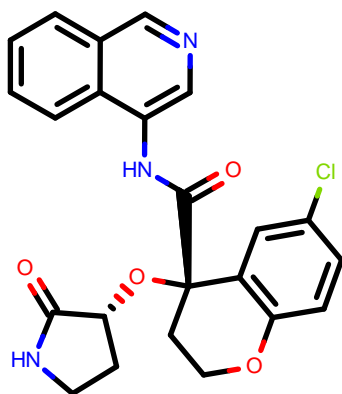
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N5C=CN=C5

RUN: RUN15017

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.23

EN300-6736413_1_2



CID: EN300-6736413_1_2

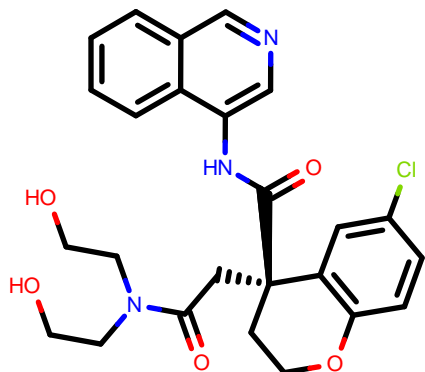
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N5CCNC5=O

RUN: RUN2163

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.17

EN300-19762_1_1



CID: EN300-19762_1_1

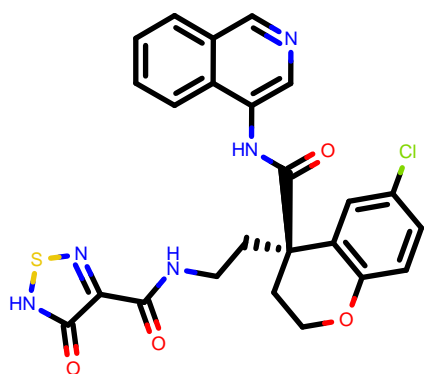
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4cc3cc4)C(=O)N5CCN(CCO)CCO

RUN: RUN5357

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.39

EN300-261859_3_1



CID: EN300-261859_3_1

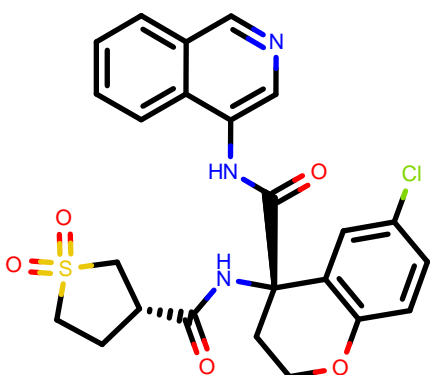
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5c(=O)[nH]n5

RUN: RUN14838

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.22

EN300-14437_1_1



CID: EN300-14437_1_1

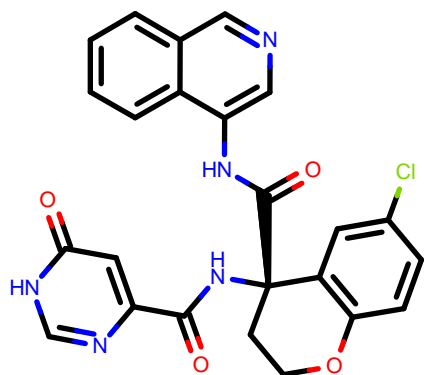
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5SCCS(=O)(=O)C5

RUN: RUN7080

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.24

EN300-817811_1_1



CID: EN300-817811_1_1

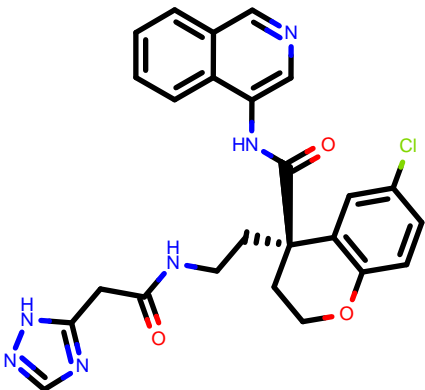
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc(=O)[nH]n5

RUN: RUN4834

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.20

EN300-96159_3_1



CID: EN300-96159_3_1

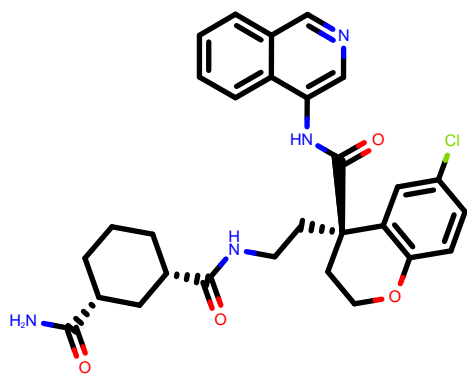
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5[nH]n5

RUN: RUN14852

DDG (kcal/mol): -1.34

dDDG (kcal/mol): 0.27

EN300-90142_3_4



CID: EN300-90142_3_4

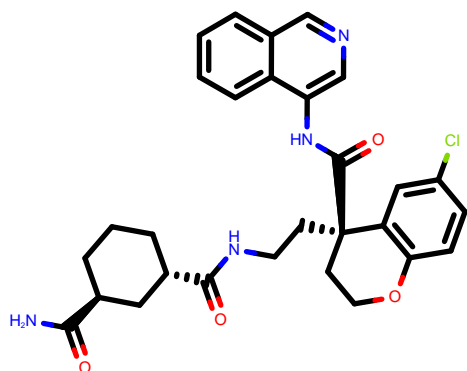
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C)CCNC(=O)C@H5CCC[C@@H](C5)Cl=O

RUN: RUN4549

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.28

EN300-90142_3_2



CID: EN300-90142_3_2

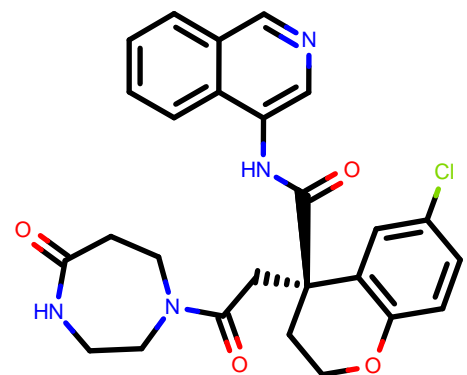
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C)CCNC(=O)C@H5CCC[C@@H](C5)Cl=O

RUN: RUN15274

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.30

EN300-69107_1_1



CID: EN300-69107_1_1

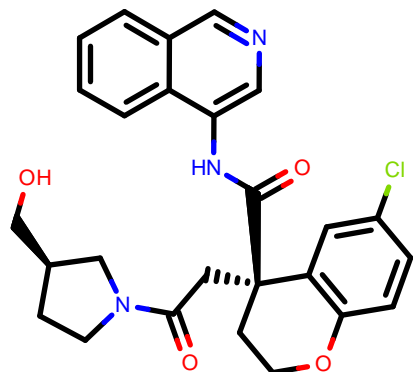
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C)CC(=O)N5CCCC(=O)NCC5

RUN: RUN9552

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.23

EN300-144970_1_1



CID: EN300-144970_1_1

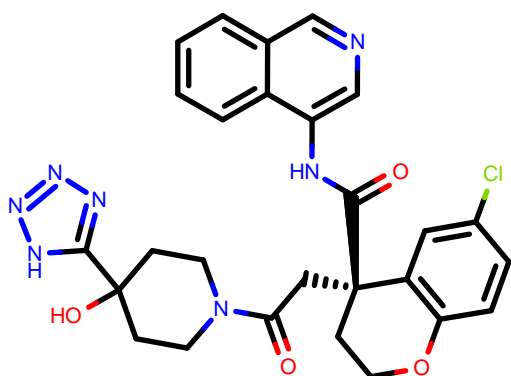
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C)CC(=O)N5CC[C@H](C5)CO

RUN: RUN5813

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.22

EN300-196160_1_1



CID: EN300-196160_1_1

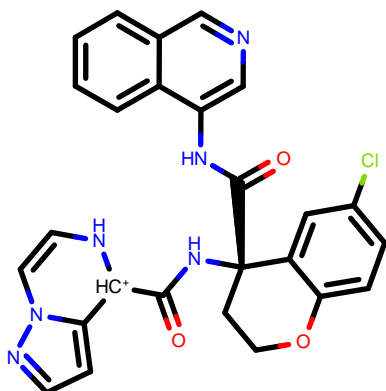
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(CS5)(c6n(n-1)nn6)O

RUN: RUN14754

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.31

EN300-359842_1_1



CID: EN300-359842_1_1

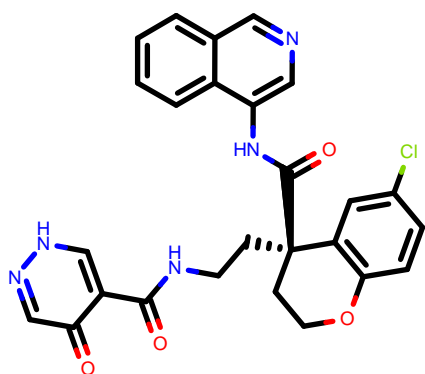
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6cnnc6cn5

RUN: RUN4966

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.20

EN300-243828_3_1



CID: EN300-243828_3_1

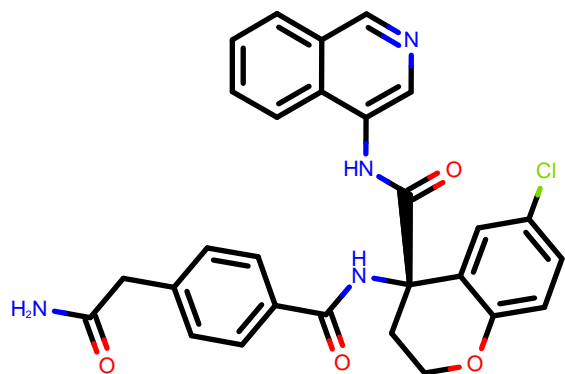
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5c[nH]nc5=O

RUN: RUN2856

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.22

EN300-2924757_1_1



CID: EN300-2924757_1_1

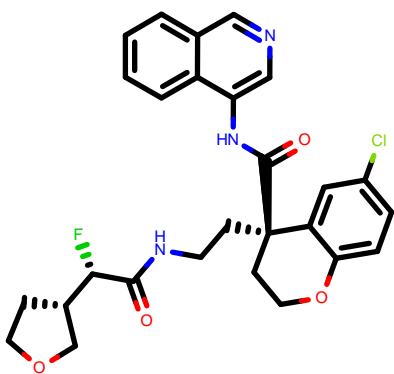
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccc(cc5)CC(=O)N

RUN: RUN627

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.22

EN300-783124_3_4



CID: EN300-783124_3_4

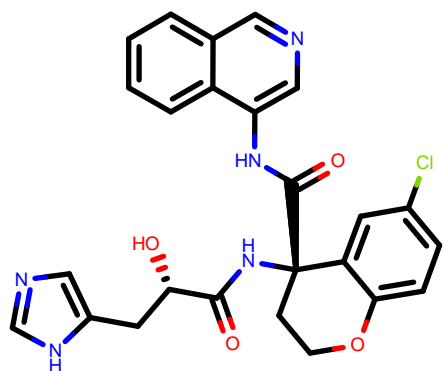
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C@H]([C@H]5CCOC5)F

RUN: RUN13536

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.28

EN300-6503811_1_1



CID: EN300-6503811_1_1

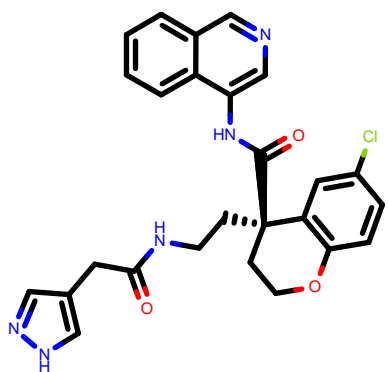
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@H]([C@H]5Ccnc[nH]5)O

RUN: RUN1577

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.24

EN300-1589101_3_1



CID: EN300-1589101_3_1

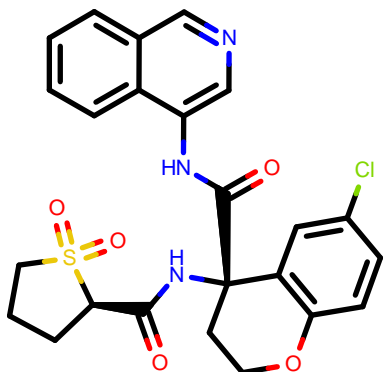
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5c[nH]ne5

RUN: RUN15307

DDG (kcal/mol): -1.33

dDDG (kcal/mol): 0.25

EN300-88656_1_2



CID: EN300-88656_1_2

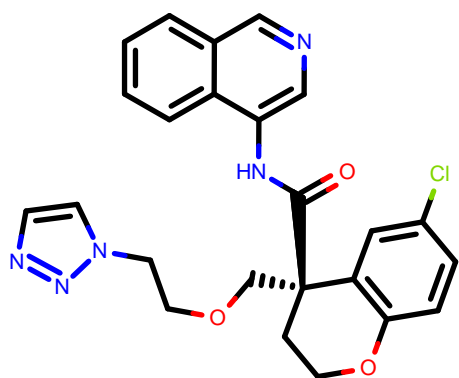
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C@H]5CCCS5(=O)=O

RUN: RUN2079

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.22

EN300-1715993_2_1



CID: EN300-1715993_2_1

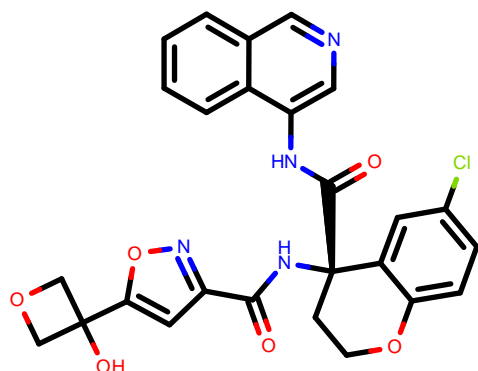
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cenn5

RUN: RUN995

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.20

EN300-365017_1_1



CID: EN300-365017_1_1

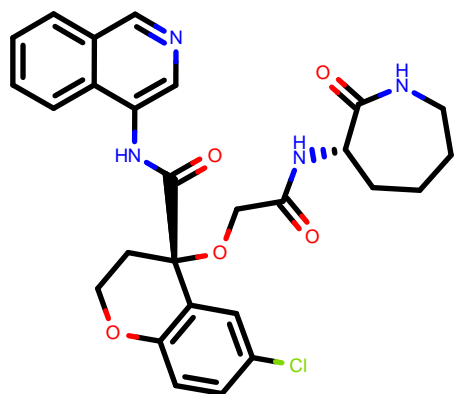
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(on5)O6(COC6)O

RUN: RUN6720

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.23

EN300-37195_1_1



CID: EN300-37195_1_1

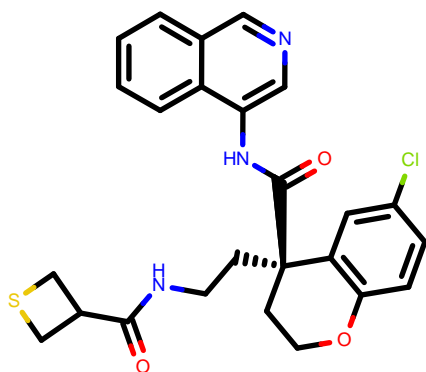
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN319

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.32

EN300-95094_3_1



CID: EN300-95094_3_1

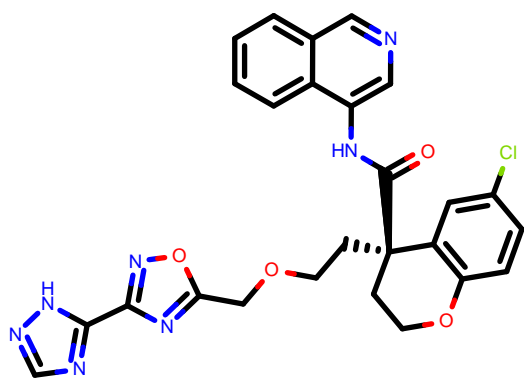
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CSC5

RUN: RUN9128

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.19

EN300-92031_3_1



CID: EN300-92031_3_1

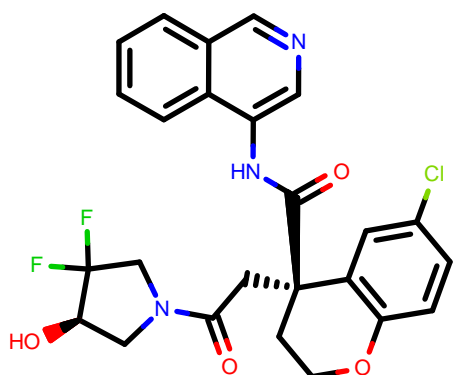
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC5nc(n5)c6[nH]n6

RUN: RUN2594

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.25

EN300-1710153_1_2



CID: EN300-1710153_1_2

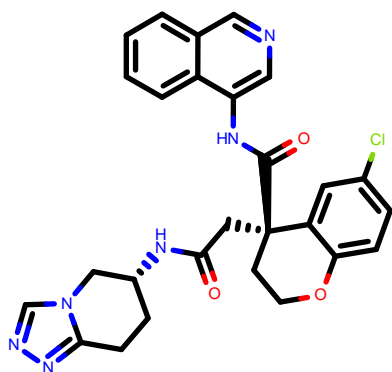
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](C5)(F)O

RUN: RUN3281

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.22

EN300-6735568_1_1



CID: EN300-6735568_1_1

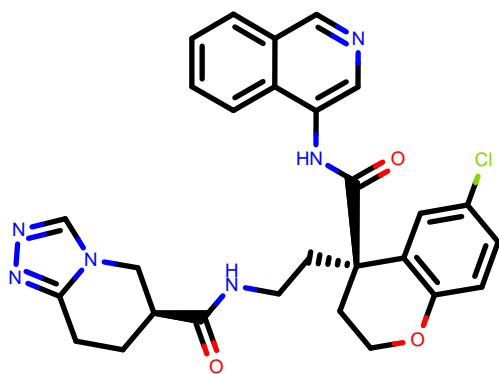
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]4H5CCc6nncn6C5

RUN: RUN4405

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.20

EN300-51350_3_2



CID: EN300-51350_3_2

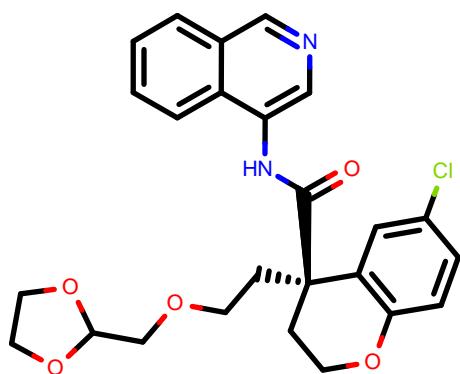
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5CCc6nncn6C5

RUN: RUN15378

DDG (kcal/mol): -1.32

dDDG (kcal/mol): 0.31

EN300-77092_3_1



CID: EN300-77092_3_1

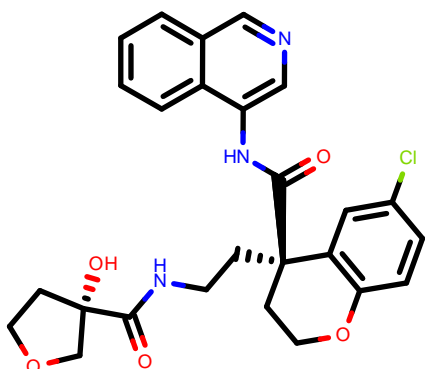
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5

RUN: RUN1728

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

EN300-148421_3_1



CID: EN300-148421_3_1

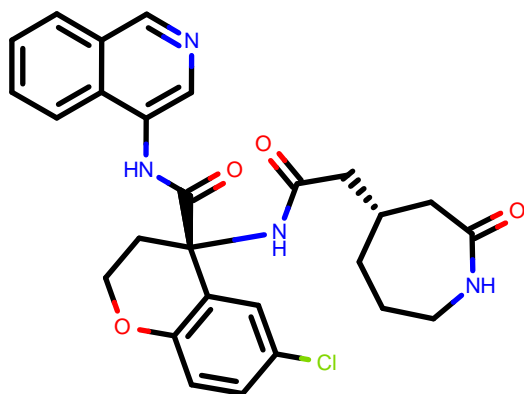
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOc5O)O

RUN: RUN4769

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.25

EN300-195590_1_1



CID: EN300-195590_1_1

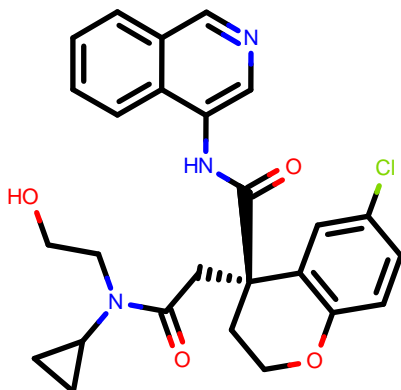
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H]5CCNC(=O)C5

RUN: RUN2982

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.26

EN300-37102_1_1



CID: EN300-37102_1_1

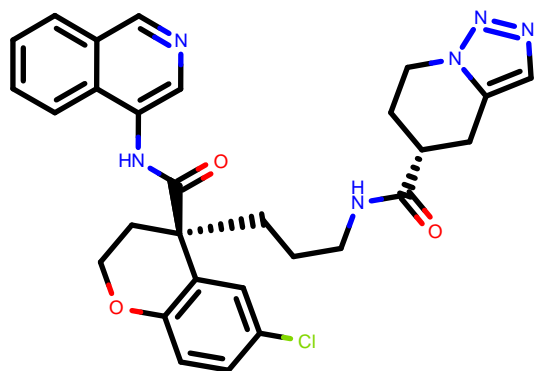
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5CC5

RUN: RUN3273

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.27

EN300-7430501_4_2



CID: EN300-7430501_4_2

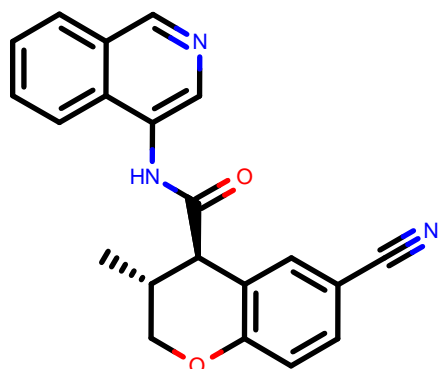
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5Cn6c(cnn6)C5

RUN: RUN11977

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.27

DAR-DIA-0d514e7d-8_1



CID: DAR-DIA-0d514e7d-8_1

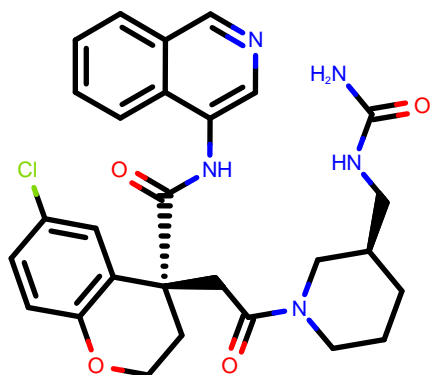
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3ncc4c3ccc4)C#N

RUN: RUN78

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.07

EN300-42195_1_1



CID: EN300-42195_1_1

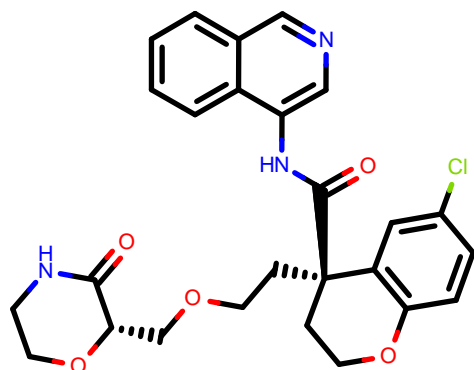
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5CNC(=O)N

RUN: RUN13222

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.32

EN300-1706036_3_1



CID: EN300-1706036_3_1

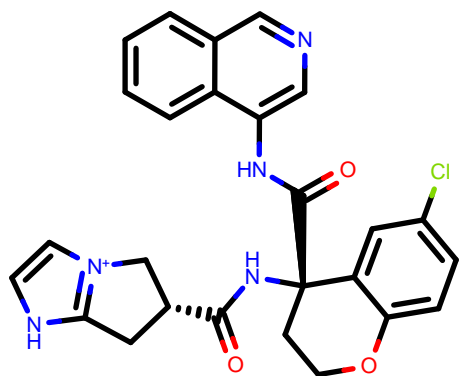
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C(=O)NCCO5

RUN: RUN2046

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.27

EN300-7385329_1_1



CID: EN300-7385329_1_1

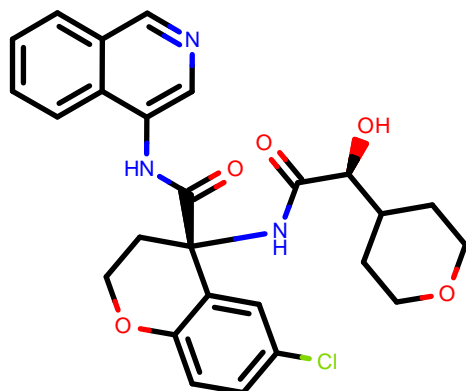
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C6[nH+]cn6C5

RUN: RUN9688

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-6792206_1_1



CID: EN300-6792206_1_1

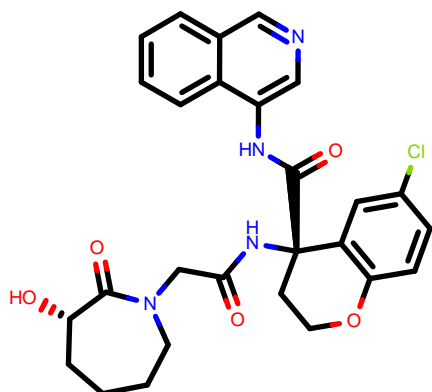
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C6COCOC5O

RUN: RUN7184

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.33

EN300-259849_1_2



CID: EN300-259849_1_2

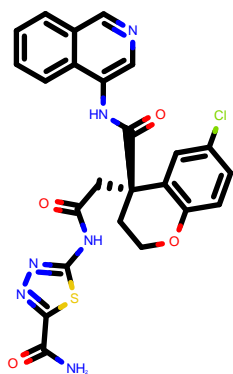
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5CCCC[C@@H]5C(=O)O

RUN: RUN9501

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.35

EN300-695831_1_1



CID: EN300-695831_1_1

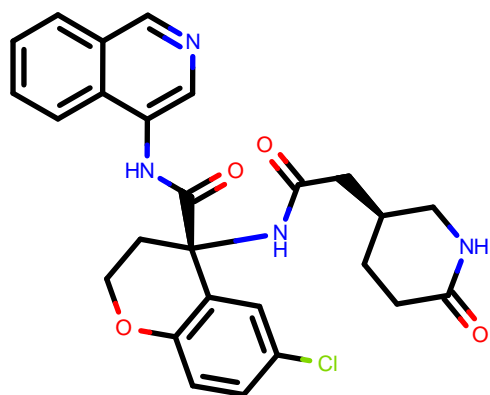
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5nnc(s5)C(=O)N

RUN: RUN4773

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.22

EN300-246992_1_1



CID: EN300-246992_1_1

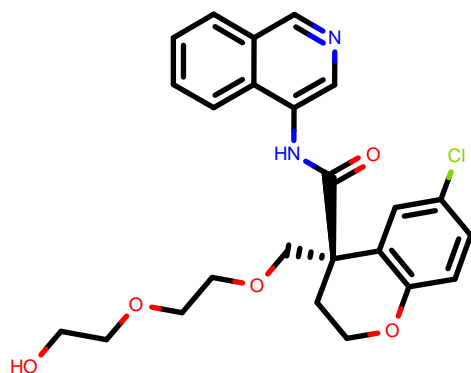
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCC(=O)NC5

RUN: RUN3922

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.24

EN300-52467_2_1



CID: EN300-52467_2_1

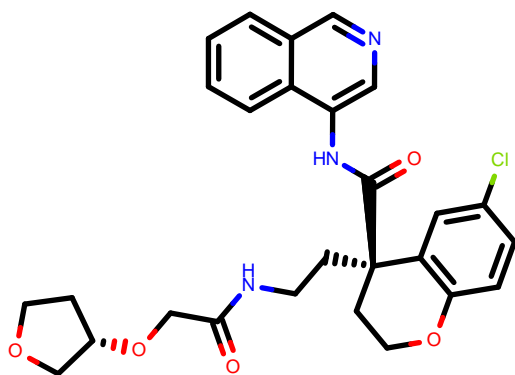
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCOCOC(O)O

RUN: RUN756

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.23

EN300-99391_3_2



CID: EN300-99391_3_2

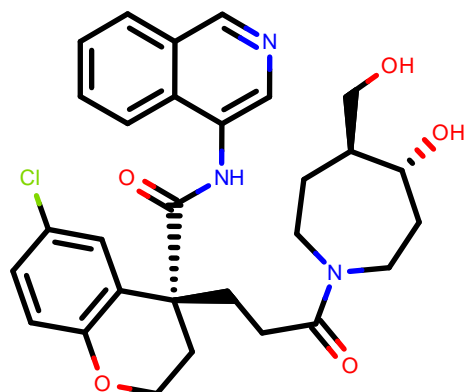
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN8083

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.28

EN300-7353672_2_4



CID: EN300-7353672_2_4

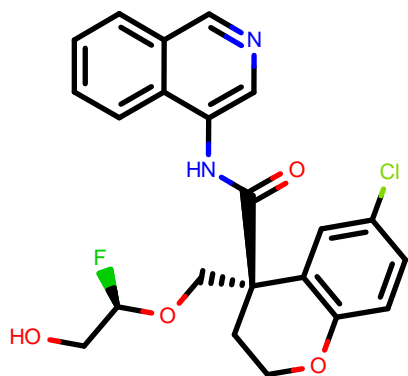
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CC(O)C[C@@H]5(CO)CCO5

RUN: RUN13053

DDG (kcal/mol): -1.31

dDDG (kcal/mol): 0.32

EN300-861925_2_2



CID: EN300-861925_2_2

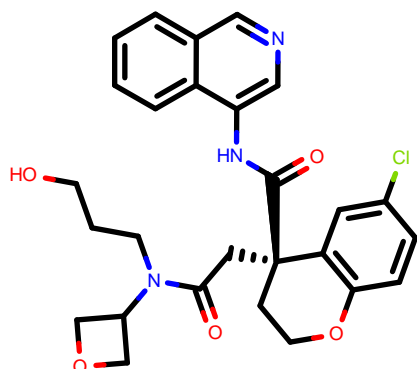
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H](CO)F

RUN: RUN268

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.23

EN300-1725529_1_1



CID: EN300-1725529_1_1

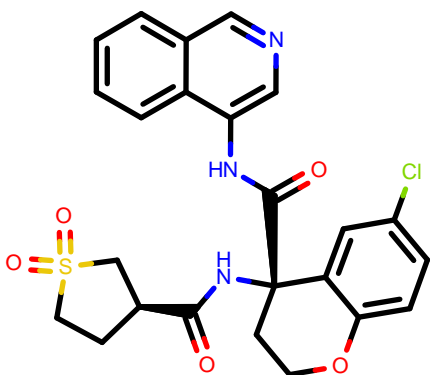
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5OCC5

RUN: RUN5657

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.38

EN300-14437_1_2



CID: EN300-14437_1_2

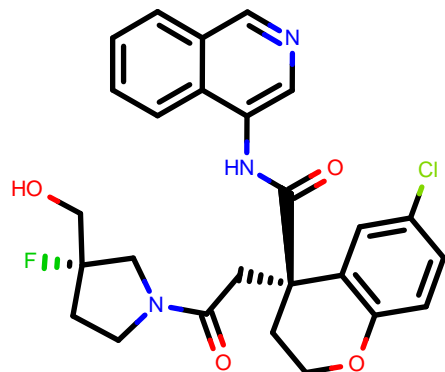
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCS(=O)(=O)C5

RUN: RUN8657

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.27

EN300-203118_1_2



CID: EN300-203118_1_2

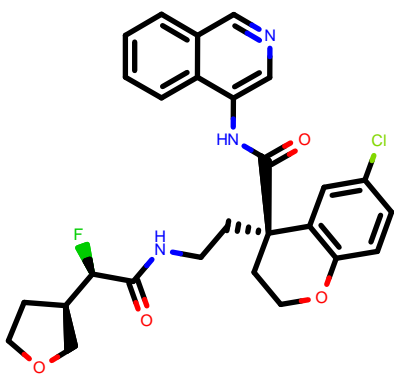
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)(CO)F

RUN: RUN9666

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.26

EN300-783124_3_1



CID: EN300-783124_3_1

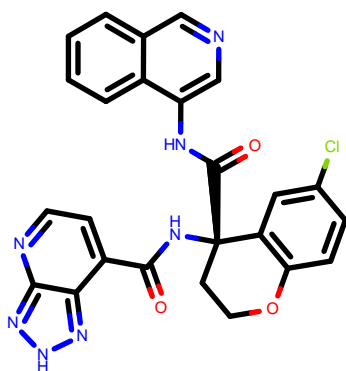
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@@H5CCOC5F

RUN: RUN8684

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.25

EN300-188377_1_1



CID: EN300-188377_1_1

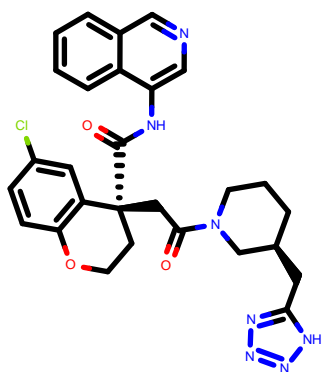
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6c5n[nH]n6

RUN: RUN4938

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.21

EN300-383891_1_2



CID: EN300-383891_1_2

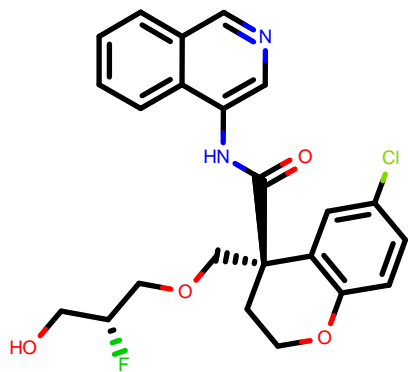
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)C6N[nH]n6

RUN: RUN11719

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.34

EN300-1600517_2_2



CID: EN300-1600517_2_2

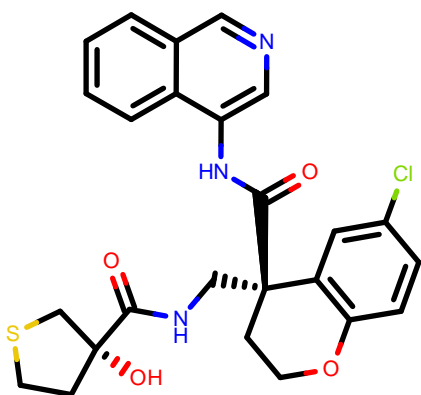
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CO)F

RUN: RUN1778

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.22

EN300-122656_2_2



CID: EN300-122656_2_2

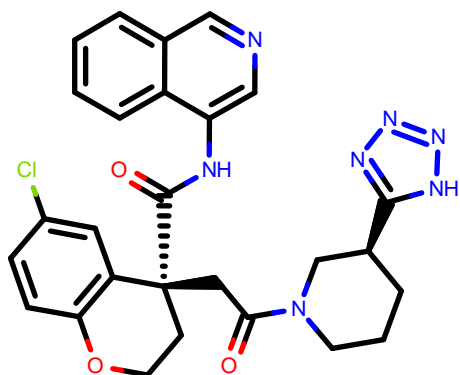
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CNC(=O)C[C@@]5(C)CCSC5)O

RUN: RUN4327

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.44

EN300-115760_1_1



CID: EN300-115760_1_1

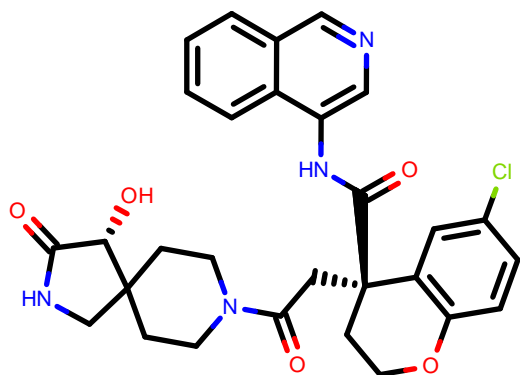
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CC(=O)N5CC[C@@]3[C@@]5(C)C6N=[N]N=C6

RUN: RUN6288

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.31

EN300-6478434_1_2



CID: EN300-6478434_1_2

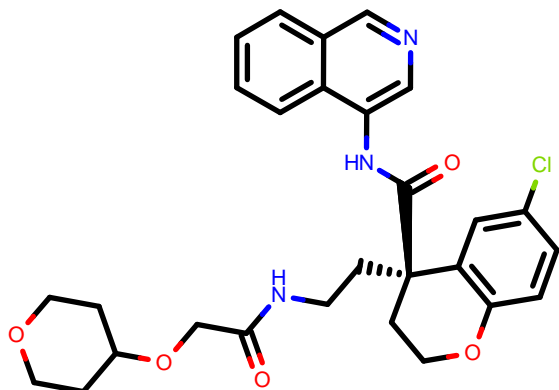
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CC(=O)N5COC6(C)CNC1=O[C@@]3[C@@]5(C)C6

RUN: RUN10483

DDG (kcal/mol): -1.30

dDDG (kcal/mol): 0.30

EN300-77520_3_1



CID: EN300-77520_3_1

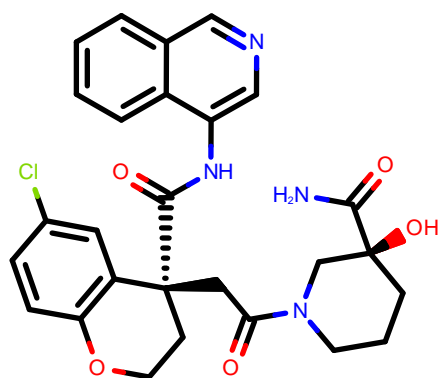
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CNC(=O)COC5COCOC5

RUN: RUN11267

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.23

EN300-210553_1_2



CID: EN300-210553_1_2

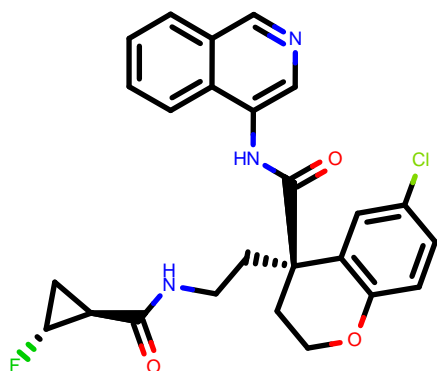
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@](C5)(C(=O)N)O

RUN: RUN5189

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.30

EN300-1654606_3_1



CID: EN300-1654606_3_1

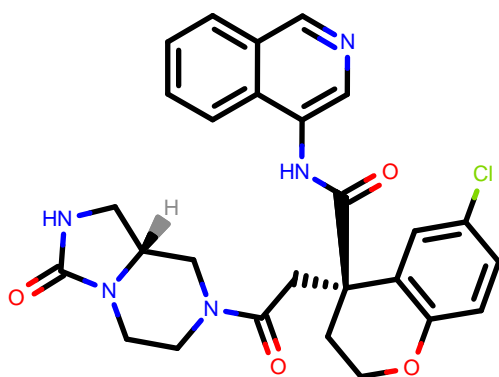
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]3(C)C(F)C

RUN: RUN15059

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.20

EN300-100765_1_2



CID: EN300-100765_1_2

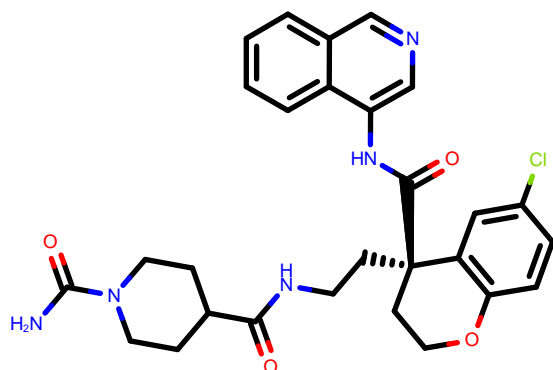
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@]3(C)C(=O)N6C

RUN: RUN8399

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.23

EN300-13489_3_1



CID: EN300-13489_3_1

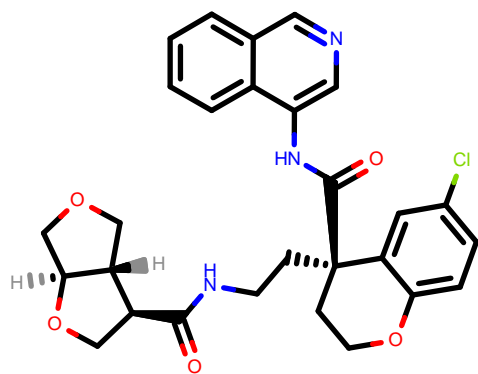
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CCN(C5)C(=O)N

RUN: RUN7191

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.35

EN300-6482296_3_4



CID: EN300-6482296_3_4

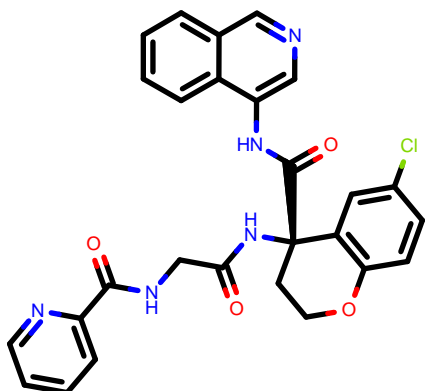
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H3CCOC4C3C(=O)C1CCNC1=O[C@@H]5COC[C@@H]6[C@@H]5COC6

RUN: RUN15133

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.26

EN300-83280_1_1



CID: EN300-83280_1_1

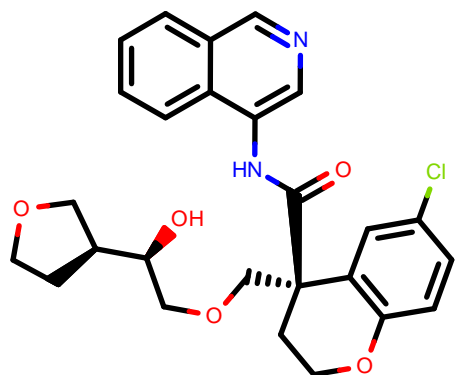
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H3CCOC4C3C(=O)C1CCNC1=O[C@@H]5COC[C@@H]6C5COC6

RUN: RUN9760

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.25

EN300-1911992_2_4



CID: EN300-1911992_2_4

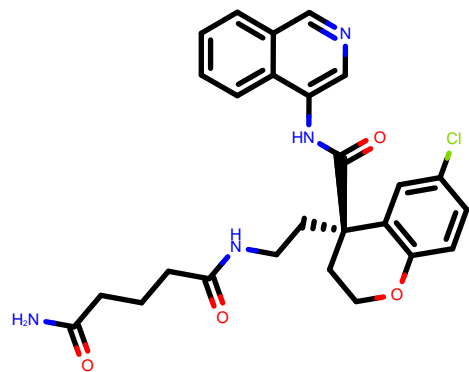
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H3CCOC4C3C(=O)C1CCNC1=O[C@@H]5COC[C@@H]6C5COC6

RUN: RUN452

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.29

EN300-59478_3_1



CID: EN300-59478_3_1

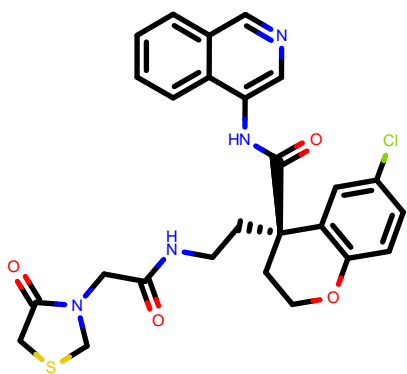
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@@H3CCOC4C3C(=O)C1CCNC1=O[C@@H]5COC[C@@H]6C5COC6

RUN: RUN3621

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.31

EN300-10747_3_1



CID: EN300-10747_3_1

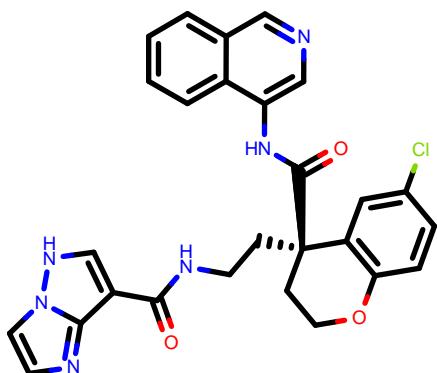
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CSCS5=O

RUN: RUN9657

DDG (kcal/mol): -1.29

dDDG (kcal/mol): 0.22

EN300-135238_3_1



CID: EN300-135238_3_1

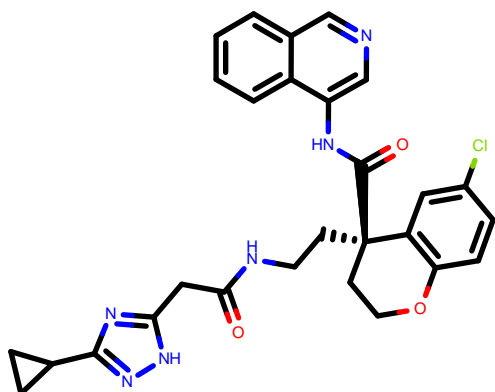
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5c[nH]n6c5nc6

RUN: RUN4789

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.22

EN300-657211_3_1



CID: EN300-657211_3_1

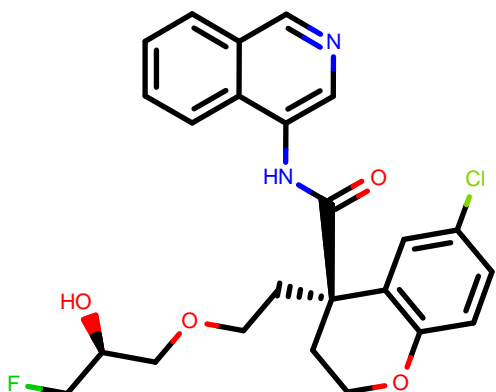
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5[nH]nc(n5)C6CC6

RUN: RUN6503

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.30

EN300-1968342_3_1



CID: EN300-1968342_3_1

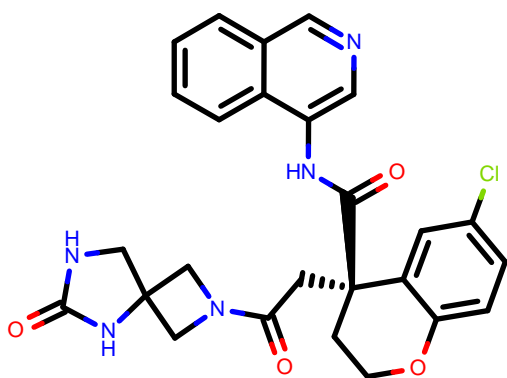
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CF)O

RUN: RUN1184

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.25

EN300-1605226_1_1



CID: EN300-1605226_1_1

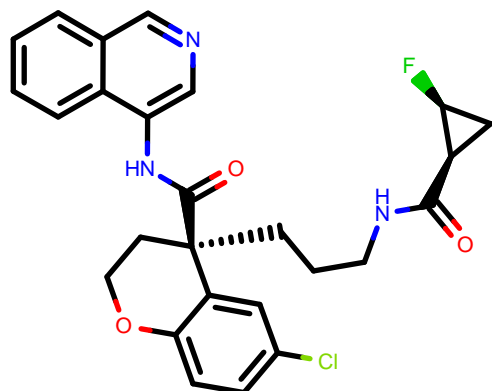
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6(C5)CNC(=O)N6

RUN: RUN13796

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.19

EN300-97300_4_3



CID: EN300-97300_4_3

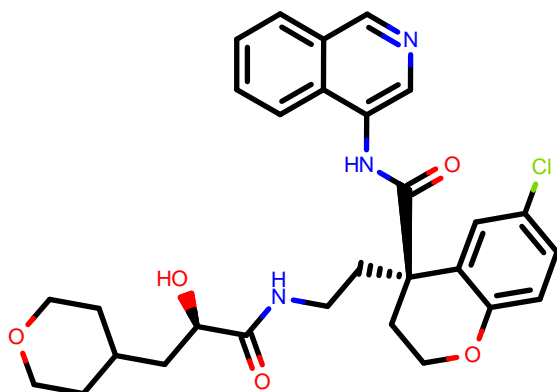
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5C[C@@]H5F

RUN: RUN12769

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.21

EN300-1452069_3_1



CID: EN300-1452069_3_1

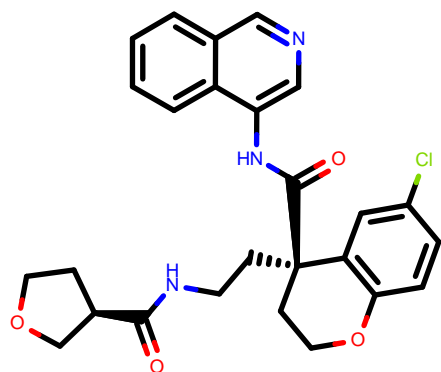
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5C[C@@]C5O

RUN: RUN11196

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.33

EN300-697519_3_1



CID: EN300-697519_3_1

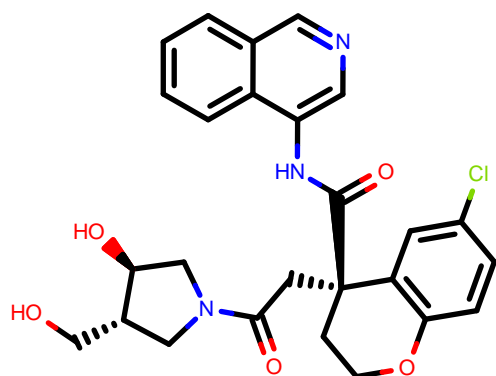
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5CCOC5

RUN: RUN4785

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.21

EN300-248521_1_1



CID: EN300-248521_1_1

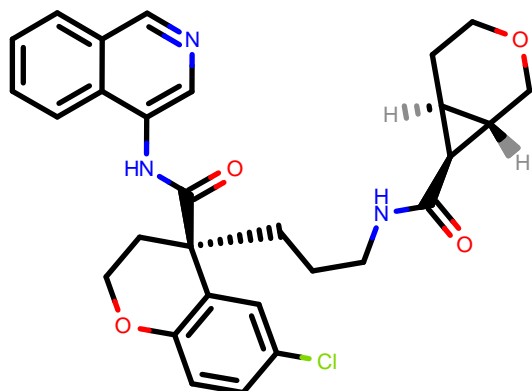
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@@H](C5)O)CO

RUN: RUN521

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.24

EN300-1644723_4_2



CID: EN300-1644723_4_2

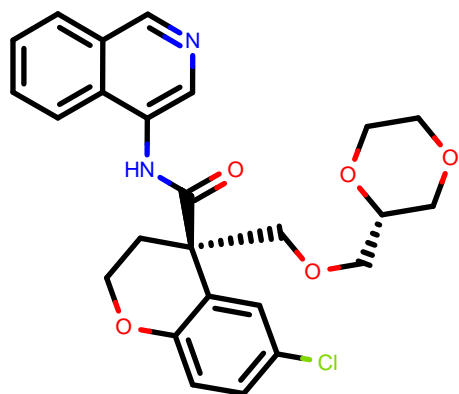
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CCN(C=O)[C@@H]5[C@@H]6[C@@H]5COCC6

RUN: RUN12921

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.23

EN300-139167_2_1



CID: EN300-139167_2_1

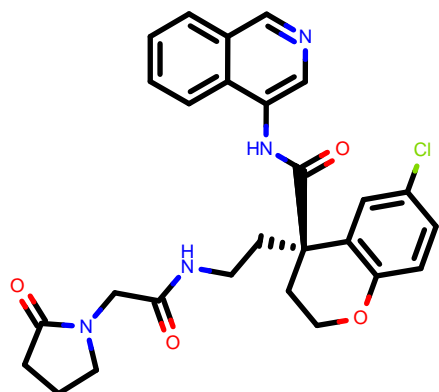
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)COC[C@@H]5COCC5O

RUN: RUN1354

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.21

EN300-11934_3_1



CID: EN300-11934_3_1

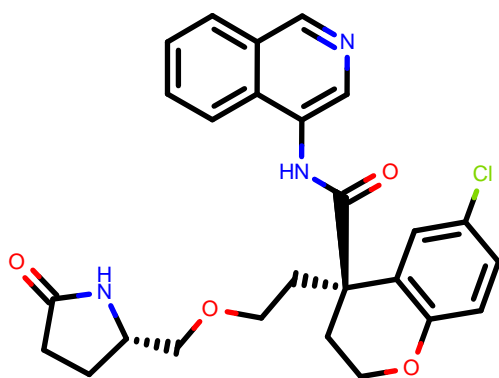
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CCNC(=O)N5CCCC5=O

RUN: RUN11691

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.25

EN300-195756_3_2



CID: EN300-195756_3_2

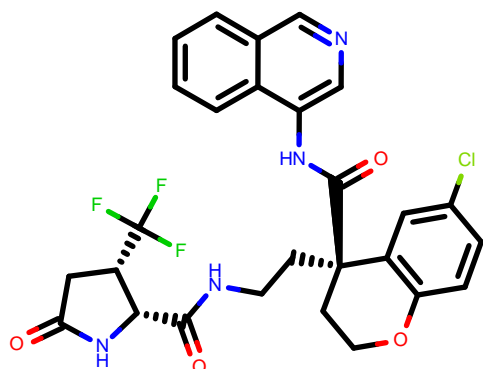
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]H5CCCC(=O)N5

RUN: RUN1927

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.25

EN300-169955_3_2



CID: EN300-169955_3_2

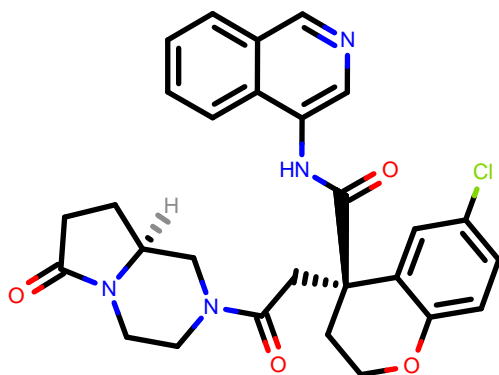
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5C(F)(F)F

RUN: RUN2933

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.22

EN300-60330_1_1



CID: EN300-60330_1_1

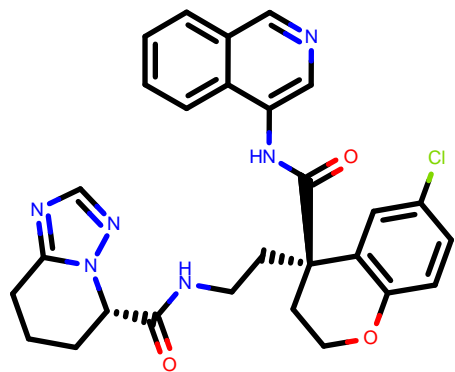
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@]H5(C5)CCC6=O

RUN: RUN12802

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.21

EN300-1273016_3_1



CID: EN300-1273016_3_1

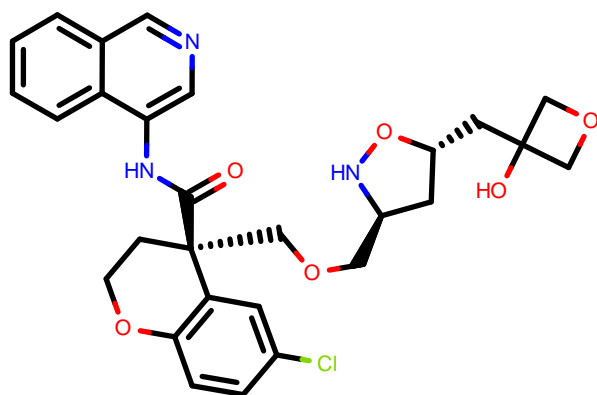
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H55CCC6n5n6

RUN: RUN5105

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.24

EN300-7457160_2_1



CID: EN300-7457160_2_1

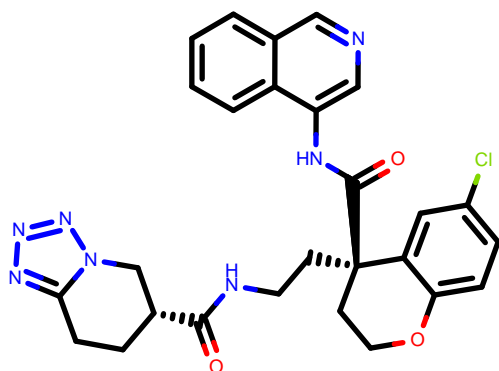
SMILES: c1ccc2c(c1)ncnc2NC(=O)C(C@@H)(COCOC4C3CC(=O)C4)CCOC5=NC(C@@H)(C5)CC6COC6O

RUN: RUN2671

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.27

EN300-269453_3_1



CID: EN300-269453_3_1

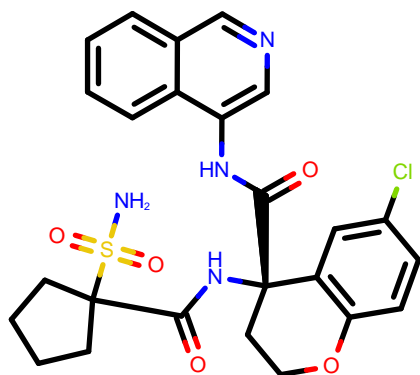
SMILES: c1ccc2c(c1)ncnc2NC(=O)C(C@@H)(COCOC4C3CC(=O)C4)CCNC(=O)C(C@@H)5CC6C6Nn6C5

RUN: RUN15359

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.25

EN300-6486793_1_1



CID: EN300-6486793_1_1

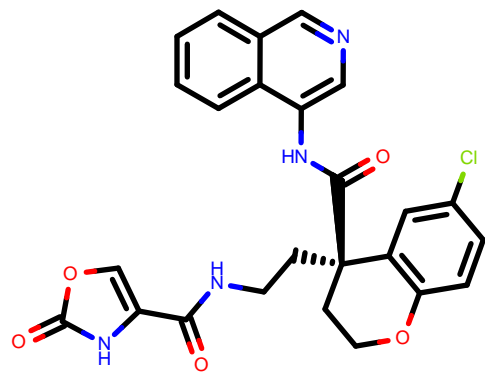
SMILES: c1ccc2c(c1)ncnc2NC(=O)C(C@@H)(COCOC4C3CC(=O)C4)NC(=O)C5(CCCC5)S(=O)(=O)N

RUN: RUN6217

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.22

EN300-246486_3_1



CID: EN300-246486_3_1

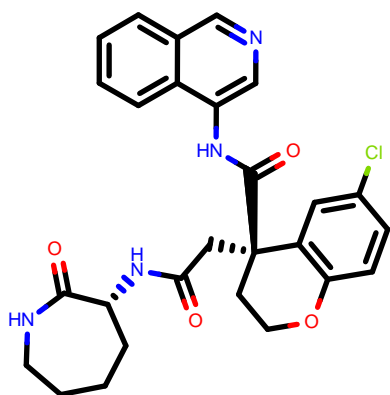
SMILES: c1ccc2c(c1)ncnc2NC(=O)C(C@@H)(COCOC4C3CC(=O)C4)CCNC(=O)c5ccoc(=O)[nH]5

RUN: RUN15505

DDG (kcal/mol): -1.28

dDDG (kcal/mol): 0.22

EN300-129384_1_2



CID: EN300-129384_1_2

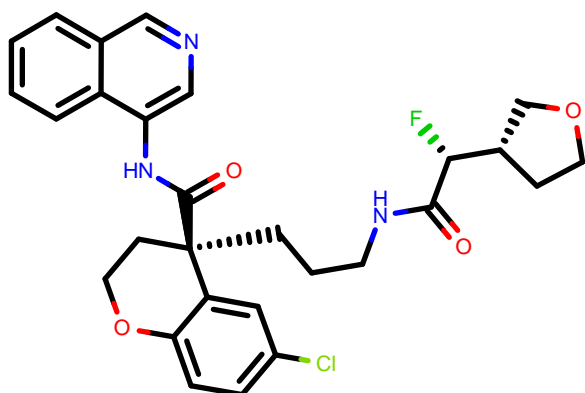
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN13478

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.20

EN300-783124_4_3



CID: EN300-783124_4_3

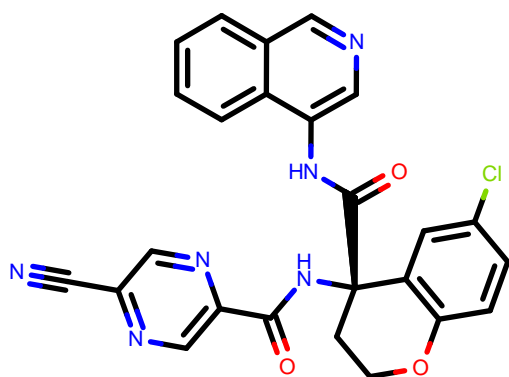
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC5F

RUN: RUN8310

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.25

EN300-149224_1_1



CID: EN300-149224_1_1

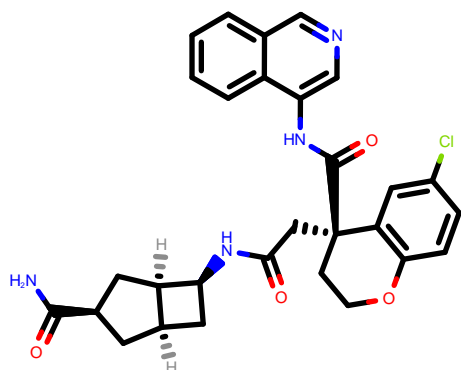
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncn(c5)C#N

RUN: RUN3054

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.19

EN300-1268016_1_10



CID: EN300-1268016_1_10

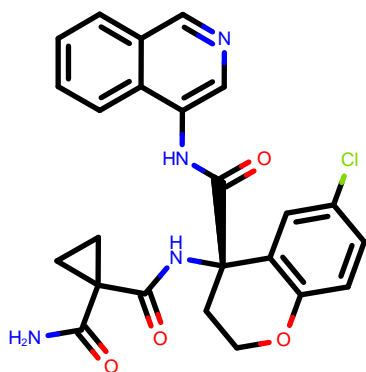
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]6[C@@H]5C[C@@H]6Cl=O

RUN: RUN4453

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.23

EN300-69070_1_1



CID: EN300-69070_1_1

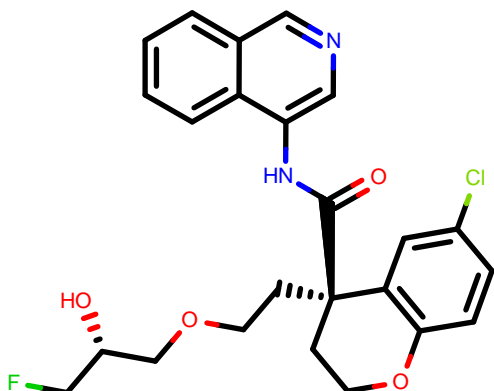
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)C(=O)N

RUN: RUN1561

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.22

EN300-1968342_3_2



CID: EN300-1968342_3_2

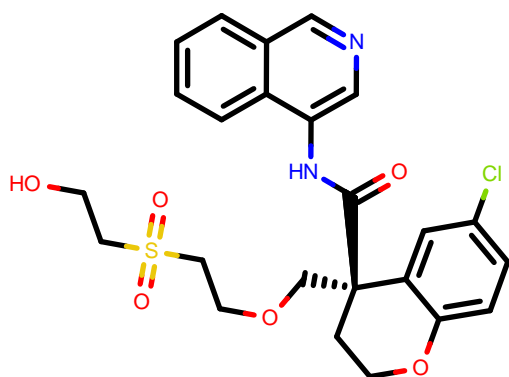
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O

RUN: RUN1168

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.27

EN300-7463171_2_1



CID: EN300-7463171_2_1

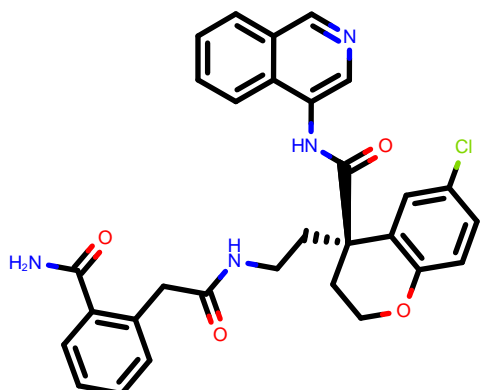
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)S(=O)(=O)O

RUN: RUN476

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.45

EN300-121144_3_1



CID: EN300-121144_3_1

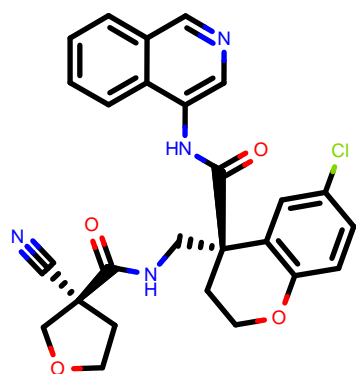
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5c5ccc5C(=O)N

RUN: RUN905

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.31

EN300-261210_2_1



CID: EN300-261210_2_1

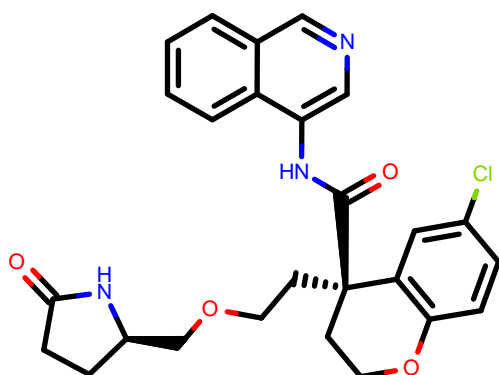
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@]5(CCOCC5)C#N

RUN: RUN4555

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.23

EN300-195756_3_1



CID: EN300-195756_3_1

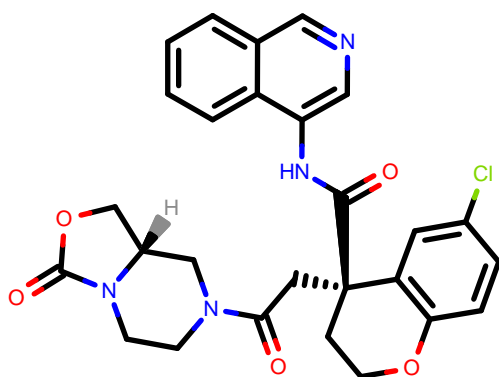
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@H]5(COCC(=O)N5)

RUN: RUN1360

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.23

EN300-109827_1_1



CID: EN300-109827_1_1

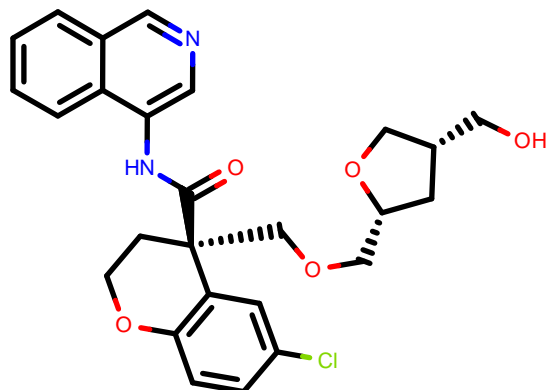
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN6[C@@H](C5)COC6=O

RUN: RUN15384

DDG (kcal/mol): -1.27

dDDG (kcal/mol): 0.24

EN300-6494158_2_3



CID: EN300-6494158_2_3

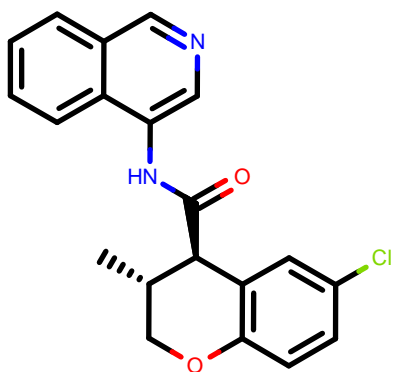
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@H]5C[C@H](CO5)CO

RUN: RUN244

DDG (kcal/mol): -1.27

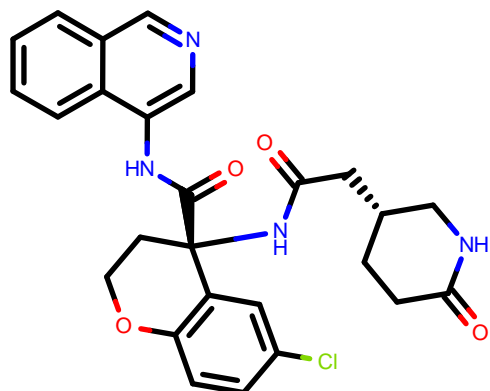
dDDG (kcal/mol): 0.24

MAT-POS-8a69d52e-4_2



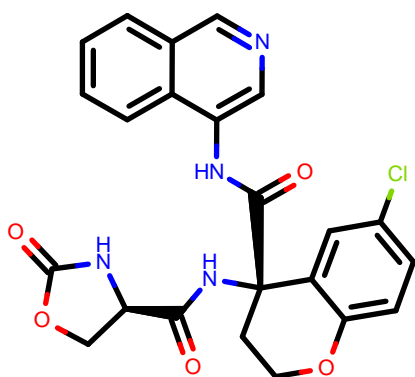
CID:	MAT-POS-8a69d52e-4_2
SMILES:	<chem>C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl</chem>
RUN:	RUN76
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.06

EN300-246992_1_2



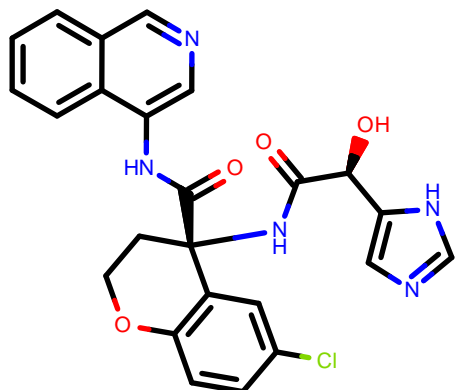
CID:	EN300-246992_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCC(=O)N5</chem>
RUN:	RUN8240
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.24

EN300-201346_1_2



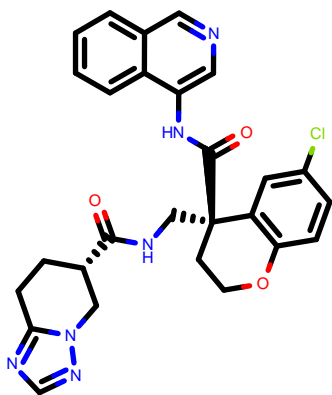
CID:	EN300-201346_1_2
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5COC(=O)N5</chem>
RUN:	RUN7204
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.20

EN300-254121_1_1



CID:	EN300-254121_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H](c5cnc[nH]5)O</chem>
RUN:	RUN7120
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.31

EN300-1662365_2_2



CID: EN300-1662365_2_2

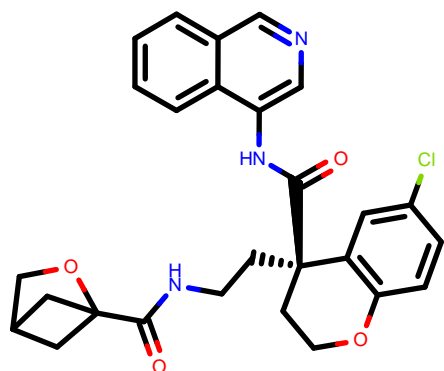
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCc6nncn6C5

RUN: RUN6394

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-2007648_3_1



CID: EN300-2007648_3_1

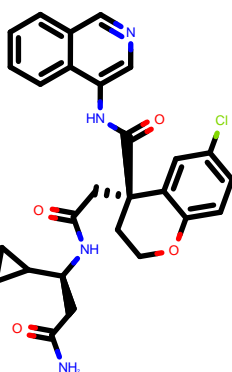
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C56CC(C5)C06

RUN: RUN2796

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.21

EN300-85413_1_2



CID: EN300-85413_1_2

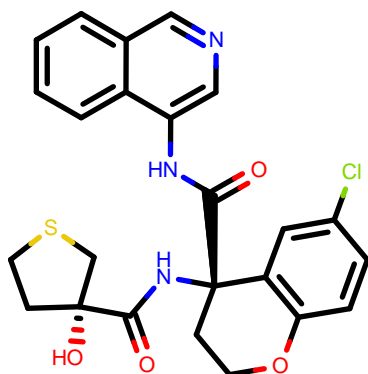
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H](C(=O)N)C5C5C5

RUN: RUN1415

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.31

EN300-122656_1_2



CID: EN300-122656_1_2

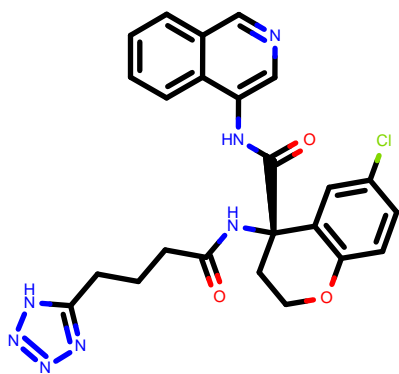
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@]5(C)CSC5O

RUN: RUN2653

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.39

EN300-134204_1_1



CID: EN300-134204_1_1

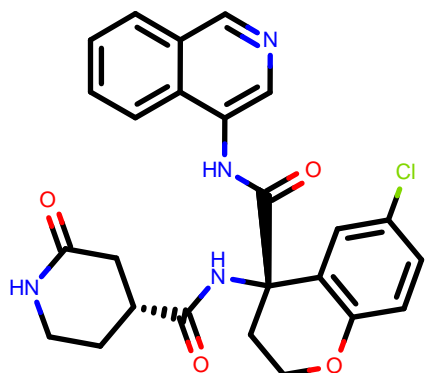
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCc5n[nH]n5

RUN: RUN8404

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.29

EN300-107493_1_2



CID: EN300-107493_1_2

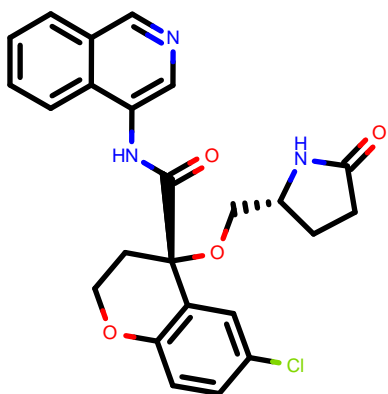
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5CCNC(=O)C5

RUN: RUN4290

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.23

EN300-195756_1_1



CID: EN300-195756_1_1

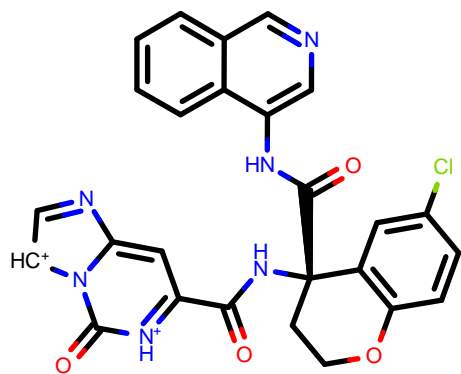
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5CCNC(=O)N5

RUN: RUN2619

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.24

EN300-7440089_1_1



CID: EN300-7440089_1_1

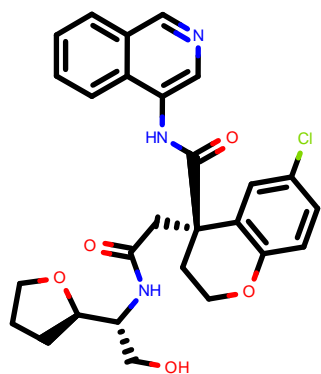
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cc6nc[nH]6(=O)[nH]5

RUN: RUN5534

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.21

EN300-190026_1_1



CID: EN300-190026_1_1

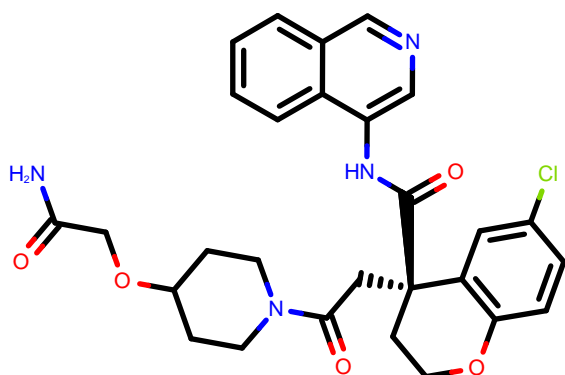
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)N(C@H)(CO)C@H)5CCCCO5

RUN: RUN10261

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.36

EN300-96808_1_1



CID: EN300-96808_1_1

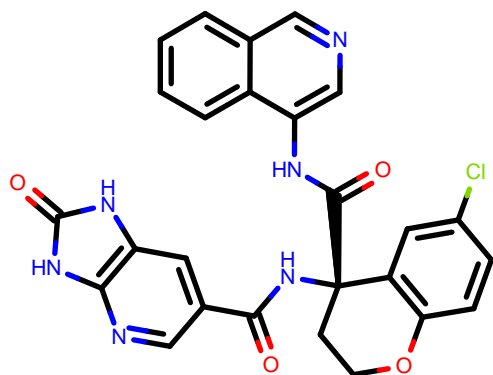
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)N(C@H)(CO)C@H)5CCCC(C(=O)O)N

RUN: RUN1231

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.24

EN300-214552_1_1



CID: EN300-214552_1_1

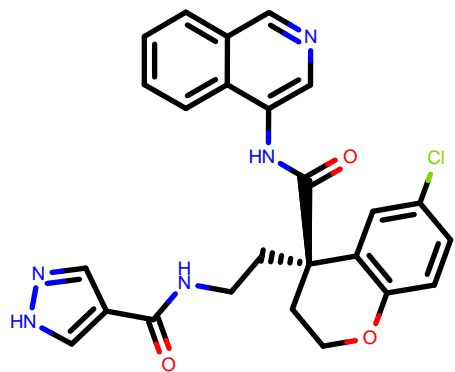
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)N(C@H)(CO)C@H)5CCCC(C(=O)N)nc5

RUN: RUN6293

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.24

EN300-41863_3_1



CID: EN300-41863_3_1

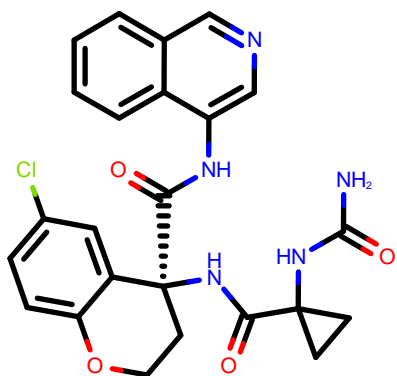
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](C(=O)O4C3CC(=O)N(C@H)(CO)C@H)5CCCC(C(=O)N)nc5

RUN: RUN15289

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.19

EN300-123614_1_1



CID: EN300-123614_1_1

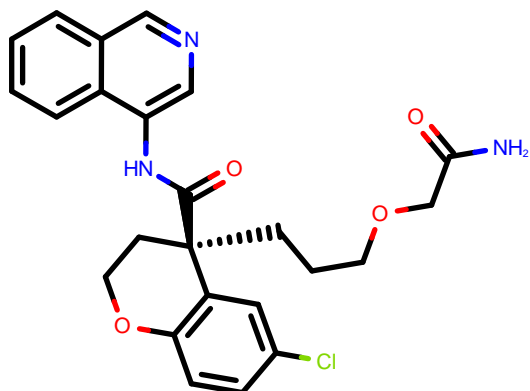
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C)C5NC(=O)N

RUN: RUN7536

DDG (kcal/mol): -1.26

dDDG (kcal/mol): 0.26

EN300-18249_4_1



CID: EN300-18249_4_1

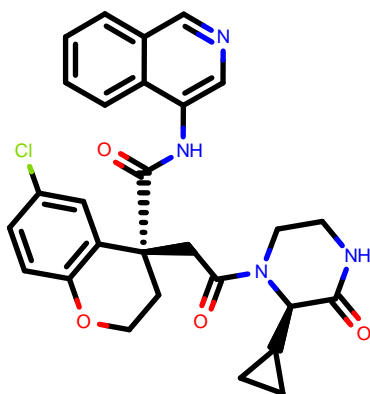
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCOCC(=O)N

RUN: RUN805

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.19

EN300-1256657_1_2



CID: EN300-1256657_1_2

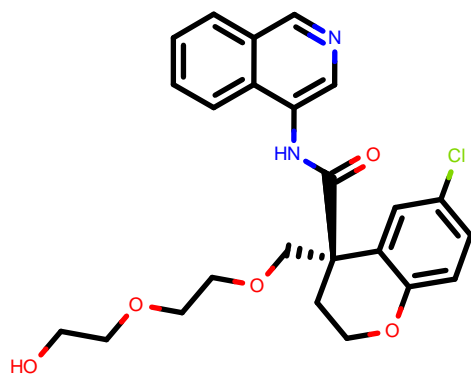
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)[C@H]5C6CC6

RUN: RUN11653

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.30

EN300-52467_2_1



CID: EN300-52467_2_1

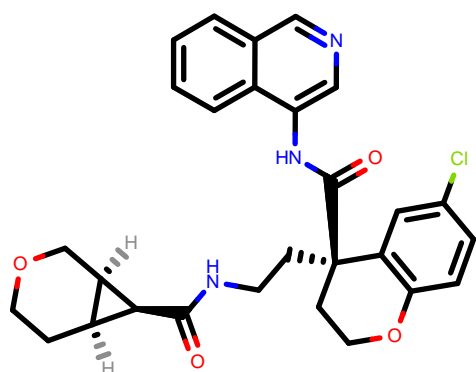
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCCOCCO

RUN: RUN764

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.20

EN300-1644723_3_6



CID: EN300-1644723_3_6

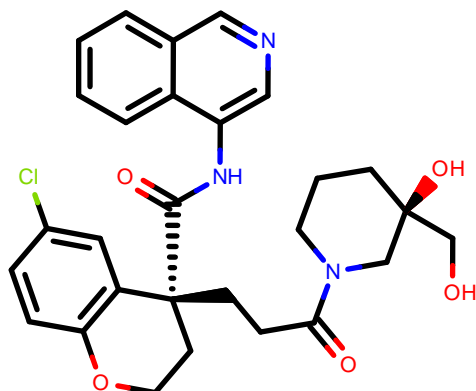
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3CCOC4C3CC(=O)C1CCNC1=O[C@@H]2[C@@H]3C#H[C@@H]3COC6

RUN: RUN14366

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.25

EN300-251396_2_1



CID: EN300-251396_2_1

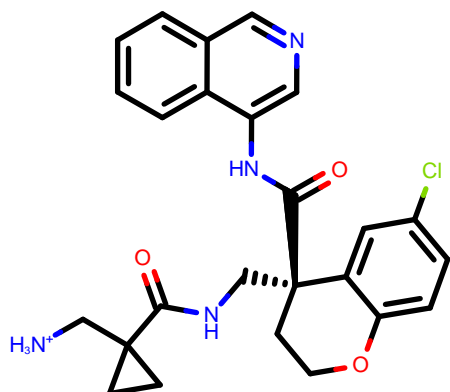
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3(CCOc4c3cc(cc4)C)CCC(=O)N5CCCC[C@@H](C5)C(O)O

RUN: RUN8991

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.35

EN300-114082_2_1



CID: EN300-114082_2_1

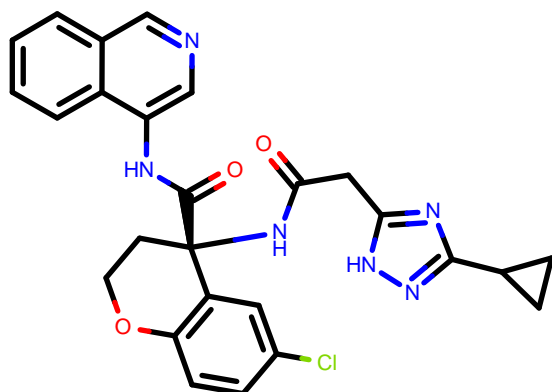
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3(CCOc4c3cc(cc4)C)CNC(=O)C5(C)C5C#N

RUN: RUN5531

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.23

EN300-657211_1_1



CID: EN300-657211_1_1

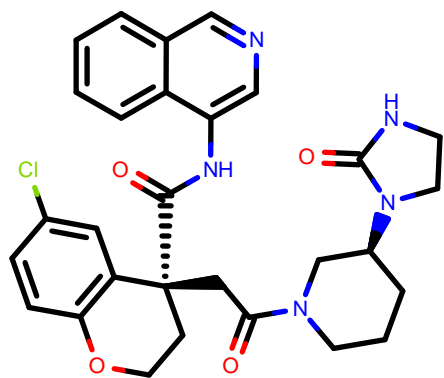
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H](C@H)3(CCOc4c3cc(cc4)C)CNC(=O)Cc5[nH]nc5C6C6

RUN: RUN7464

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.26

EN300-55087_1_1



CID: EN300-55087_1_1

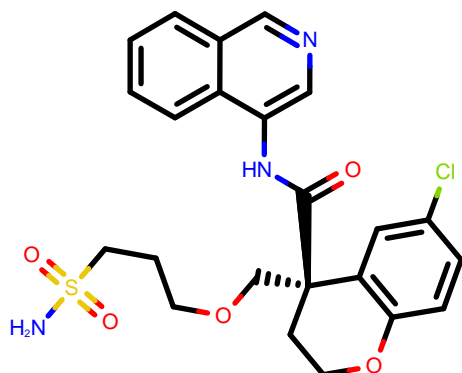
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC6=O

RUN: RUN12560

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.30

EN300-79588_2_1



CID: EN300-79588_2_1

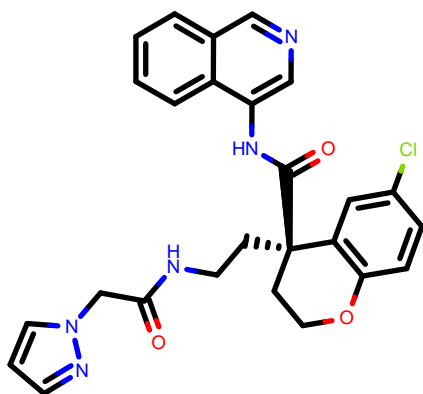
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N

RUN: RUN1218

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.27

EN300-23942_3_1



CID: EN300-23942_3_1

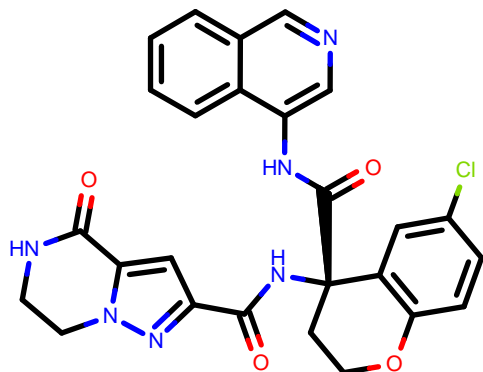
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cccn5

RUN: RUN15064

DDG (kcal/mol): -1.25

dDDG (kcal/mol): 0.21

EN300-200426_1_1



CID: EN300-200426_1_1

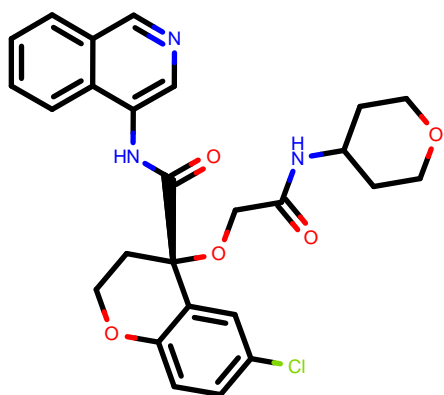
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)c5cc6n(n5)CCNC6=O

RUN: RUN8633

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.23

EN300-67573_1_1



CID: EN300-67573_1_1

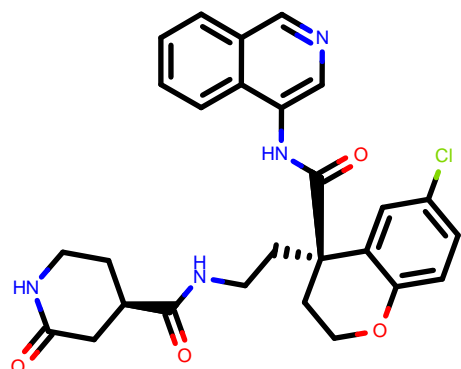
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCOCC5

RUN: RUN1293

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.25

EN300-107493_3_2



CID: EN300-107493_3_2

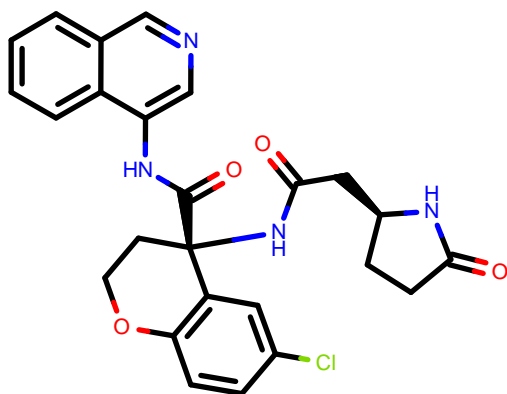
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5CCNCC5

RUN: RUN14844

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.27

EN300-68203_1_2



CID: EN300-68203_1_2

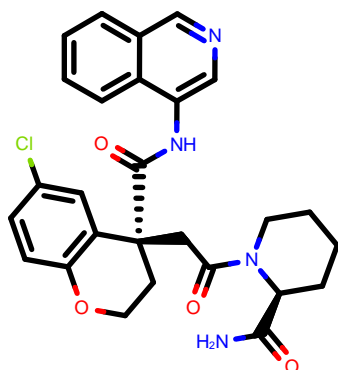
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5CCN5

RUN: RUN5706

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.23

EN300-34542_1_1



CID: EN300-34542_1_1

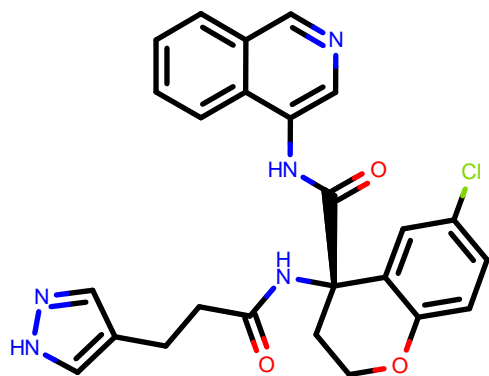
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@]5C(=O)N

RUN: RUN9687

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.23

EN300-250836_1_1



CID: EN300-250836_1_1

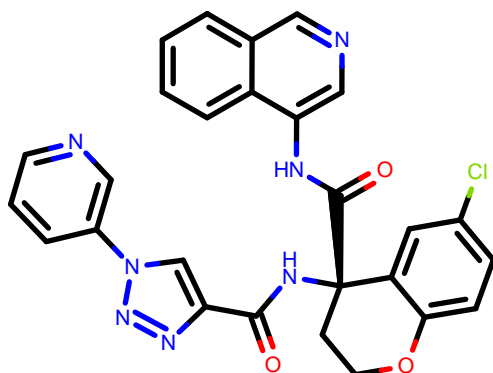
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5c[nH]je5

RUN: RUN5030

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.21

EN300-151330_1_1



CID: EN300-151330_1_1

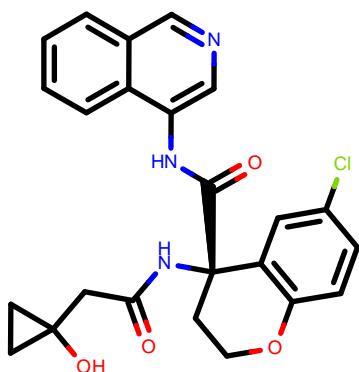
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]c6ccnc6

RUN: RUN2103

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.17

EN300-207873_1_1



CID: EN300-207873_1_1

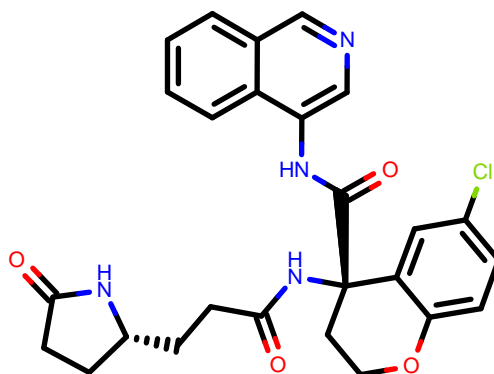
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CC5)O

RUN: RUN699

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.21

EN300-104592_1_2



CID: EN300-104592_1_2

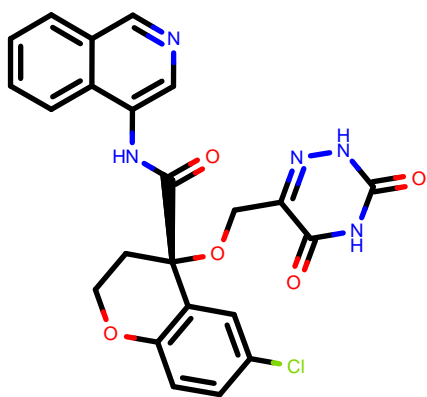
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@@]4HJ5CCC(=O)N5

RUN: RUN4258

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.24

EN300-761746_1_1



CID: EN300-761746_1_1

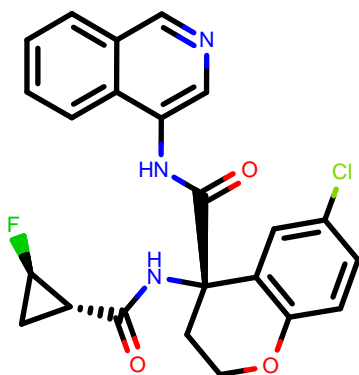
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c(=O)[nH]c(=O)[nH]5

RUN: RUN1828

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.18

EN300-1654606_1_1



CID: EN300-1654606_1_1

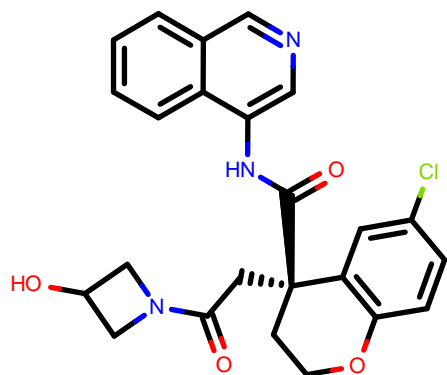
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5F

RUN: RUN5842

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.17

EN300-65115_1_1



CID: EN300-65115_1_1

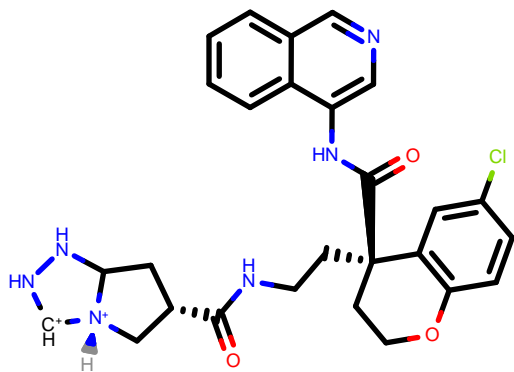
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)O

RUN: RUN11761

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.18

EN300-6745453_3_2



CID: EN300-6745453_3_2

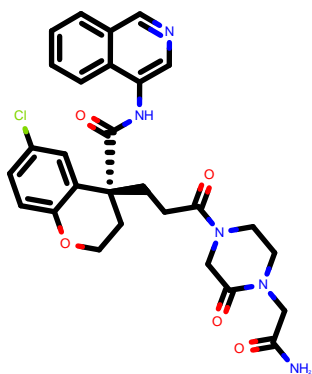
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C6nncn6C5

RUN: RUN15413

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.23

EN300-251571_2_1



CID: EN300-251571_2_1

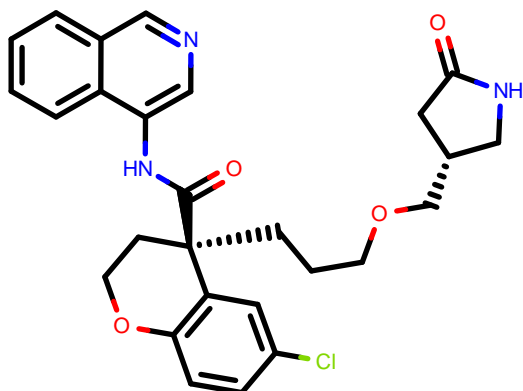
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCN(C(=O)C5)CC(=O)N

RUN: RUN5060

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.28

EN300-246747_4_1



CID: EN300-246747_4_1

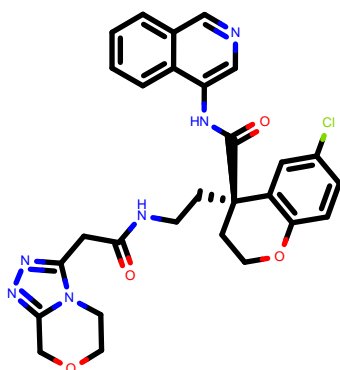
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5C(=O)N5

RUN: RUN1978

DDG (kcal/mol): -1.24

dDDG (kcal/mol): 0.21

EN300-1718836_3_1



CID: EN300-1718836_3_1

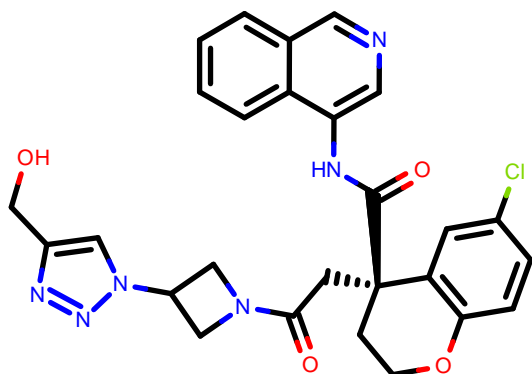
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5nnc6n5CCOC6

RUN: RUN11996

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.38

EN300-1664105_1_1



CID: EN300-1664105_1_1

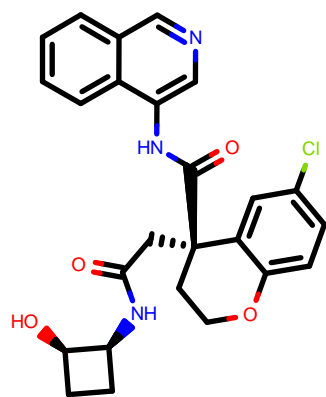
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)n6cc(nn6)CO

RUN: RUN361

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.23

EN300-129424_1_2



CID: EN300-129424_1_2

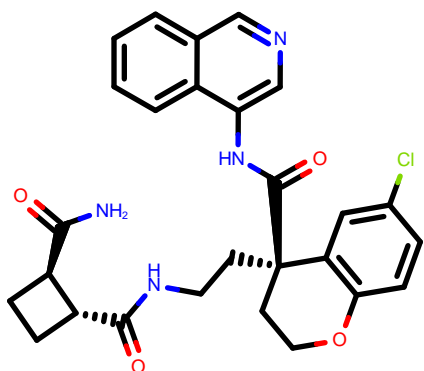
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5C[C@H]5O

RUN: RUN10119

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.21

EN300-217107_3_1



CID: EN300-217107_3_1

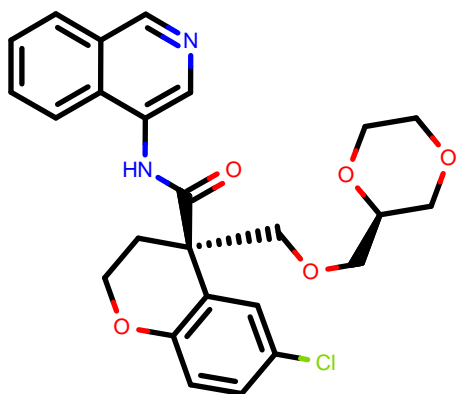
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)N[C@@H]5C[C@H]5O=N

RUN: RUN13680

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.23

EN300-139167_2_2



CID: EN300-139167_2_2

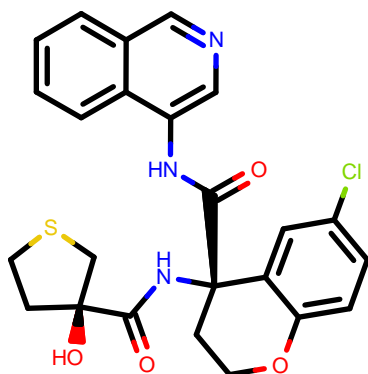
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@H]5COC5O

RUN: RUN916

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.20

EN300-122656_1_1



CID: EN300-122656_1_1

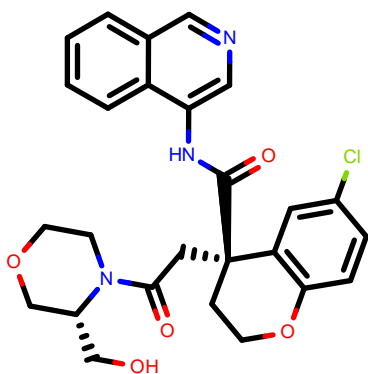
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5(CCS)S5O

RUN: RUN8104

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.45

EN300-173903_1_1



CID: EN300-173903_1_1

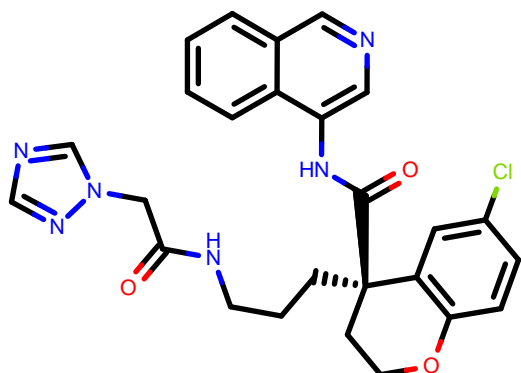
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO

RUN: RUN11559

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.34

EN300-06654_4_1



CID: EN300-06654_4_1

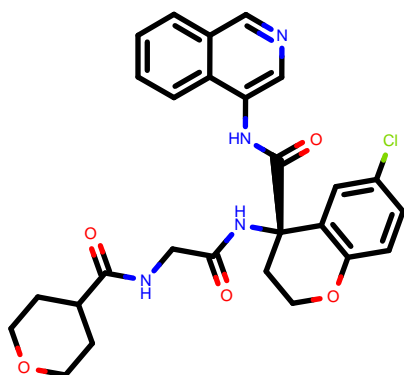
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnnc5

RUN: RUN8150

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.24

EN300-74167_1_1



CID: EN300-74167_1_1

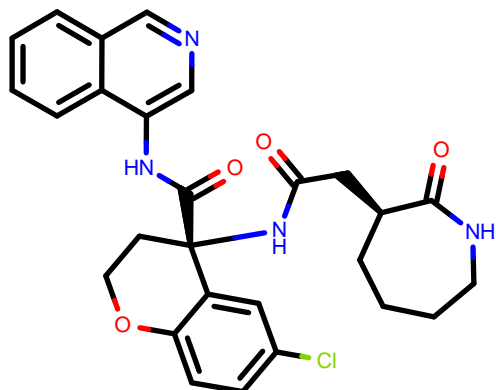
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)C5CCCC5

RUN: RUN8420

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.28

EN300-198633_1_2



CID: EN300-198633_1_2

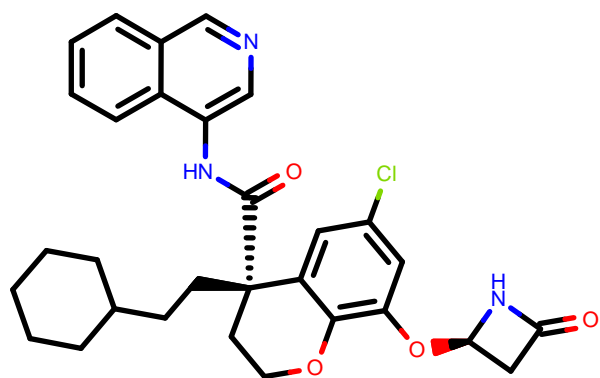
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCCNC5=O

RUN: RUN9229

DDG (kcal/mol): -1.23

dDDG (kcal/mol): 0.27

VLA-UCB-05e51b3f-12_1



CID: VLA-UCB-05e51b3f-12_1

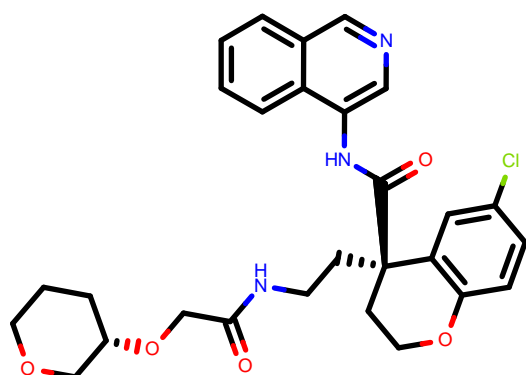
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@H]5CC(=O)N5)C1CCC6CCCC6

RUN: RUN208

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.33

EN300-1627945_3_2



CID: EN300-1627945_3_2

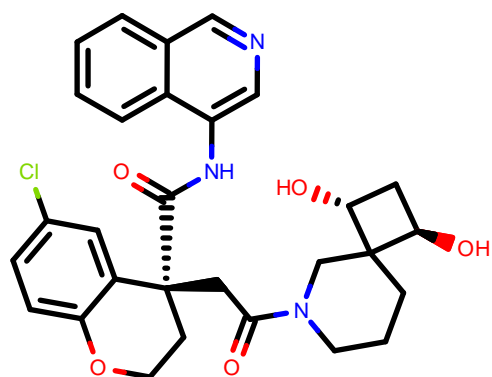
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C1)CCNC(=O)C1[C@@H]5CCOC5

RUN: RUN8644

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-7445890_1_2



CID: EN300-7445890_1_2

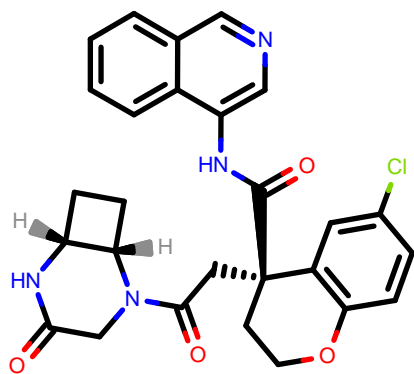
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C1)CC(=O)N5CCOC6(C5)C[C@@H]7C[C@@H]8O

RUN: RUN6639

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.28

EN300-6499164_1_3



CID: EN300-6499164_1_3

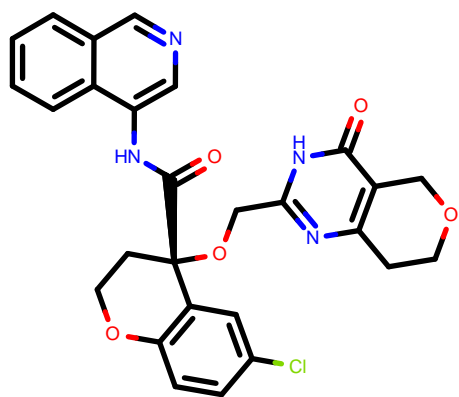
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C1)CC(=O)N5CC(=O)N[C@@H]6C[C@@H]5O6

RUN: RUN9484

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.21

EN300-343103_1_1



CID: EN300-343103_1_1

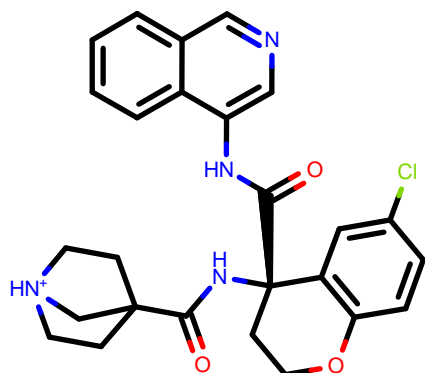
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5[nH]c(=O)c6c(n5)CCOC6

RUN: RUN2814

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-313366_1_1



CID: EN300-313366_1_1

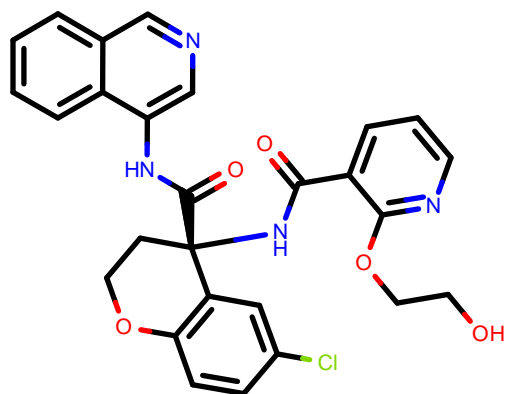
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C56C[NH+]C5)CC6

RUN: RUN4090

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.31

EN300-85043_1_1



CID: EN300-85043_1_1

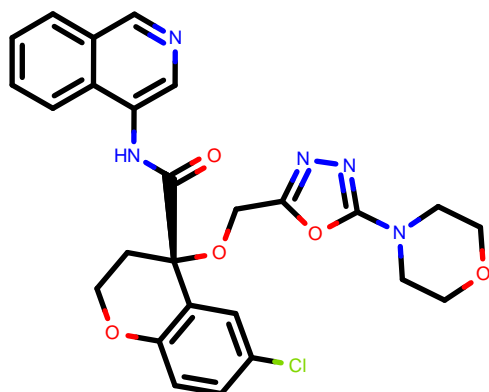
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cccnc5OCCO

RUN: RUN5194

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-6486576_1_1



CID: EN300-6486576_1_1

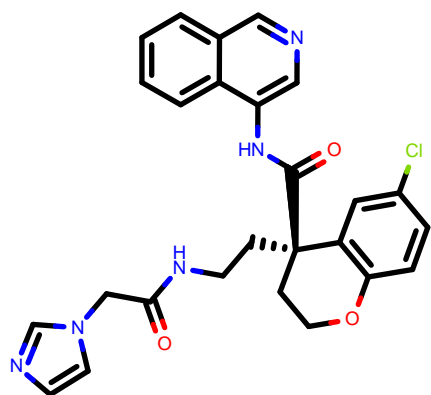
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCc5nnc(o5)NCCOCC6

RUN: RUN1509

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.26

EN300-38979_3_1



CID: EN300-38979_3_1

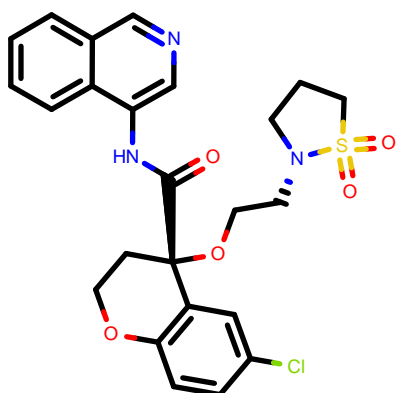
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc5

RUN: RUN15215

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.24

EN300-114134_1_2



CID: EN300-114134_1_2

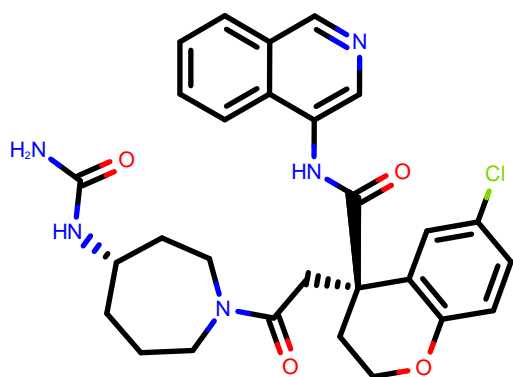
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN(S(=O)(=O)O)O

RUN: RUN2020

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.32

EN300-6759972_1_1



CID: EN300-6759972_1_1

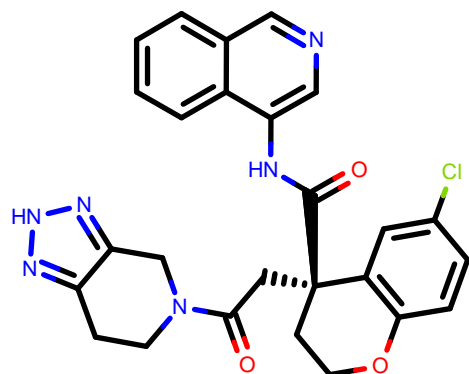
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@]3H[C@@]5NC(=O)N

RUN: RUN3141

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.27

EN300-90293_1_1



CID: EN300-90293_1_1

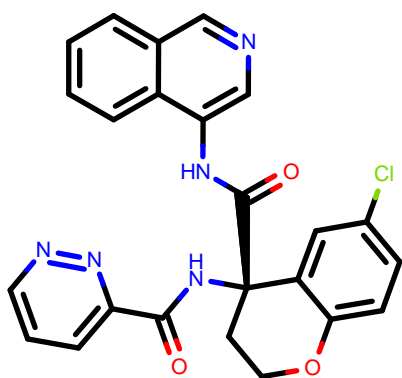
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c(n[nH]6)C5

RUN: RUN12598

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.23

EN300-79022_1_1



CID: EN300-79022_1_1

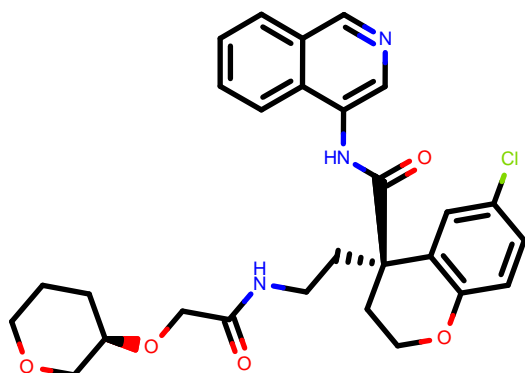
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5

RUN: RUN2998

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.17

EN300-1627945_3_1



CID: EN300-1627945_3_1

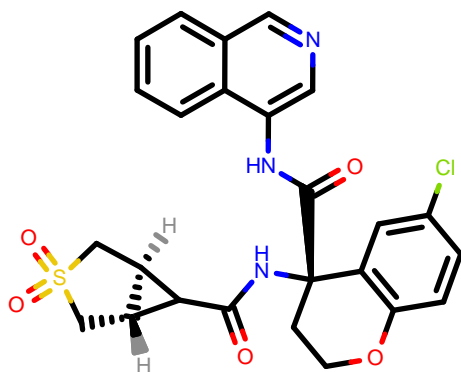
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5

RUN: RUN2756

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.22

EN300-6779469_1_3



CID: EN300-6779469_1_3

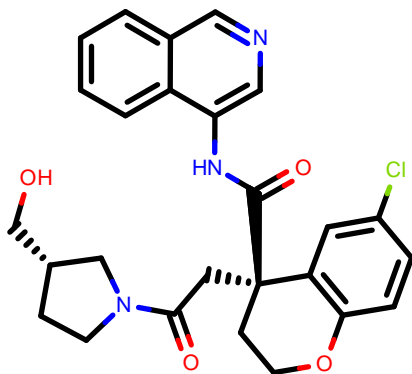
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C(=O)S(=O)(=O)C)C[C@H]5C[C@@H](O)N5

RUN: RUN9329

DDG (kcal/mol): -1.22

dDDG (kcal/mol): 0.22

EN300-88131_1_1



CID: EN300-88131_1_1

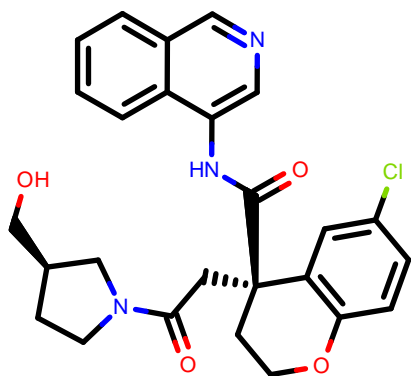
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN5577

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.20

EN300-144970_1_1



CID: EN300-144970_1_1

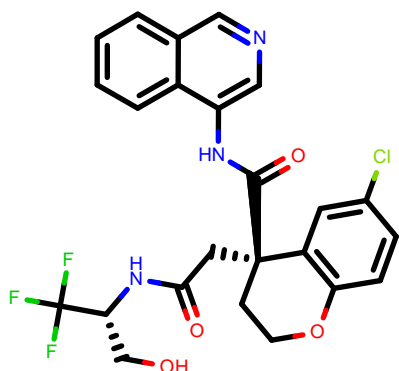
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)CO

RUN: RUN5817

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.21

EN300-139403_1_1



CID: EN300-139403_1_1

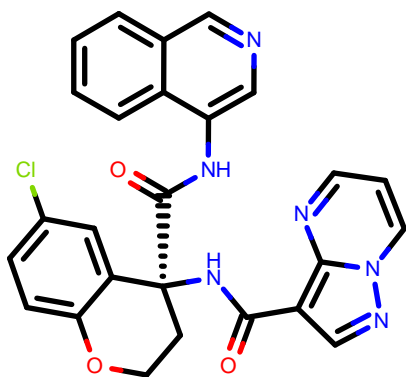
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CC(=O)N(C)C@H(CO)(F)F

RUN: RUN8555

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.34

EN300-29520_1_1



CID: EN300-29520_1_1

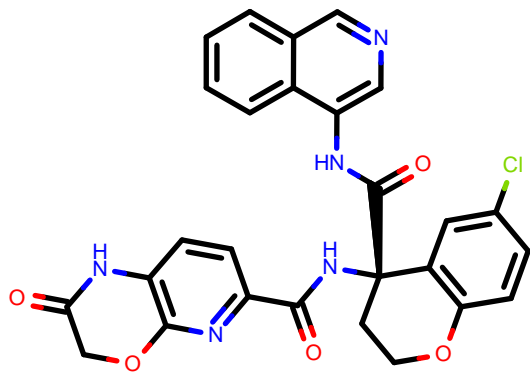
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)NC(=O)c5cnc6c5nccc6

RUN: RUN2199

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.21

EN300-2726690_1_1



CID: EN300-2726690_1_1

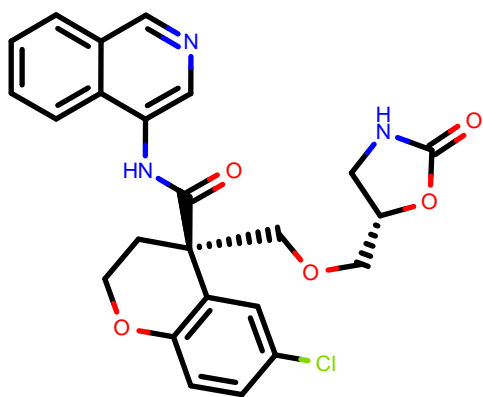
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)NC(=O)c5ccc6c(n5)OCC(=O)N6

RUN: RUN9904

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.21

EN300-203293_2_2



CID: EN300-203293_2_2

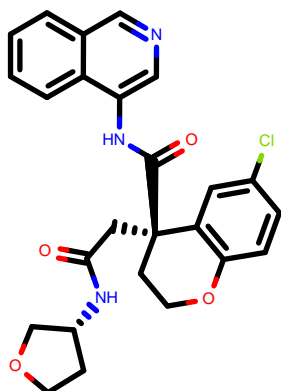
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]H5CNC(=O)O5

RUN: RUN804

DDG (kcal/mol): -1.21

dDDG (kcal/mol): 0.24

EN300-171752_1_1



CID: EN300-171752_1_1

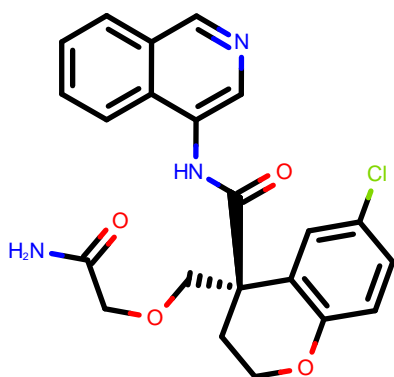
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5CCOC5

RUN: RUN5693

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.22

EN300-18249_2_1



CID: EN300-18249_2_1

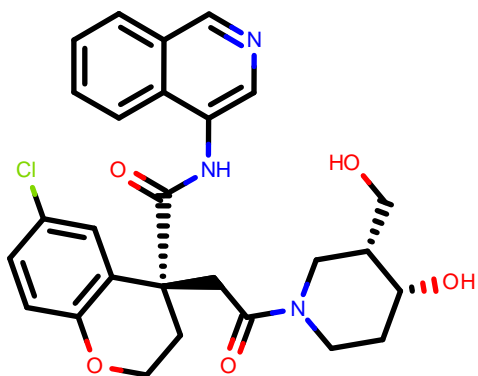
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N

RUN: RUN2056

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.14

EN300-233678_1_2



CID: EN300-233678_1_2

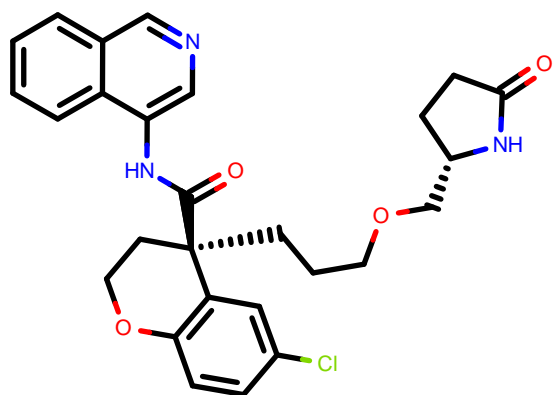
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C[C@@H](C5)CO)O

RUN: RUN1223

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.24

EN300-195756_4_2



CID: EN300-195756_4_2

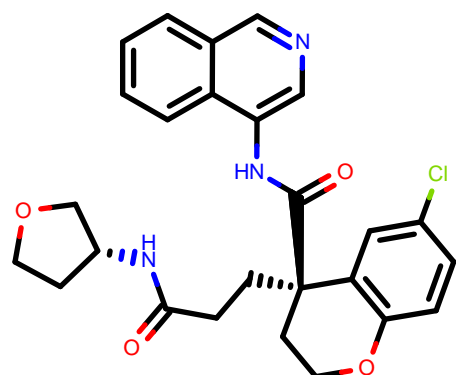
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5H5CCC(=O)N5

RUN: RUN813

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.23

EN300-256939_2_1



CID: EN300-256939_2_1

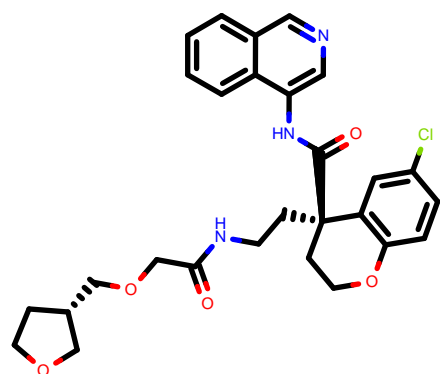
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5CCOC5

RUN: RUN3600

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.28

EN300-80522_3_2



CID: EN300-80522_3_2

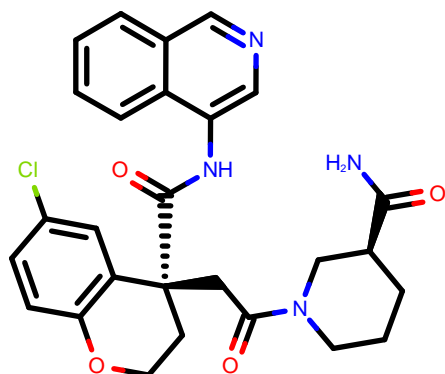
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@@]5H5CCOC5

RUN: RUN8768

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-18610_1_1



CID: EN300-18610_1_1

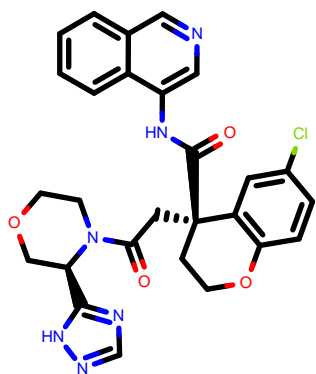
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@]5H(C5)C(=O)N

RUN: RUN12248

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.22

EN300-205616_1_2



CID: EN300-205616_1_2

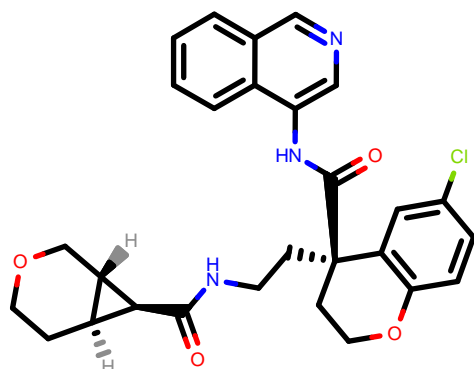
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@]H5c6[nH]n6

RUN: RUN9961

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.27

EN300-1644723_3_2



CID: EN300-1644723_3_2

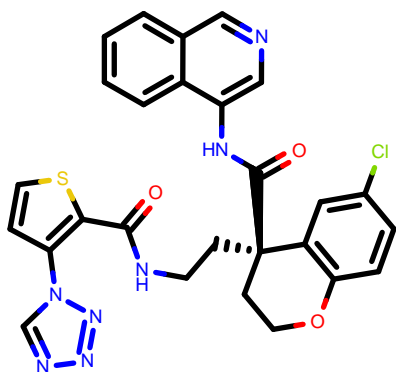
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5[C@@]H5c6c6

RUN: RUN15358

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.23

EN300-36731_3_1



CID: EN300-36731_3_1

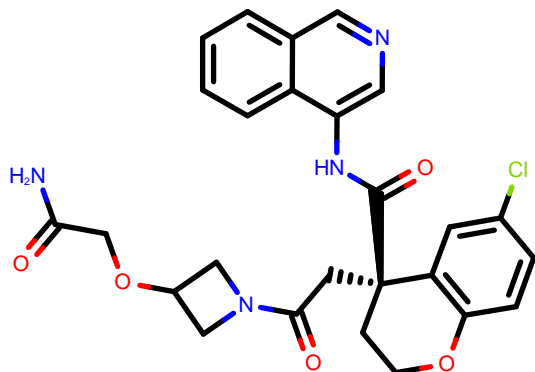
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5c(ccs5)n6cnn6

RUN: RUN14302

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.25

EN300-1081256_1_1



CID: EN300-1081256_1_1

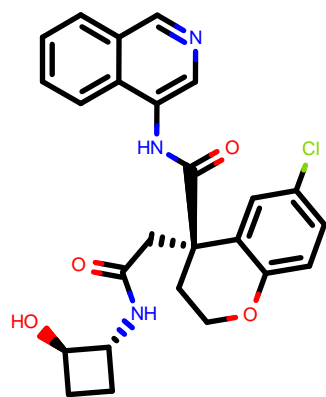
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)OCC(=O)N

RUN: RUN7471

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.22

EN300-129424_1_1



CID: EN300-129424_1_1

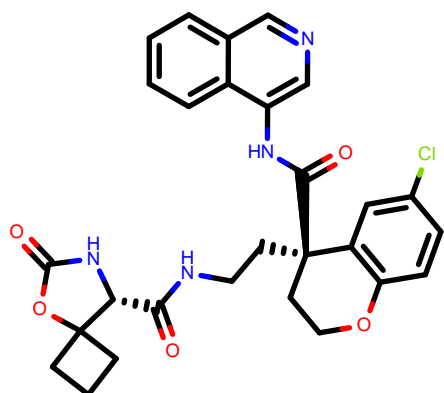
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@H]5O

RUN: RUN1703

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.21

EN300-7432415_3_1



CID: EN300-7432415_3_1

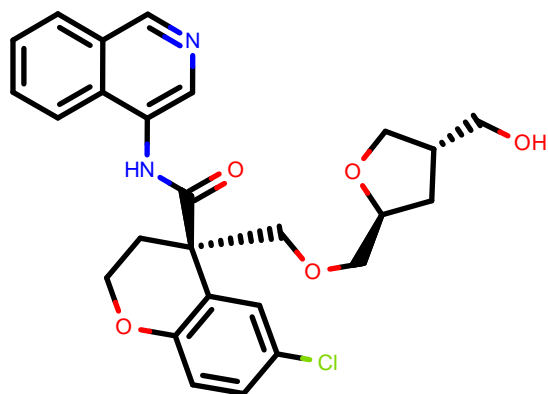
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C6(CCC6)OC1=O5

RUN: RUN12052

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.25

EN300-6494158_2_4



CID: EN300-6494158_2_4

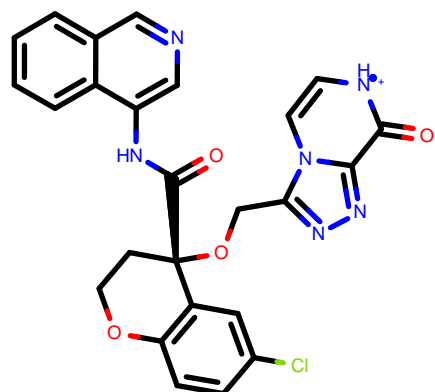
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@]4[C@@H]5C[C@H](CO)5O4

RUN: RUN2025

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.25

EN300-378316_1_1



CID: EN300-378316_1_1

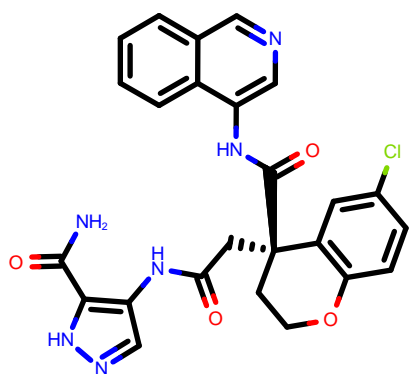
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nnc6[nH]c6=O

RUN: RUN1621

DDG (kcal/mol): -1.20

dDDG (kcal/mol): 0.22

EN300-175220_1_1



CID: EN300-175220_1_1

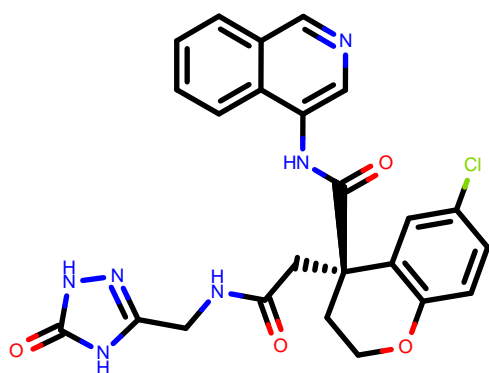
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5c[nH]c5C(=O)N

RUN: RUN14858

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.21

EN300-98038_1_1



CID: EN300-98038_1_1

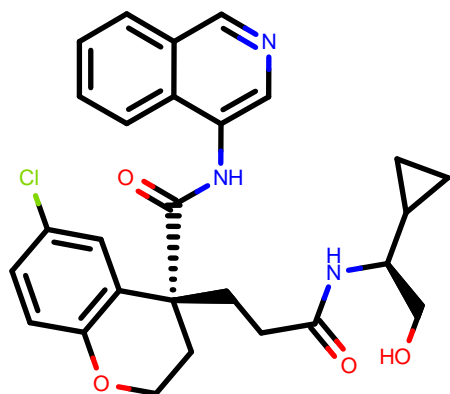
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5[nH]c5[nH]n5

RUN: RUN12306

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.20

EN300-77885_2_1



CID: EN300-77885_2_1

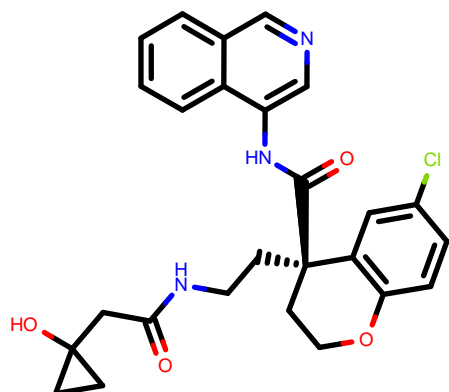
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CO)C5C5C5

RUN: RUN6998

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.33

EN300-207873_3_1



CID: EN300-207873_3_1

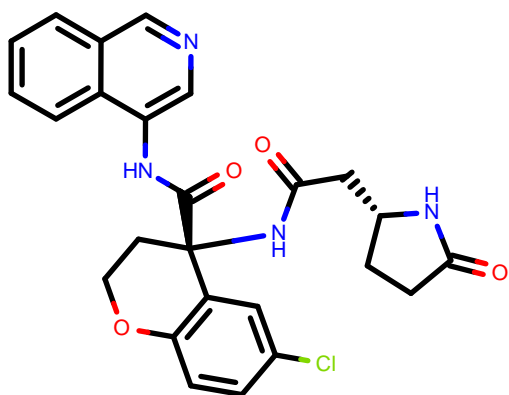
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CC5)O

RUN: RUN13788

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.21

EN300-68203_1_1



CID: EN300-68203_1_1

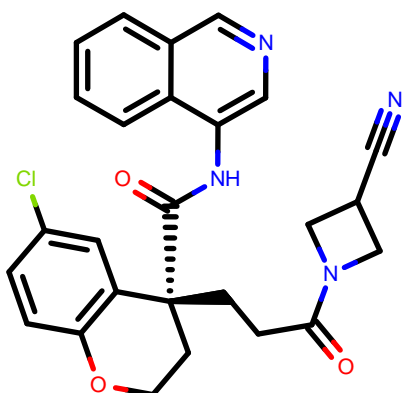
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)N5

RUN: RUN899

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.23

EN300-206282_2_1



CID: EN300-206282_2_1

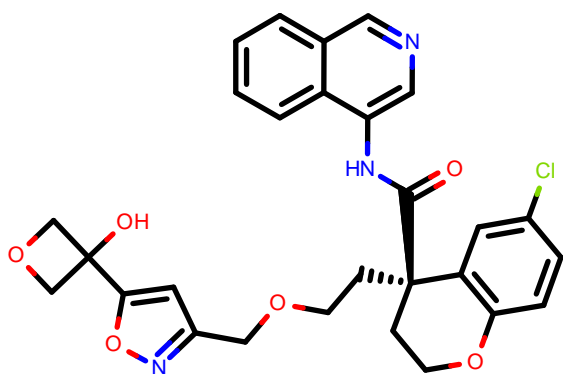
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C#N

RUN: RUN14295

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.22

EN300-7457159_3_1



CID: EN300-7457159_3_1

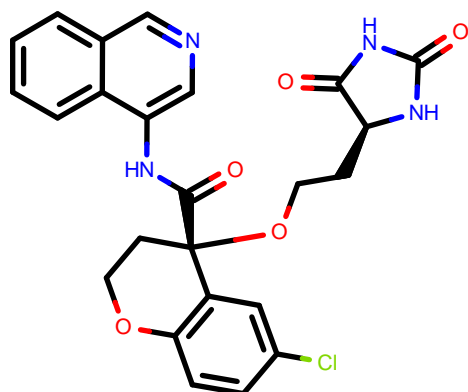
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cc(on5)C6(COC6)O

RUN: RUN2615

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.28

EN300-6498856_1_1



CID: EN300-6498856_1_1

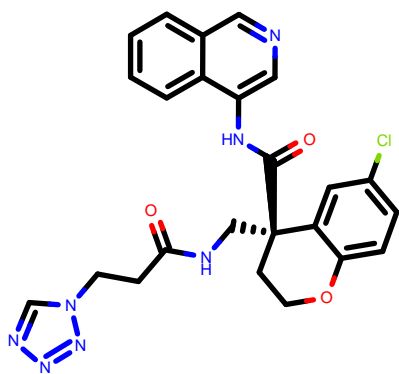
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[C@H]5C(=O)NC(=O)N5

RUN: RUN959

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.23

EN300-191904_2_1



CID: EN300-191904_2_1

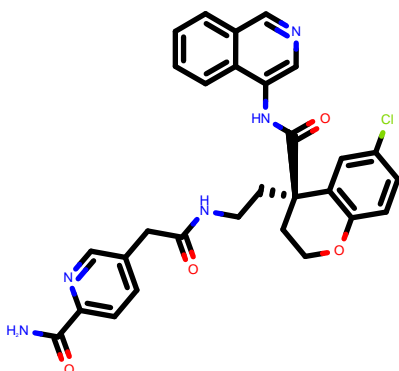
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5cncn5

RUN: RUN5599

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.23

EN300-322332_3_1



CID: EN300-322332_3_1

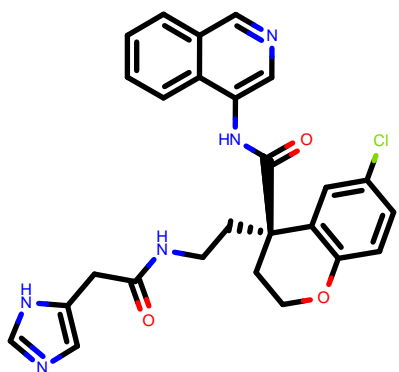
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(nc5)C(=O)N

RUN: RUN2165

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.27

EN300-342226_3_1



CID: EN300-342226_3_1

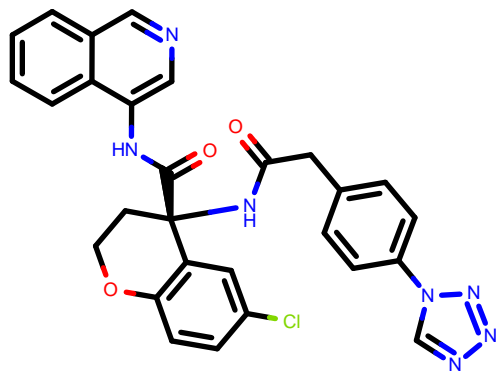
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnc[nH]5

RUN: RUN15272

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.24

EN300-31970_1_1



CID: EN300-31970_1_1

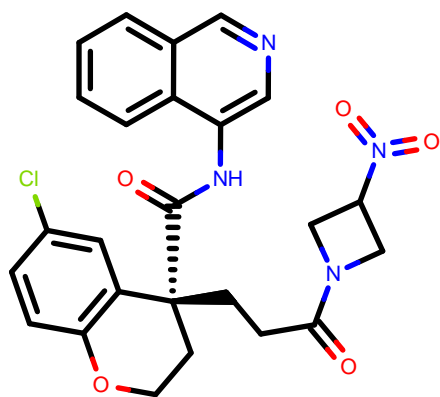
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5ccc(cc5)n6cncn6

RUN: RUN9868

DDG (kcal/mol): -1.19

dDDG (kcal/mol): 0.30

EN300-7461023_2_1



CID: EN300-7461023_2_1

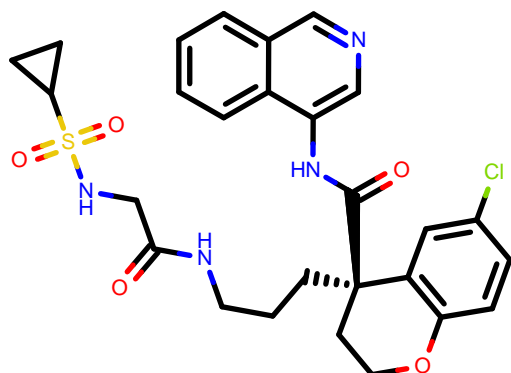
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)N(=O)=O

RUN: RUN14507

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.21

EN300-203853_4_1



CID: EN300-203853_4_1

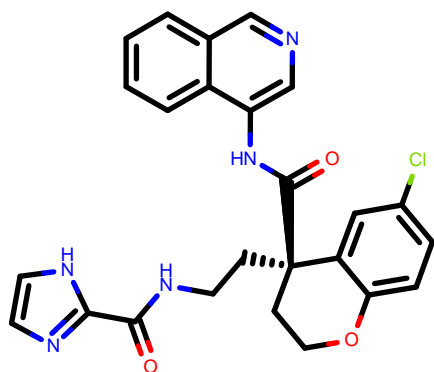
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CNS(=O)(=O)C5CC5

RUN: RUN8522

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.42

EN300-315836_3_1



CID: EN300-315836_3_1

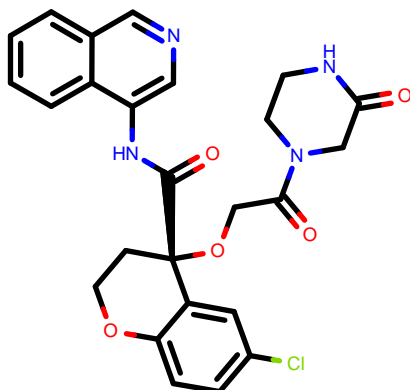
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5[nH]cn5

RUN: RUN15242

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.20

EN300-22884_1_1



CID: EN300-22884_1_1

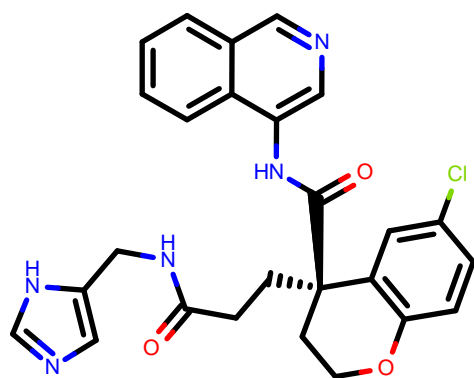
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCNC(=O)C5

RUN: RUN503

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.23

EN300-82476_2_1



CID: EN300-82476_2_1

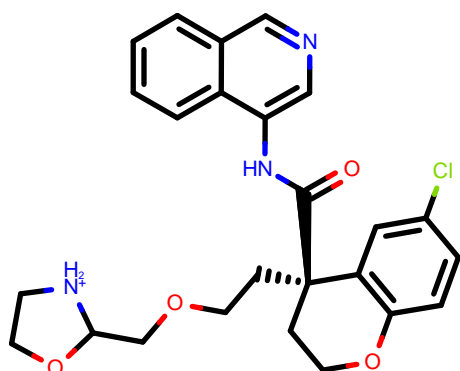
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5nc[nH]5

RUN: RUN4204

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.33

EN300-317555_3_1



CID: EN300-317555_3_1

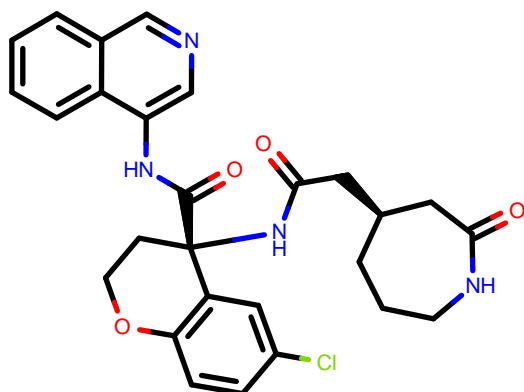
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5

RUN: RUN1248

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.20

EN300-195590_1_2



CID: EN300-195590_1_2

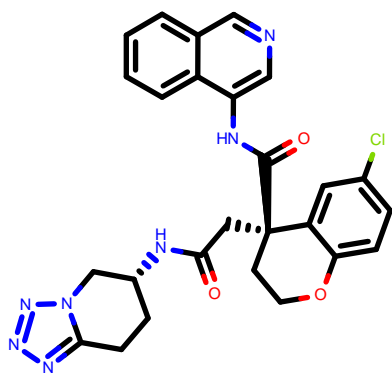
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5H5CCCNC(=O)C5

RUN: RUN3746

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.29

EN300-7444106_1_1



CID: EN300-7444106_1_1

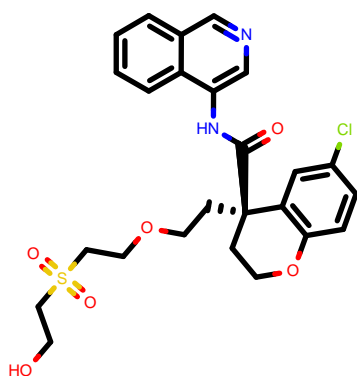
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5CCc6nnn6C5

RUN: RUN4617

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.25

EN300-7463171_3_1



CID: EN300-7463171_3_1

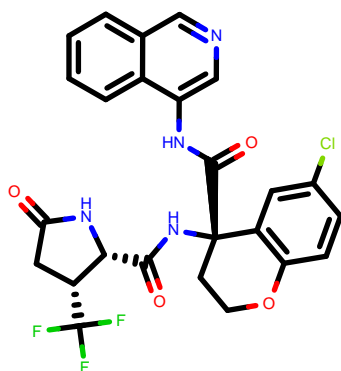
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCS(=O)(=O)CO

RUN: RUN993

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.48

EN300-169955_1_3



CID: EN300-169955_1_3

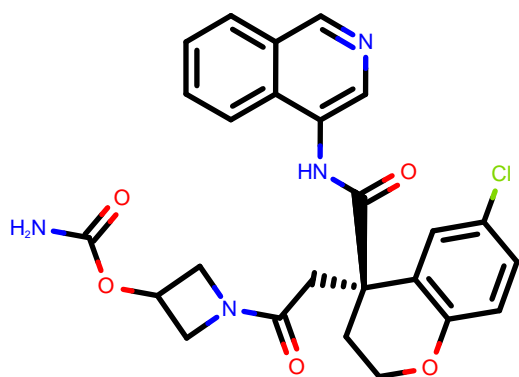
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)NC(=O)C@H5(C@H)CC(=O)N5)C(F)(F)F

RUN: RUN6724

DDG (kcal/mol): -1.18

dDDG (kcal/mol): 0.20

EN300-1707774_1_1



CID: EN300-1707774_1_1

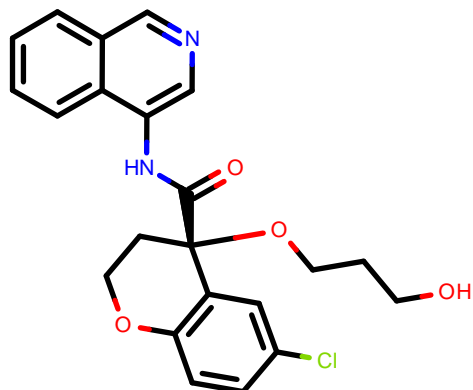
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)OC(=O)N

RUN: RUN13734

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.22

EN300-221518_1_1



CID: EN300-221518_1_1

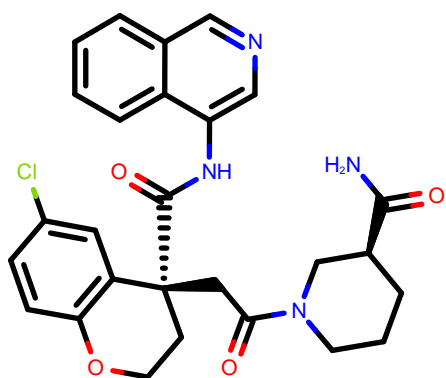
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCCO

RUN: RUN1709

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.15

EN300-18610_1_1



CID: EN300-18610_1_1

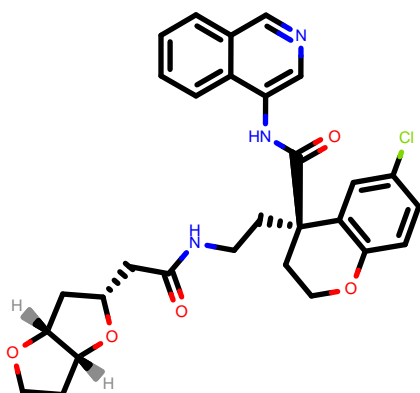
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)C(=O)N

RUN: RUN12250

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.22

EN300-7355519_3_5



CID: EN300-7355519_3_5

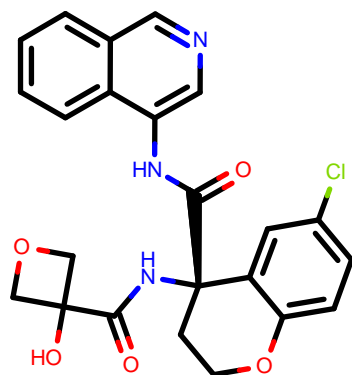
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)C(=O)N

RUN: RUN8824

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.29

EN300-101443_1_1



CID: EN300-101443_1_1

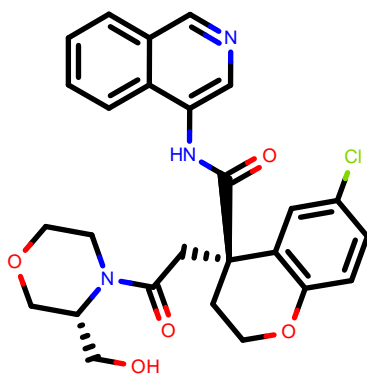
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)C(=O)N

RUN: RUN2822

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.21

EN300-173903_1_1



CID: EN300-173903_1_1

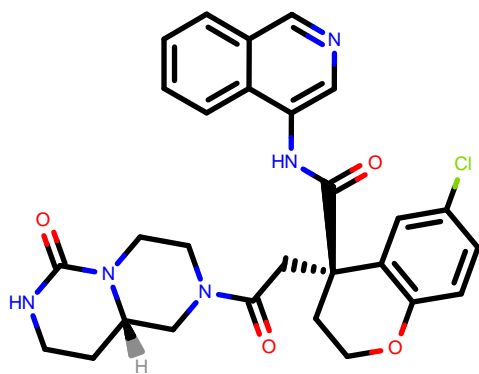
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)C(=O)N

RUN: RUN11561

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.28

EN300-6474647_1_1



CID: EN300-6474647_1_1

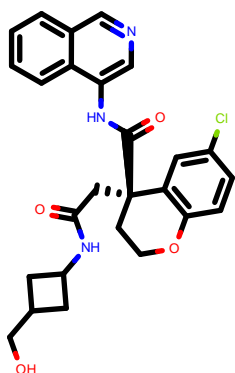
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@H](C5)CCNC6=O

RUN: RUN4281

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.22

EN300-309235_1_1



CID: EN300-309235_1_1

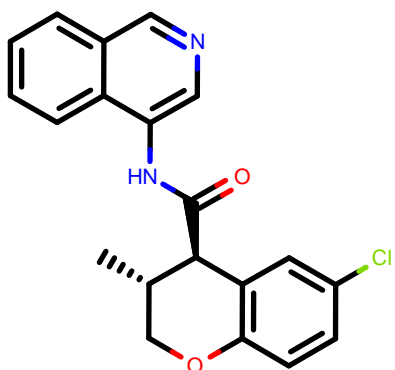
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)CO

RUN: RUN10205

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.21

MAT-POS-8a69d52e-4_2



CID: MAT-POS-8a69d52e-4_2

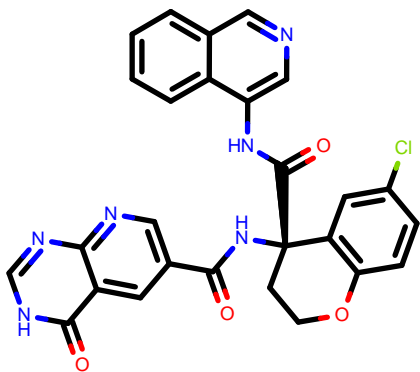
SMILES: C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN75

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.06

EN300-7494115_1_1



CID: EN300-7494115_1_1

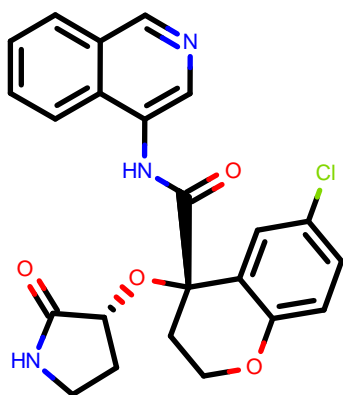
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(=O)[nH]cnc6n5

RUN: RUN3518

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.22

EN300-6736413_1_2



CID: EN300-6736413_1_2

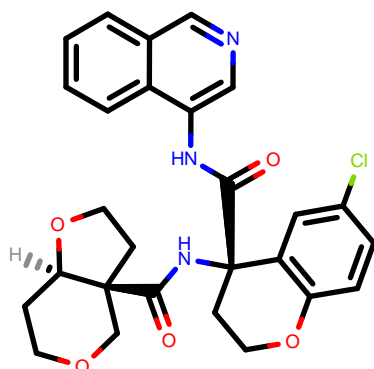
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCNC5=O

RUN: RUN2171

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.16

EN300-341337_1_1



CID: EN300-341337_1_1

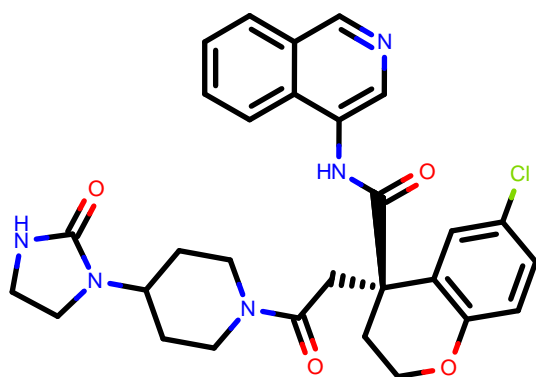
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]56CCO[C@@H]5CCOC6

RUN: RUN8973

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.25

EN300-49777_1_1



CID: EN300-49777_1_1

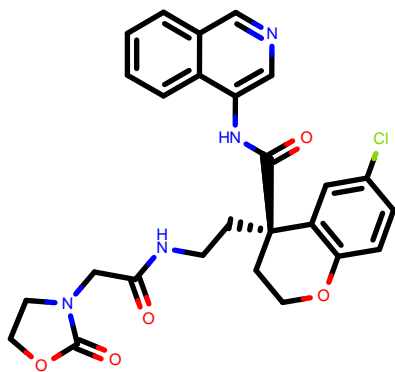
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C(C)5)N6CCNC6=O

RUN: RUN10475

DDG (kcal/mol): -1.17

dDDG (kcal/mol): 0.26

EN300-172179_3_1



CID: EN300-172179_3_1

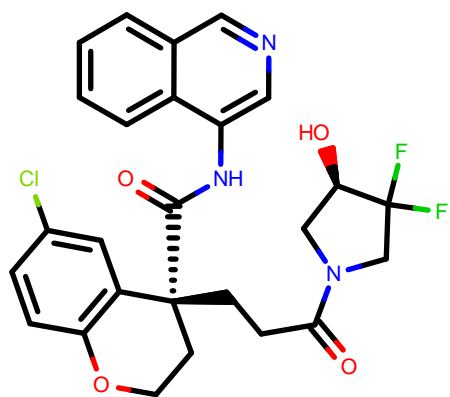
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCOC5=O

RUN: RUN11799

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.24

EN300-1710153_2_2



CID: EN300-1710153_2_2

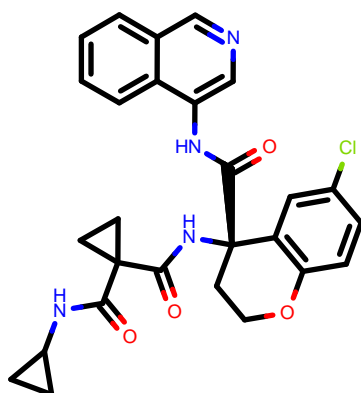
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5C[C@H](C(C5)(F)F)O

RUN: RUN14665

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.26

EN300-61636_1_1



CID: EN300-61636_1_1

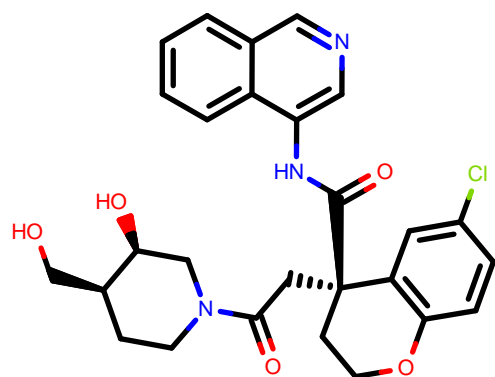
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(C(C5)O)NC6CC6

RUN: RUN7688

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.23

EN300-95639_1_2



CID: EN300-95639_1_2

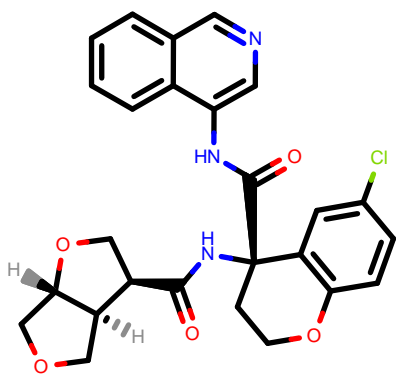
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C[C@H](C5)O)CO

RUN: RUN3505

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.30

EN300-6482296_1_3



CID: EN300-6482296_1_3

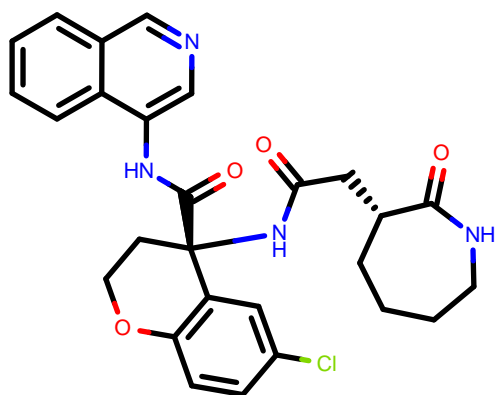
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]4(C[C@@]4(C)O)CO

RUN: RUN9613

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.22

EN300-198633_1_1



CID: EN300-198633_1_1

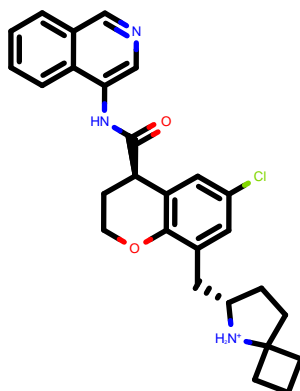
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@H]5CCCCNC5=O

RUN: RUN8865

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.30

DAR-DIA-23e5a6a0-6_2



CID: DAR-DIA-23e5a6a0-6_2

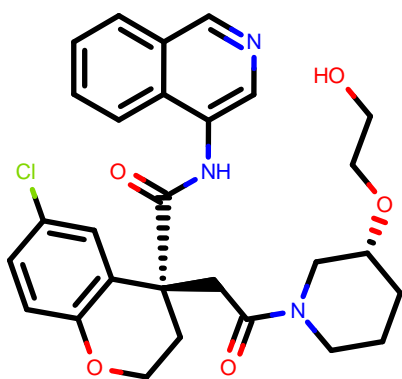
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6([NH2+][5])OCC6)Cl

RUN: RUN162

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.28

EN300-157830_1_2



CID: EN300-157830_1_2

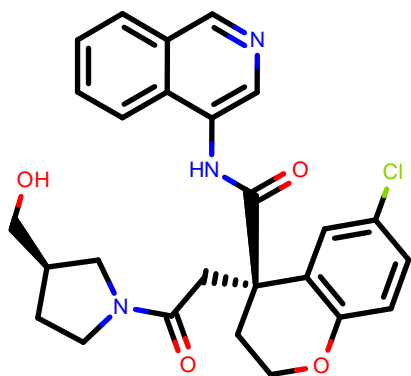
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)OCCO

RUN: RUN9376

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.35

EN300-144970_1_1



CID: EN300-144970_1_1

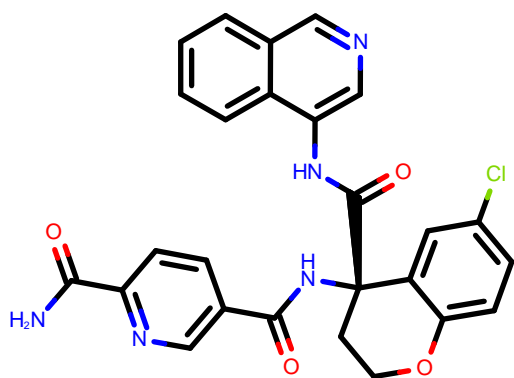
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN5821

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.21

EN300-58864_1_1



CID: EN300-58864_1_1

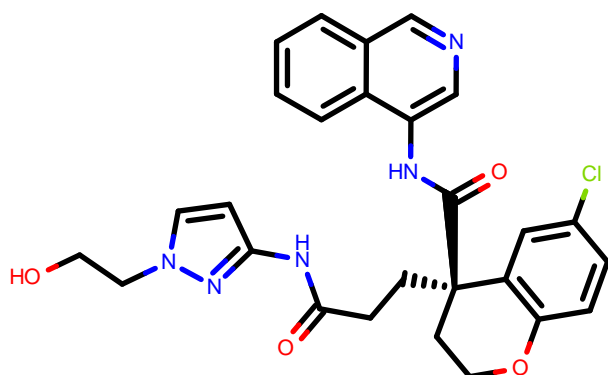
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(nc5)C(=O)N

RUN: RUN6864

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.21

EN300-70815_2_1



CID: EN300-70815_2_1

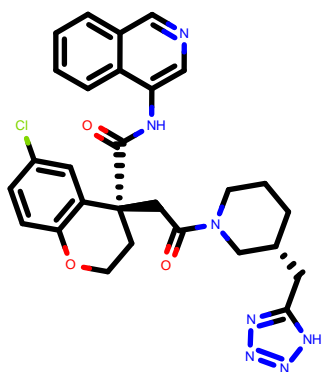
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)Nc5cn(n5)CCO

RUN: RUN6199

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.24

EN300-383891_1_1



CID: EN300-383891_1_1

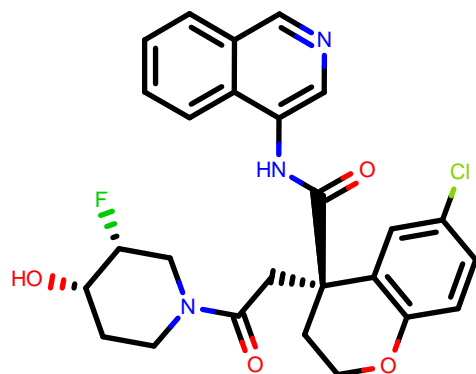
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3([H])C5C6N=CN6

RUN: RUN6368

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.33

EN300-741926_1_3



CID: EN300-741926_1_3

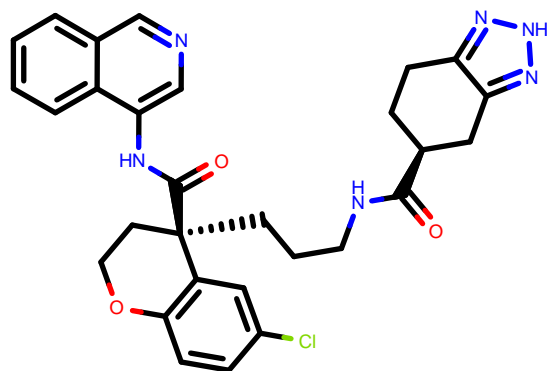
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3([H])C6=C(F)C=C6O

RUN: RUN12262

DDG (kcal/mol): -1.16

dDDG (kcal/mol): 0.26

EN300-185729_4_1



CID: EN300-185729_4_1

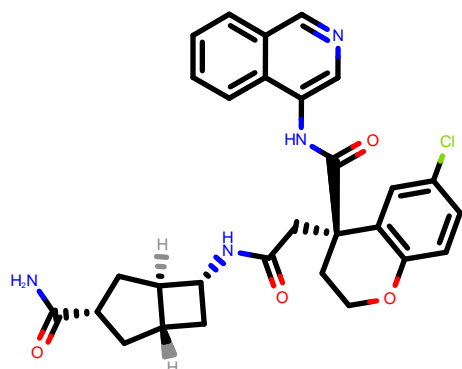
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCNC(=O)[C@H]5CCc6c(n[nH]6)C5

RUN: RUN12573

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.26

EN300-1091489_1_1



CID: EN300-1091489_1_1

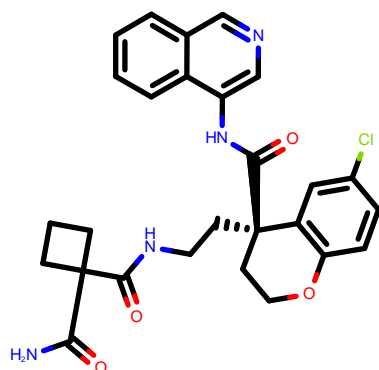
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C[C@@H]5C[C@H]6[C@H]5C6[C@H]6)C1=O

RUN: RUN2253

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.25

EN300-68747_3_1



CID: EN300-68747_3_1

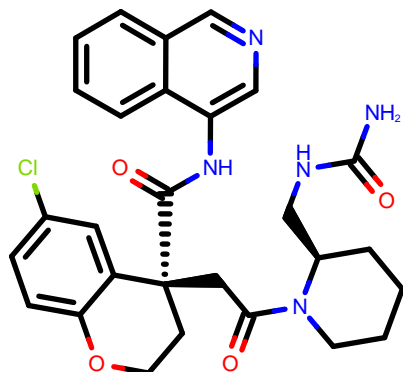
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CCC5)C(=O)N

RUN: RUN14110

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.27

EN300-62166_1_1



CID: EN300-62166_1_1

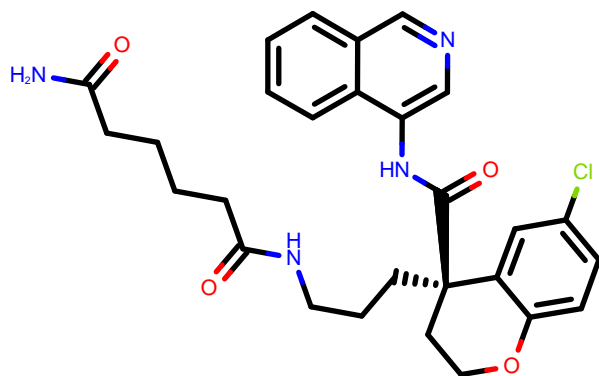
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@]3(C)N5CNC(=O)N

RUN: RUN6727

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.25

EN300-142412_4_1



CID: EN300-142412_4_1

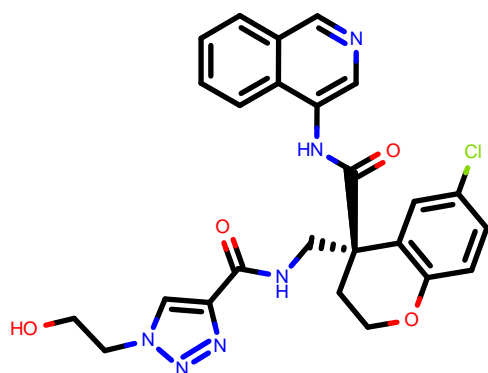
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCC(=O)N

RUN: RUN11015

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.28

EN300-52193_2_1



CID: EN300-52193_2_1

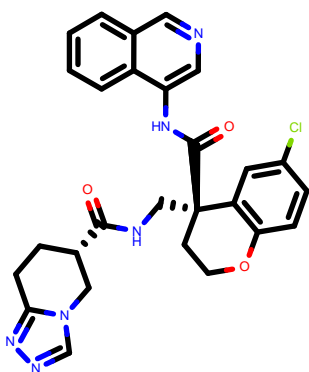
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)CO

RUN: RUN8922

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.25

EN300-51350_2_2



CID: EN300-51350_2_2

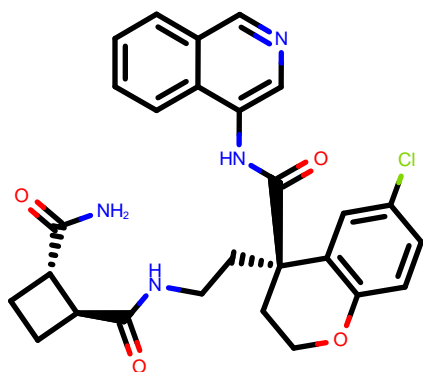
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCc6nnc65

RUN: RUN7261

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.24

EN300-217107_3_4



CID: EN300-217107_3_4

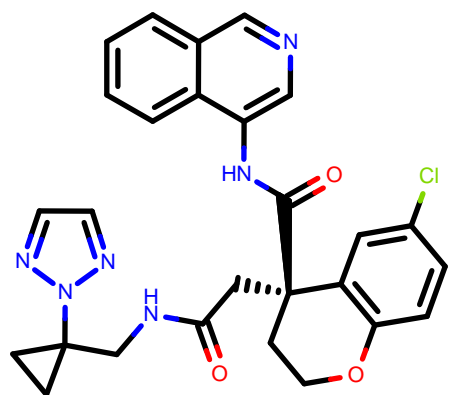
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC[C@@]5H5Cl=O

RUN: RUN2475

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.25

EN300-1722016_1_1



CID: EN300-1722016_1_1

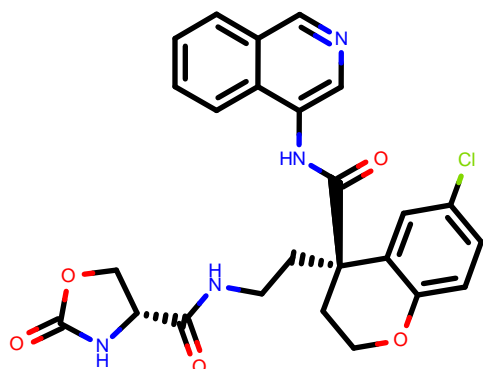
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC5(CC5)n6ncn6

RUN: RUN12614

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.23

EN300-201346_3_2



CID: EN300-201346_3_2

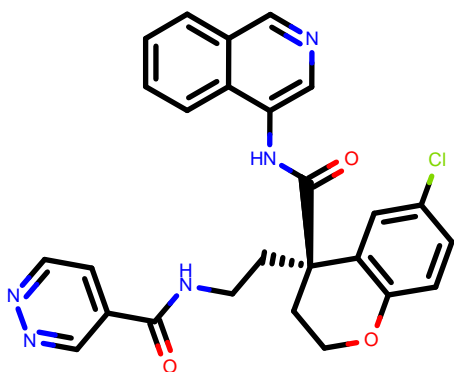
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5COC(=O)N5

RUN: RUN15265

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.22

EN300-75875_3_1



CID: EN300-75875_3_1

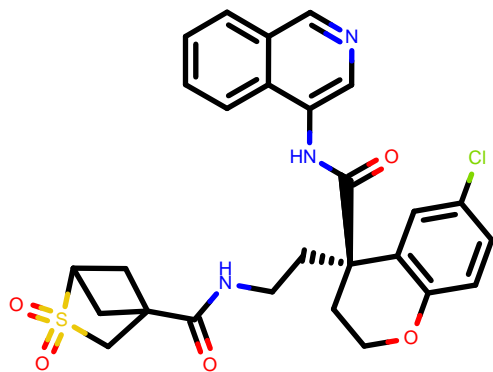
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccnnc5

RUN: RUN15493

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.23

EN300-7354033_3_1



CID: EN300-7354033_3_1

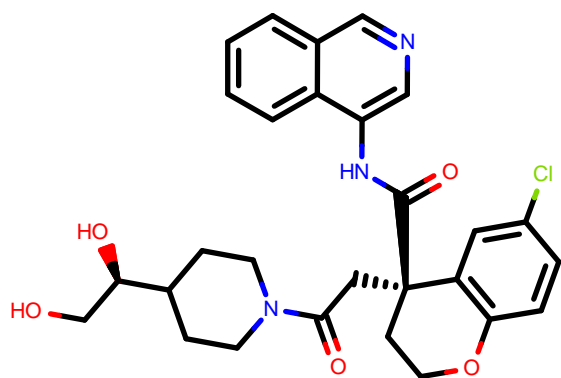
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C56CC(C5)S(=O)(=O)C6

RUN: RUN2913

DDG (kcal/mol): -1.15

dDDG (kcal/mol): 0.22

EN300-1699332_1_1



CID: EN300-1699332_1_1

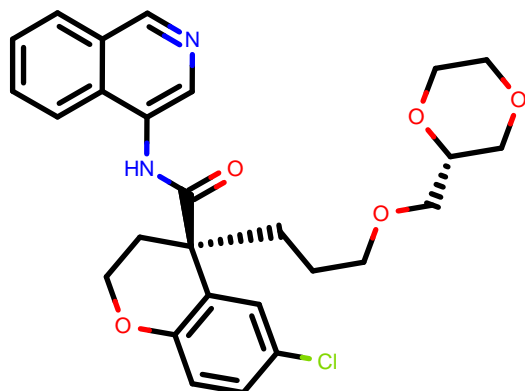
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(C5)[C@@H](CO)O

RUN: RUN5213

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.28

EN300-139167_4_1



CID: EN300-139167_4_1

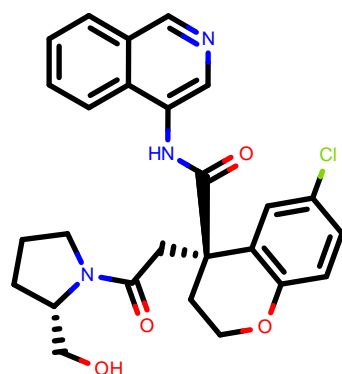
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCOC5

RUN: RUN1938

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.22

EN300-70033_1_1



CID: EN300-70033_1_1

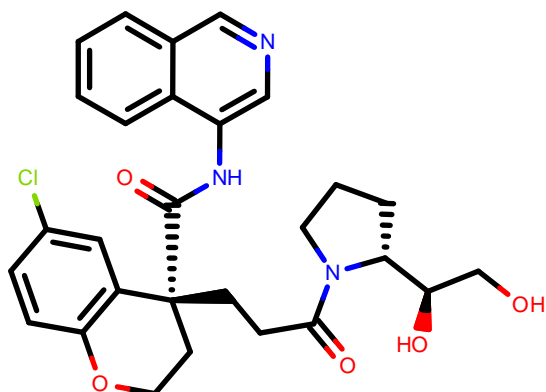
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5CO

RUN: RUN6073

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.23

EN300-7459540_2_1



CID: EN300-7459540_2_1

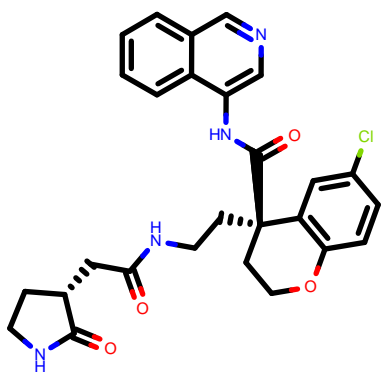
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5(CO)O

RUN: RUN3988

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.29

EN300-343474_3_1



CID: EN300-343474_3_1

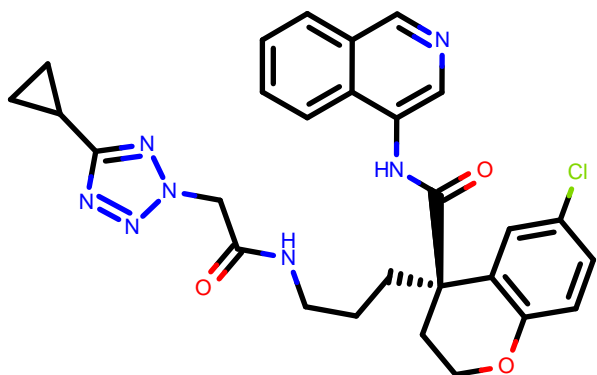
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@H]5CCNC5=O

RUN: RUN13106

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.25

EN300-1719432_4_1



CID: EN300-1719432_4_1

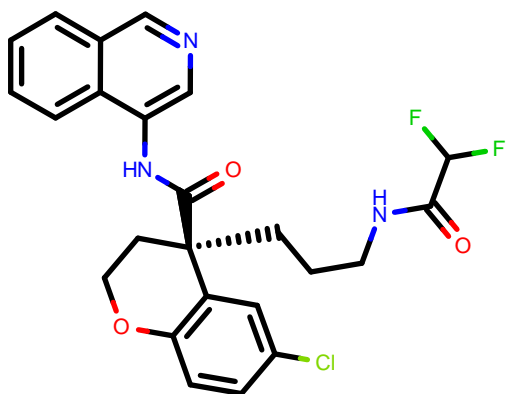
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5nc(nc5)C6CC6

RUN: RUN9614

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.24

EN300-19507_4_1



CID: EN300-19507_4_1

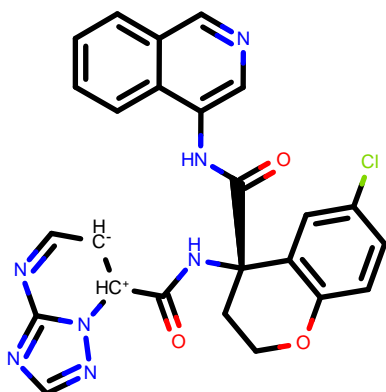
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C(F)F

RUN: RUN12989

DDG (kcal/mol): -1.14

dDDG (kcal/mol): 0.16

EN300-28262_1_1



CID: EN300-28262_1_1

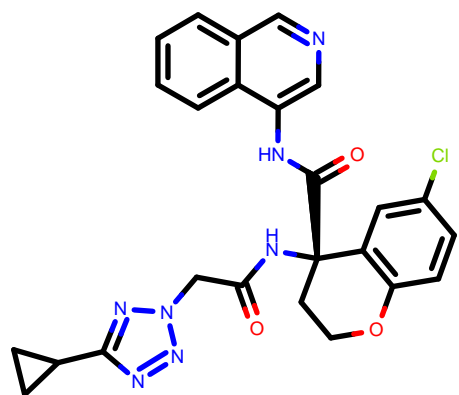
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cncn5n6

RUN: RUN5050

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.24

EN300-1719432_1_1



CID: EN300-1719432_1_1

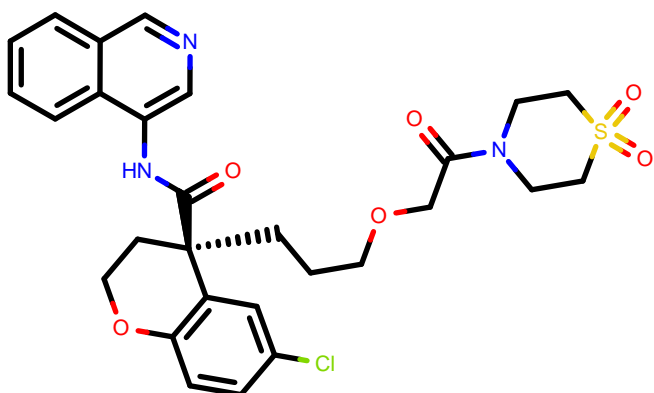
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5nc(n5)C6CC6

RUN: RUN9233

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.24

EN300-1265948_4_1



CID: EN300-1265948_4_1

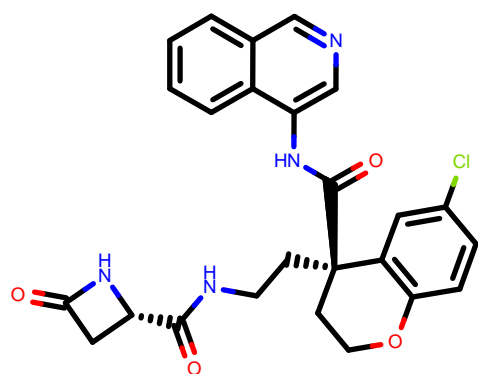
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN541

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.28

EN300-101505_3_1



CID: EN300-101505_3_1

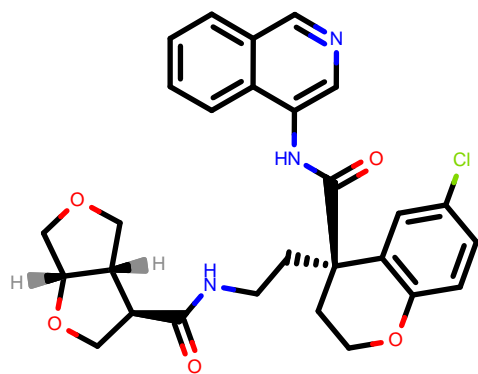
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)N5

RUN: RUN15206

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.24

EN300-6482296_3_2



CID: EN300-6482296_3_2

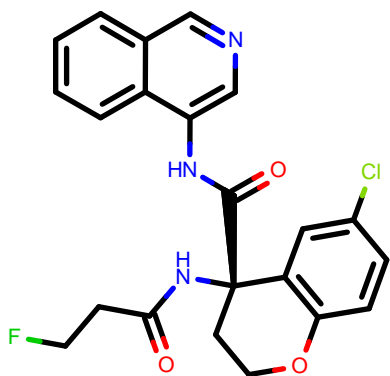
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H5CO[C@@H]5COO6

RUN: RUN2981

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.24

EN300-97758_1_1



CID: EN300-97758_1_1

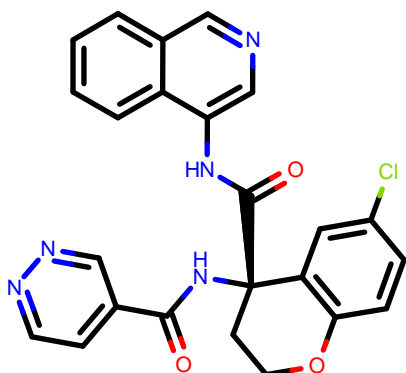
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCF

RUN: RUN1840

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.18

EN300-75875_1_1



CID: EN300-75875_1_1

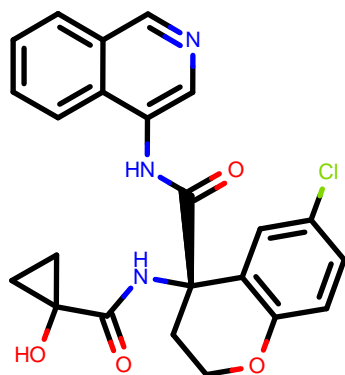
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5

RUN: RUN5542

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.18

EN300-25702_1_1



CID: EN300-25702_1_1

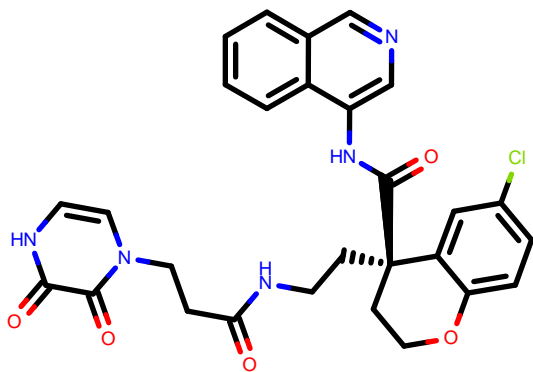
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)O

RUN: RUN2595

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.20

EN300-65383_3_1



CID: EN300-65383_3_1

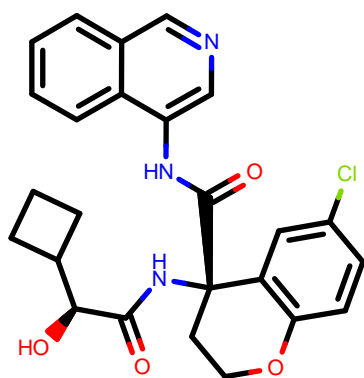
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5c[nH]c1=O)c5=O

RUN: RUN14870

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.39

EN300-249764_1_2



CID: EN300-249764_1_2

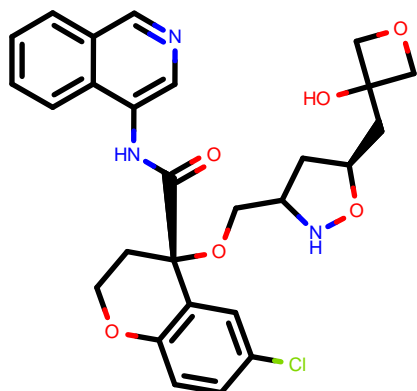
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C@H](C5CC5)O

RUN: RUN979

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.22

EN300-7457160_1_1



CID: EN300-7457160_1_1

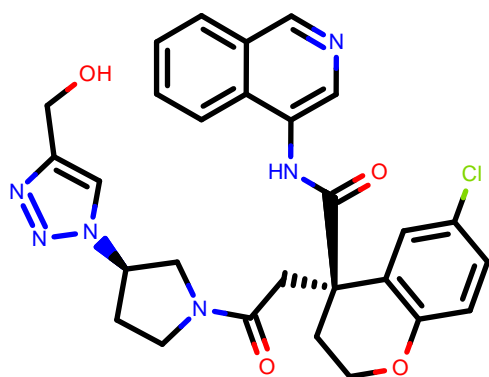
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NO[C@H](C5)CC6(COC6)O

RUN: RUN471

DDG (kcal/mol): -1.13

dDDG (kcal/mol): 0.27

EN300-234362_1_2



CID: EN300-234362_1_2

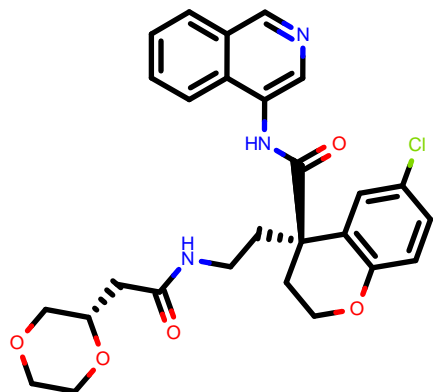
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)n6cc(nn6)CO

RUN: RUN12920

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.26

EN300-731622_3_1



CID: EN300-731622_3_1

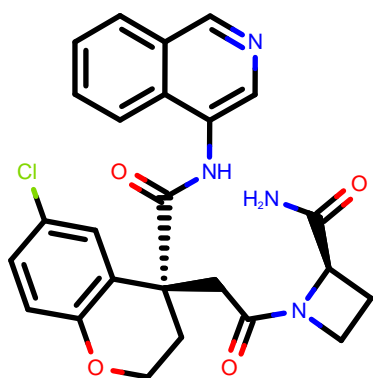
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5COCOC5

RUN: RUN13352

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.26

EN300-862094_1_2



CID: EN300-862094_1_2

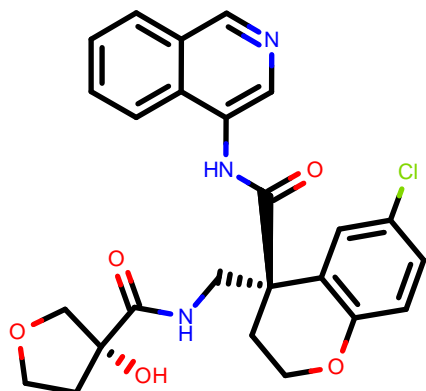
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4Cl)CC(=O)N5CC[C@H]5C(=O)N

RUN: RUN1886

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.20

EN300-148421_2_2



CID: EN300-148421_2_2

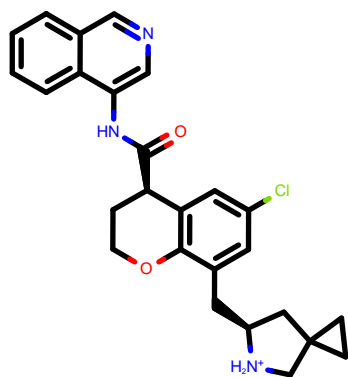
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4Cl)CNC(=O)[C@H]5(C)COC5O

RUN: RUN4591

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.24

DAR-DIA-23e5a6a0-9_1



CID: DAR-DIA-23e5a6a0-9_1

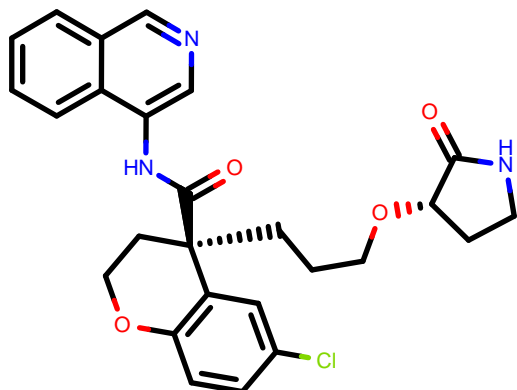
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4Cl)C[C@H]5CC6(C)C6C[NH2+]5Cl

RUN: RUN191

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.25

EN300-6736413_4_1



CID: EN300-6736413_4_1

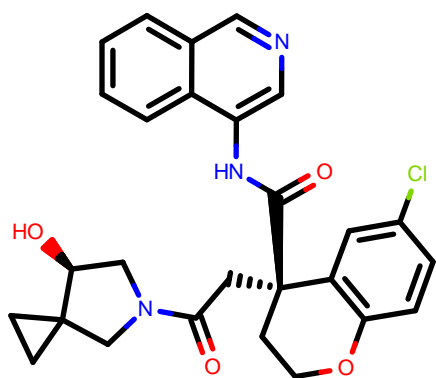
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4c3cc(cc4Cl)CCCO[C@H]5CCNC5=O

RUN: RUN933

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.20

EN300-142333_1_1



CID: EN300-142333_1_1

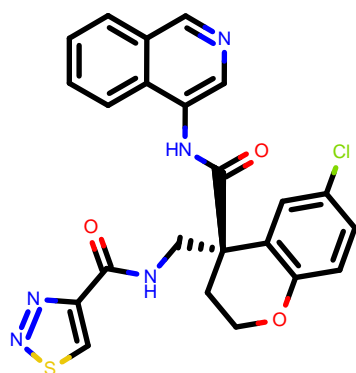
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5[C@@H](C6(C)C5)CC6)O

RUN: RUN6268

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.26

EN300-24297_2_1



CID: EN300-24297_2_1

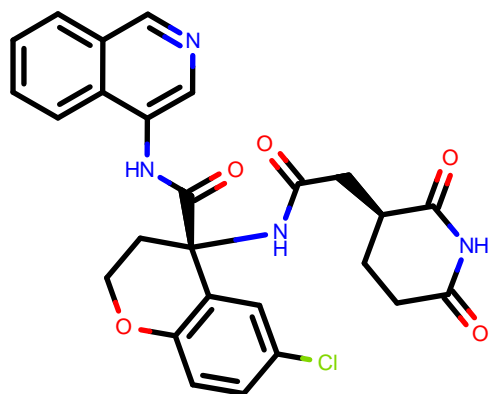
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5csnn5

RUN: RUN2743

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.23

EN300-3451857_1_2



CID: EN300-3451857_1_2

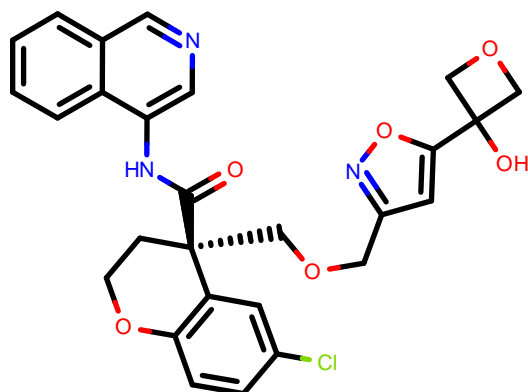
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)NC5=O

RUN: RUN955

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.25

EN300-7457159_2_1



CID: EN300-7457159_2_1

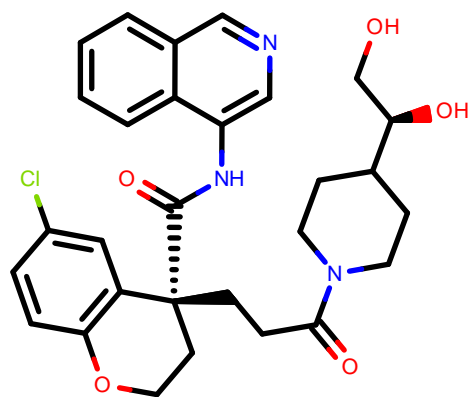
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cc(O)C6(COC6)O

RUN: RUN2701

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.28

EN300-1699332_2_1



CID: EN300-1699332_2_1

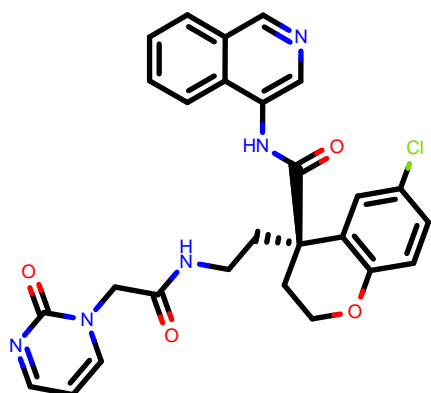
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCCC(CS5)[C@@H](CO)O

RUN: RUN14291

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.35

EN300-35789_3_1



CID: EN300-35789_3_1

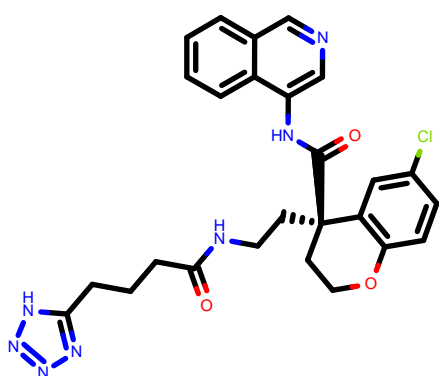
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ccoc5=O

RUN: RUN9744

DDG (kcal/mol): -1.12

dDDG (kcal/mol): 0.25

EN300-134204_3_1



CID: EN300-134204_3_1

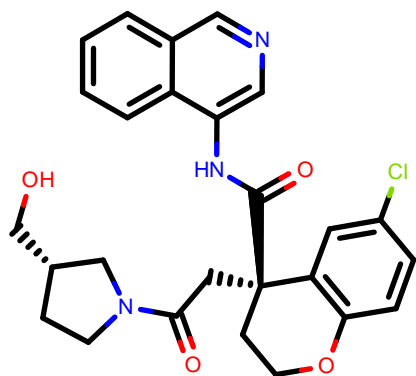
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCc5cn[nH]n5

RUN: RUN15175

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.34

EN300-88131_1_1



CID: EN300-88131_1_1

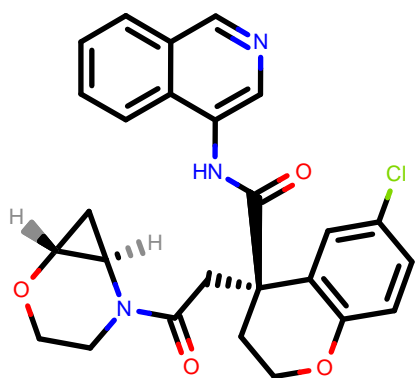
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN5581

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.21

EN300-91609_1_1



CID: EN300-91609_1_1

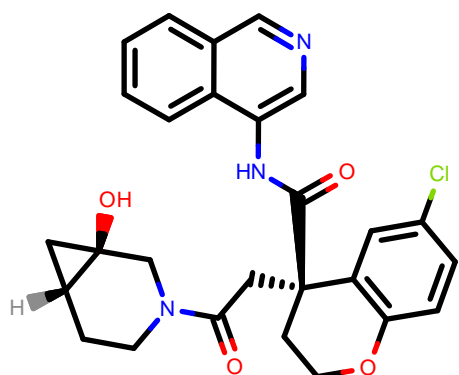
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@@H]6[C@@H]5C6

RUN: RUN10127

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.20

EN300-1267093_1_1



CID: EN300-1267093_1_1

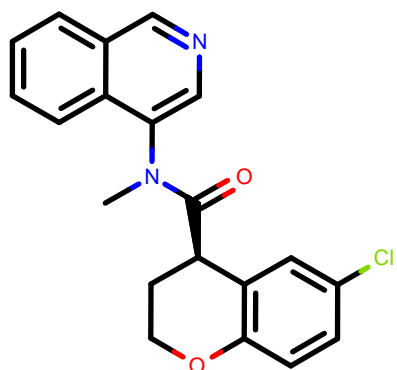
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(O)N5CCO[C@@H]6[C@@H]5C6O

RUN: RUN10585

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

MAK-UNK-3875bbc8-2_1



CID: MAK-UNK-3875bbc8-2_1

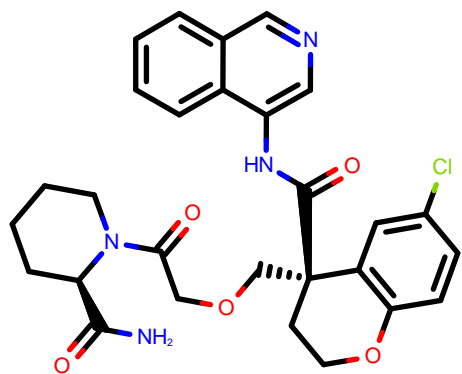
SMILES: CN(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)C)C1

RUN: RUN77

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.08

EN300-22879_2_2



CID: EN300-22879_2_2

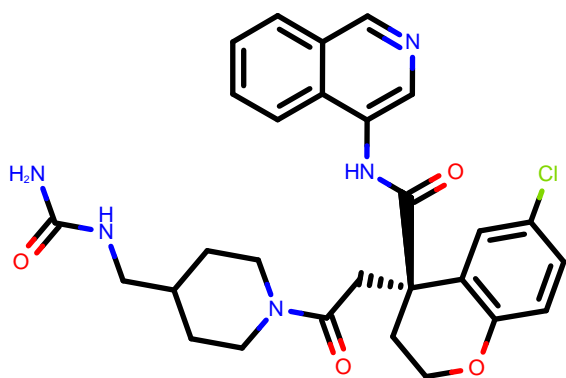
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)N5CCCC[C@@H]5C(=O)N

RUN: RUN1258

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.28

EN300-41549_1_1



CID: EN300-41549_1_1

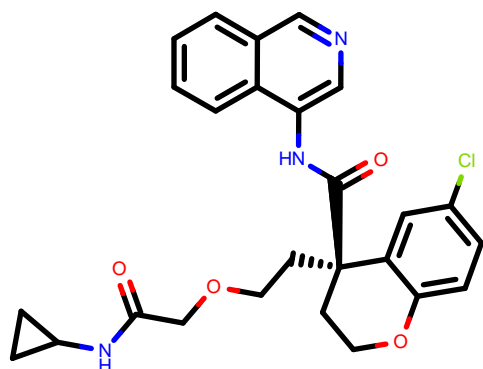
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(C5)CNC(=O)N

RUN: RUN5833

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.27

EN300-1253178_3_1



CID: EN300-1253178_3_1

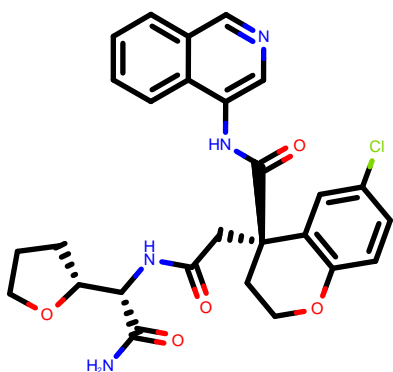
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NC5CC5

RUN: RUN1991

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.20

EN300-191187_1_2



CID: EN300-191187_1_2

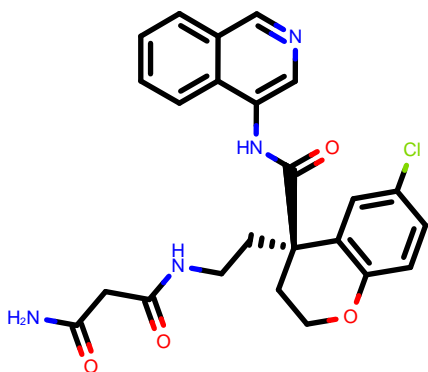
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CO)CCO5

RUN: RUN13304

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.23

EN300-82179_3_1



CID: EN300-82179_3_1

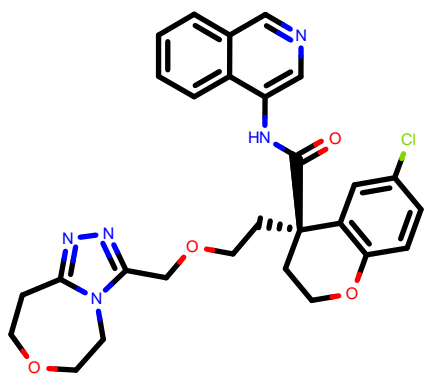
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)N

RUN: RUN12670

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.23

EN300-310888_3_1



CID: EN300-310888_3_1

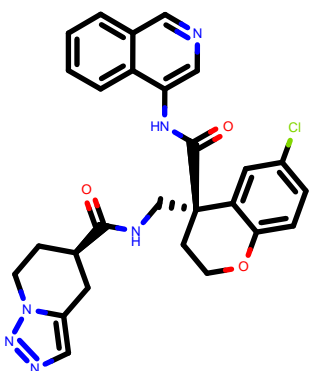
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5nnC6n5COCOC6

RUN: RUN2329

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.34

EN300-7430501_2_2



CID: EN300-7430501_2_2

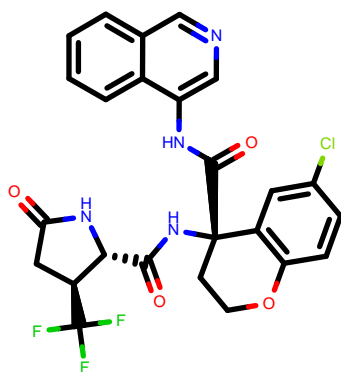
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4[C@@]4(H)5C6n6c(cnn6)C5

RUN: RUN6741

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.26

EN300-169955_1_1



CID: EN300-169955_1_1

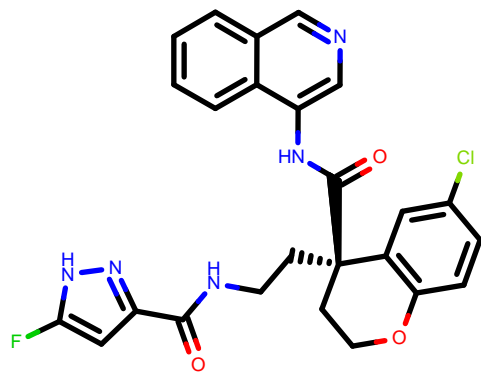
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4[C@@]4(H)5C6C(F)(F)F6

RUN: RUN9133

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.22

EN300-150212_3_1



CID: EN300-150212_3_1

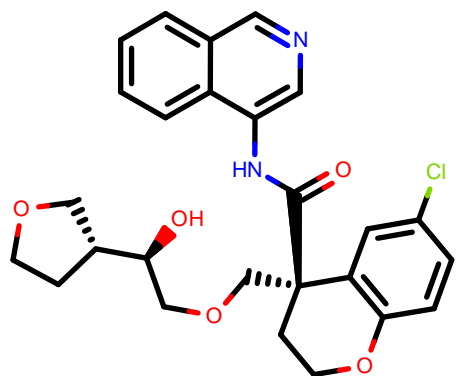
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc([nH]n5)F

RUN: RUN15506

DDG (kcal/mol): -1.11

dDDG (kcal/mol): 0.22

EN300-1911992_2_2



CID: EN300-1911992_2_2

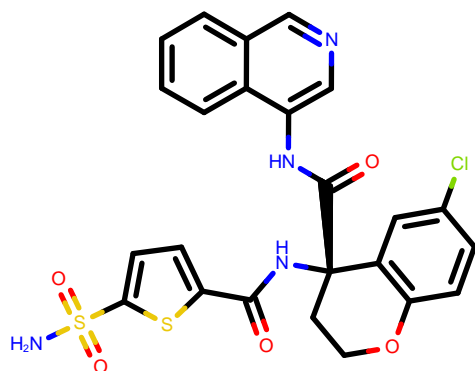
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]([C@@H]5CCOC5)O

RUN: RUN980

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.27

EN300-59386_1_1



CID: EN300-59386_1_1

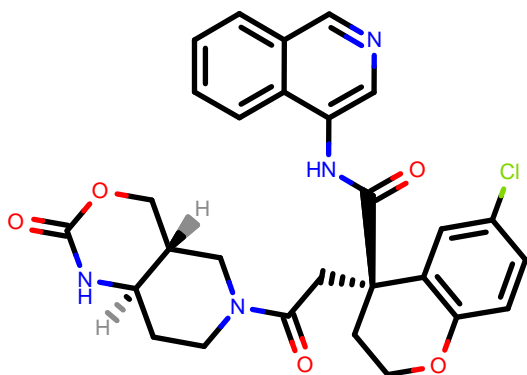
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(s5)S(=O)(=O)N

RUN: RUN6393

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.26

EN300-7500524_1_1



CID: EN300-7500524_1_1

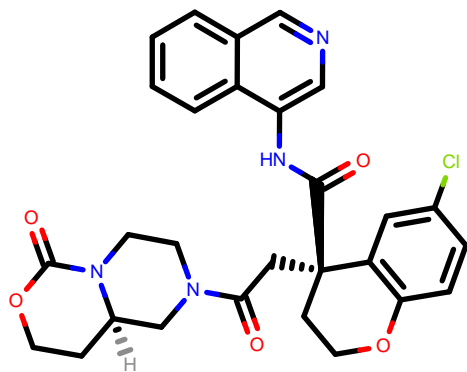
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CC[C@H]([C@@H]6C5)COC1=O)N6

RUN: RUN6511

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.25

EN300-121939_1_2



CID: EN300-121939_1_2

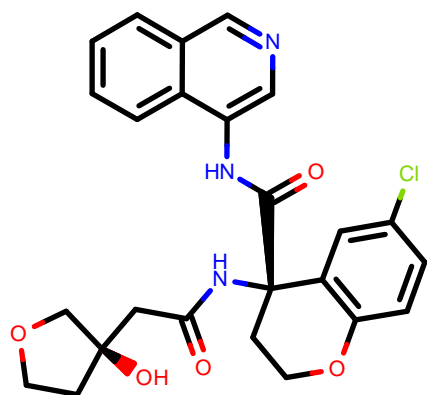
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CCN6[C@@H]([C@@H]5)COC6=O

RUN: RUN10263

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.25

EN300-360157_1_1



CID: EN300-360157_1_1

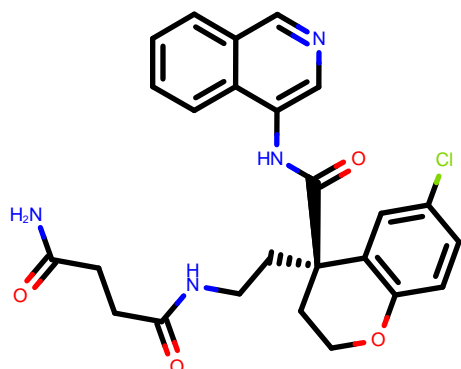
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]5(CCOC5)O

RUN: RUN6904

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.24

EN300-178515_3_1



CID: EN300-178515_3_1

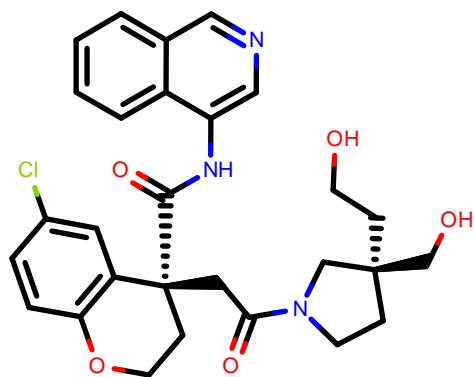
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCC(=O)N

RUN: RUN12356

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.31

EN300-1707870_1_2



CID: EN300-1707870_1_2

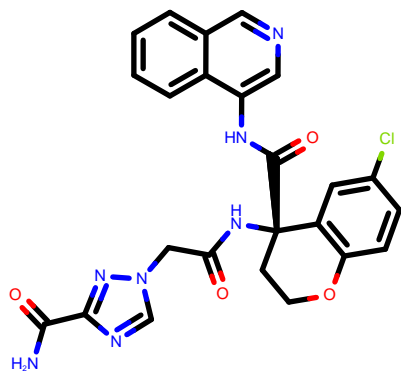
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]3(C5)CCO)CO

RUN: RUN5841

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.25

EN300-262604_1_1



CID: EN300-262604_1_1

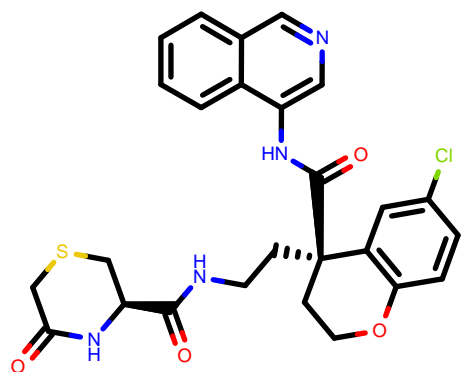
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5ncnc5)C(=O)N

RUN: RUN9473

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.25

EN300-657320_3_1



CID: EN300-657320_3_1

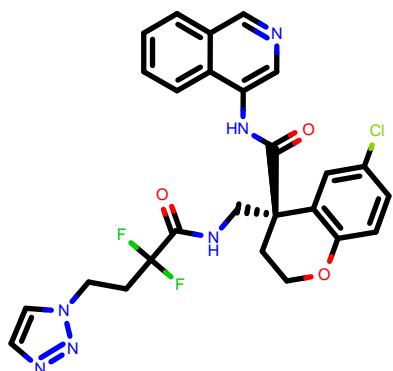
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CSCC(=O)N5

RUN: RUN9184

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.24

EN300-6474220_2_1



CID: EN300-6474220_2_1

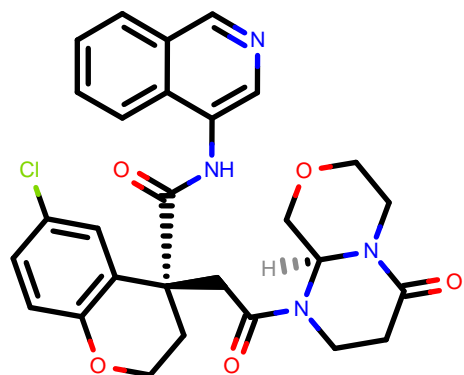
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C1C(Cn5cnn5)F1F

RUN: RUN3951

DDG (kcal/mol): -1.10

dDDG (kcal/mol): 0.33

EN300-1608240_1_2



CID: EN300-1608240_1_2

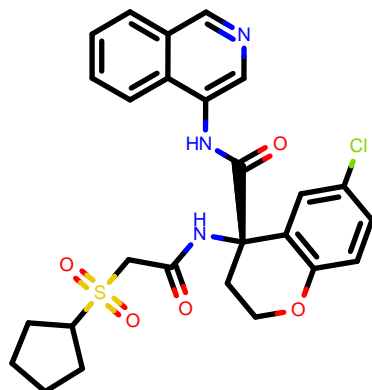
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC1(=O)N6C@H]5COC6

RUN: RUN13904

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.29

EN300-42154_1_1



CID: EN300-42154_1_1

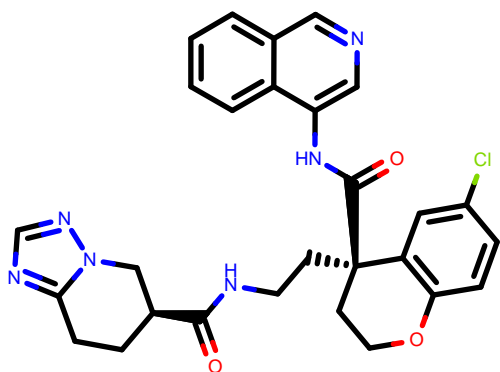
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CS(=O)(=O)C5CCCC5

RUN: RUN4534

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.27

EN300-1662365_3_2



CID: EN300-1662365_3_2

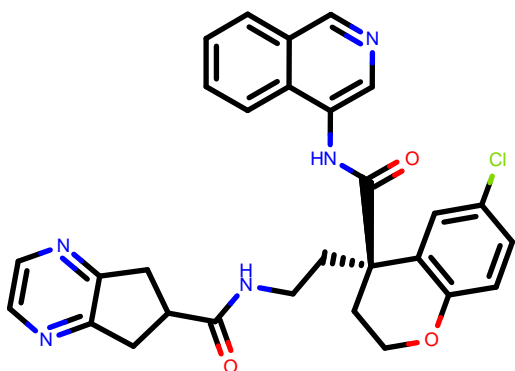
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCc6nncn6C5

RUN: RUN15393

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.25

EN300-2011576_3_1



CID: EN300-2011576_3_1

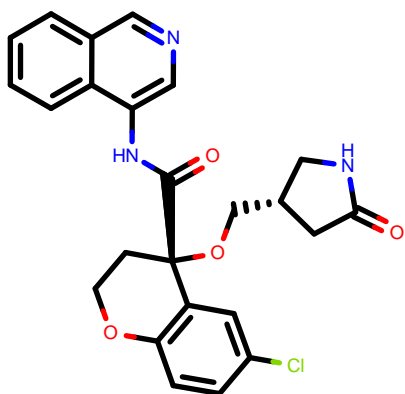
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C6c6nccn6C5

RUN: RUN15416

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.26

EN300-246747_1_2



CID: EN300-246747_1_2

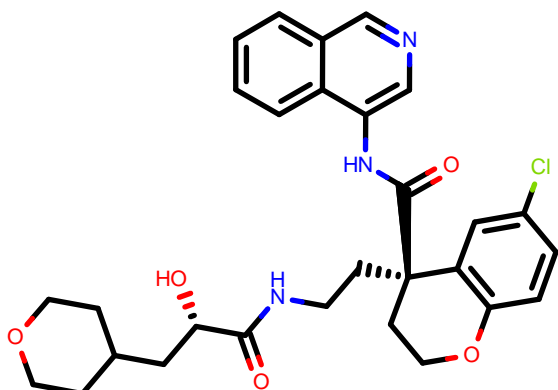
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CC(=O)NC5

RUN: RUN1541

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.23

EN300-1452069_3_2



CID: EN300-1452069_3_2

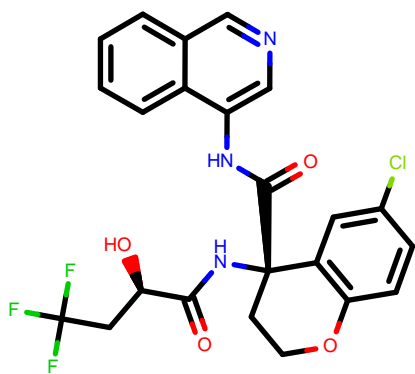
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](CC5COCC5)O

RUN: RUN13416

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.34

EN300-1932013_1_1



CID: EN300-1932013_1_1

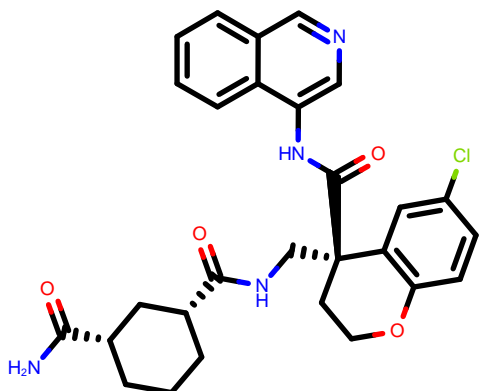
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CC(F)(F)F)O

RUN: RUN3754

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.28

EN300-90142_2_1



CID: EN300-90142_2_1

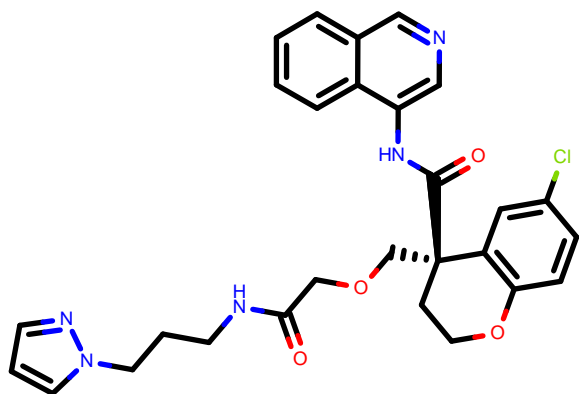
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5CCCC5)N

RUN: RUN5703

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.31

EN300-47500_2_1



CID: EN300-47500_2_1

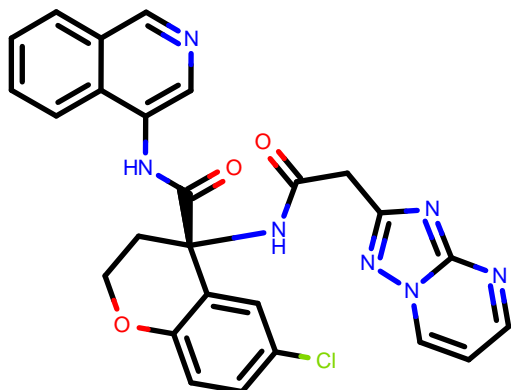
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NCCCn5cccn5

RUN: RUN2240

DDG (kcal/mol): -1.09

dDDG (kcal/mol): 0.32

EN300-39826_1_1



CID: EN300-39826_1_1

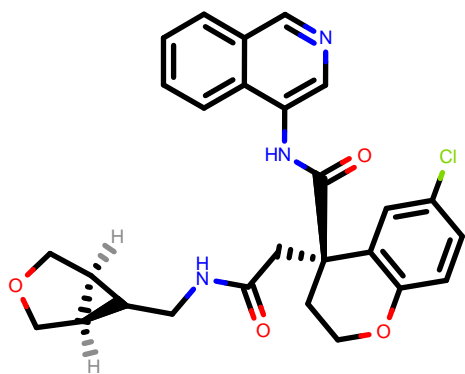
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nc6ncccn6n5

RUN: RUN9754

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.25

EN300-210089_1_1



CID: EN300-210089_1_1

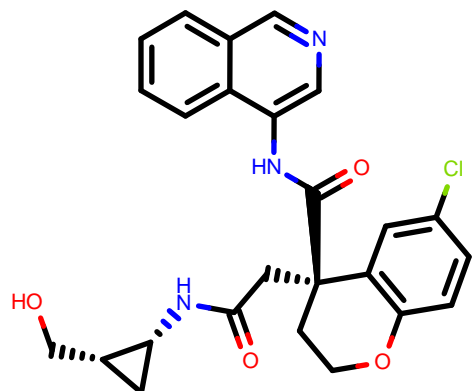
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5[C@H]6[C@@H]5COC6

RUN: RUN6815

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.19

EN300-196962_1_1



CID: EN300-196962_1_1

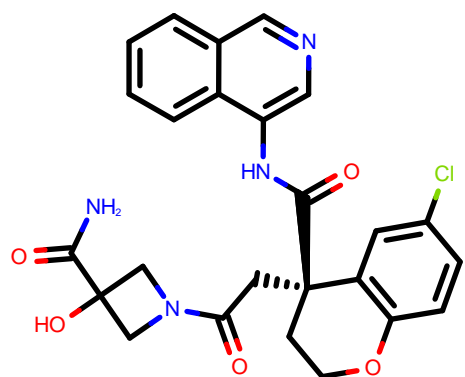
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4[C@H]5[C@@]4[C@H]5CO

RUN: RUN5161

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.23

EN300-316171_1_1



CID: EN300-316171_1_1

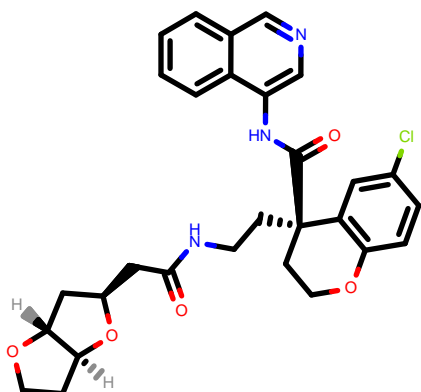
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C(=O)NO

RUN: RUN12644

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.23

EN300-7355519_3_2



CID: EN300-7355519_3_2

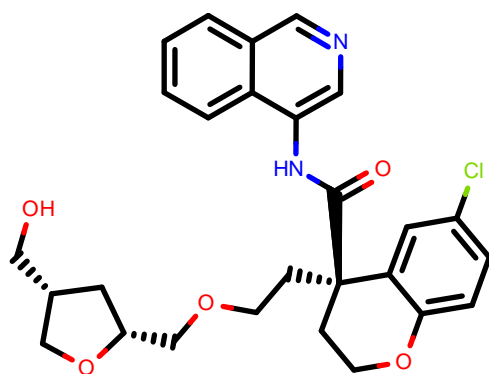
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4[C@H]5[C@@]4[C@H]5COC6

RUN: RUN15007

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.27

EN300-6494158_3_3



CID: EN300-6494158_3_3

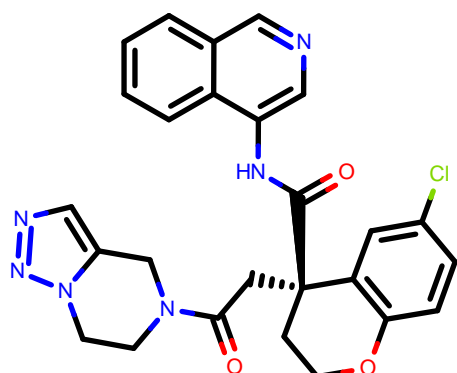
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C[C@H](CO)5CO

RUN: RUN2070

DDG (kcal/mol): -1.08

dDDG (kcal/mol): 0.28

EN300-29228_1_1



CID: EN300-29228_1_1

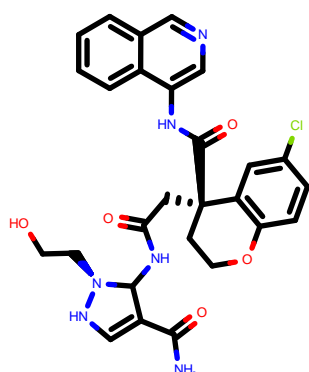
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6C(CN6)C5

RUN: RUN13070

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-80245_1_1



CID: EN300-80245_1_1

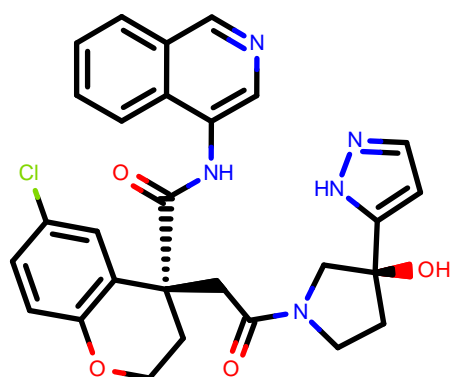
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5c(cnn5CCO)C(=O)N

RUN: RUN15022

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.29

EN300-1609922_1_2



CID: EN300-1609922_1_2

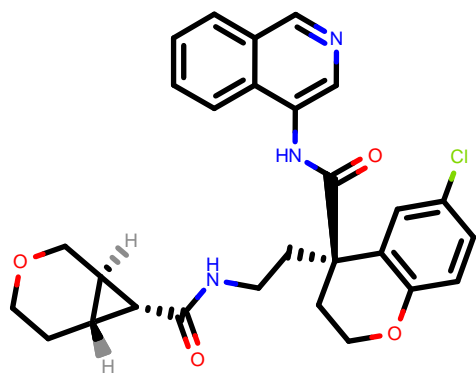
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]5(C)C6CN(CN6)O

RUN: RUN12848

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.27

EN300-1644723_3_7



CID: EN300-1644723_3_7

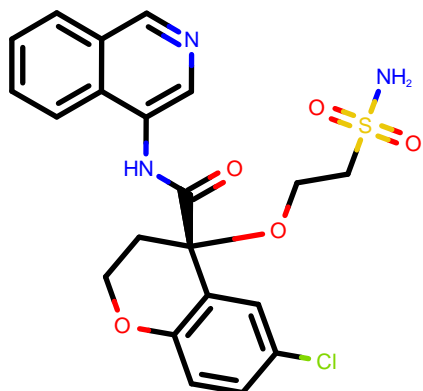
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5H5C@H[C@@H]5COCC6

RUN: RUN15332

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.23

EN300-270710_1_1



CID: EN300-270710_1_1

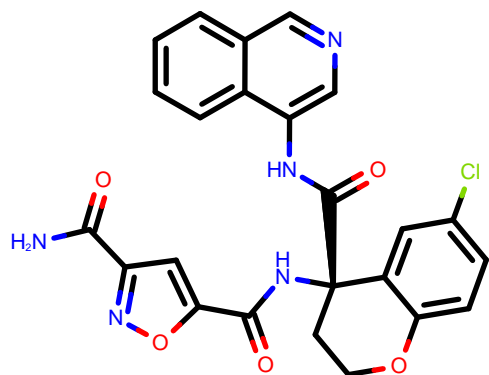
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)OCCS(=O)(=O)N

RUN: RUN2051

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.23

EN300-127156_1_1



CID: EN300-127156_1_1

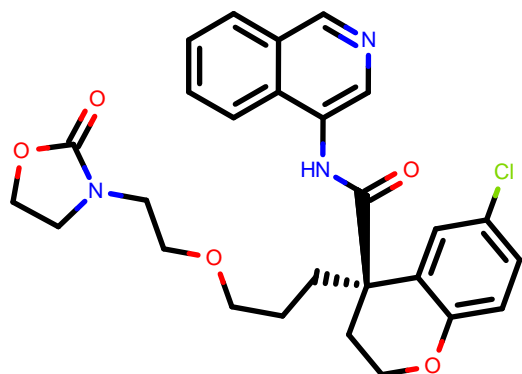
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)c5cc(nc5)C(=O)N

RUN: RUN3126

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.20

EN300-370967_4_1



CID: EN300-370967_4_1

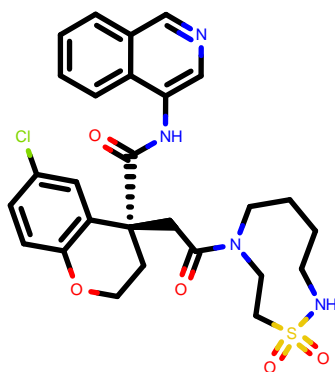
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCOC5N5COC5=O

RUN: RUN1187

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-6743781_1_1



CID: EN300-6743781_1_1

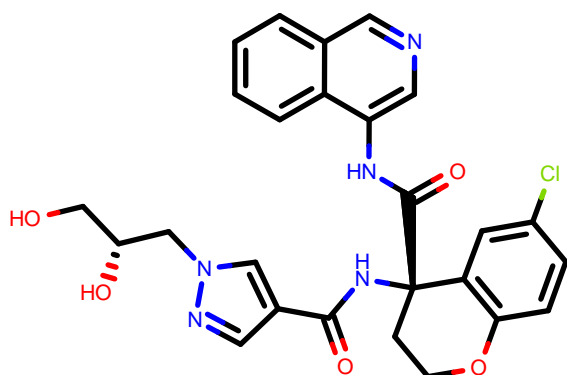
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCCNS(=O)(=O)CC5

RUN: RUN7847

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.32

EN300-246178_1_1



CID: EN300-246178_1_1

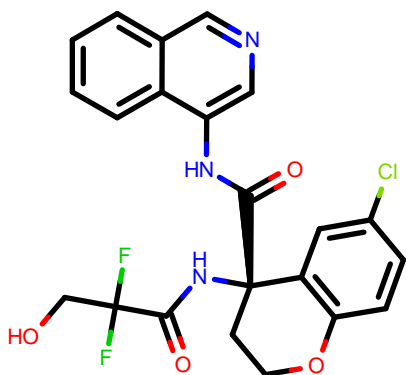
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnnc5C[C@@H](CO)O

RUN: RUN1505

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.35

EN300-123489_1_1



CID: EN300-123489_1_1

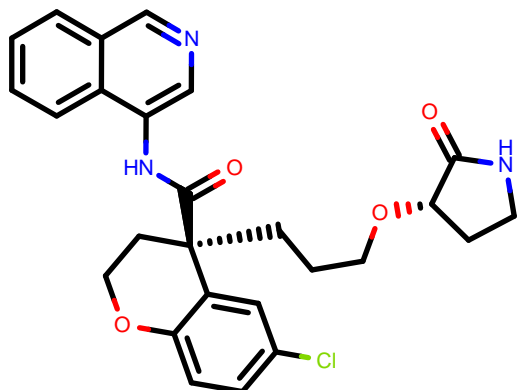
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CO)(F)F

RUN: RUN1209

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.25

EN300-6736413_4_1



CID: EN300-6736413_4_1

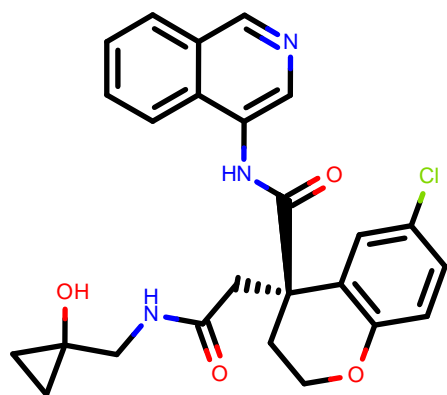
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN941

DDG (kcal/mol): -1.07

dDDG (kcal/mol): 0.22

EN300-1644703_1_1



CID: EN300-1644703_1_1

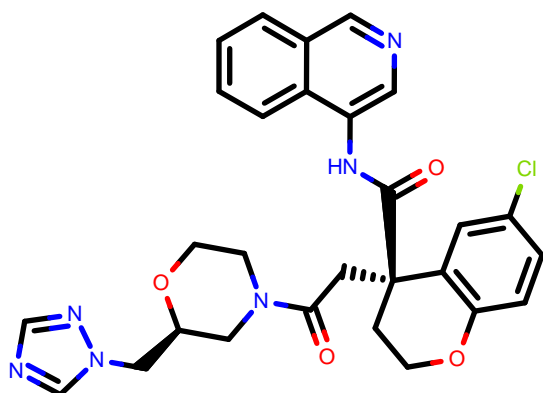
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(C)CC5O

RUN: RUN3305

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.24

EN300-80241_1_1



CID: EN300-80241_1_1

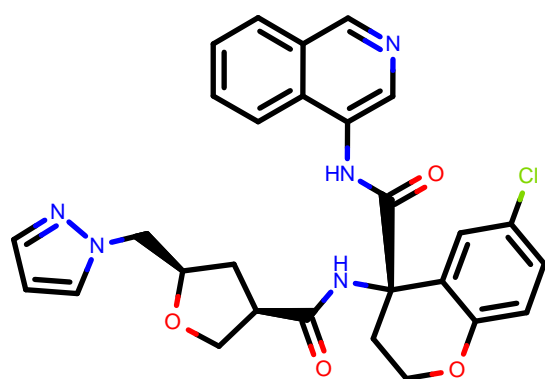
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]3[H](C5)Cn6cnc6

RUN: RUN9504

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.31

EN300-6494859_1_3



CID: EN300-6494859_1_3

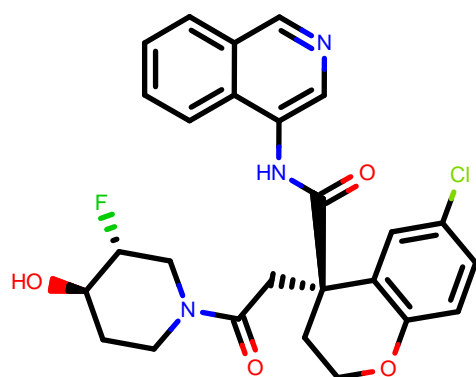
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)N(C)C(=O)C@@H]5C[C@@H](C5)F6cnc6

RUN: RUN8472

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.28

EN300-741926_1_4



CID: EN300-741926_1_4

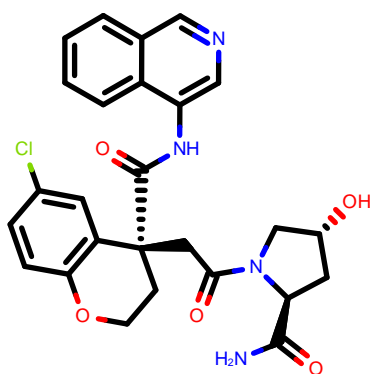
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)F)O

RUN: RUN3809

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.24

EN300-07752_1_2



CID: EN300-07752_1_2

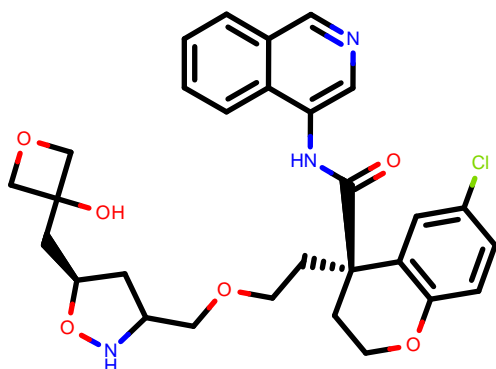
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N5O

RUN: RUN7055

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-7457160_3_2



CID: EN300-7457160_3_2

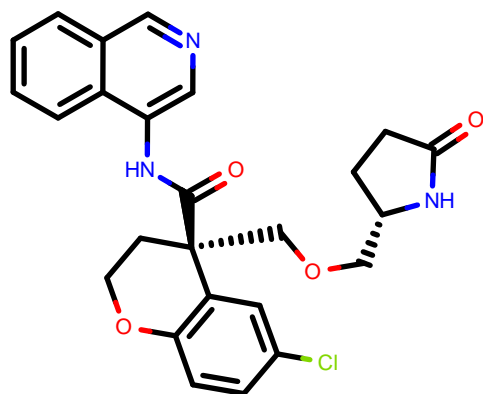
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N5O

RUN: RUN834

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.33

EN300-195756_2_2



CID: EN300-195756_2_2

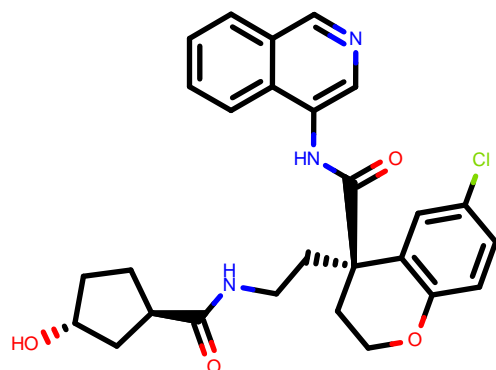
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N5

RUN: RUN1953

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.23

EN300-321597_3_1



CID: EN300-321597_3_1

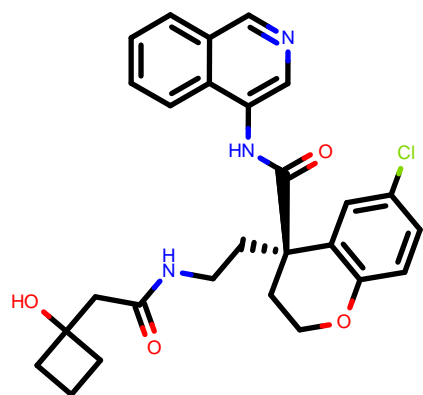
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N5

RUN: RUN5009

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.24

EN300-246423_3_1



CID: EN300-246423_3_1

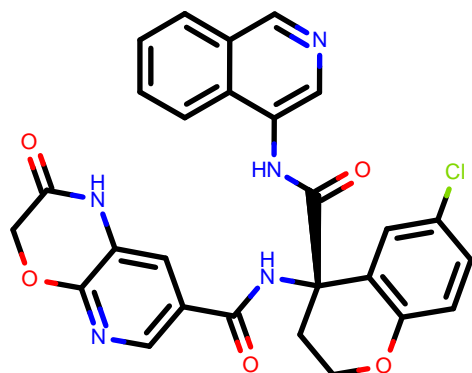
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)CC5(CCC5)O

RUN: RUN7543

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-103979_1_1



CID: EN300-103979_1_1

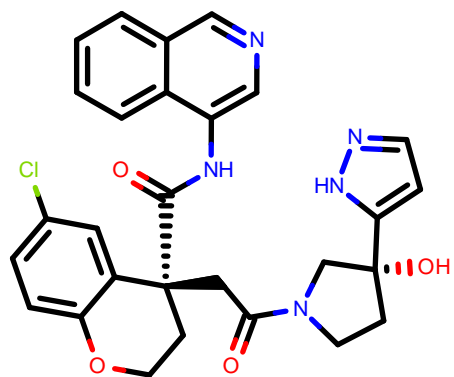
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)c5cc6c(nc5)OCC(=O)N6

RUN: RUN7248

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.23

EN300-1609922_1_1



CID: EN300-1609922_1_1

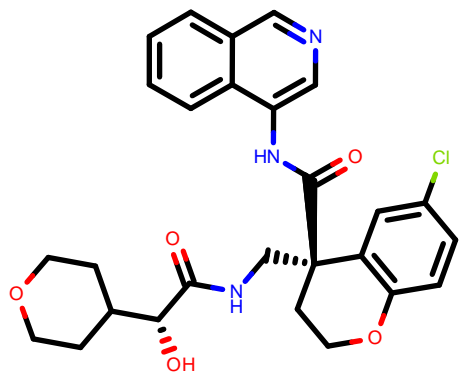
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)N5CC[C@H]5)C6=CN=CN6

RUN: RUN6531

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-79180_2_1



CID: EN300-79180_2_1

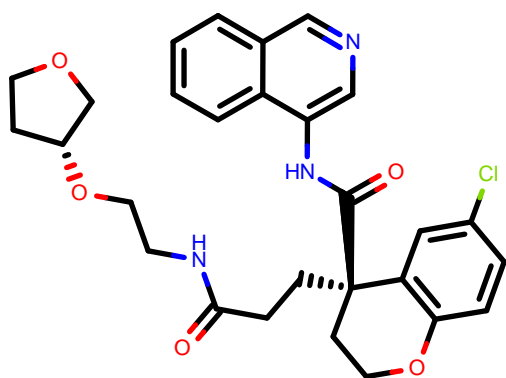
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@@H]5COCOC5)O

RUN: RUN7081

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.26

EN300-702062_2_1



CID: EN300-702062_2_1

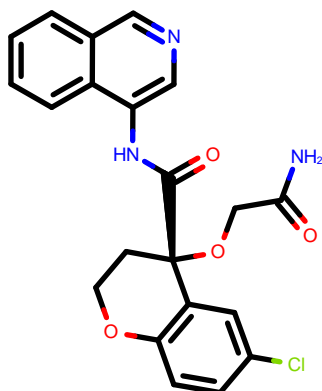
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCO[C@@]5CCOC5

RUN: RUN9980

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.30

EN300-18249_1_1



CID: EN300-18249_1_1

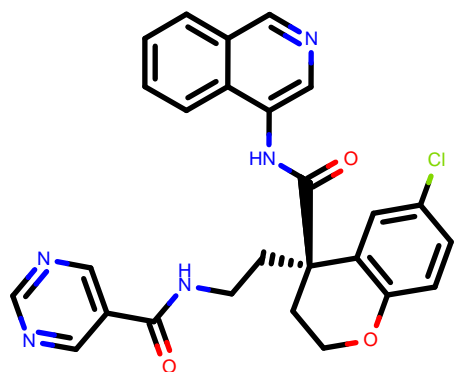
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N

RUN: RUN1629

DDG (kcal/mol): -1.06

dDDG (kcal/mol): 0.14

EN300-64297_3_1



CID: EN300-64297_3_1

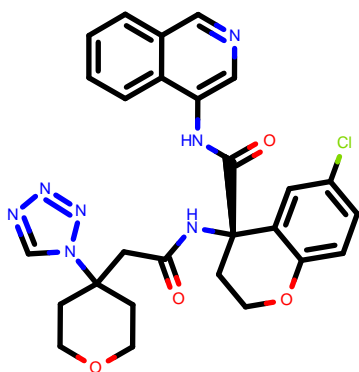
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5nncn5

RUN: RUN15418

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.20

EN300-306097_1_1



CID: EN300-306097_1_1

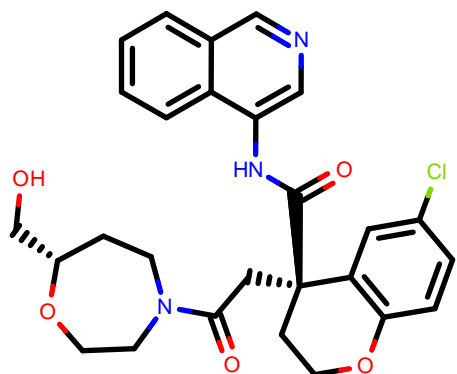
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCOCC5)n6cnm6

RUN: RUN2574

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-2007620_1_1



CID: EN300-2007620_1_1

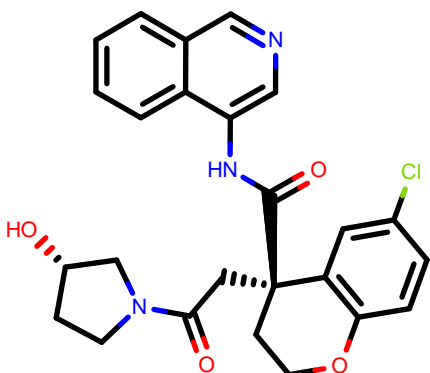
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](OCC5)CO

RUN: RUN3137

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.26

EN300-69312_1_1



CID: EN300-69312_1_1

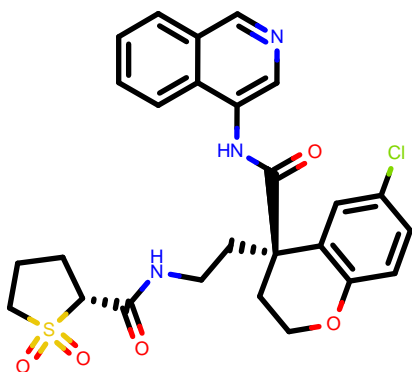
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O

RUN: RUN3357

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.21

EN300-88656_3_2



CID: EN300-88656_3_2

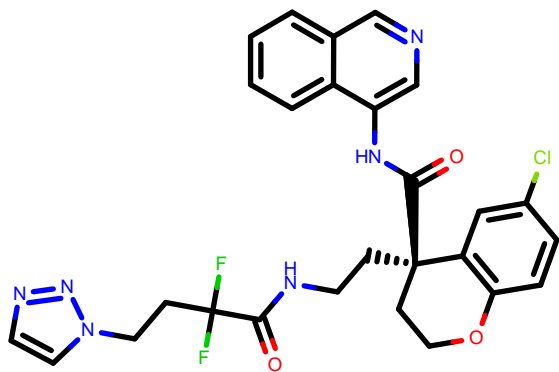
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5SCC(S5)=O

RUN: RUN2941

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.25

EN300-6474220_3_1



CID: EN300-6474220_3_1

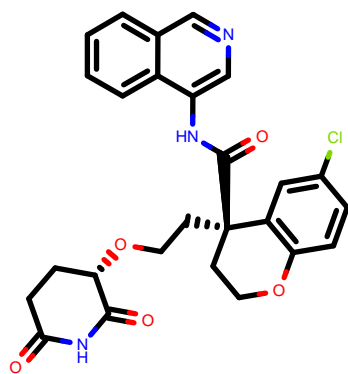
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(Cn5cnn5)F

RUN: RUN4493

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.27

EN300-120920_3_1



CID: EN300-120920_3_1

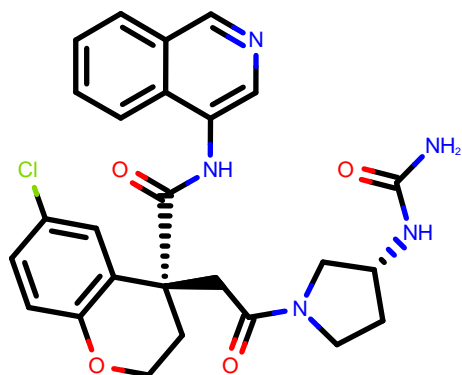
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@@H]5CCCC(=O)NC5=O

RUN: RUN2270

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.24

EN300-118869_1_2



CID: EN300-118869_1_2

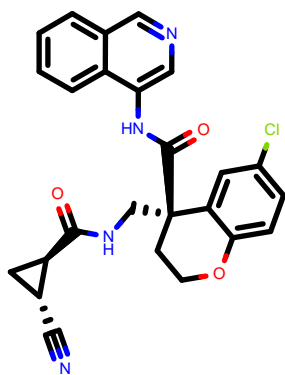
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)NC(=O)N

RUN: RUN4077

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.32

EN300-1588617_2_1



CID: EN300-1588617_2_1

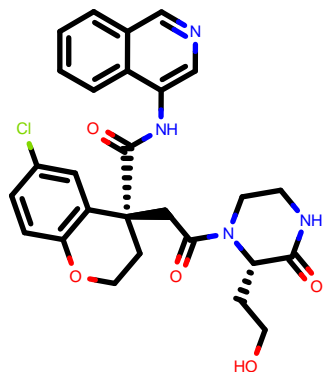
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5C[C@H]5C#N

RUN: RUN6869

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.24

EN300-1587691_1_1



CID: EN300-1587691_1_1

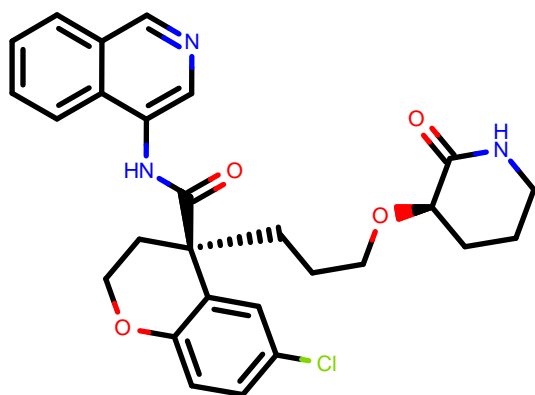
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)[C@@]6C[C@H]5CO

RUN: RUN5293

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.30

EN300-107267_4_2



CID: EN300-107267_4_2

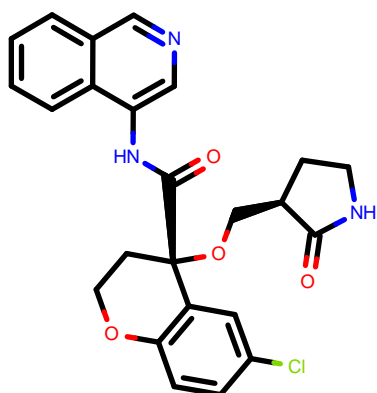
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O

RUN: RUN605

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.27

EN300-246248_1_1



CID: EN300-246248_1_1

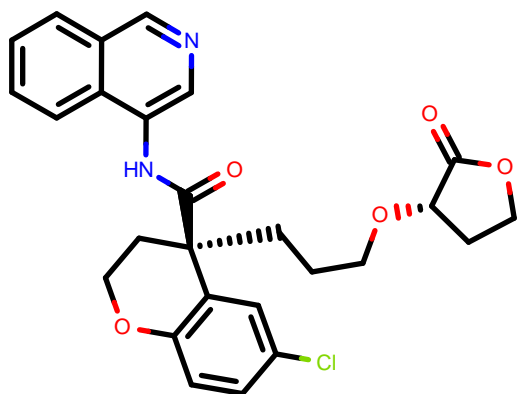
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCNC5=O

RUN: RUN1852

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.19

EN300-20496_4_1



CID: EN300-20496_4_1

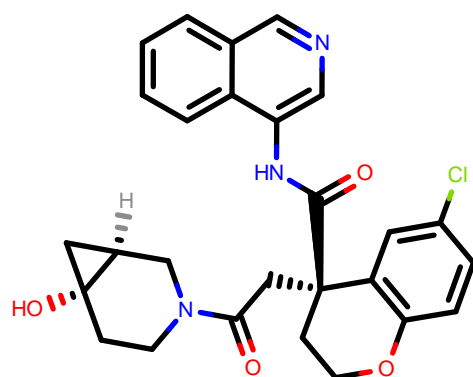
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCOC5=O

RUN: RUN1107

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.21

EN300-303908_1_1



CID: EN300-303908_1_1

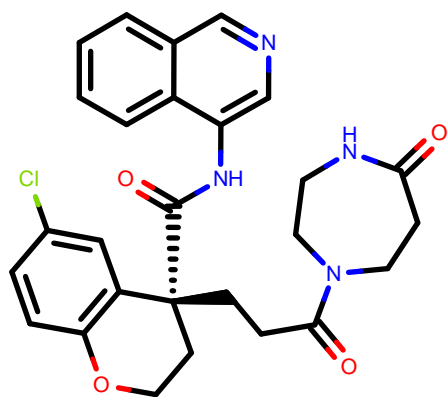
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]6(C)[C@@H]6C5=O

RUN: RUN3177

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.29

EN300-69107_2_1



CID: EN300-69107_2_1

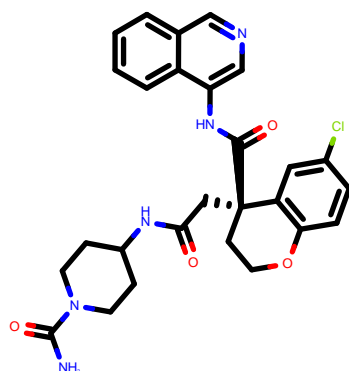
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCCC(=O)NCC5

RUN: RUN10190

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.23

EN300-25791_1_1



CID: EN300-25791_1_1

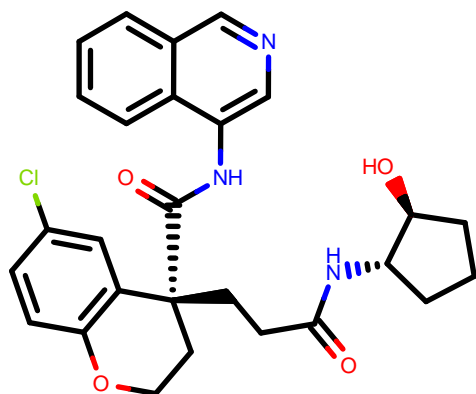
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5CCN(CC5)C(=O)N

RUN: RUN11024

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.29

EN300-344121_2_1



CID: EN300-344121_2_1

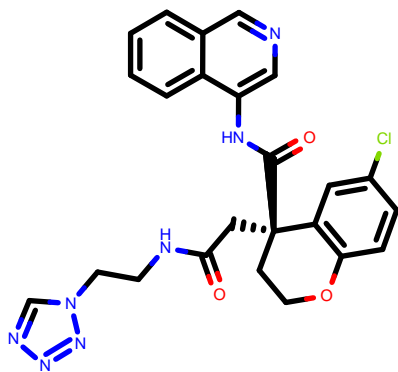
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CC[C@]3([H])O

RUN: RUN5484

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.26

EN300-108022_1_1



CID: EN300-108022_1_1

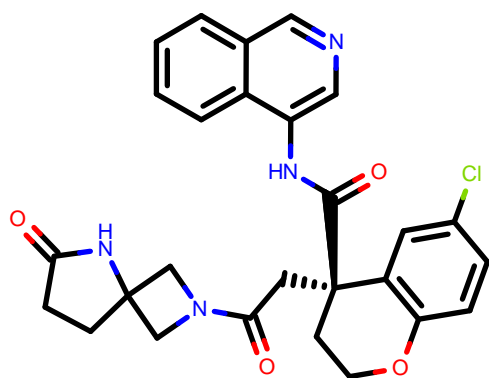
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCn5cnnn5

RUN: RUN9771

DDG (kcal/mol): -1.05

dDDG (kcal/mol): 0.21

EN300-2010267_1_1



CID: EN300-2010267_1_1

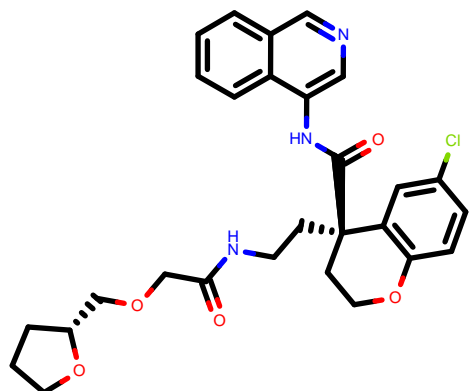
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CCC(=O)N6

RUN: RUN12272

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.20

EN300-60033_3_1



CID: EN300-60033_3_1

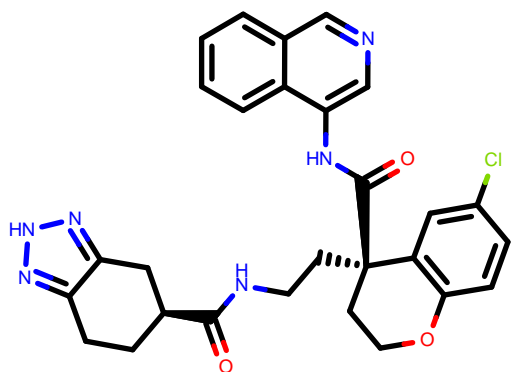
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@H]5CCCC5

RUN: RUN11194

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.22

EN300-185729_3_1



CID: EN300-185729_3_1

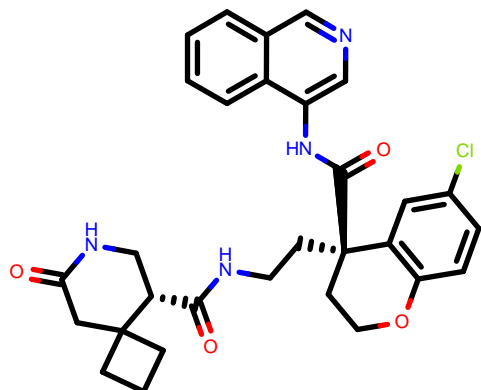
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCc6c(n[nH]n6)C5

RUN: RUN15433

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-1704404_3_2



CID: EN300-1704404_3_2

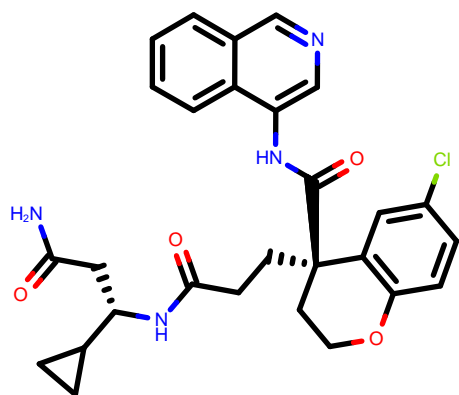
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CNC1=C(O)CC56CCO6

RUN: RUN15182

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.28

EN300-85413_2_2



CID: EN300-85413_2_2

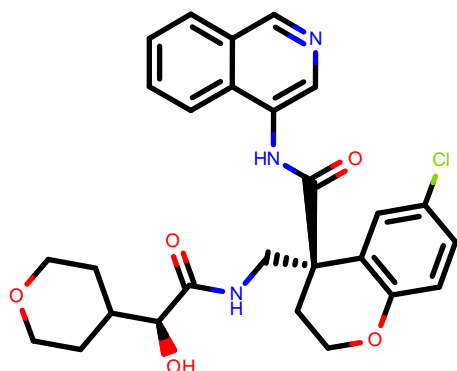
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H](CC(=O)N)C5CC5

RUN: RUN2180

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.31

EN300-79180_2_2



CID: EN300-79180_2_2

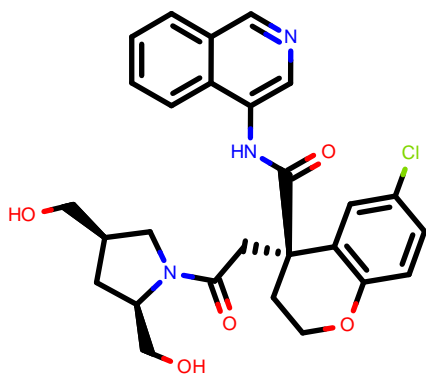
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H](C5CCOCC5)O

RUN: RUN6059

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.32

EN300-1212400_1_2



CID: EN300-1212400_1_2

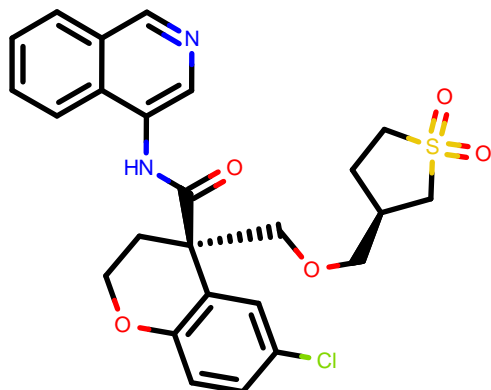
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H](C)C@H5CO)CO

RUN: RUN497

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.24

EN300-1448603_2_2



CID: EN300-1448603_2_2

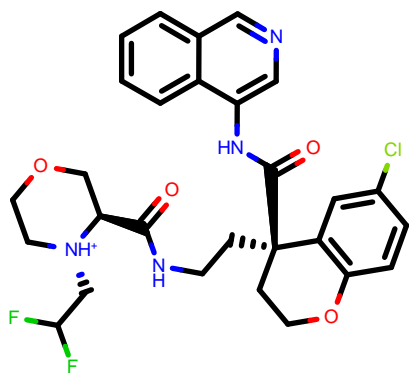
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN1138

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.28

EN300-140582_3_1



CID: EN300-140582_3_1

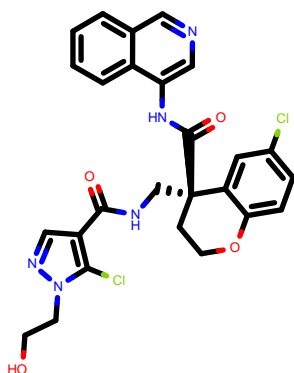
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CNC(=O)[C@@H]5COC(=O)C(F)F

RUN: RUN12010

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.29

EN300-333468_2_1



CID: EN300-333468_2_1

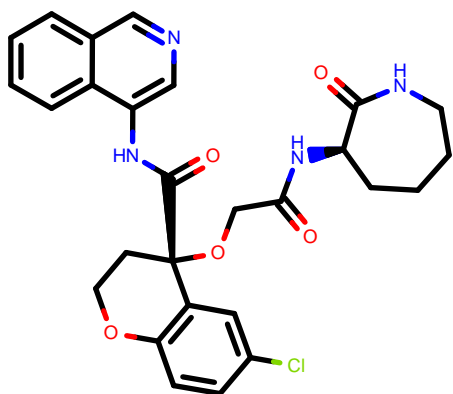
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CNC(=O)Nc5cnc(Cl)CO

RUN: RUN8866

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.26

EN300-37195_1_2



CID: EN300-37195_1_2

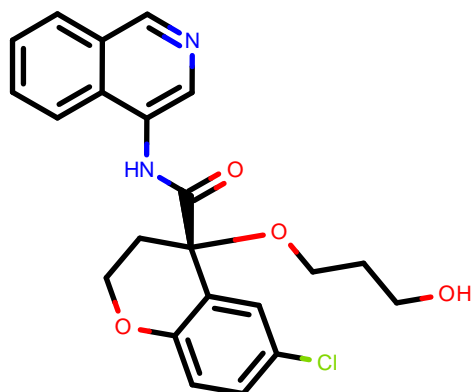
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)OCC(=O)N[C@@H]5COC(=O)C5=O

RUN: RUN1501

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.26

EN300-221518_1_1



CID: EN300-221518_1_1

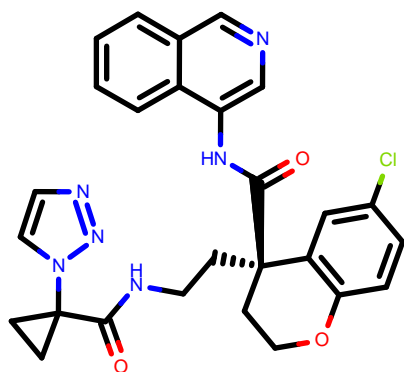
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)OCCCCO

RUN: RUN1701

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.15

EN300-658559_3_1



CID: EN300-658559_3_1

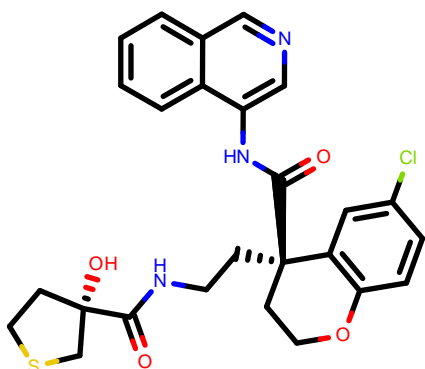
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)C5(C)C5n6ccn6

RUN: RUN2897

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.26

EN300-122656_3_1



CID: EN300-122656_3_1

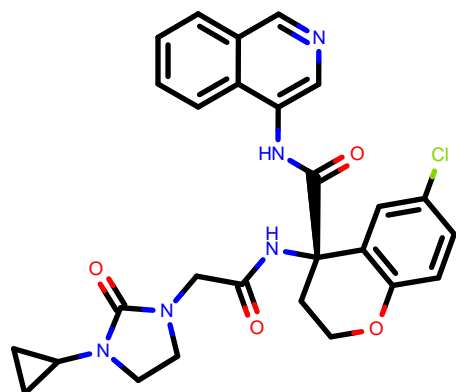
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(C)CSCS5O

RUN: RUN8511

DDG (kcal/mol): -1.04

dDDG (kcal/mol): 0.38

EN300-304771_1_1



CID: EN300-304771_1_1

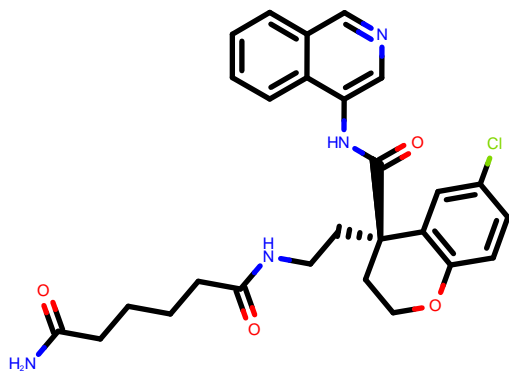
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)NC(=O)CN5CCN(C5=O)C6CC6

RUN: RUN9631

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.31

EN300-142412_3_1



CID: EN300-142412_3_1

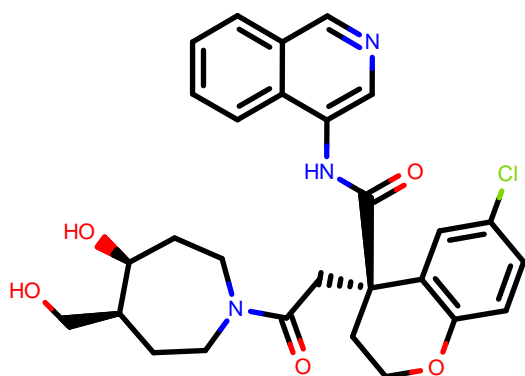
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)C)CCNC(=O)CCCC(=O)N

RUN: RUN937

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.30

EN300-7353672_1_2



CID: EN300-7353672_1_2

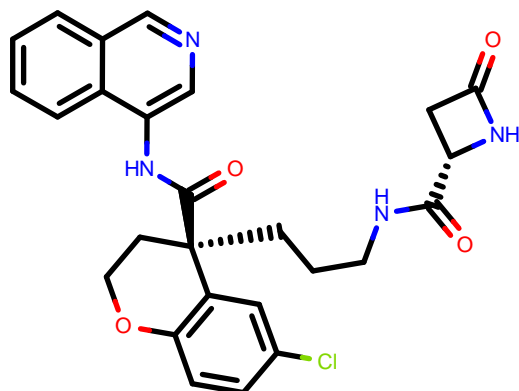
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CC(=O)N5C[C@@H](C5)CO

RUN: RUN10091

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.36

EN300-103219_4_1



CID: EN300-103219_4_1

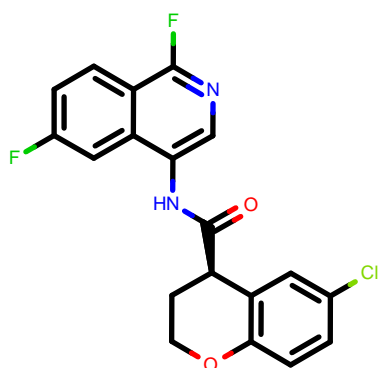
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CCCNC(=O)[C@@]4NCC(=O)N4

RUN: RUN13499

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.23

JOH-SUS-a69c159d-5_1



CID: JOH-SUS-a69c159d-5_1

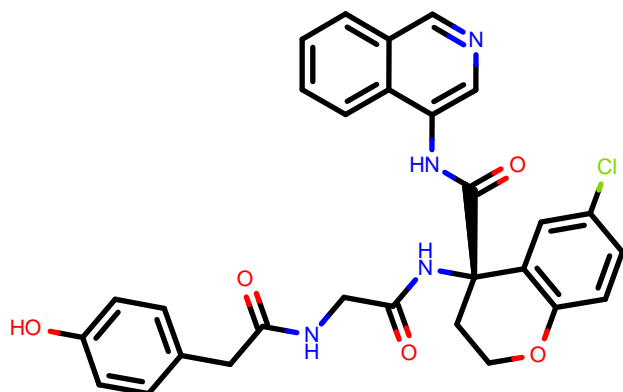
SMILES: c1cc2c(c1)c(cnc2F)NC(=O)[C@@]3(CCOc4c3cc(c4)C)F

RUN: RUN11

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.07

EN300-65253_1_1



CID: EN300-65253_1_1

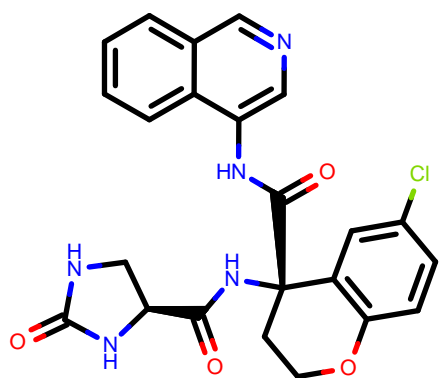
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)NC(=O)CNC(=O)Cc5ccc(O)c5

RUN: RUN8945

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.27

EN300-66461_1_1



CID: EN300-66461_1_1

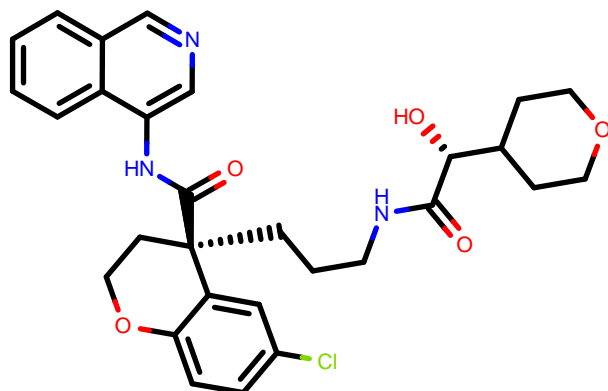
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5CN(C=O)N5

RUN: RUN3470

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.19

EN300-79180_4_1



CID: EN300-79180_4_1

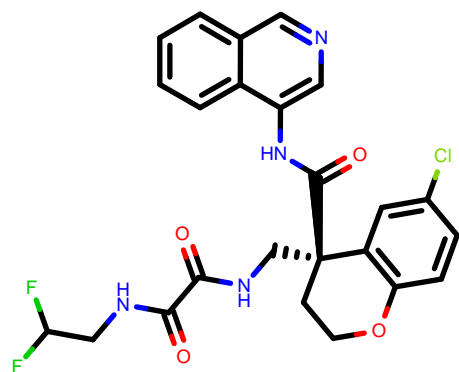
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H[C@H]5COCOC5O

RUN: RUN9581

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.26

EN300-128277_2_1



CID: EN300-128277_2_1

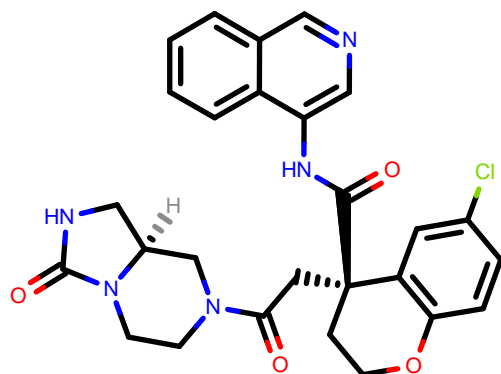
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(=O)NCC(F)F

RUN: RUN7313

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.25

EN300-100765_1_1



CID: EN300-100765_1_1

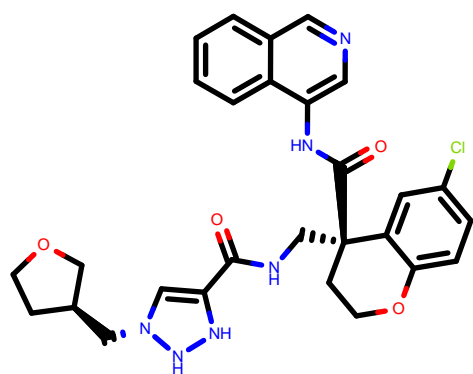
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@]H[C@H](C5)CNC6=O

RUN: RUN10683

DDG (kcal/mol): -1.03

dDDG (kcal/mol): 0.23

EN300-317272_2_2



CID: EN300-317272_2_2

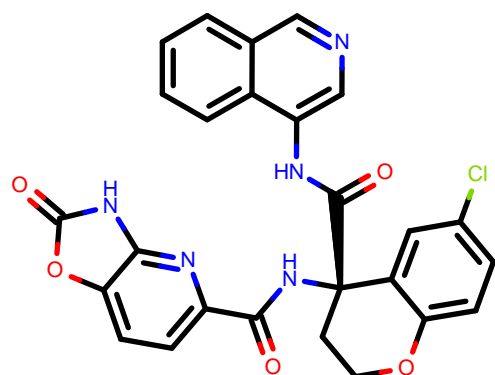
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(n5)C[C@@H]6CCOC6

RUN: RUN9330

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.36

EN300-188174_1_1



CID: EN300-188174_1_1

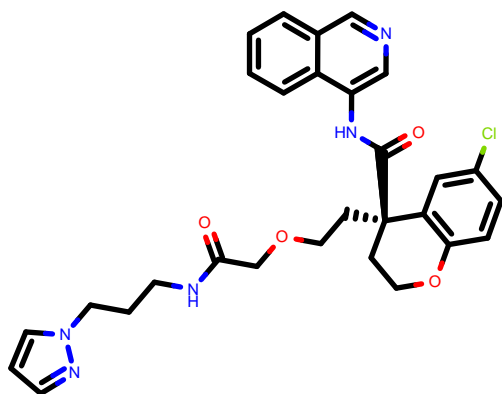
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)[nH]c(=O)o6

RUN: RUN6440

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.21

EN300-47500_3_1



CID: EN300-47500_3_1

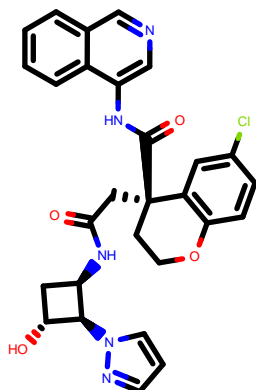
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCCCn5cccn5

RUN: RUN818

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.31

EN300-260696_1_3



CID: EN300-260696_1_3

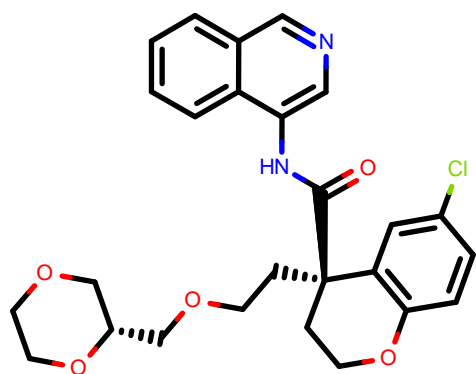
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[C@@H]5C[C@@H]6[C@@]3(C)C[C@H]56

RUN: RUN12654

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.30

EN300-139167_3_1



CID: EN300-139167_3_1

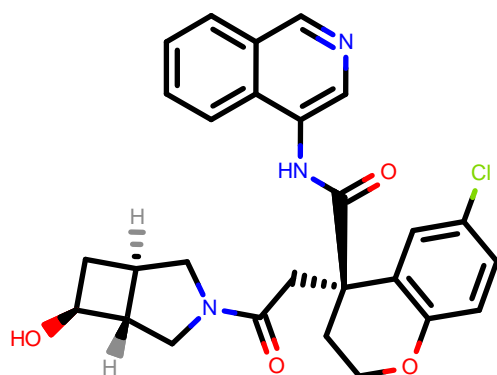
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COC(CO)5

RUN: RUN1943

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.24

EN300-305294_1_6



CID: EN300-305294_1_6

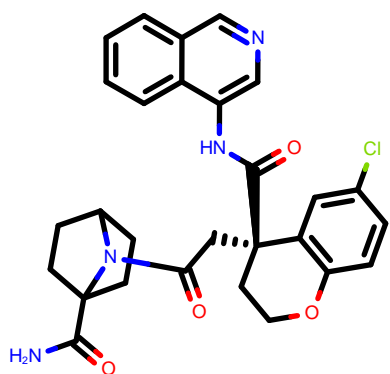
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](O)[C@@H](O)5

RUN: RUN9995

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.22

EN300-637522_1_1



CID: EN300-637522_1_1

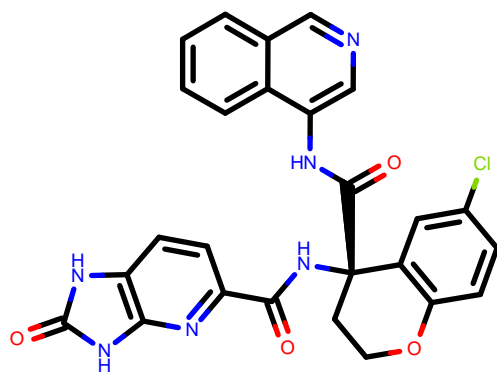
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6CCC5(C)C(=O)N

RUN: RUN12104

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.29

EN300-203402_1_1



CID: EN300-203402_1_1

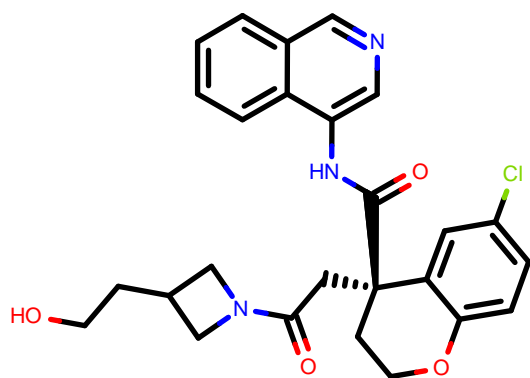
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)[nH]c(=O)[nH]6

RUN: RUN571

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.21

EN300-7413100_1_1



CID: EN300-7413100_1_1

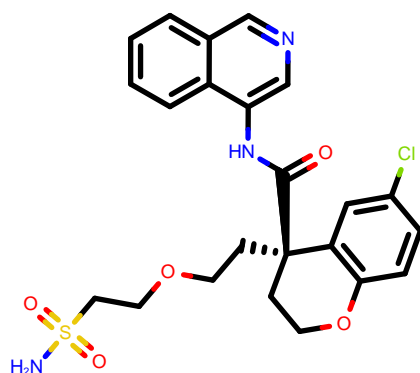
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CCO

RUN: RUN5973

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.23

EN300-270710_3_1



CID: EN300-270710_3_1

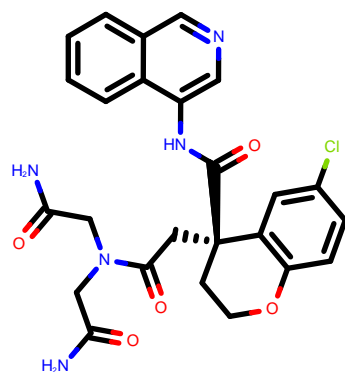
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)N

RUN: RUN1680

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.28

EN300-66290_1_1



CID: EN300-66290_1_1

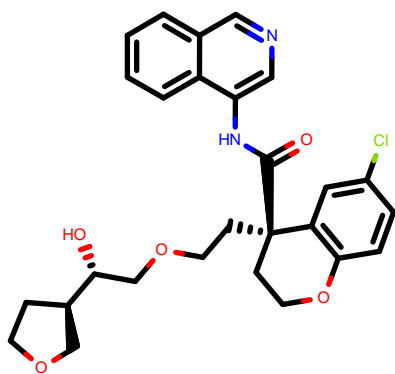
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)CC(=O)N

RUN: RUN3165

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.26

EN300-1911992_3_1



CID: EN300-1911992_3_1

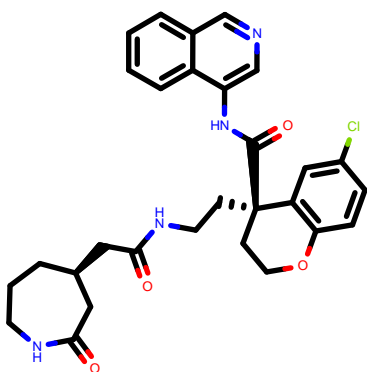
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](C)[C@@H]5CCOC5O

RUN: RUN2182

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.31

EN300-195590_3_2



CID: EN300-195590_3_2

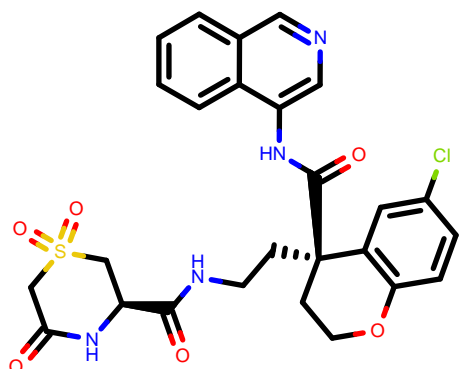
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)C[C@@]HJ5CCCC(=O)C5

RUN: RUN6153

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.27

EN300-702756_3_1



CID: EN300-702756_3_1

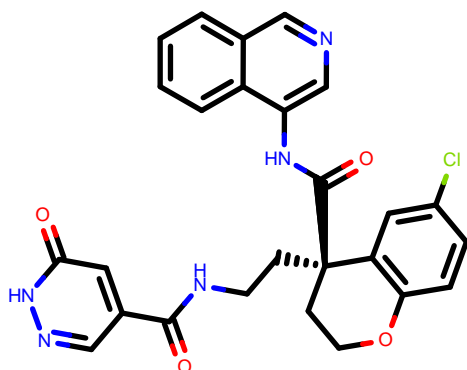
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)C[C@@]HJ5CS(=O)C(=O)C1=CN=C1

RUN: RUN15163

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.26

EN300-159634_3_1



CID: EN300-159634_3_1

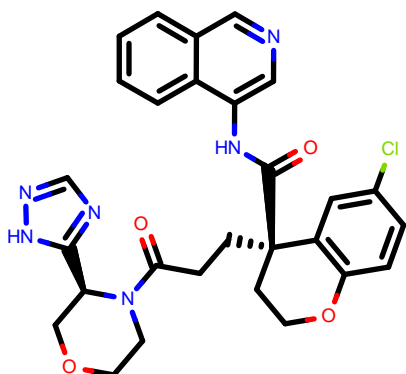
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)c5cc(=O)[nH]nc5

RUN: RUN15466

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.21

EN300-205616_2_1



CID: EN300-205616_2_1

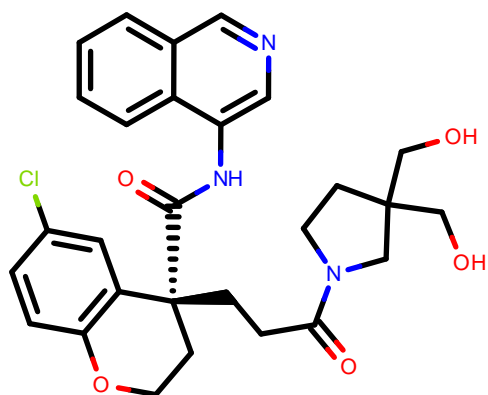
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCC(=O)N5CCOC[C@@]HJ5c6[nH]nc6

RUN: RUN3444

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.26

EN300-306144_2_1



CID: EN300-306144_2_1

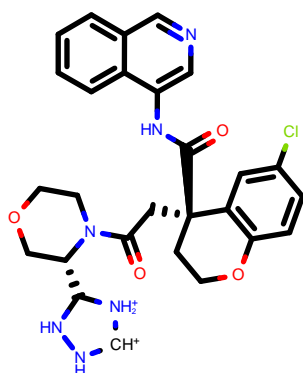
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)(CO)CO

RUN: RUN13005

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.28

EN300-205616_1_1



CID: EN300-205616_1_1

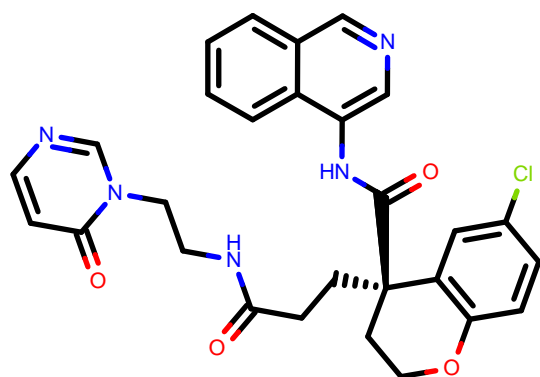
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5c6[nH]n6

RUN: RUN5445

DDG (kcal/mol): -1.02

dDDG (kcal/mol): 0.27

EN300-258326_2_1



CID: EN300-258326_2_1

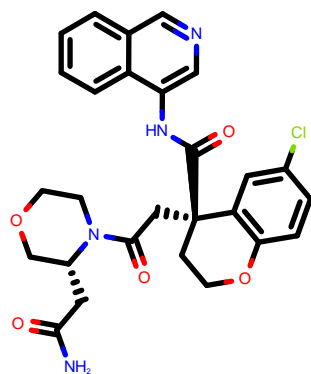
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)Nc5ccncc5=O

RUN: RUN3532

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.26

EN300-249093_1_2



CID: EN300-249093_1_2

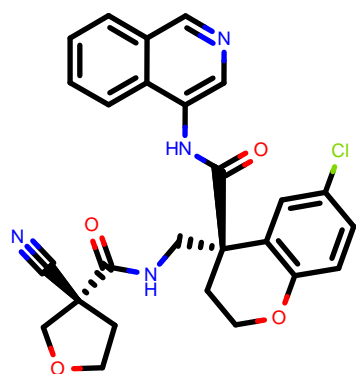
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5C(=O)N

RUN: RUN9702

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.39

EN300-261210_2_2



CID: EN300-261210_2_2

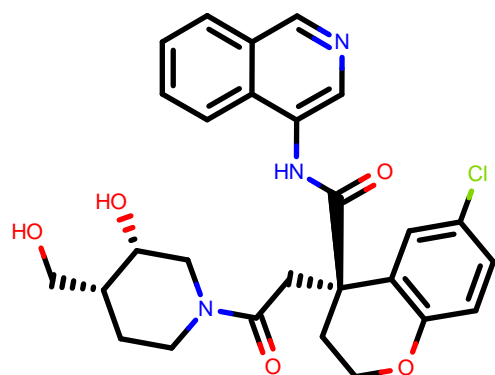
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOCC5)C#N

RUN: RUN5699

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.26

EN300-95639_1_3



CID: EN300-95639_1_3

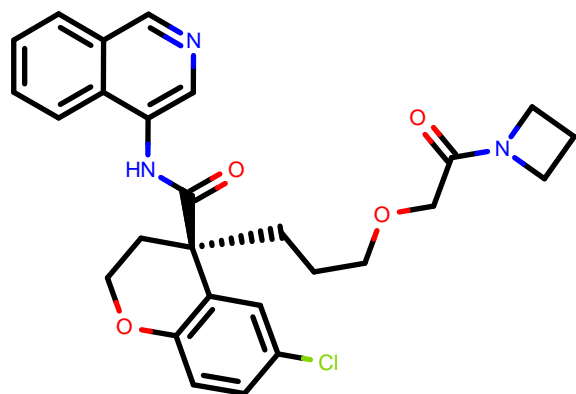
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5OCCO

RUN: RUN3421

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.28

EN300-11195_4_1



CID: EN300-11195_4_1

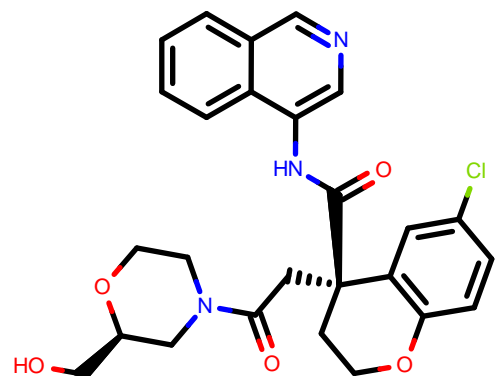
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCO5

RUN: RUN1004

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.20

EN300-175487_1_1



CID: EN300-175487_1_1

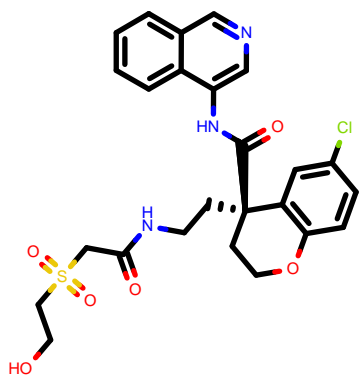
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H]5OCCO

RUN: RUN5197

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.26

EN300-4293814_3_1



CID: EN300-4293814_3_1

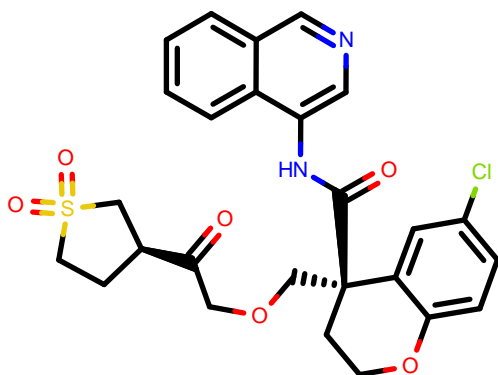
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)CCO

RUN: RUN3557

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.45

EN300-226314_2_2



CID: EN300-226314_2_2

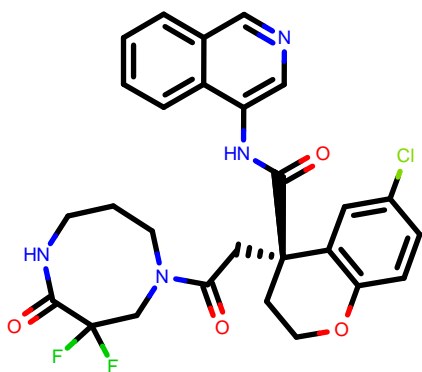
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)[C@H]5CCS(=O)(=O)C5

RUN: RUN324

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.39

EN300-1273202_1_1



CID: EN300-1273202_1_1

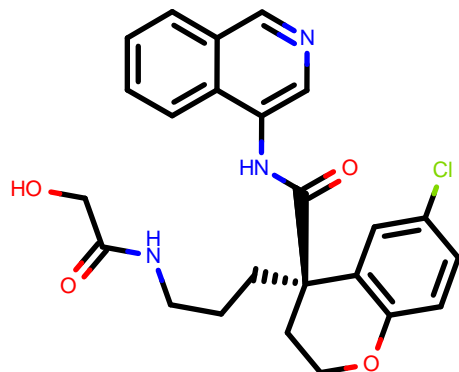
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)C(C5)(F)F

RUN: RUN6527

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.24

EN300-19242_4_1



CID: EN300-19242_4_1

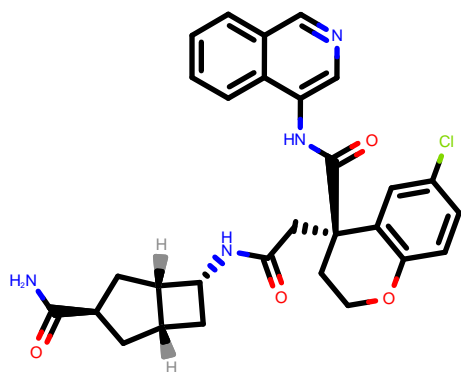
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO

RUN: RUN3376

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.19

EN300-1268016_1_15



CID: EN300-1268016_1_15

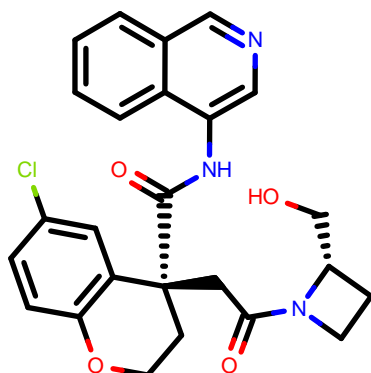
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc4)C(C)C(=O)N[C@@]H5[C@@]H6[C@@]H5[C@@]H(C6)C1=O

RUN: RUN5881

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.30

EN300-154332_1_2



CID: EN300-154332_1_2

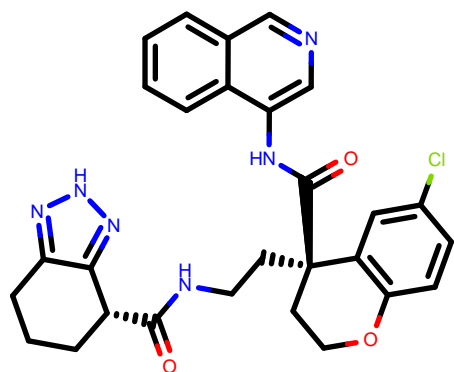
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc4)C(C)CC(=O)N5C[C@@]H5CO

RUN: RUN11617

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.22

EN300-208236_3_1



CID: EN300-208236_3_1

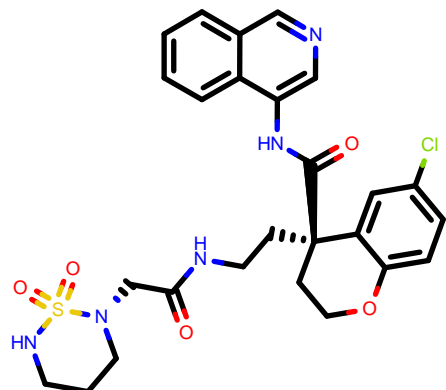
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc4)C(C)CCNC(=O)[C@@]H5C[C@@]6c5n(H)H6

RUN: RUN9240

DDG (kcal/mol): -1.01

dDDG (kcal/mol): 0.24

EN300-4726186_3_2



CID: EN300-4726186_3_2

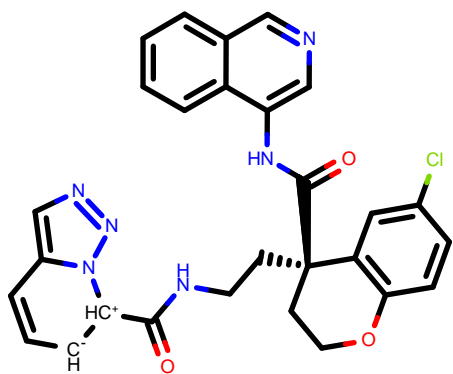
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4cc3cc4)C(C)CCNC(=O)[C@@]H5CCN(S(=O)=O)=O

RUN: RUN4393

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.35

EN300-2010167_3_1



CID: EN300-2010167_3_1

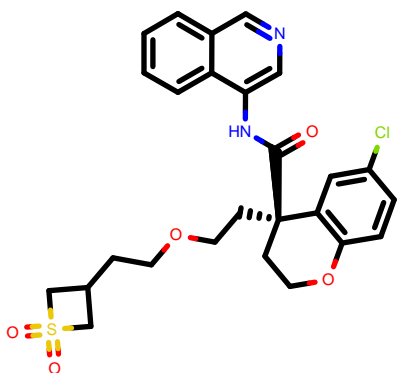
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccccc6n5nnc6

RUN: RUN15092

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.28

EN300-189563_3_1



CID: EN300-189563_3_1

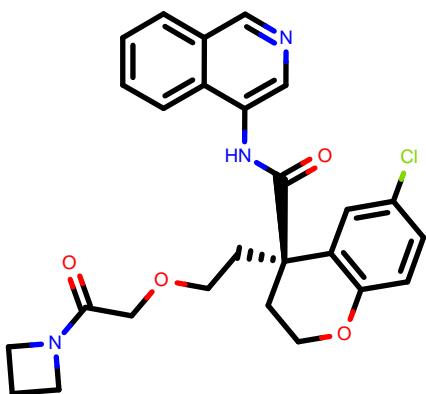
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCSC(=O)(=O)C5

RUN: RUN2230

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.27

EN300-11195_3_1



CID: EN300-11195_3_1

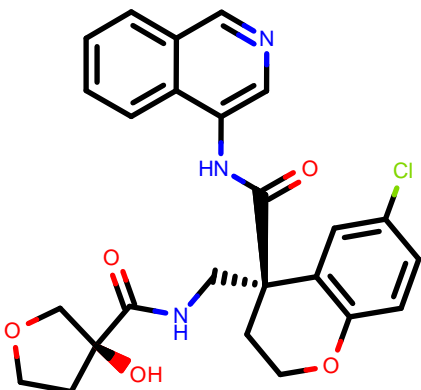
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CC5

RUN: RUN1640

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.20

EN300-148421_2_1



CID: EN300-148421_2_1

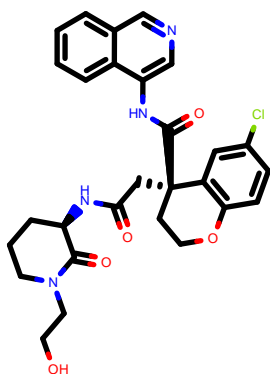
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOCS)O

RUN: RUN4739

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.24

EN300-141480_1_2



CID: EN300-141480_1_2

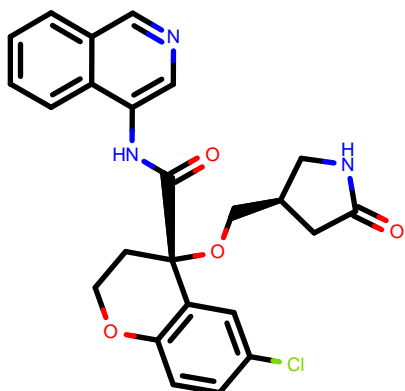
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5CCCC(C5=O)CCO

RUN: RUN8055

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.27

EN300-246747_1_1



CID: EN300-246747_1_1

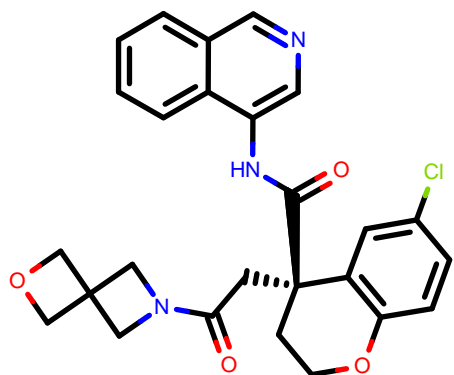
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]H5CC(=O)NCS

RUN: RUN1685

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.25

EN300-81038_1_1



CID: EN300-81038_1_1

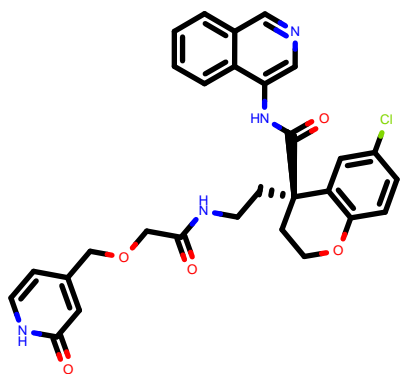
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)COC6

RUN: RUN12954

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.21

EN300-316258_3_1



CID: EN300-316258_3_1

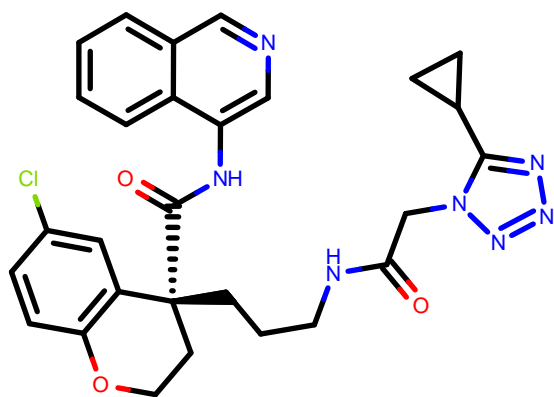
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COCc5cc(nH)c(=O)c5

RUN: RUN11184

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.25

EN300-872798_4_1



CID: EN300-872798_4_1

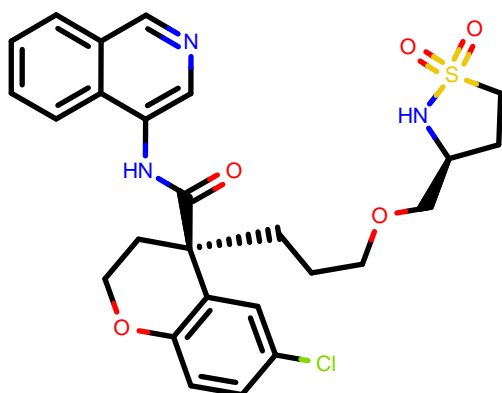
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCCN(C(=O)Cn5c1nn5)C6CC6

RUN: RUN11408

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.29

EN300-1699871_4_2



CID: EN300-1699871_4_2

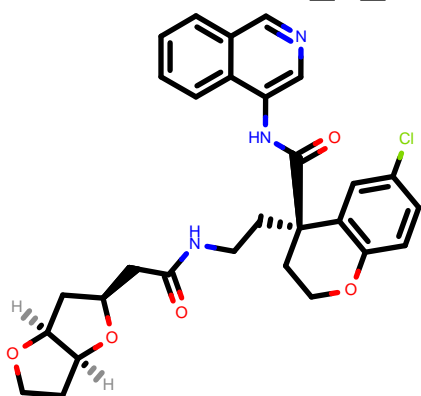
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCOC[C@@]5(C)SCCS(=O)N5

RUN: RUN965

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.26

EN300-7355519_3_4



CID: EN300-7355519_3_4

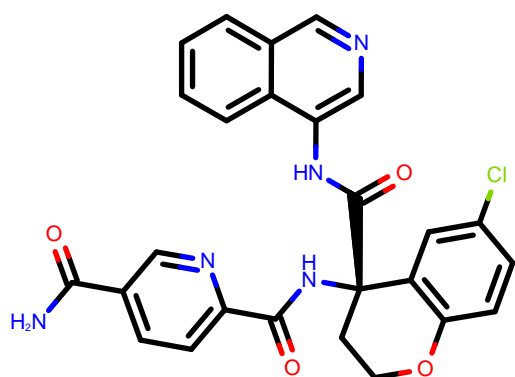
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCN(C(=O)C[C@@H]5OC[C@H]5)C6CC6

RUN: RUN14700

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.28

EN300-58880_1_1



CID: EN300-58880_1_1

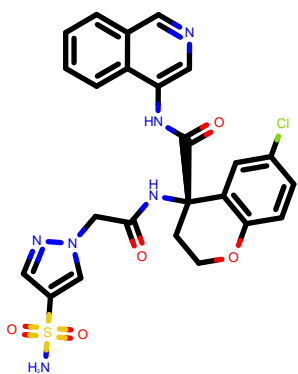
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cn5)C(=O)N

RUN: RUN323

DDG (kcal/mol): -1.00

dDDG (kcal/mol): 0.20

EN300-60514_1_1



CID: EN300-60514_1_1

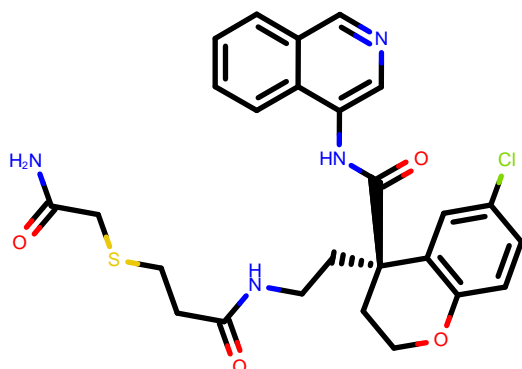
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccn5S(=O)(=O)N

RUN: RUN9748

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.28

EN300-31015_3_1



CID: EN300-31015_3_1

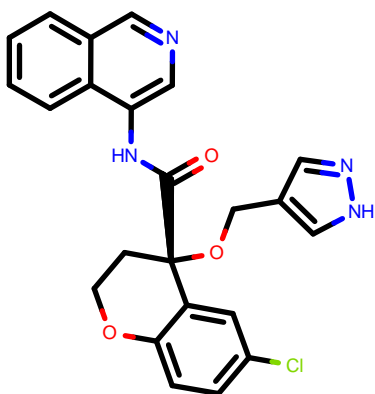
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCSCC(=O)N

RUN: RUN14106

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EDJ-MED-28ec730d-4_1



CID: EDJ-MED-28ec730d-4_1

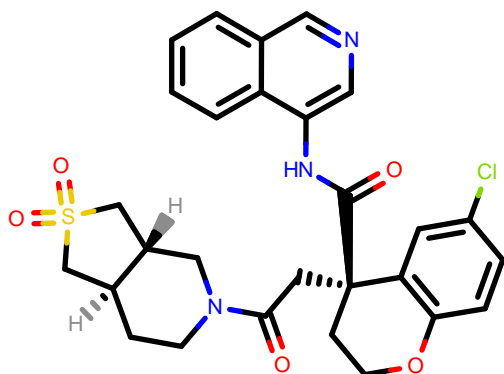
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5

RUN: RUN231

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.17

EN300-365993_1_4



CID: EN300-365993_1_4

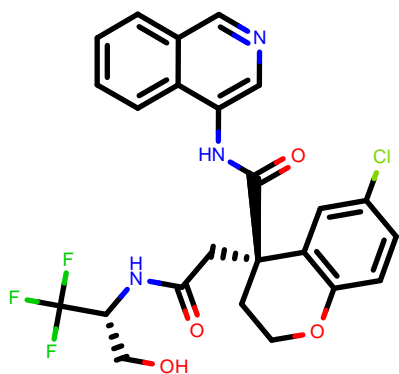
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N6CC[C@H]8CS(=O)(=O)C[C@@]8([H])C5

RUN: RUN15434

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.30

EN300-139403_1_1



CID: EN300-139403_1_1

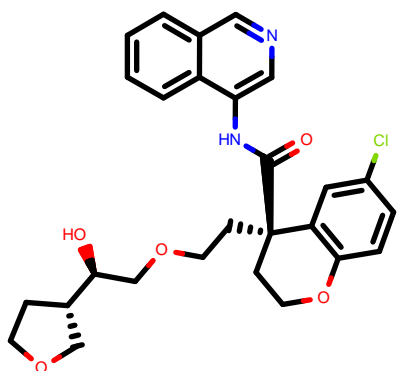
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)C(F)(F)F

RUN: RUN8559

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.37

EN300-1911992_3_4



CID: EN300-1911992_3_4

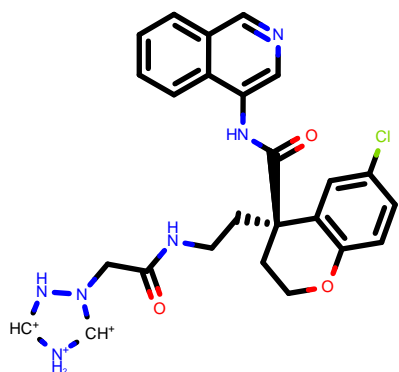
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CO)C5COCCO5

RUN: RUN2094

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.39

EN300-06654_3_1



CID: EN300-06654_3_1

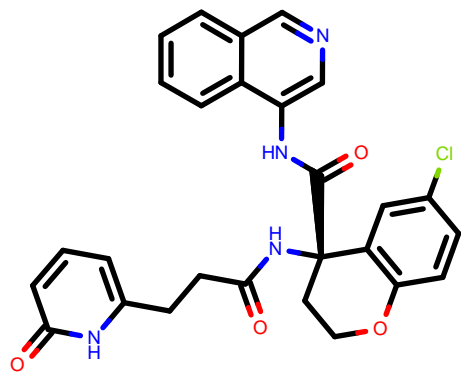
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cn5

RUN: RUN15158

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.22

EN300-6491697_1_1



CID: EN300-6491697_1_1

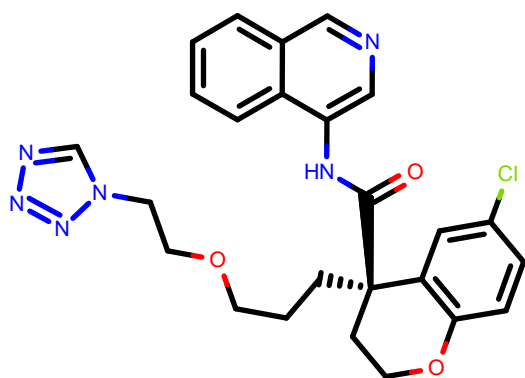
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5ccc(O)=N5

RUN: RUN3978

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.23

EN300-364679_4_1



CID: EN300-364679_4_1

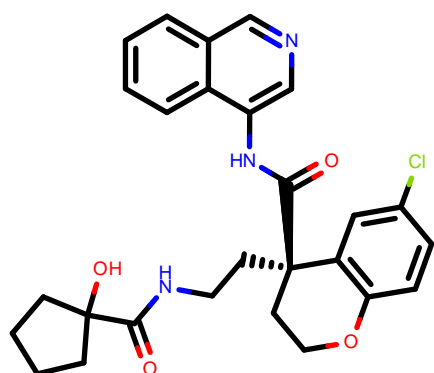
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCCCOCCn5cnnn5

RUN: RUN1499

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.23

EN300-25960_3_1



CID: EN300-25960_3_1

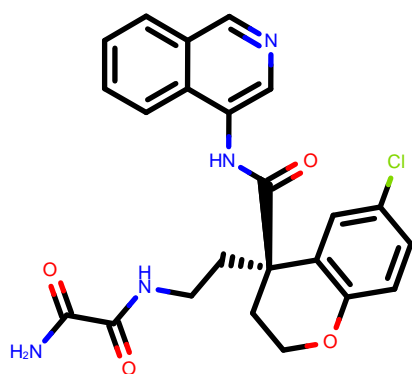
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C5(CCCC5)O

RUN: RUN4361

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.25

EN300-113507_3_1



CID: EN300-113507_3_1

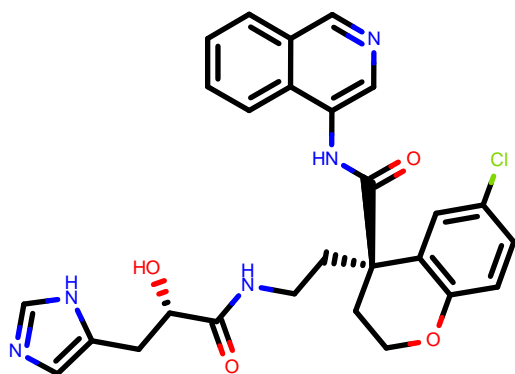
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C(=O)N

RUN: RUN15105

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.19

EN300-6503811_3_1



CID: EN300-6503811_3_1

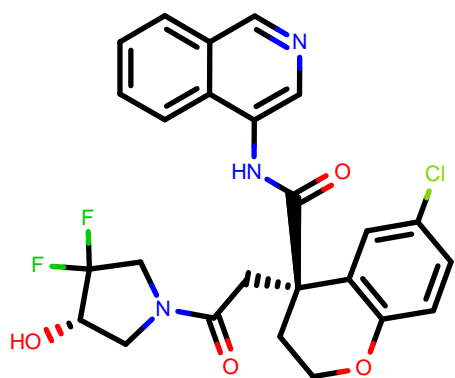
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@H](C5cnc[nH]5)O

RUN: RUN2377

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.29

EN300-1710153_1_1



CID: EN300-1710153_1_1

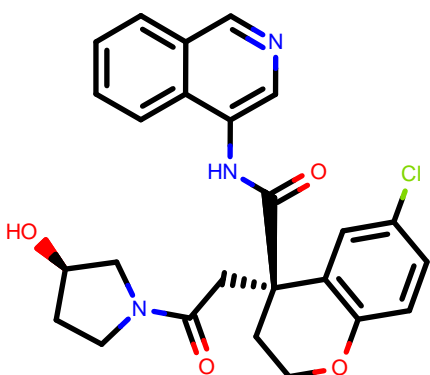
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]@H](C(C5)(F)F)O

RUN: RUN3761

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.20

EN300-69313_1_1



CID: EN300-69313_1_1

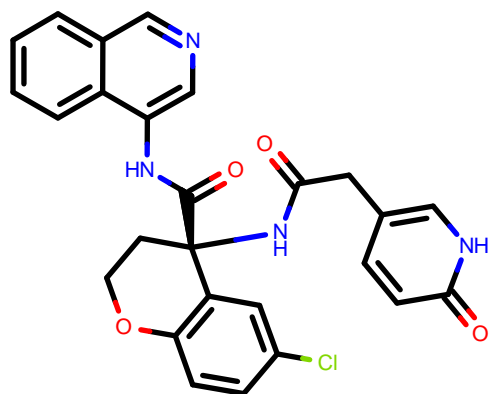
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]@H](C5)O

RUN: RUN1671

DDG (kcal/mol): -0.99

dDDG (kcal/mol): 0.21

EN300-189672_1_1



CID: EN300-189672_1_1

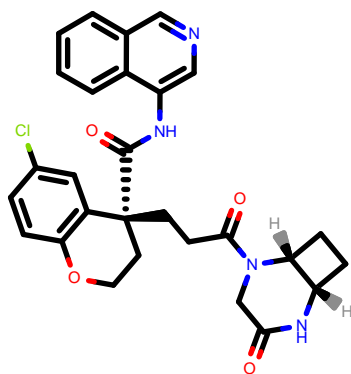
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(=O)[nH]c5

RUN: RUN9643

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-6499164_2_2



CID: EN300-6499164_2_2

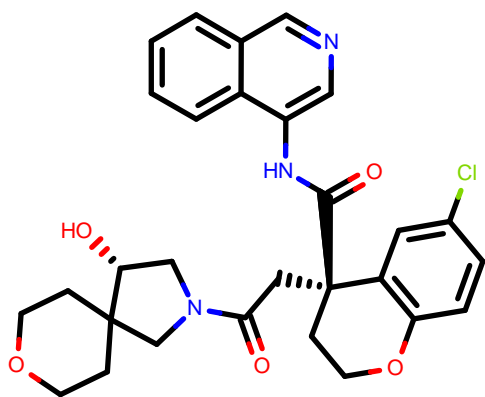
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@]@H](C@H)(C@H)C5=O

RUN: RUN2244

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-7435482_1_2



CID: EN300-7435482_1_2

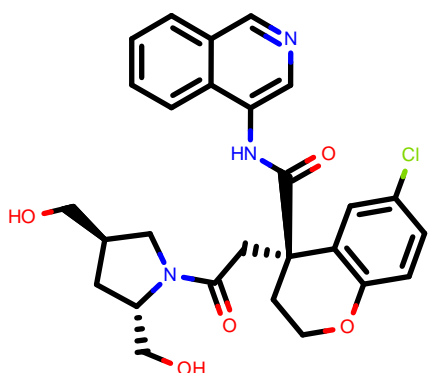
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC4C3cc(cc4)Cl)CC(=O)N5C[C@@H](C6(C5)COCOC6)O

RUN: RUN15333

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.23

EN300-1212400_1_4



CID: EN300-1212400_1_4

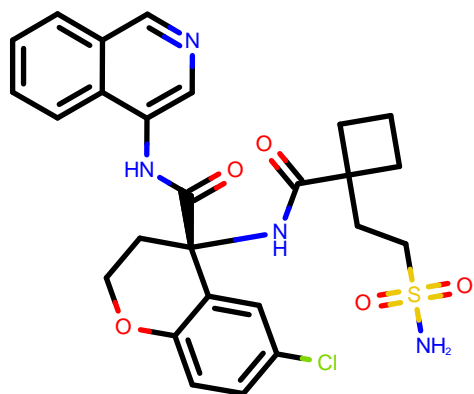
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC4C3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H]5CO)CO

RUN: RUN6851

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.34

EN300-7438227_1_1



CID: EN300-7438227_1_1

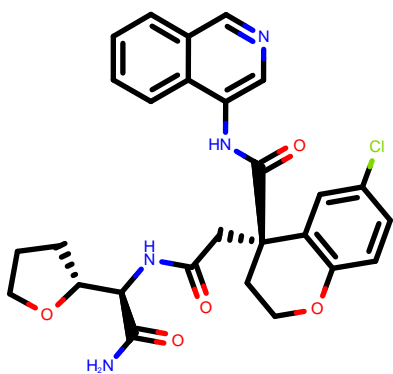
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC4C3cc(cc4)Cl)NC(=O)C5(CCC5)CCS(=O)(=O)N

RUN: RUN9045

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-191187_1_1



CID: EN300-191187_1_1

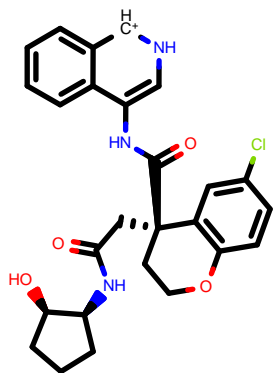
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC4C3cc(cc4)Cl)CC(=O)N[C@@H](C5(COC5)Cl)O

RUN: RUN13748

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.27

EN300-61592_1_1



CID: EN300-61592_1_1

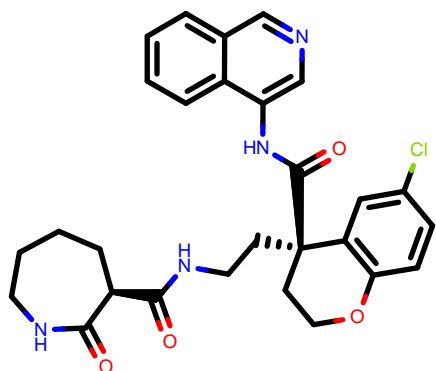
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCC[C@@H]5O

RUN: RUN10605

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.23

EN300-6737762_3_1



CID: EN300-6737762_3_1

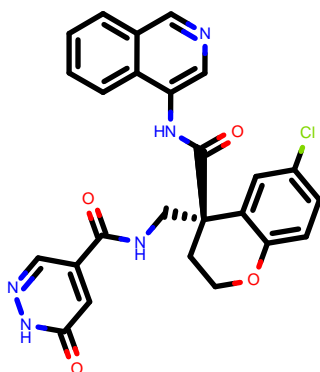
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCCNC5=O

RUN: RUN14958

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.25

EN300-159634_2_1



CID: EN300-159634_2_1

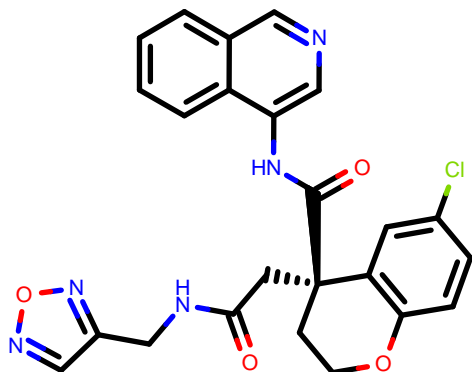
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(=O)[nH]jnc5

RUN: RUN8577

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.24

EN300-1068239_1_1



CID: EN300-1068239_1_1

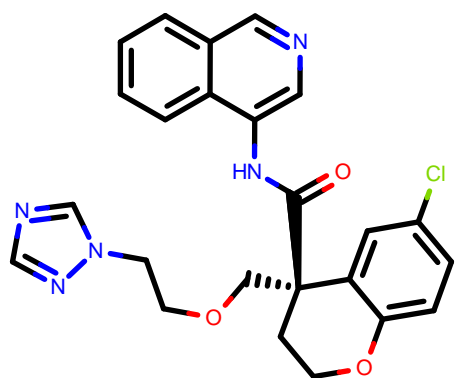
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C=CN5

RUN: RUN4349

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.18

EN300-6255179_2_1



CID: EN300-6255179_2_1

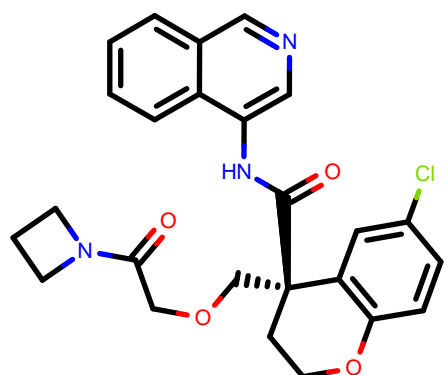
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cncn5

RUN: RUN740

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.20

EN300-11195_2_1



CID: EN300-11195_2_1

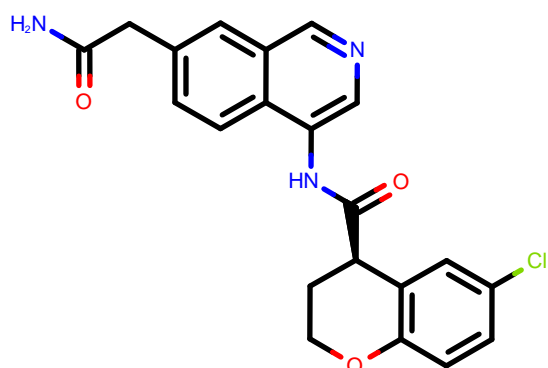
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC5

RUN: RUN1019

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.19

MAK-UNK-8be7dca9-2_1



CID: MAK-UNK-8be7dca9-2_1

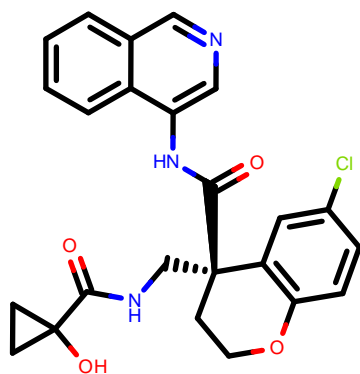
SMILES: c1cc2c(cc1CC(=O)N)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN61

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.11

EN300-25702_2_1



CID: EN300-25702_2_1

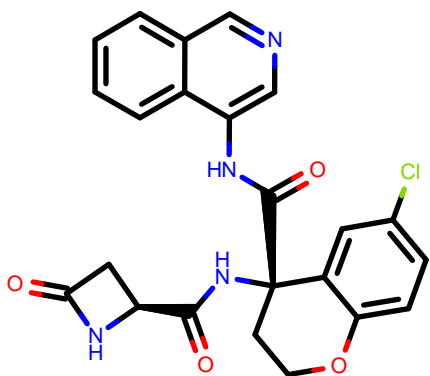
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)O

RUN: RUN3619

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.21

EN300-101505_1_1



CID: EN300-101505_1_1

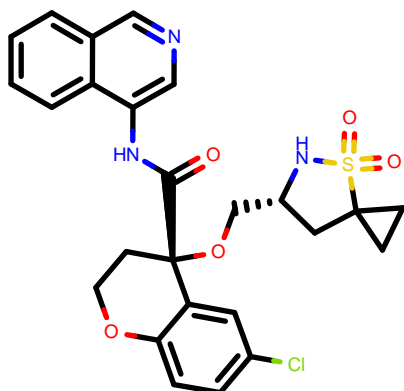
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC(=O)N5

RUN: RUN1161

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.19

EN300-6504697_1_1



CID: EN300-6504697_1_1

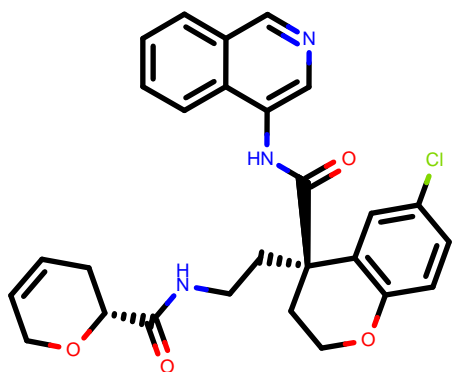
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CC6(CC6)S(=O)(=O)N5

RUN: RUN759

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.32

EN300-378044_3_2



CID: EN300-378044_3_2

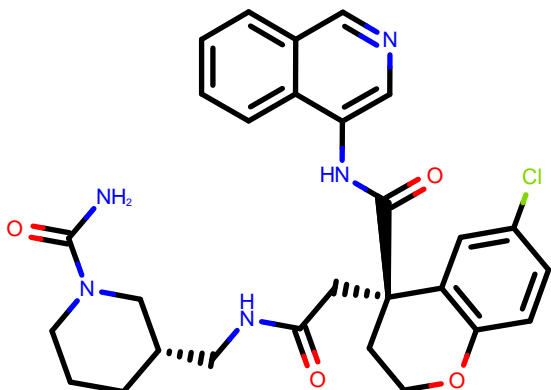
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC=CCO5

RUN: RUN4861

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-212381_1_1



CID: EN300-212381_1_1

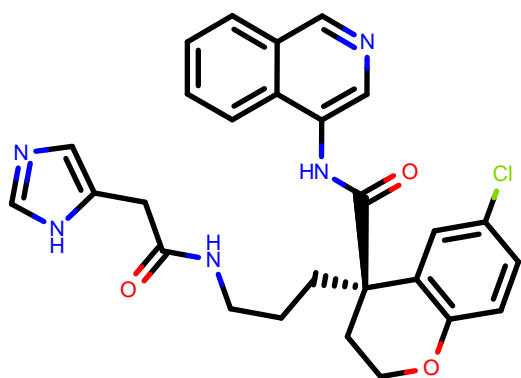
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCCN(C5)C(=O)N

RUN: RUN10575

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.27

EN300-342226_4_1



CID: EN300-342226_4_1

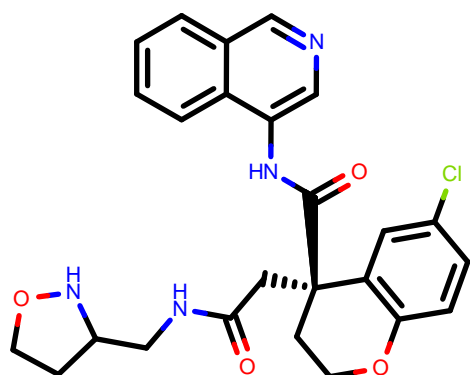
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnc[nH]5

RUN: RUN7846

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.27

EN300-1720418_1_1



CID: EN300-1720418_1_1

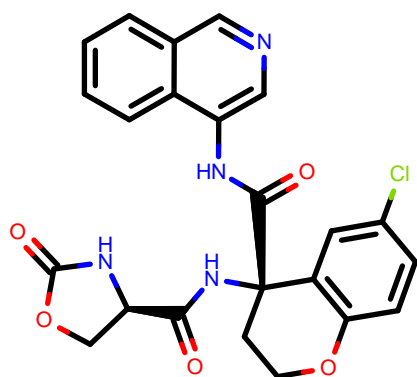
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)CC(=O)NCC5=NOCC5

RUN: RUN10075

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.18

EN300-201346_1_2



CID: EN300-201346_1_2

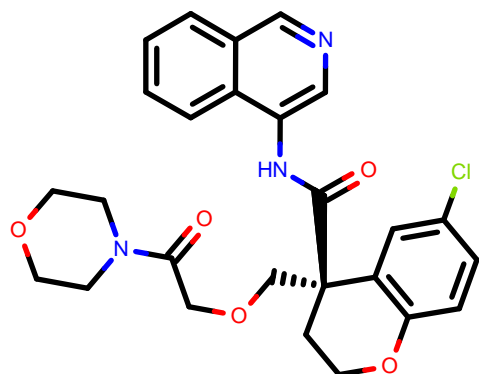
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COC(=O)N5

RUN: RUN7200

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.20

EN300-1241327_2_1



CID: EN300-1241327_2_1

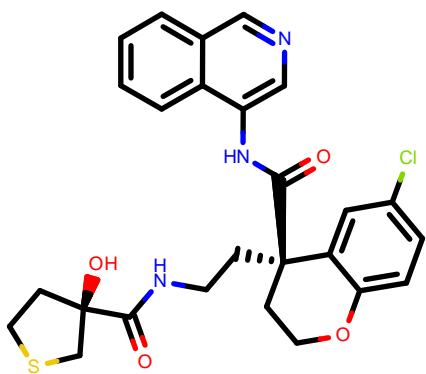
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOc4c3cc(cc4)Cl)COC(=O)N5CCOCC5

RUN: RUN836

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.21

EN300-122656_3_2



CID: EN300-122656_3_2

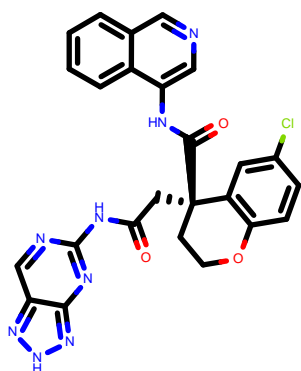
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(C)CCSC5O

RUN: RUN13570

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.39

EN300-821186_1_1



CID: EN300-821186_1_1

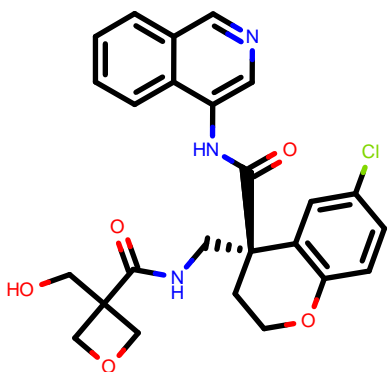
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nc6c(n5)[nH]n6

RUN: RUN15467

DDG (kcal/mol): -0.98

dDDG (kcal/mol): 0.22

EN300-105693_2_1



CID: EN300-105693_2_1

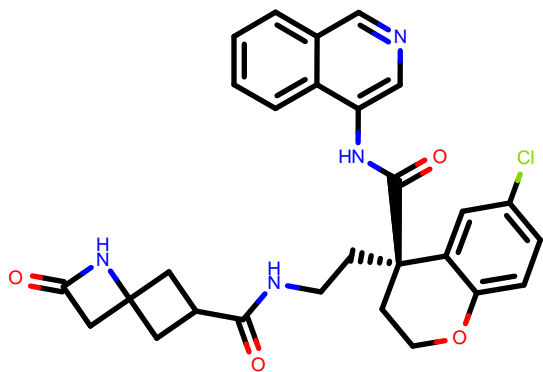
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(C)COC5O

RUN: RUN5959

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.23

EN300-1700760_3_1



CID: EN300-1700760_3_1

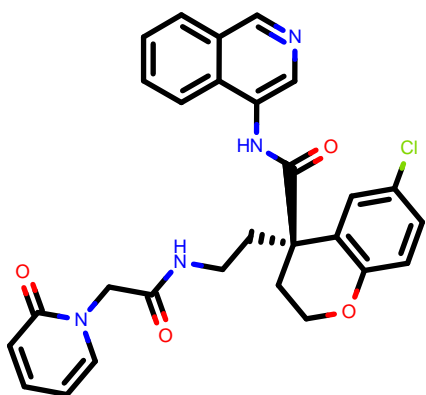
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN15409

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.30

EN300-11714_3_1



CID: EN300-11714_3_1

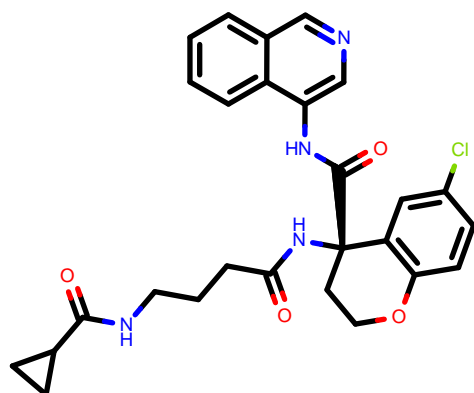
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ccccc5=O

RUN: RUN10049

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.30

EN300-36850_1_1



CID: EN300-36850_1_1

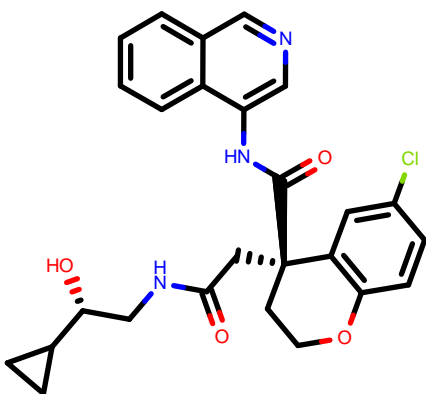
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCNC(=O)C5CC5

RUN: RUN2533

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.27

EN300-67533_1_1



CID: EN300-67533_1_1

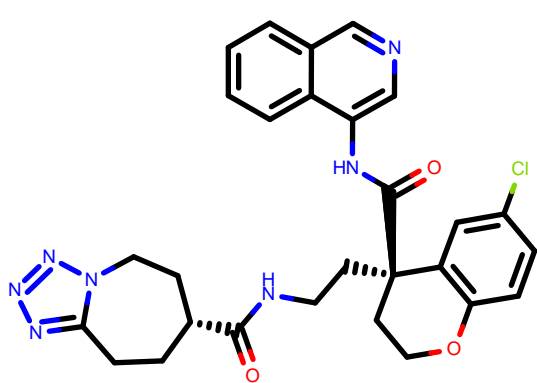
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H](C5CC5)O

RUN: RUN7291

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.24

EN300-253571_3_1



CID: EN300-253571_3_1

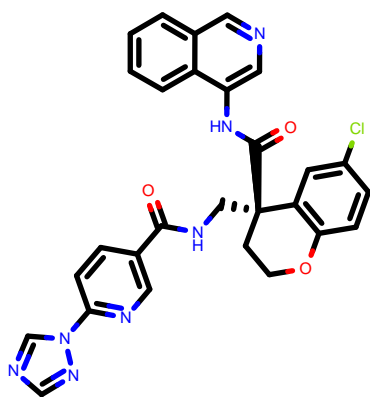
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@]4H5CCc6nncn6C5

RUN: RUN15138

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.24

EN300-27261_2_1



CID: EN300-27261_2_1

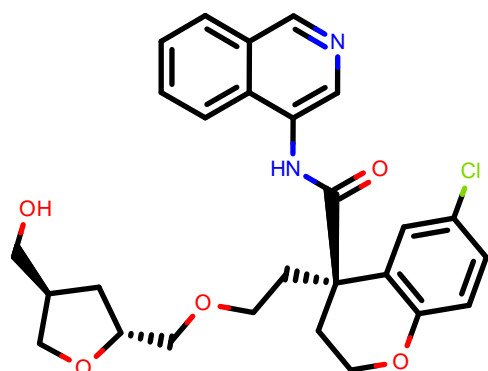
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5ccc(nc5)n6cncn6

RUN: RUN9526

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.32

EN300-6494158_3_1



CID: EN300-6494158_3_1

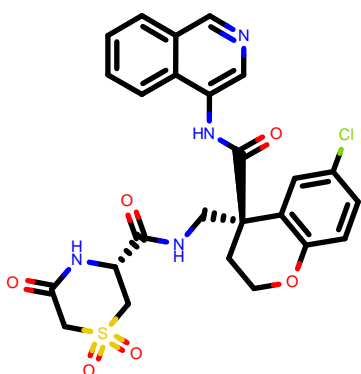
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5C[C@@H](CO)O5

RUN: RUN2300

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.28

EN300-702756_2_1



CID: EN300-702756_2_1

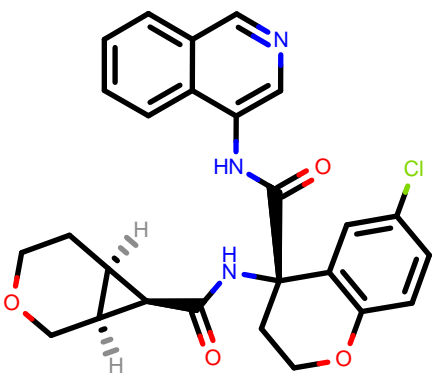
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[S@@]5(=O)O=C1=NO1

RUN: RUN8565

DDG (kcal/mol): -0.97

dDDG (kcal/mol): 0.29

EN300-1644723_1_3



CID: EN300-1644723_1_3

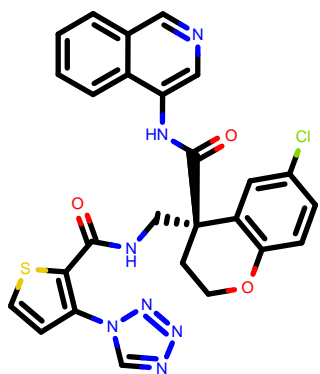
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5[C@@H]6[C@@H](C)OCC6

RUN: RUN9265

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.19

EN300-36731_2_1



CID: EN300-36731_2_1

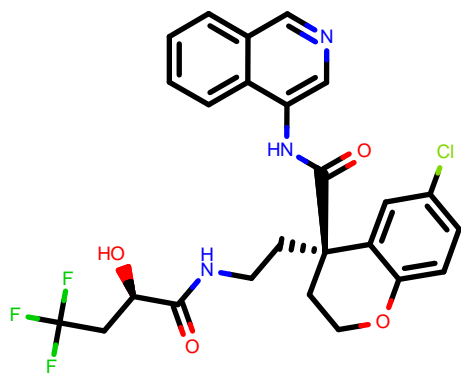
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4c3cc(cc4)Cl)CNC(=O)C5C(CCS5)N6C=CN6

RUN: RUN8325

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.29

EN300-1932013_3_1



CID: EN300-1932013_3_1

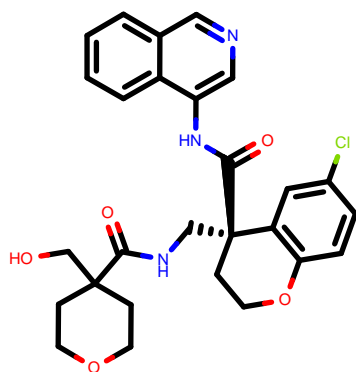
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C(F)(F)F)O

RUN: RUN14138

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.39

EN300-244909_2_1



CID: EN300-244909_2_1

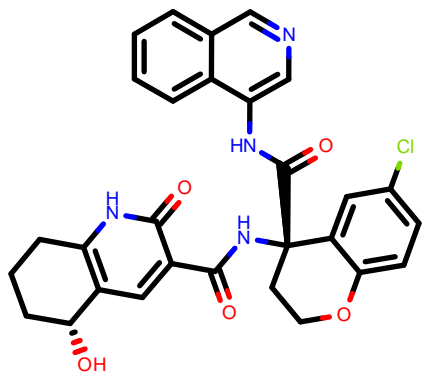
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4c3cc(cc4)Cl)CNC(=O)C5(COCC5)CO

RUN: RUN5851

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.28

EN300-238234_1_2



CID: EN300-238234_1_2

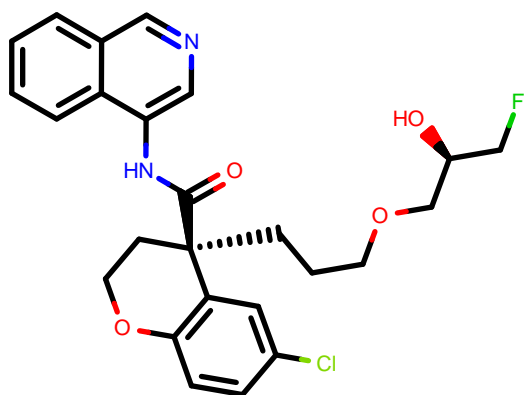
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3[C@@H](COCc4c3cc(cc4)Cl)CNC(=O)C5C(COCC5)N6C=CN6

RUN: RUN6988

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.31

EN300-1968342_4_2



CID: EN300-1968342_4_2

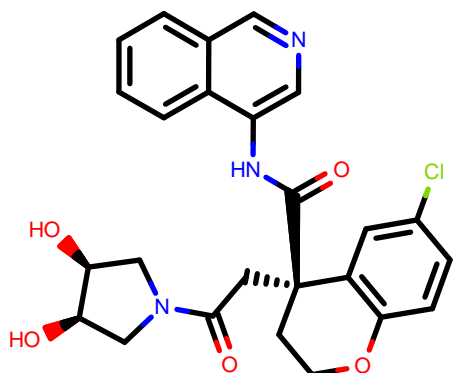
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCOC[C@H](CF)O

RUN: RUN421

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.24

EN300-96037_1_1



CID: EN300-96037_1_1

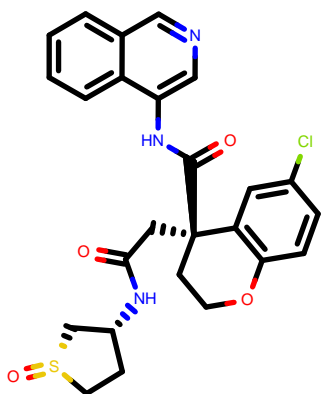
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C[C@H](C5)O)O

RUN: RUN11631

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.23

EN300-93574_1_1



CID: EN300-93574_1_1

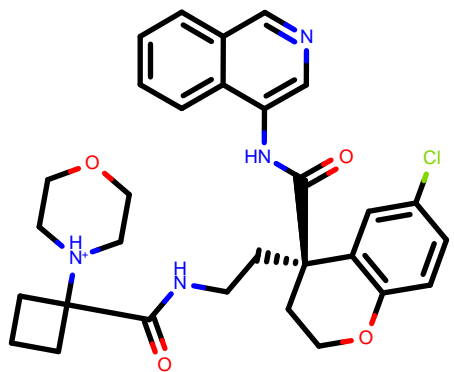
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[S@H](=O)C5

RUN: RUN6747

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.25

EN300-124365_3_1



CID: EN300-124365_3_1

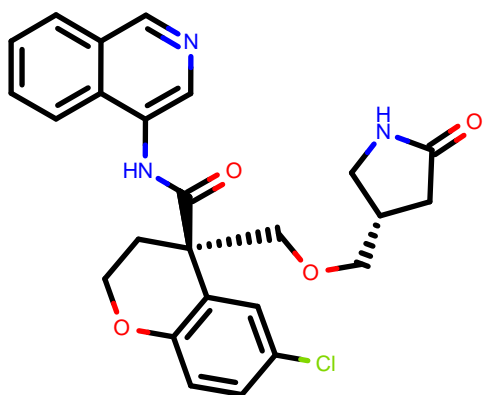
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)[NH+]6COC6

RUN: RUN14200

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.38

EN300-246747_2_2



CID: EN300-246747_2_2

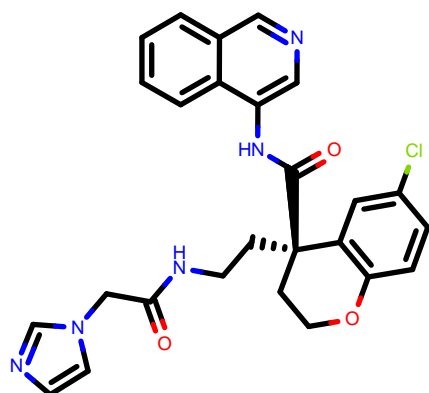
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CC(=O)NCS

RUN: RUN1666

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.21

EN300-38979_3_1



CID: EN300-38979_3_1

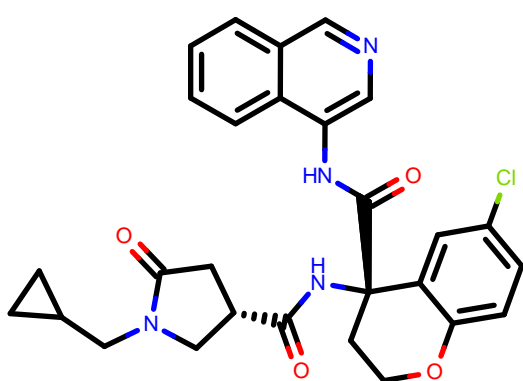
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccnc5

RUN: RUN15214

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.22

EN300-31969_1_2



CID: EN300-31969_1_2

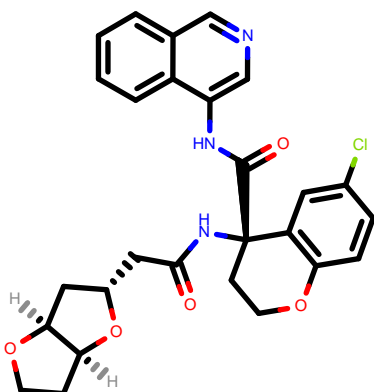
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N(C5)OC6CC6

RUN: RUN8576

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.26

EN300-7355519_1_3



CID: EN300-7355519_1_3

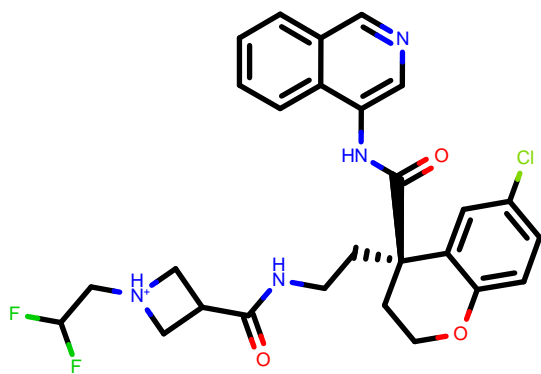
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5C[C@@H]6[C@@H](O5)CCO6

RUN: RUN9389

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.24

EN300-182579_3_1



CID: EN300-182579_3_1

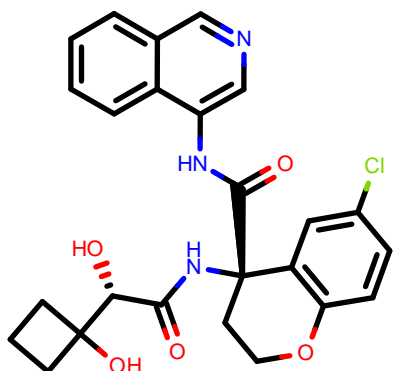
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCNC(=O)C5CN(C5)CC(F)F

RUN: RUN10952

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.27

EN300-1073320_1_2



CID: EN300-1073320_1_2

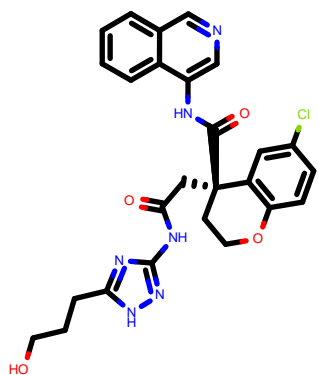
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5(CCC5)O)O

RUN: RUN491

DDG (kcal/mol): -0.96

dDDG (kcal/mol): 0.29

EN300-02623_1_1



CID: EN300-02623_1_1

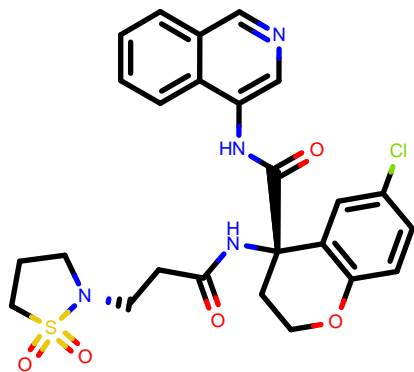
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)Nc5nc([nH]n5)CCCO

RUN: RUN13910

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.24

EN300-44873_1_2



CID: EN300-44873_1_2

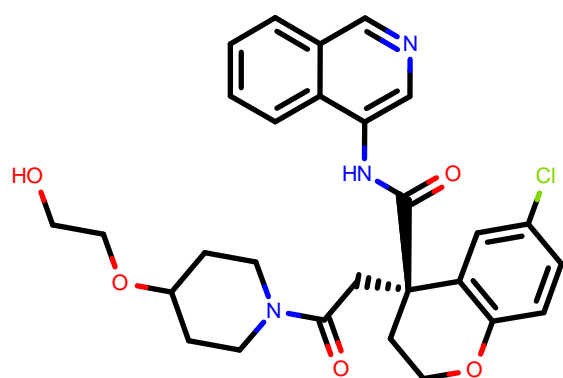
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)CN@5SCCS5(=O)=O

RUN: RUN4198

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.36

EN300-104088_1_1



CID: EN300-104088_1_1

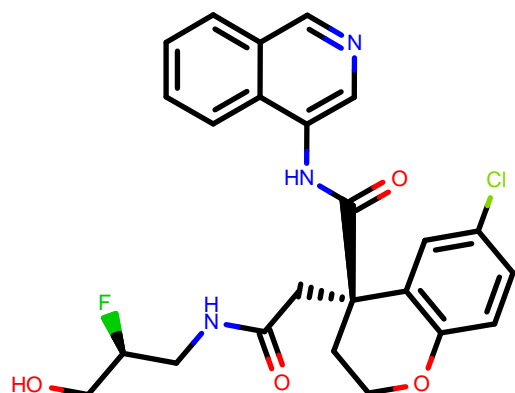
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C)(C5)OCCO

RUN: RUN3049

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.26

EN300-7353971_1_1



CID: EN300-7353971_1_1

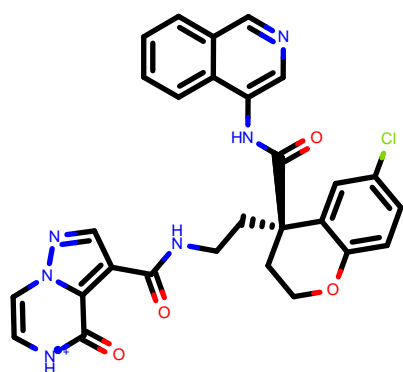
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H](CO)F

RUN: RUN10399

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-7463176_3_1



CID: EN300-7463176_3_1

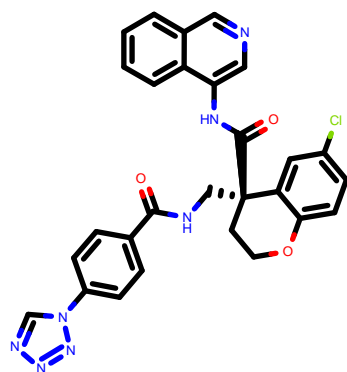
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5nnn6c5c(=O)[nH]c6

RUN: RUN11419

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.24

EN300-06030_2_1



CID: EN300-06030_2_1

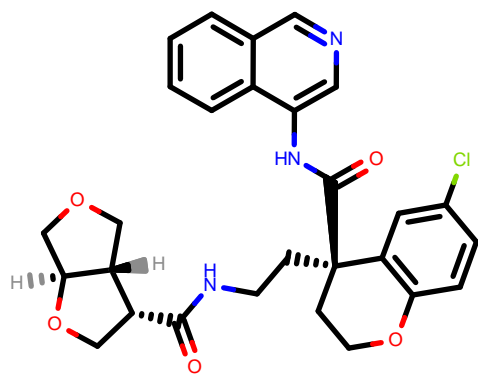
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5ccoc(cc5)n6cnn6

RUN: RUN9518

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.22

EN300-6482296_3_3



CID: EN300-6482296_3_3

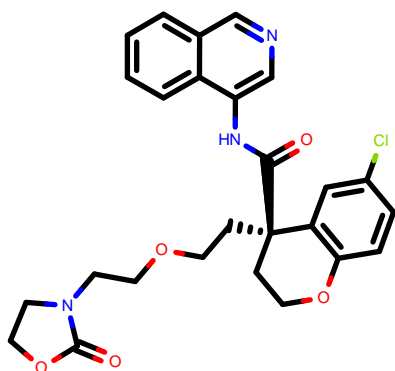
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCO4c3ccc(O)CCNC(=O)[C@@H]5C[C@@H]6[C@@H]5COC6

RUN: RUN15239

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-370967_3_1



CID: EN300-370967_3_1

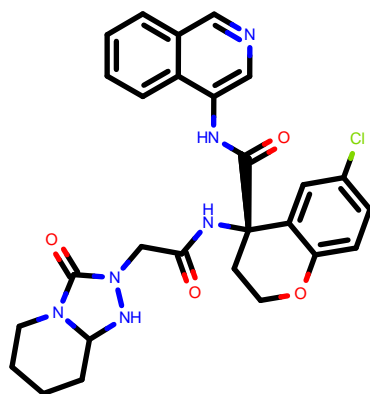
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCO4c3ccc(O)C1CCOCCN5COC5=O

RUN: RUN2142

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.27

EN300-263346_1_1



CID: EN300-263346_1_1

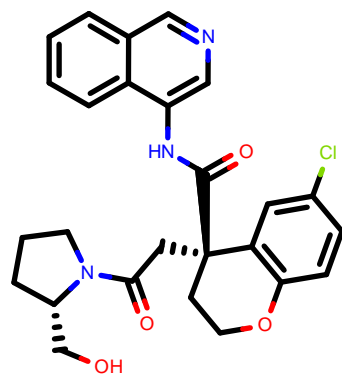
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCO4c3ccc(O)C1NC(=O)Cn5c(O)n6c(n5)COC6

RUN: RUN6281

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

EN300-70033_1_1



CID: EN300-70033_1_1

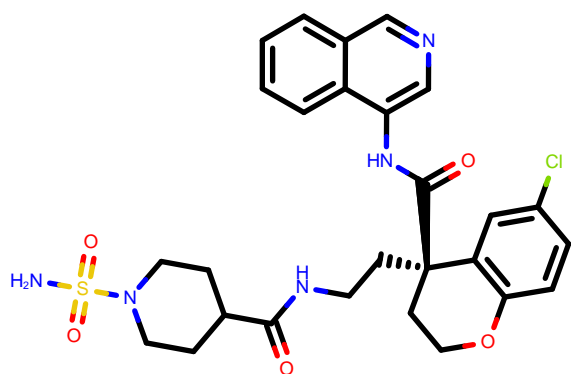
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCO4c3ccc(O)C1CC(=O)N5CC[C@H]5CO

RUN: RUN6069

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.28

EN300-31102_3_1



CID: EN300-31102_3_1

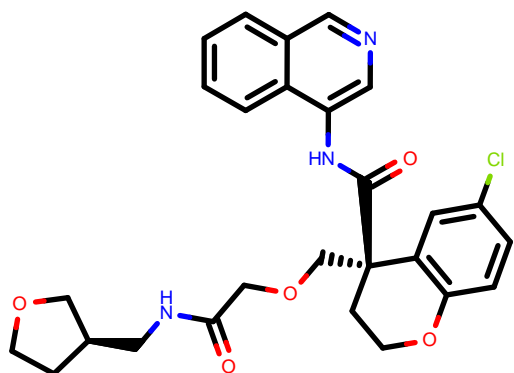
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CCN(CC5)S(=O)(=O)N

RUN: RUN1926

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.40

EN300-46832_2_2



CID: EN300-46832_2_2

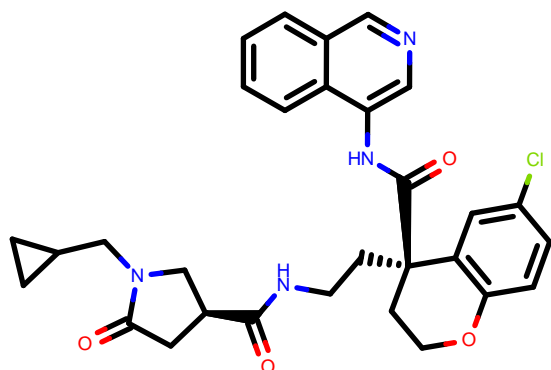
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC[C@@H]5CCOC5

RUN: RUN1122

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.25

EN300-31969_3_2



CID: EN300-31969_3_2

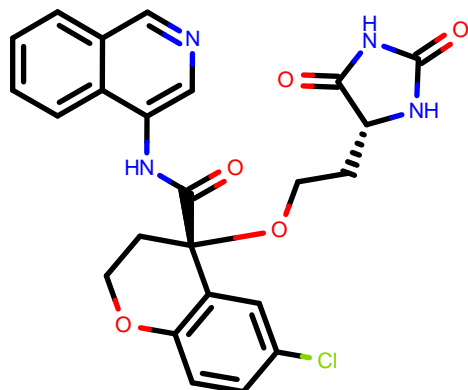
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CCN(C5)C6CC6

RUN: RUN12798

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.32

EN300-6498856_1_2



CID: EN300-6498856_1_2

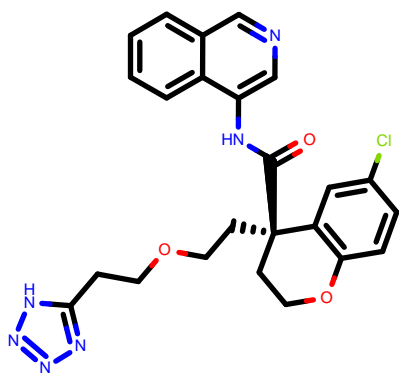
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[C@@H]5C(=O)NC(=O)N5

RUN: RUN623

DDG (kcal/mol): -0.95

dDDG (kcal/mol): 0.23

EN300-183231_3_1



CID: EN300-183231_3_1

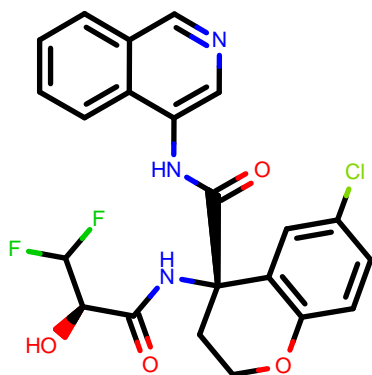
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5n[n-]nn5

RUN: RUN2078

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-1932780_1_2



CID: EN300-1932780_1_2

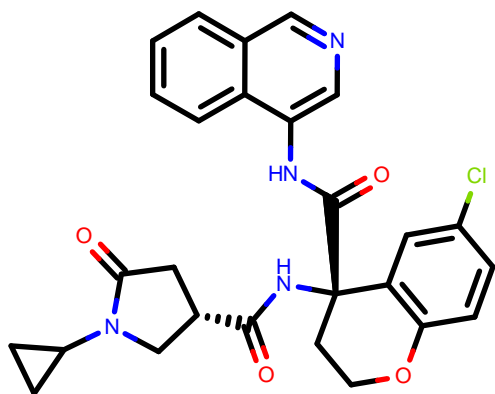
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C(F)F)O

RUN: RUN4722

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-12440_1_2



CID: EN300-12440_1_2

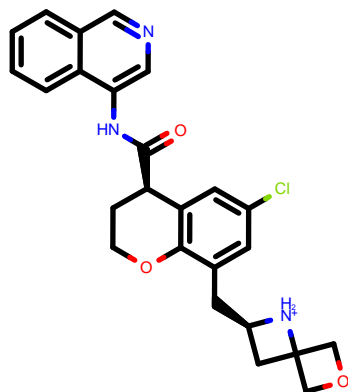
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N(C5)C6CC6

RUN: RUN9261

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.24

DAR-DIA-23e5a6a0-8_2



CID: DAR-DIA-23e5a6a0-8_2

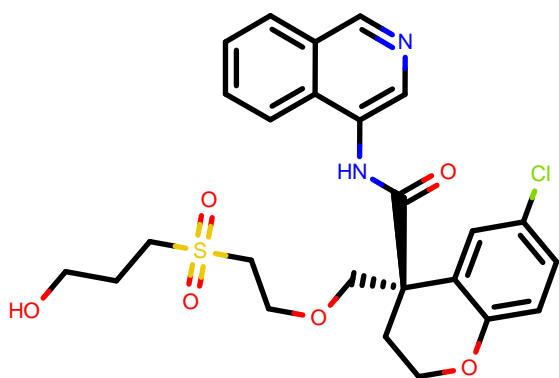
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[C@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN179

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.25

EN300-7456499_2_1



CID: EN300-7456499_2_1

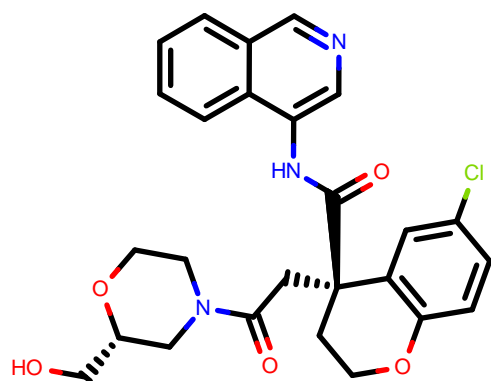
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)O)CCO

RUN: RUN1514

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.35

EN300-175485_1_1



CID: EN300-175485_1_1

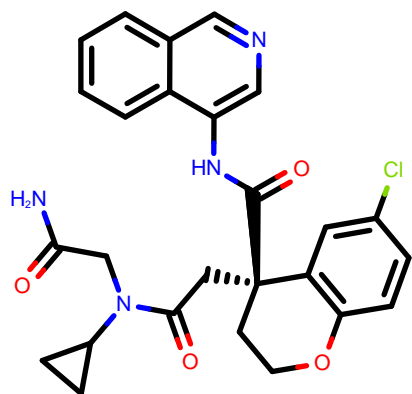
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CO

RUN: RUN9795

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.22

EN300-112500_1_1



CID: EN300-112500_1_1

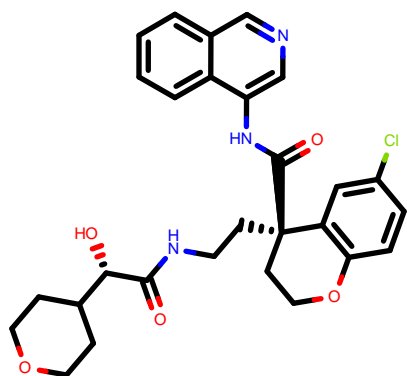
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)C5CC5

RUN: RUN5621

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.28

EN300-79180_3_2



CID: EN300-79180_3_2

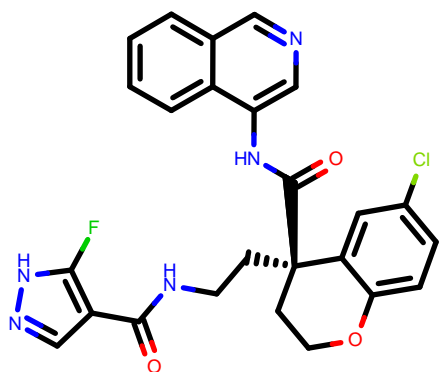
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5COCOC5)O

RUN: RUN4673

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.31

EN300-7121836_3_1



CID: EN300-7121836_3_1

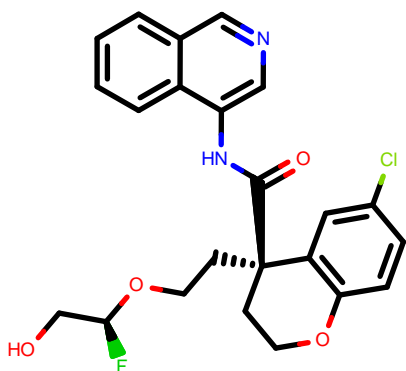
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cn[nH]c5F

RUN: RUN4733

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.19

EN300-861925_3_1



CID: EN300-861925_3_1

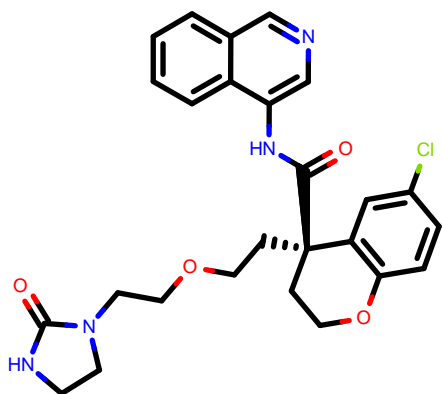
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCO[C@H](CO)F

RUN: RUN1112

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.24

EN300-214800_3_1



CID: EN300-214800_3_1

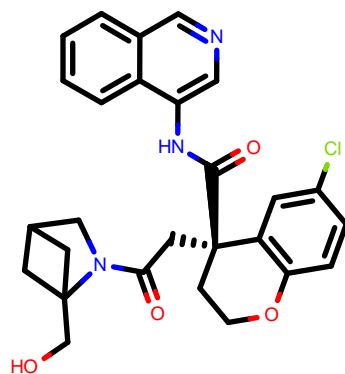
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCCN5CCNC5=O

RUN: RUN2102

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.30

EN300-298031_1_1



CID: EN300-298031_1_1

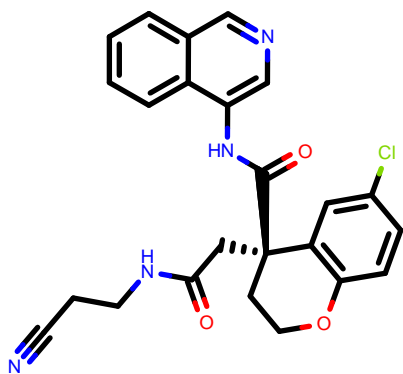
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6CC5(C6)CO

RUN: RUN1783

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.22

EN300-183001_1_1



CID: EN300-183001_1_1

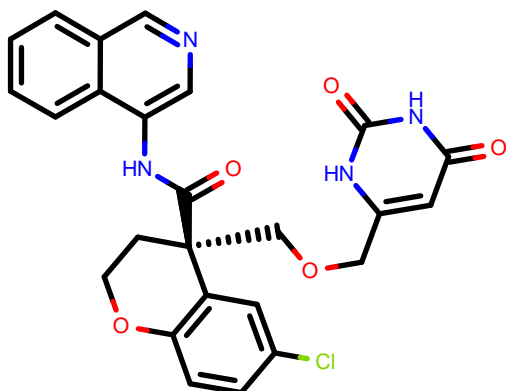
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCC#N

RUN: RUN11731

DDG (kcal/mol): -0.94

dDDG (kcal/mol): 0.20

EN300-11300_2_1



CID: EN300-11300_2_1

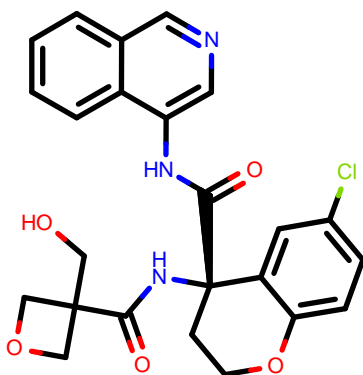
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN252

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.22

EN300-105693_1_1



CID: EN300-105693_1_1

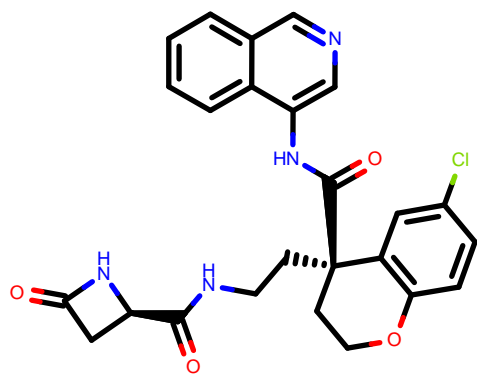
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COC5)CO

RUN: RUN3078

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.19

EN300-101505_3_2



CID: EN300-101505_3_2

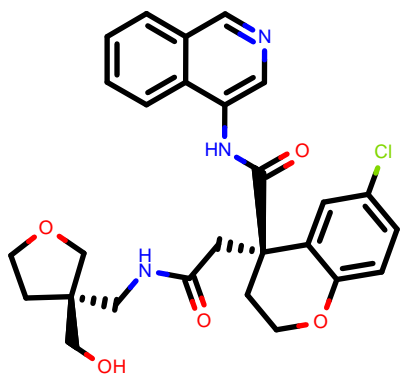
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)N5

RUN: RUN15156

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.22

EN300-682529_1_1



CID: EN300-682529_1_1

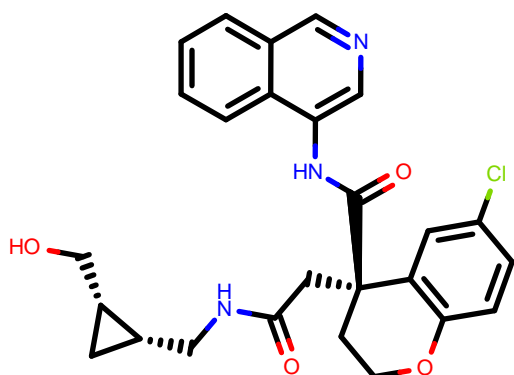
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCOc5)CO

RUN: RUN2349

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-1277662_1_1



CID: EN300-1277662_1_1

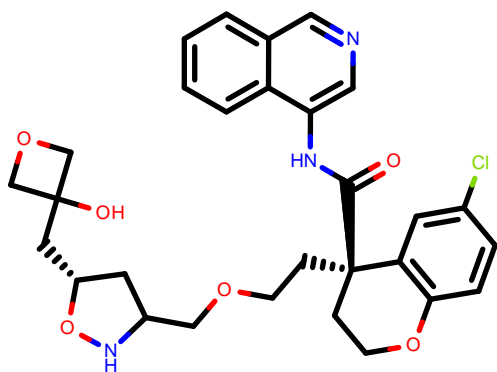
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5H5C[C@@]5H5CO

RUN: RUN9536

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.20

EN300-7457160_3_1



CID: EN300-7457160_3_1

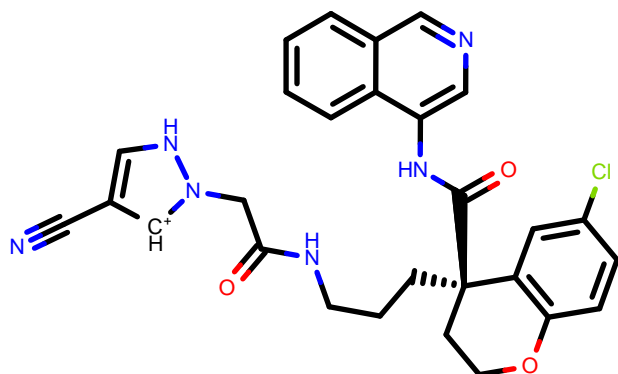
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5=NC[C@@]6(C)COC6CO

RUN: RUN842

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.35

EN300-1590388_4_1



CID: EN300-1590388_4_1

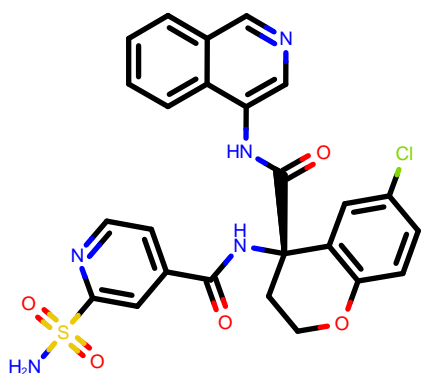
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(en5)C#N

RUN: RUN8659

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.28

EN300-141628_1_1



CID: EN300-141628_1_1

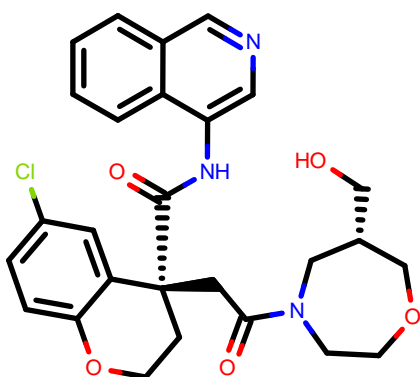
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)S(=O)(=O)N

RUN: RUN6261

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.31

EN300-6478054_1_1



CID: EN300-6478054_1_1

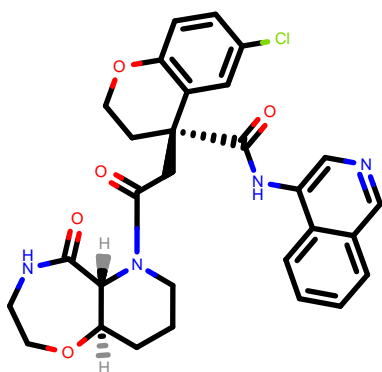
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)CO

RUN: RUN9496

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.32

EN300-364612_1_3



CID: EN300-364612_1_3

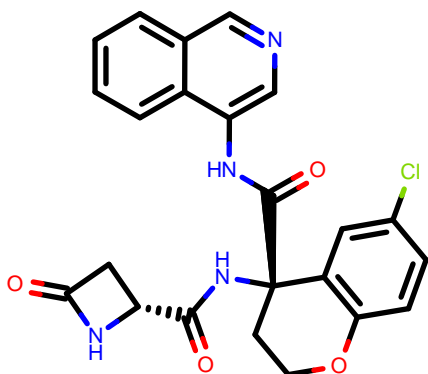
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]6[C@@H]5C(=O)NCCO6

RUN: RUN9088

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.23

EN300-101505_1_2



CID: EN300-101505_1_2

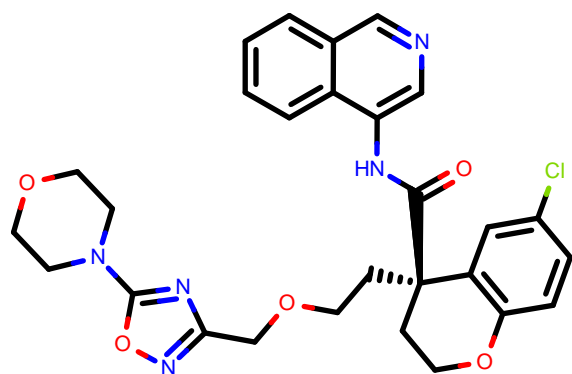
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5

RUN: RUN3574

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.21

EN300-1608590_3_1



CID: EN300-1608590_3_1

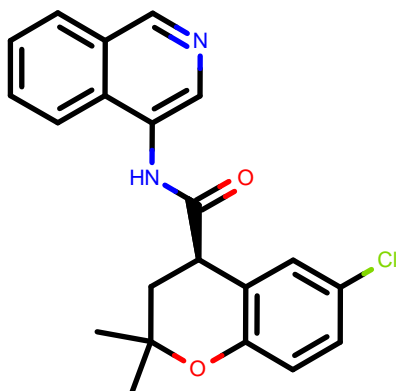
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC5nc(on5)N6COCOC6

RUN: RUN858

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.30

ADA-UCB-dc2b944c-16_1



CID: ADA-UCB-dc2b944c-16_1

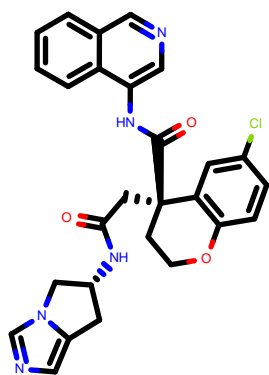
SMILES: CC1(C)[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3cccc4)C

RUN: RUN41

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.08

EN300-244100_1_1



CID: EN300-244100_1_1

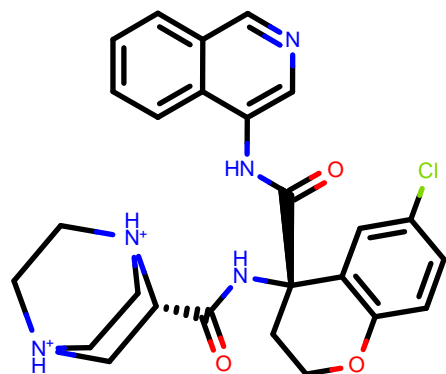
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5CNC6ncn6C5

RUN: RUN8275

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.22

EN300-1605566_1_1



CID: EN300-1605566_1_1

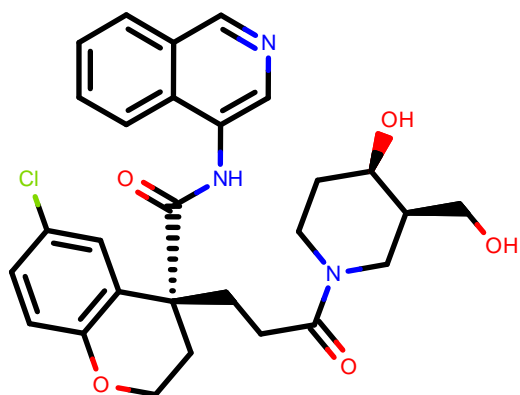
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5CN6CC[NH+]5CC6

RUN: RUN8076

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.26

EN300-233678_2_2



CID: EN300-233678_2_2

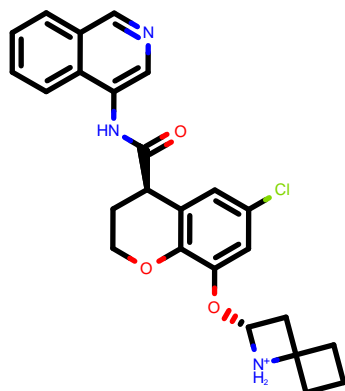
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4cc3cc4C)CC(=O)N5CCC@HC5CO

RUN: RUN3768

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.38

DAR-DIA-23e5a6a0-2_1



CID: DAR-DIA-23e5a6a0-2_1

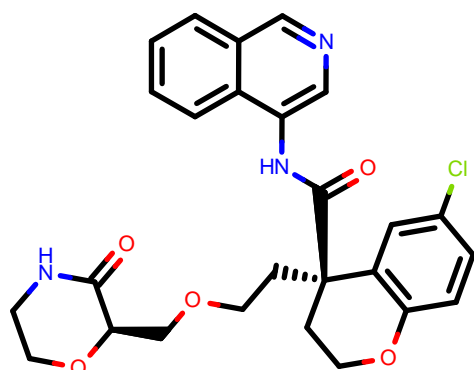
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@@]5C6C([NH2+][5])CC6)Cl

RUN: RUN4

DDG (kcal/mol): -0.93

dDDG (kcal/mol): 0.33

EN300-1706036_3_2



CID: EN300-1706036_3_2

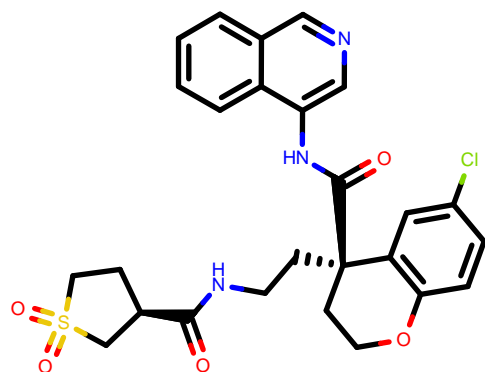
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCOC[C@@]5C6C([NH2+][5])NCC6)O

RUN: RUN2222

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.26

EN300-14437_3_1



CID: EN300-14437_3_1

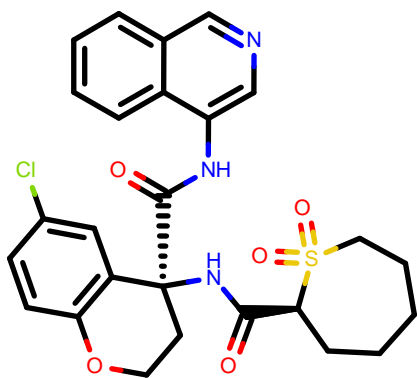
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCNC(=O)[C@@]5C6C([NH2+][5])SCS6(=O)=O)C5

RUN: RUN14978

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.30

EN300-6499531_1_1



CID: EN300-6499531_1_1

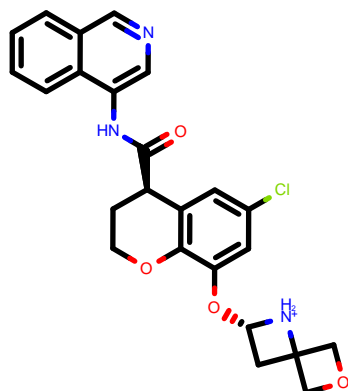
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)NC(=O)[C@@]H5CCCCSS(=O)=O

RUN: RUN3022

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.29

DAR-DIA-23e5a6a0-3_2



CID: DAR-DIA-23e5a6a0-3_2

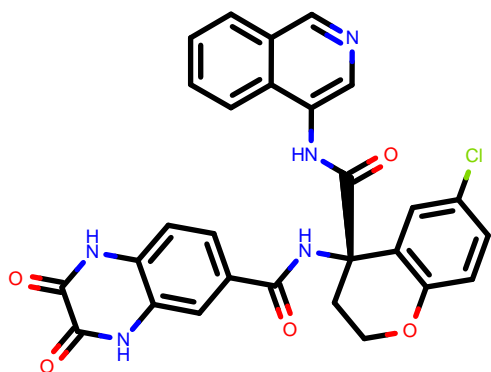
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]H3CCOc4c3cc(cc4O)[C@@]H5CC6([NH2+][5]O)O6Cl

RUN: RUN59

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.29

EN300-07268_1_1



CID: EN300-07268_1_1

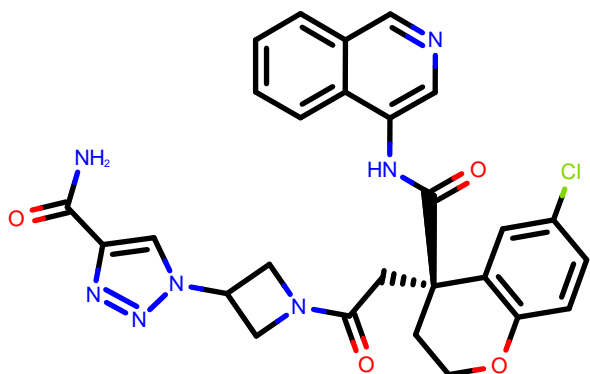
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)NC(=O)c5ccc6c(c5)[nH+]c7c(O)nc7[nH]6

RUN: RUN9913

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.27

EN300-136080_1_1



CID: EN300-136080_1_1

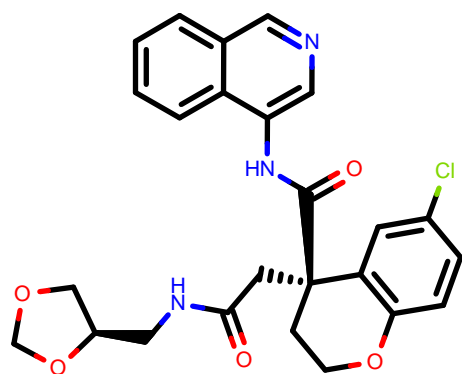
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4Cl)CC(=O)N5CC(C5)n6cc(nn6)C(=O)N

RUN: RUN14910

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.22

EN300-253187_1_2



CID: EN300-253187_1_2

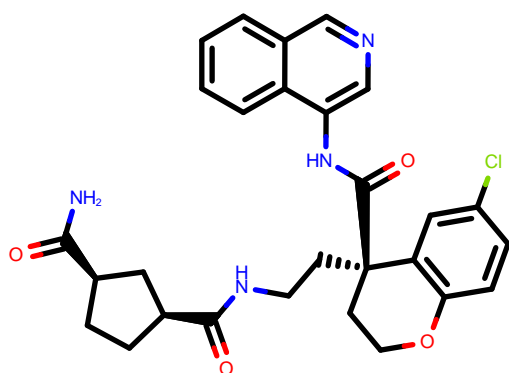
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5COCOC5

RUN: RUN7607

DDG (kcal/mol): -0.92

dDDG (kcal/mol): 0.23

EN300-370753_3_1



CID: EN300-370753_3_1

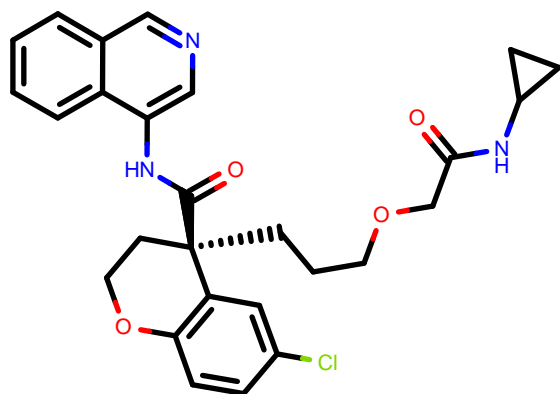
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@H](C5)Cl=ON

RUN: RUN4189

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.25

EN300-1253178_4_1



CID: EN300-1253178_4_1

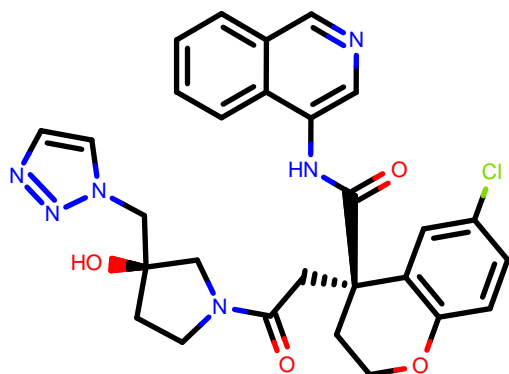
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC5C5

RUN: RUN1051

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-269627_1_1



CID: EN300-269627_1_1

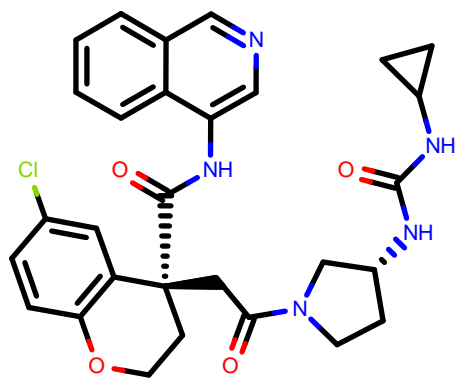
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSCC[C@@]5(C)Cn6cnrn6O

RUN: RUN2261

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.29

EN300-135393_1_2



CID: EN300-135393_1_2

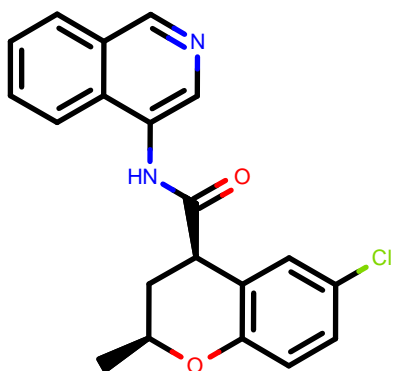
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](C)C(=O)C1=CC=C(C=C1)C(=O)N5CC[C@H](C5)NC(=O)NC6CC6

RUN: RUN329

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.28

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

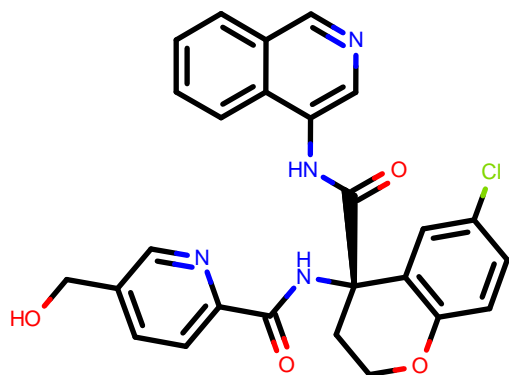
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN81

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.08

EN300-1270299_1_1



CID: EN300-1270299_1_1

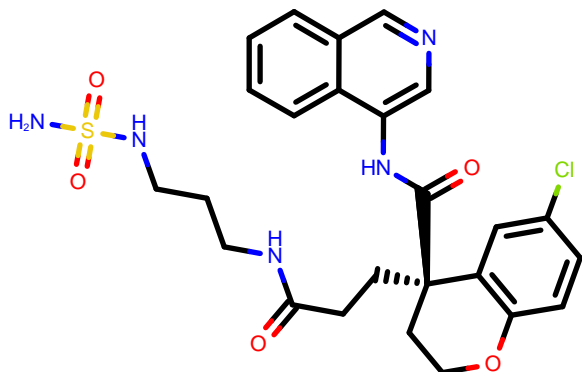
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](C)C(=O)C1=CC=C(C=C1)C(=O)N5CC[C@H](C5)NC(=O)N6CO

RUN: RUN1489

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.19

EN300-6504325_2_1



CID: EN300-6504325_2_1

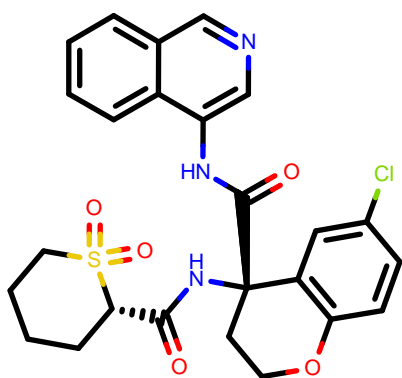
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@H](C)C(=O)C1=CC=C(C=C1)C(=O)N5CC[C@H](C5)NC(=O)N6S(=O)(=O)N

RUN: RUN6064

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.58

EN300-107435_1_1



CID: EN300-107435_1_1

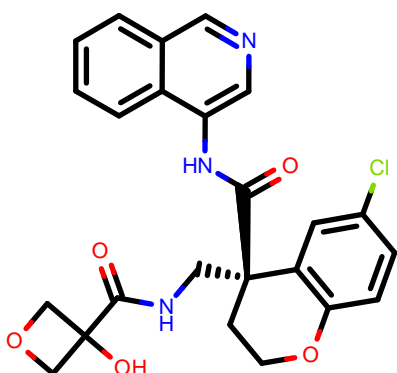
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCCS5(=O)=O

RUN: RUN6660

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-101443_2_1



CID: EN300-101443_2_1

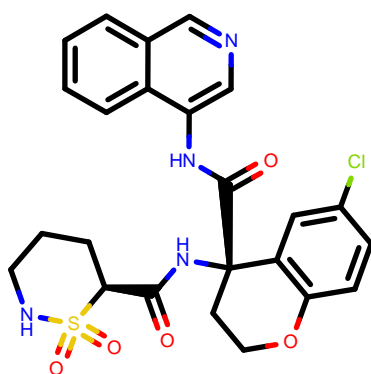
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CNC(=O)C5(COC5)O

RUN: RUN4151

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.21

EN300-1587757_1_1



CID: EN300-1587757_1_1

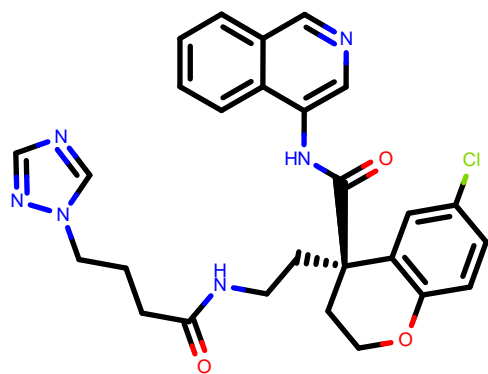
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCCNS5(=O)=O

RUN: RUN6868

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.24

EN300-316216_3_1



CID: EN300-316216_3_1

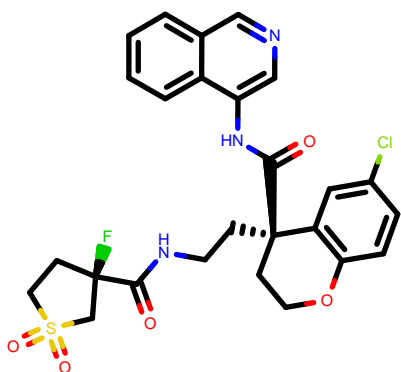
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCN5enon5

RUN: RUN11212

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.28

EN300-311920_3_2



CID: EN300-311920_3_2

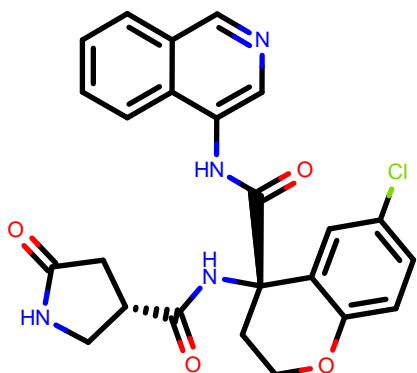
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@]5(CCS(=O)=O)C5F

RUN: RUN2836

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.23

EN300-59487_1_2



CID: EN300-59487_1_2

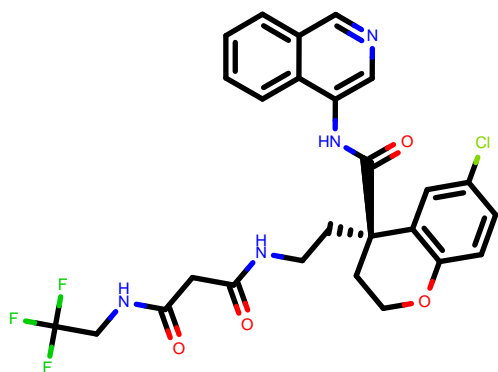
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC(=O)NCS

RUN: RUN4770

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.21

EN300-128715_3_1



CID: EN300-128715_3_1

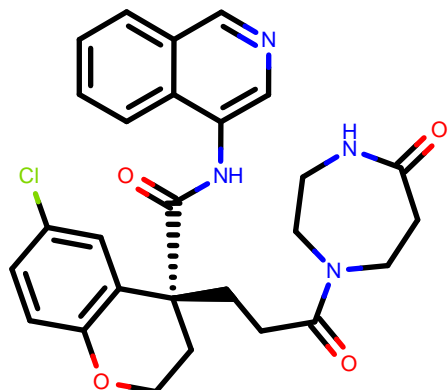
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC(=O)NCC(F)(F)F

RUN: RUN7591

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.27

EN300-69107_2_1



CID: EN300-69107_2_1

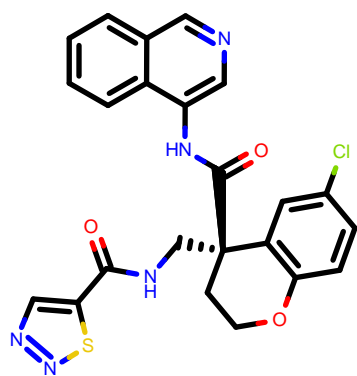
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCCC(=O)NCCS

RUN: RUN10188

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.26

EN300-42269_2_1



CID: EN300-42269_2_1

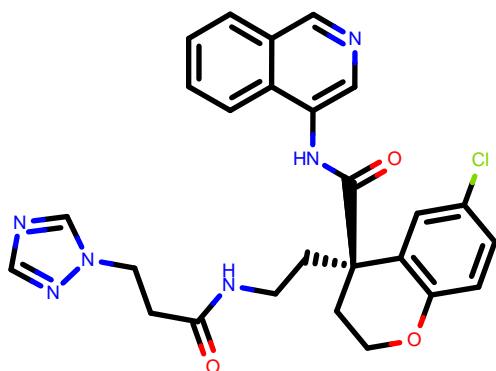
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnns5

RUN: RUN8401

DDG (kcal/mol): -0.91

dDDG (kcal/mol): 0.25

EN300-26147_3_1



CID: EN300-26147_3_1

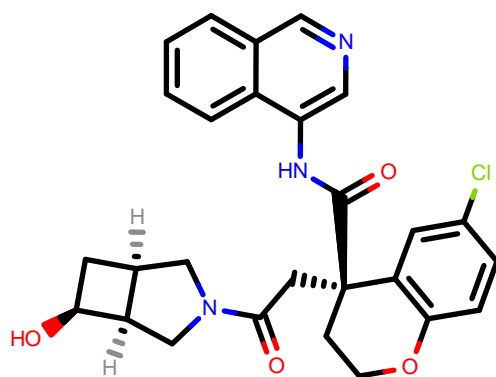
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cnns5

RUN: RUN4005

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.28

EN300-305294_1_2



CID: EN300-305294_1_2

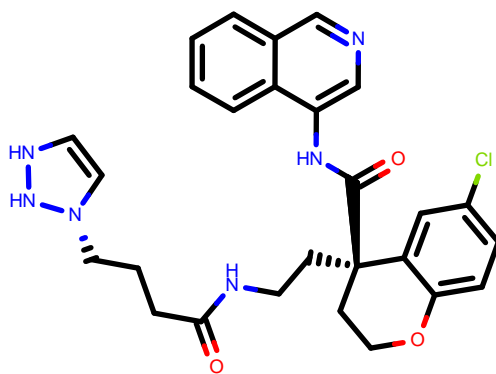
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5C6C7C8C5C6C7C8O

RUN: RUN3097

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.24

EN300-124301_3_1



CID: EN300-124301_3_1

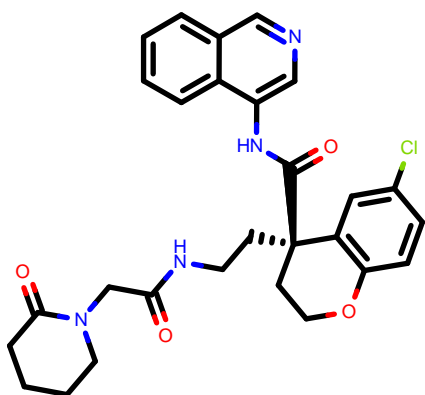
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cnns5

RUN: RUN11188

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.26

EN300-36111_3_1



CID: EN300-36111_3_1

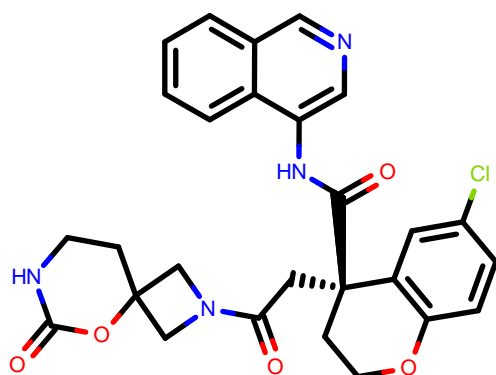
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5NCCCCC5=O

RUN: RUN13296

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.26

EN300-658355_1_1



CID: EN300-658355_1_1

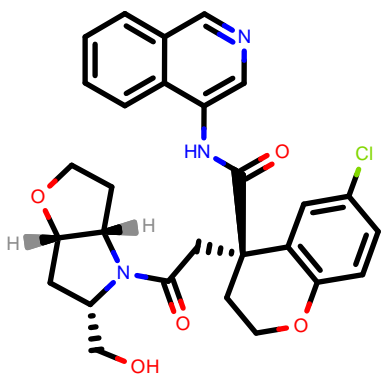
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC6(C5)CCNC(=O)O6

RUN: RUN9651

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.24

EN300-1588907_1_1



CID: EN300-1588907_1_1

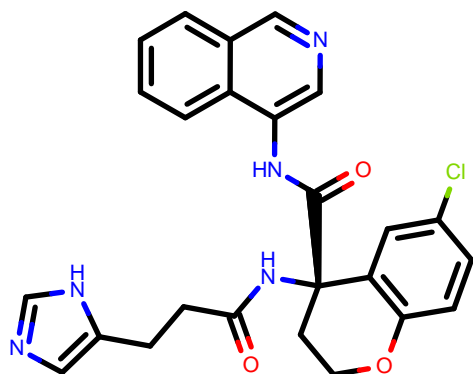
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C@H(CCO)C@H9C@H9CO

RUN: RUN3157

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.26

EN300-145616_1_1



CID: EN300-145616_1_1

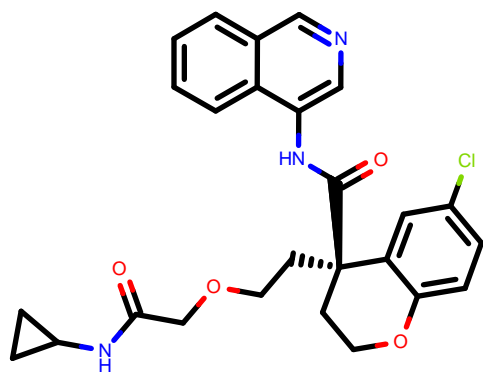
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)CCc5nc[nH]5)

RUN: RUN8484

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.23

EN300-1253178_3_1



CID: EN300-1253178_3_1

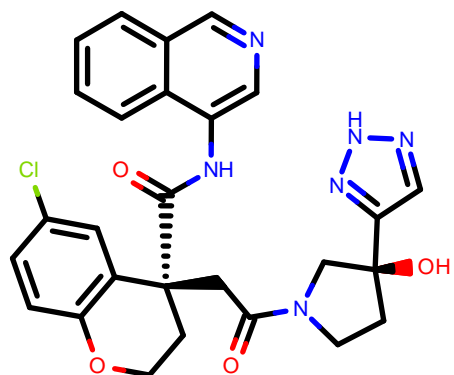
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NC5OC5

RUN: RUN1999

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.21

EN300-221122_1_2



CID: EN300-221122_1_2

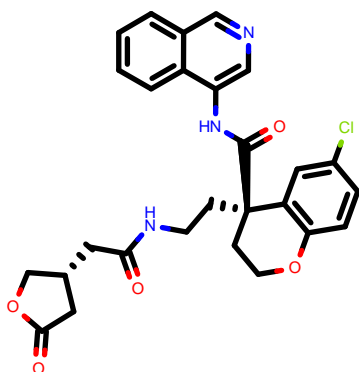
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]5(C)C6CN([NH]6)O

RUN: RUN2229

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.27

EN300-109535_3_1



CID: EN300-109535_3_1

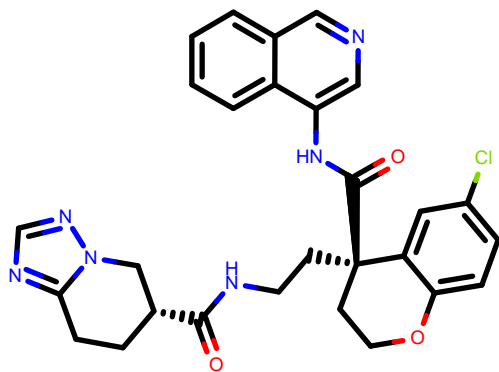
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CC(=O)OC5

RUN: RUN14942

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.24

EN300-1662365_3_1



CID: EN300-1662365_3_1

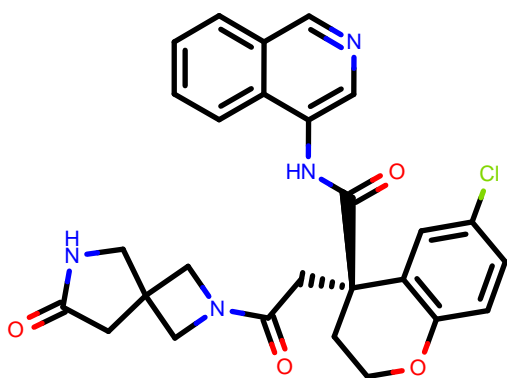
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC6N6C6

RUN: RUN15346

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.29

EN300-1722713_1_1



CID: EN300-1722713_1_1

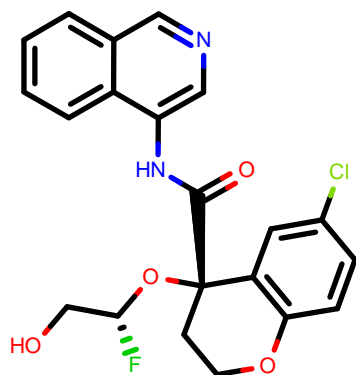
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CC(=O)N6

RUN: RUN12346

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.20

EN300-861925_1_2



CID: EN300-861925_1_2

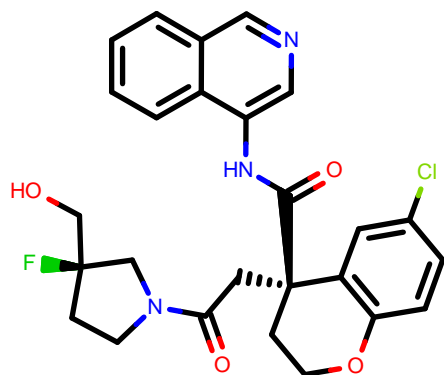
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H](CO)F

RUN: RUN807

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.21

EN300-203118_1_1



CID: EN300-203118_1_1

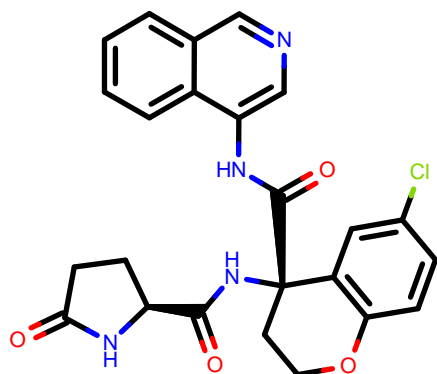
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3(C5)(CO)F

RUN: RUN1311

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.24

EN300-72896_1_1



CID: EN300-72896_1_1

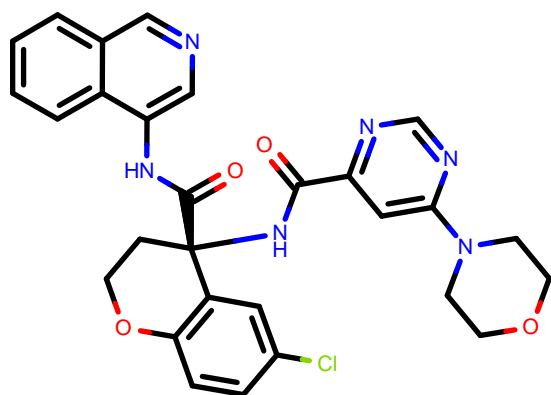
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN1769

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.18

EN300-313410_1_1



CID: EN300-313410_1_1

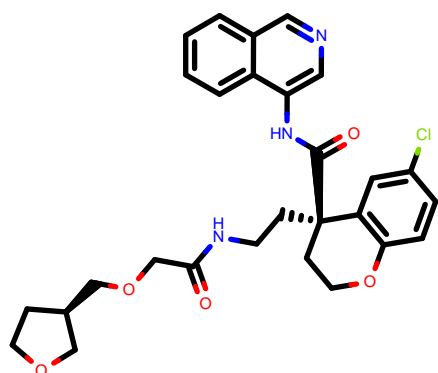
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N(C(=O)c5cc(nn5)N6CCOCC6

RUN: RUN3142

DDG (kcal/mol): -0.90

dDDG (kcal/mol): 0.18

EN300-80522_3_1



CID: EN300-80522_3_1

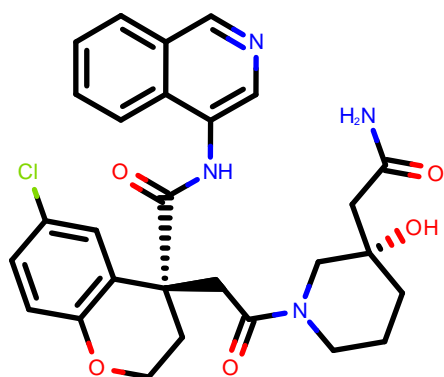
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCN(C(=O)COC[C@@]5H5CCOCC5

RUN: RUN11260

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.24

EN300-259060_1_1



CID: EN300-259060_1_1

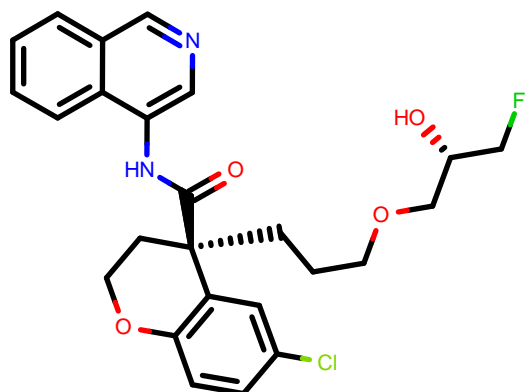
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@]6(C)C(=O)N5O

RUN: RUN5133

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.29

EN300-1968342_4_1



CID: EN300-1968342_4_1

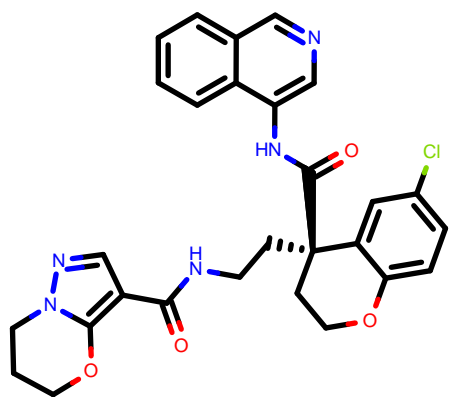
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@]5H5(CF)O

RUN: RUN365

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.21

EN300-103722_3_1



CID: EN300-103722_3_1

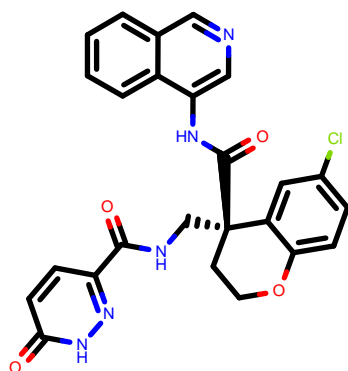
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnc6c5OCC6

RUN: RUN15026

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-04614_2_1



CID: EN300-04614_2_1

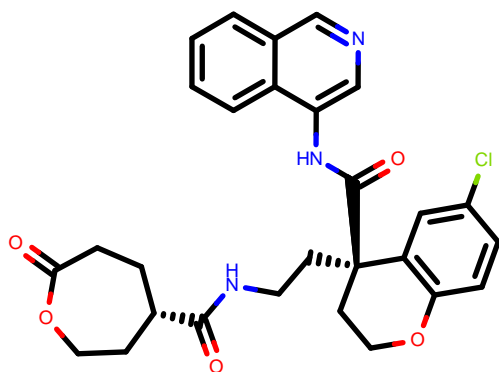
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnc6c5O[nH]n5

RUN: RUN3215

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.23

EN300-2011083_3_2



CID: EN300-2011083_3_2

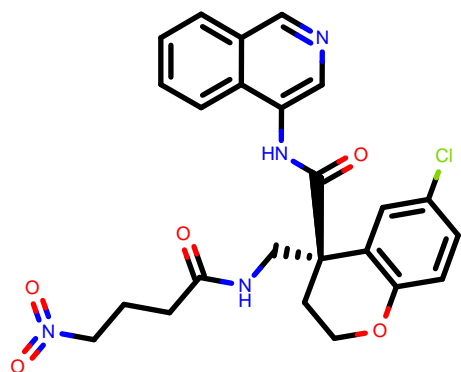
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5OCC(=O)OCC5

RUN: RUN14648

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.26

EN300-143449_2_1



CID: EN300-143449_2_1

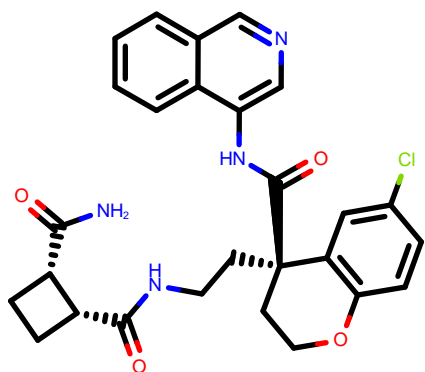
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCN(=O)=O

RUN: RUN1604

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.28

EN300-217107_3_3



CID: EN300-217107_3_3

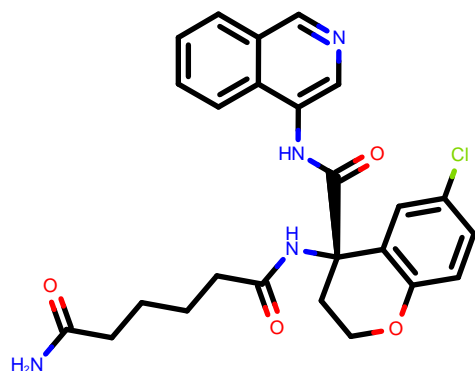
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@@]5SC[C@@]5[F]Cl=O

RUN: RUN13602

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-142412_1_1



CID: EN300-142412_1_1

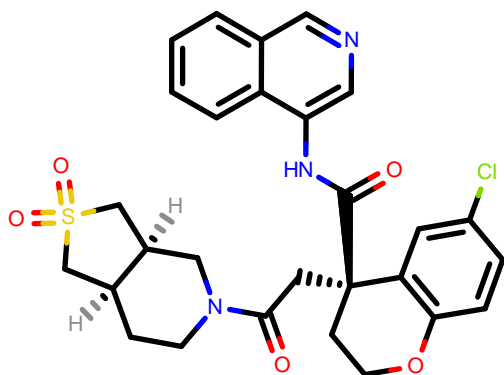
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCCC(=O)N

RUN: RUN3946

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.28

EN300-365993_1_2



CID: EN300-365993_1_2

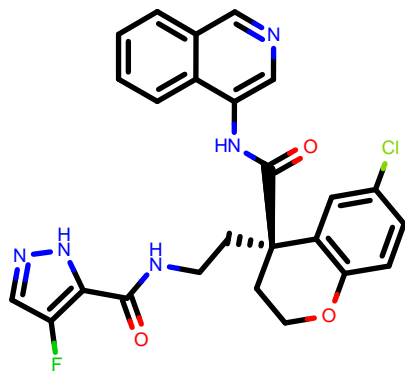
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)NSC(=O)N[C@@]5CCN(C5)S(=O)(=O)C

RUN: RUN12352

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.23

EN300-98143_3_1



CID: EN300-98143_3_1

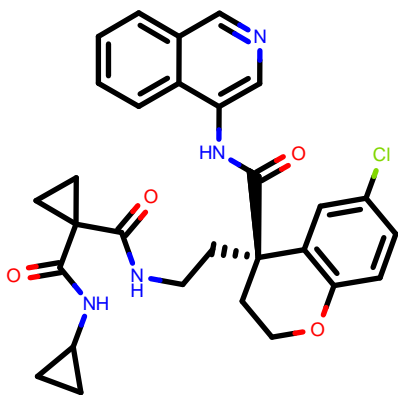
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5c[nH]c5F

RUN: RUN4829

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.21

EN300-61636_3_1



CID: EN300-61636_3_1

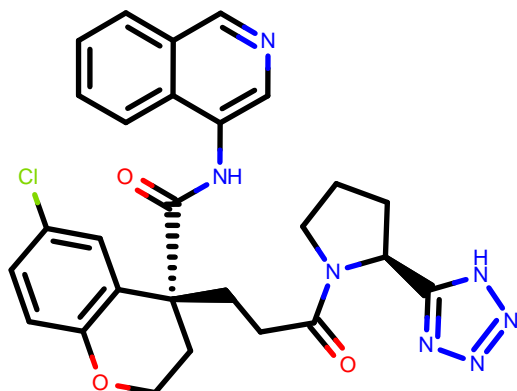
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)C(=O)N6C6C6

RUN: RUN11377

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.29

EN300-43282_2_1



CID: EN300-43282_2_1

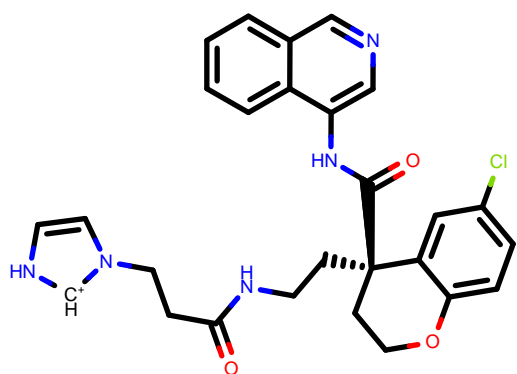
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5c6n[n-]n6

RUN: RUN6383

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.28

EN300-75342_3_1



CID: EN300-75342_3_1

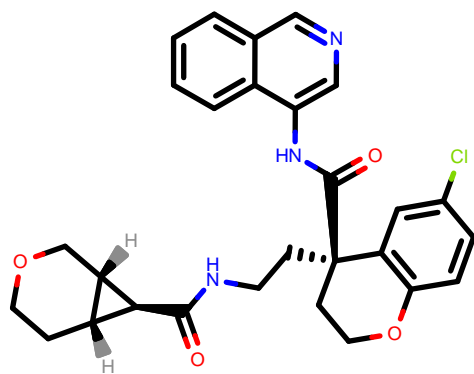
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc5

RUN: RUN8095

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.25

EN300-1644723_3_4



CID: EN300-1644723_3_4

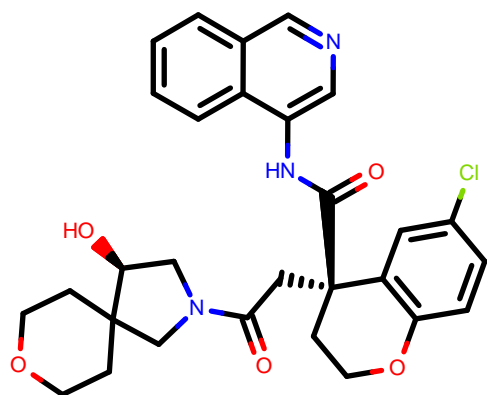
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5[C@@H]6C@@H5CO6C6

RUN: RUN13946

DDG (kcal/mol): -0.89

dDDG (kcal/mol): 0.24

EN300-7435482_1_1



CID: EN300-7435482_1_1

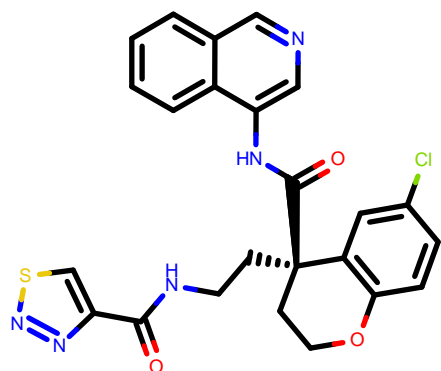
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H](C6)C5CCCC6O

RUN: RUN7175

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.25

EN300-24297_3_1



CID: EN300-24297_3_1

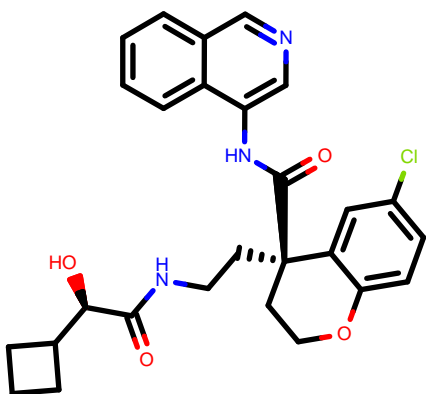
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5csnn5

RUN: RUN15297

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.20

EN300-249764_3_1



CID: EN300-249764_3_1

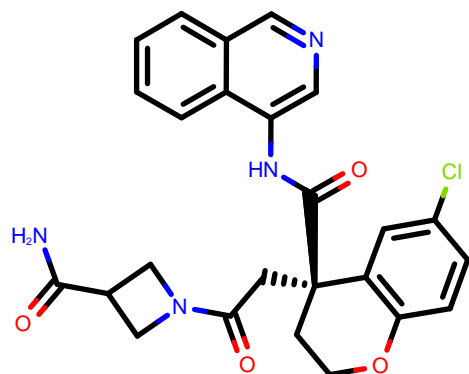
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H](C5)C5C5O

RUN: RUN2173

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.24

EN300-365106_1_1



CID: EN300-365106_1_1

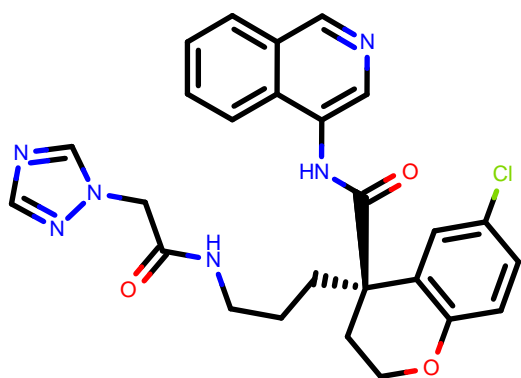
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)C(=O)N

RUN: RUN13110

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.21

EN300-06654_4_1



CID: EN300-06654_4_1

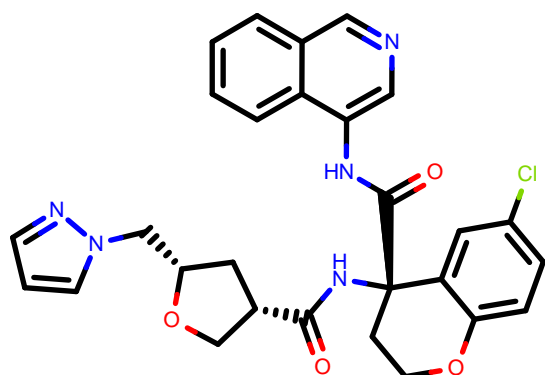
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)Cn5cnns5

RUN: RUN8146

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.22

EN300-6494859_1_2



CID: EN300-6494859_1_2

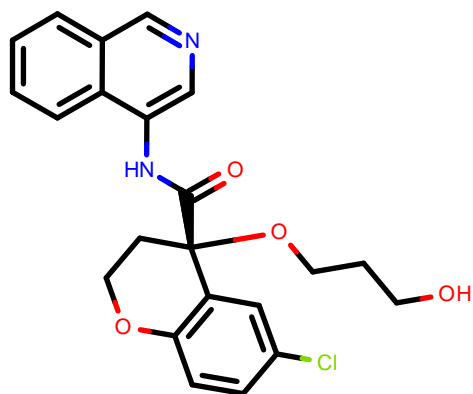
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)N[C@@H]5C[C@H](O)C5

RUN: RUN7104

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.28

EN300-221518_1_1



CID: EN300-221518_1_1

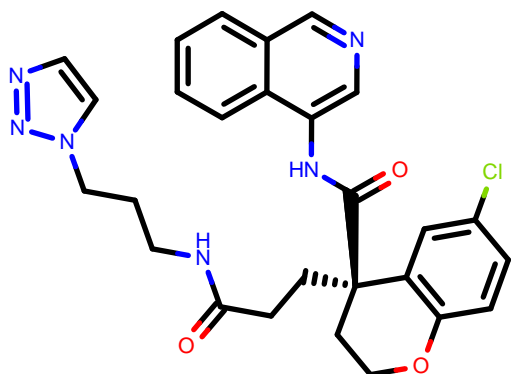
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCCO

RUN: RUN1693

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.16

EN300-1698650_2_1



CID: EN300-1698650_2_1

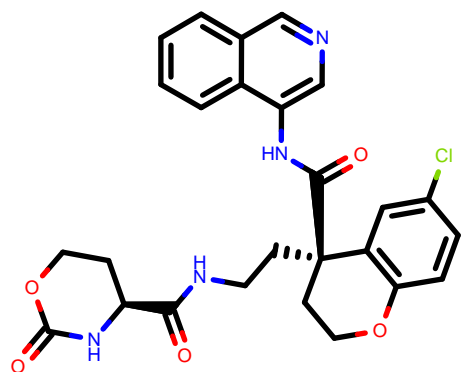
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCCn5cnns5

RUN: RUN8739

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.24

EN300-249804_3_1



CID: EN300-249804_3_1

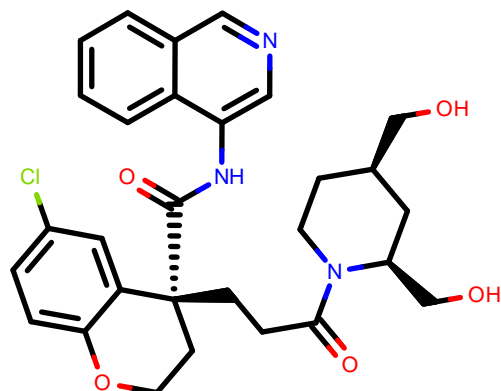
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCOC(=O)N5

RUN: RUN15122

DDG (kcal/mol): -0.88

dDDG (kcal/mol): 0.22

EN300-7470991_2_1



CID: EN300-7470991_2_1

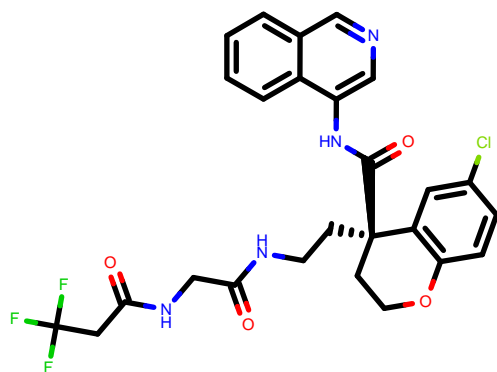
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H]6C[C@@H]6O)CO

RUN: RUN3968

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.31

EN300-43939_3_1



CID: EN300-43939_3_1

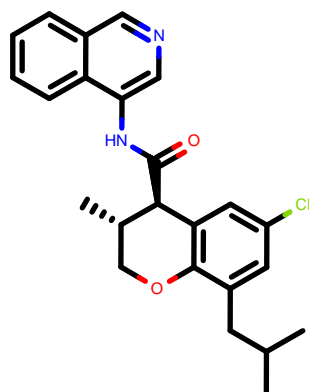
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)CNC(F)(F)F

RUN: RUN13562

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.25

DAR-DIA-0d514e7d-24_1



CID: DAR-DIA-0d514e7d-24_1

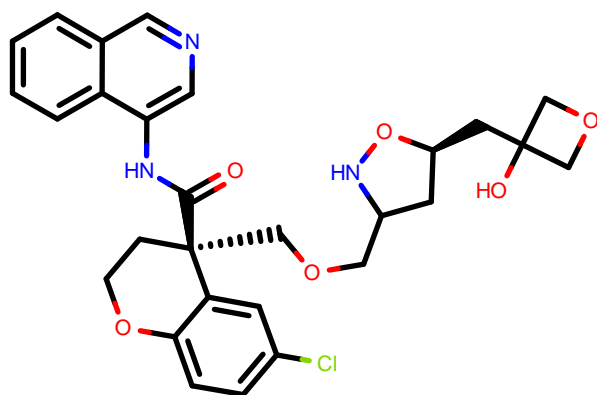
SMILES: C[C@@H]1COc2c(cc(cc2[C@@]3[H]1C(=O)Nc3cnc4c3ccc4)C)CC(C)C

RUN: RUN154

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.18

EN300-7457160_2_2



CID: EN300-7457160_2_2

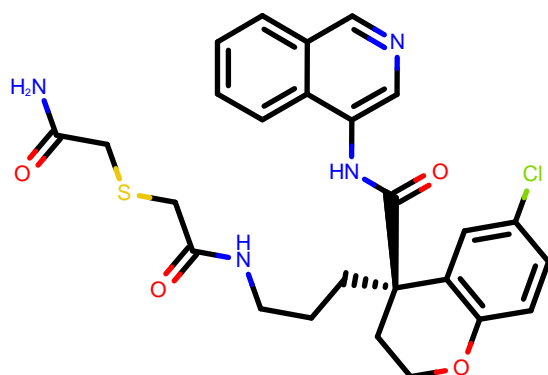
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4Cl)COCc5=NO[C@H](C5)Cc6(COC6)O

RUN: RUN2713

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.30

EN300-33513_4_1



CID: EN300-33513_4_1

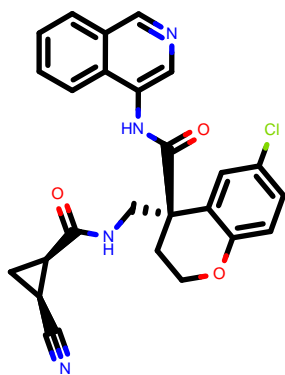
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4Cl)C)CCNC(=O)CSCC(=O)N

RUN: RUN11021

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.24

EN300-1600363_2_1



CID: EN300-1600363_2_1

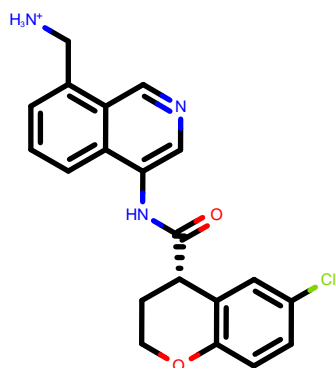
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4Cl)C)CNC(=O)[C@@]3[C@@]3(C)C#N

RUN: RUN3579

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.20

MAK-UNK-8be7dca9-6_2



CID: MAK-UNK-8be7dca9-6_2

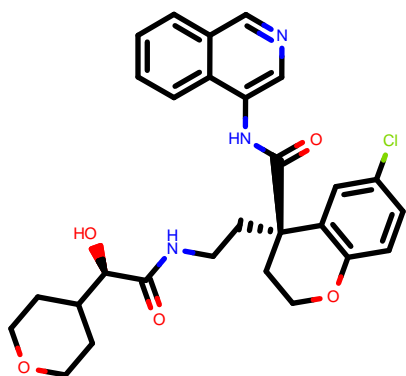
SMILES: c1cc(c2cncc(c2c1)NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4Cl)C)[NH3+]

RUN: RUN166

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.19

EN300-79180_3_1



CID: EN300-79180_3_1

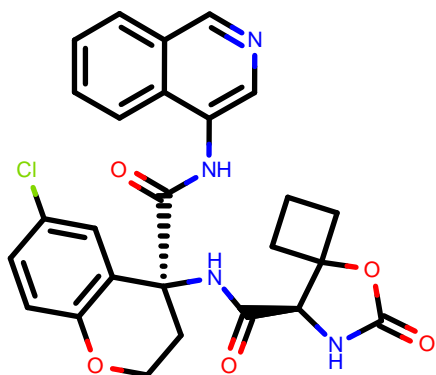
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H[C5CCOCC5]O

RUN: RUN15038

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-7432415_1_2



CID: EN300-7432415_1_2

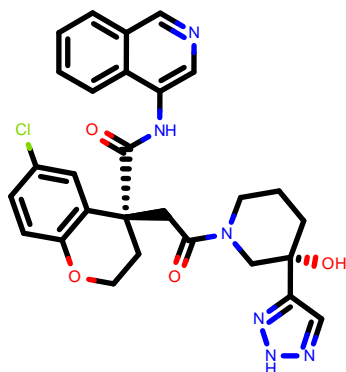
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H[C5C6(CCC6)OC(=O)N5]

RUN: RUN9700

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.24

EN300-222120_1_2



CID: EN300-222120_1_2

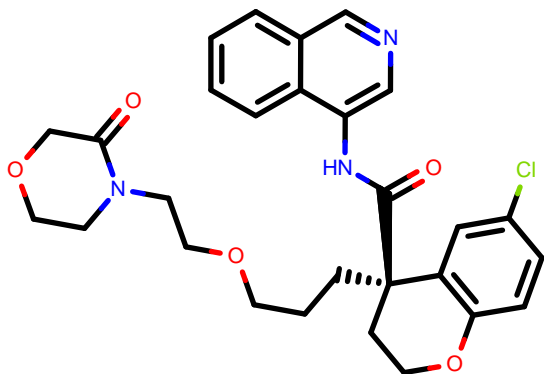
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@]3(C5)(c6cn[nH]n6)O

RUN: RUN9524

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.26

EN300-219330_4_1



CID: EN300-219330_4_1

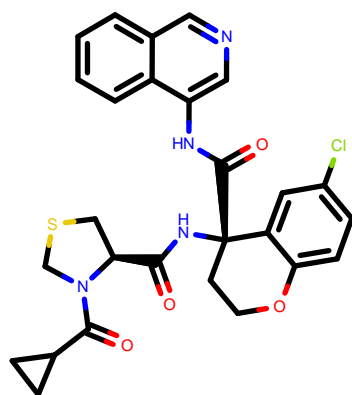
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOCC5=O

RUN: RUN1755

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.27

EN300-18928_1_1



CID: EN300-18928_1_1

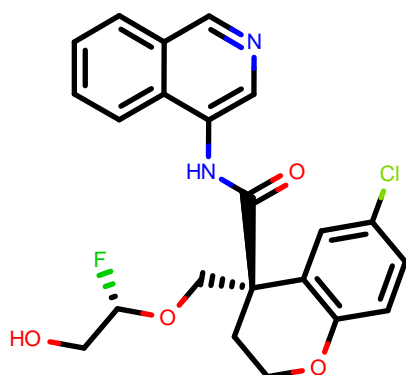
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]H5CSCN5C(=O)C6CC6

RUN: RUN9529

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.23

EN300-861925_2_1



CID: EN300-861925_2_1

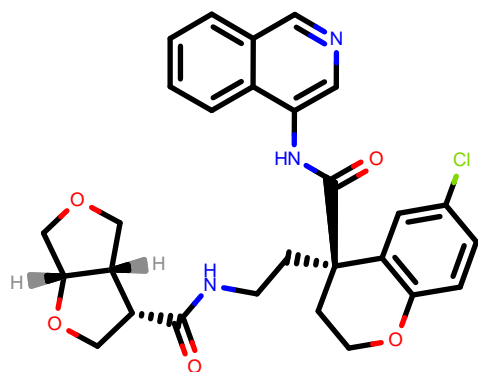
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H](CO)F

RUN: RUN1050

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.22

EN300-6482296_3_1



CID: EN300-6482296_3_1

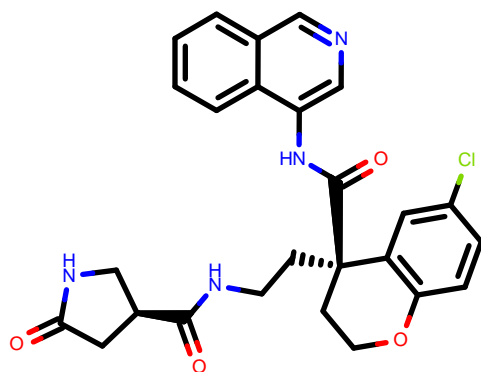
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5CO[C@H]5C

RUN: RUN14979

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.28

EN300-59487_3_2



CID: EN300-59487_3_2

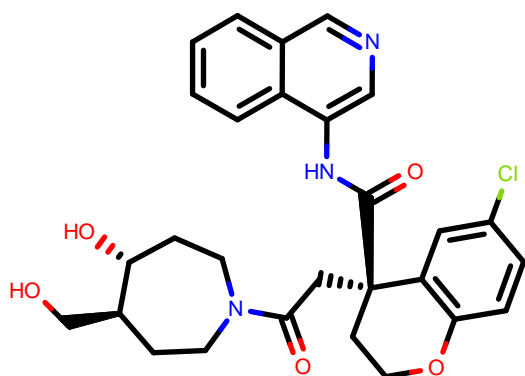
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5CC(=O)NC5

RUN: RUN4993

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.24

EN300-7353672_1_4



CID: EN300-7353672_1_4

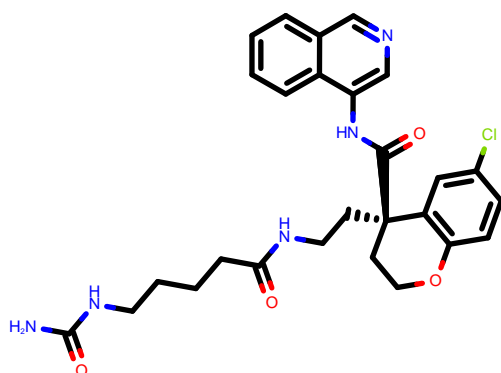
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C@@)CC5O)CO

RUN: RUN12208

DDG (kcal/mol): -0.87

dDDG (kcal/mol): 0.30

EN300-13499_3_1



CID: EN300-13499_3_1

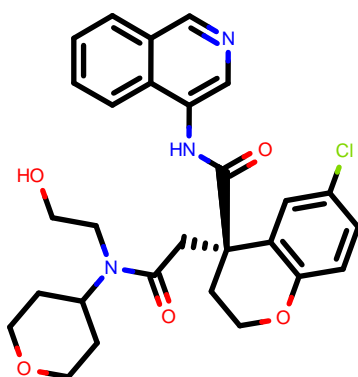
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCCNC(=O)N

RUN: RUN14290

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.36

EN300-154191_1_1



CID: EN300-154191_1_1

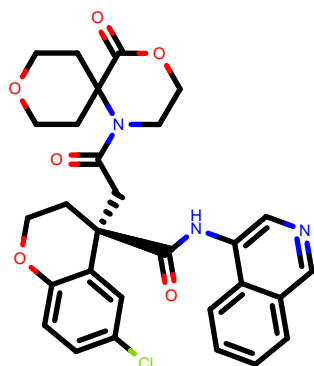
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5CCOCC5

RUN: RUN7763

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.33

EN300-1071014_1_1



CID: EN300-1071014_1_1

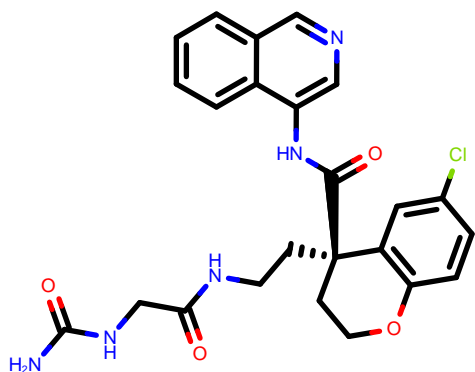
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC(=O)C56COC6

RUN: RUN13006

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.34

EN300-10397_3_1



CID: EN300-10397_3_1

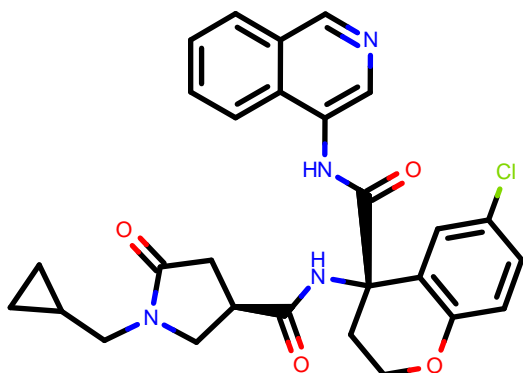
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)C)CNC(=O)CNC(=O)N

RUN: RUN8491

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.22

EN300-31969_1_1



CID: EN300-31969_1_1

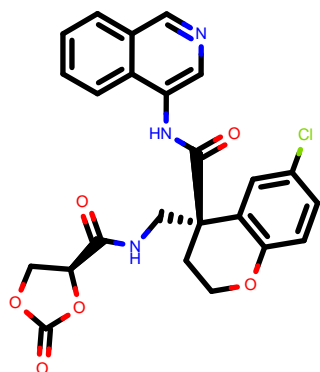
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)C)N(C(=O)O)C@H5CC1=ON(C5)COC6C6

RUN: RUN7700

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.26

EN300-5253939_2_1



CID: EN300-5253939_2_1

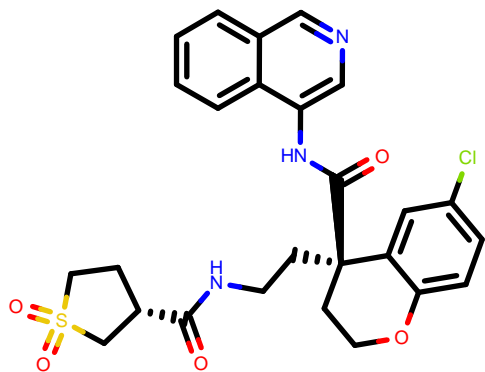
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)C)CNC(=O)[C@@H]5COC(=O)O5

RUN: RUN6989

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.26

EN300-14437_3_2



CID: EN300-14437_3_2

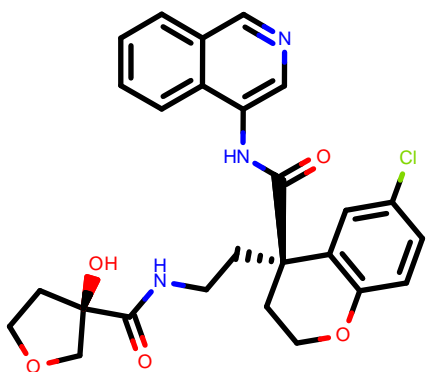
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCO4c3cc(cc4O)C)CNC(=O)[C@@H]5SCCS(=O)(=O)C5

RUN: RUN15019

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.27

EN300-148421_3_2



CID: EN300-148421_3_2

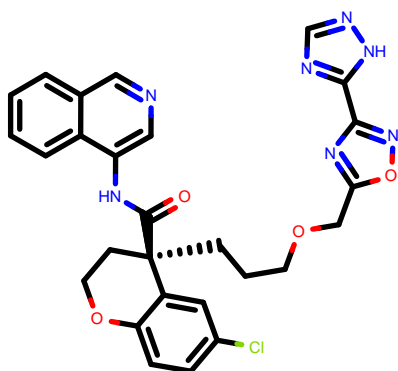
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOCS)O

RUN: RUN14440

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.29

EN300-92031_4_1



CID: EN300-92031_4_1

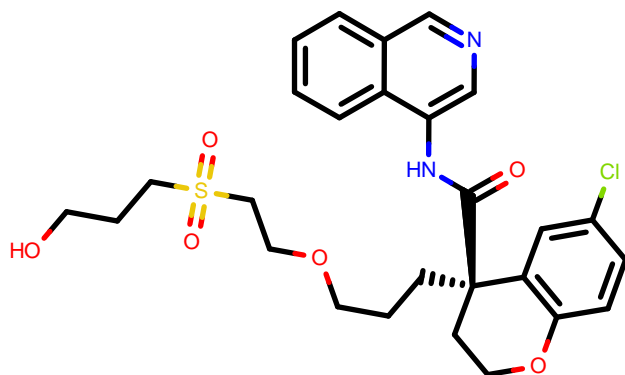
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nc(n6)[nH]n6

RUN: RUN1747

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.24

EN300-7456499_4_1



CID: EN300-7456499_4_1

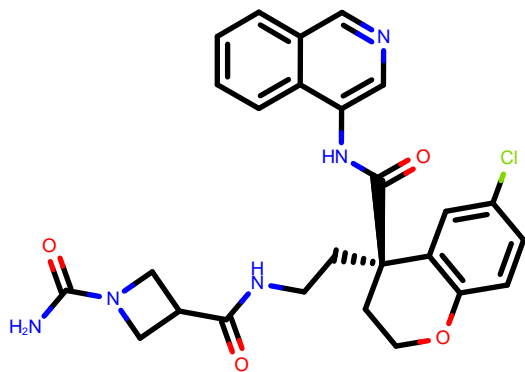
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)C(O)C

RUN: RUN437

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.32

EN300-1248250_3_1



CID: EN300-1248250_3_1

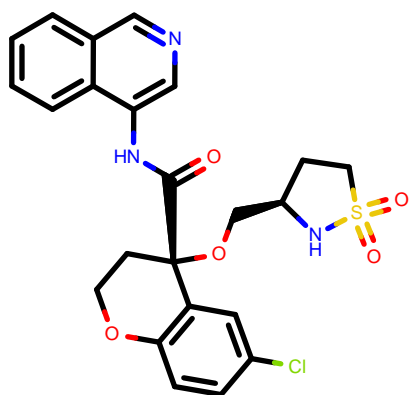
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CN(C5)C(=O)N

RUN: RUN15526

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.23

EN300-1699871_1_1



CID: EN300-1699871_1_1

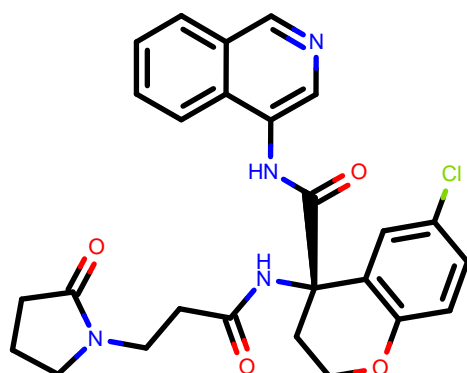
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCS(=O)(=O)N5

RUN: RUN1277

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.26

EN300-67191_1_1



CID: EN300-67191_1_1

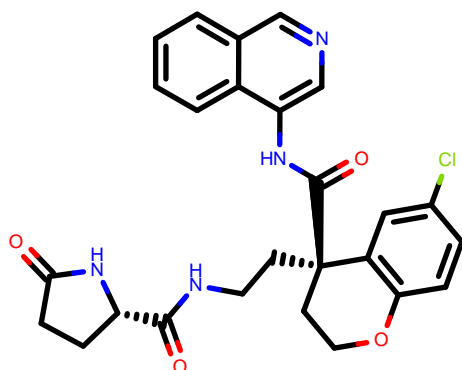
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O

RUN: RUN5566

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.27

EN300-72896_3_1



CID: EN300-72896_3_1

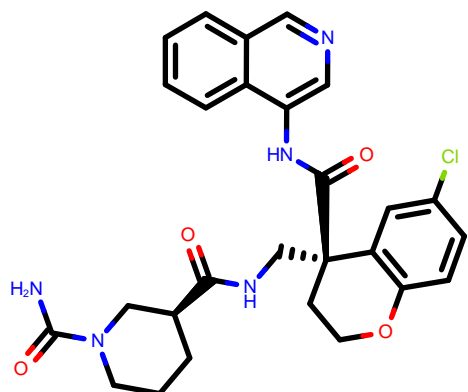
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]3[C@@]3C5CCN5

RUN: RUN14444

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.24

EN300-14767_2_2



CID: EN300-14767_2_2

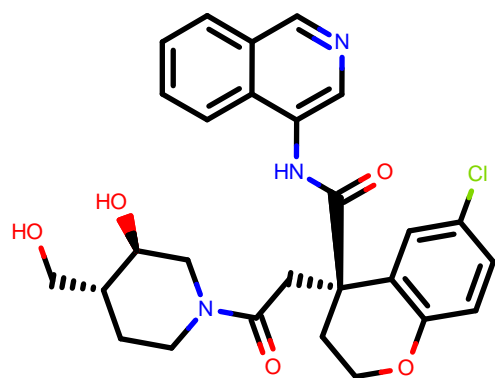
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCN(C5)C(=O)N

RUN: RUN6047

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.27

EN300-95639_1_1



CID: EN300-95639_1_1

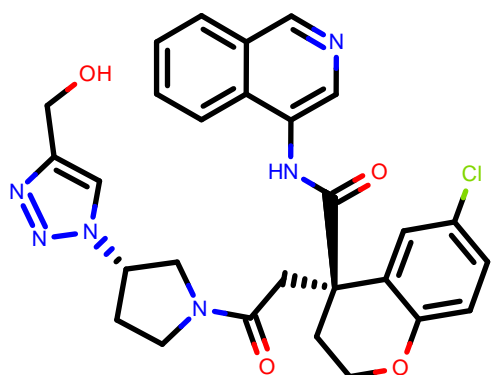
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)C(C)CC(=O)N5CC[C@@H]3[C@H](C5)O

RUN: RUN3053

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.24

EN300-234362_1_1



CID: EN300-234362_1_1

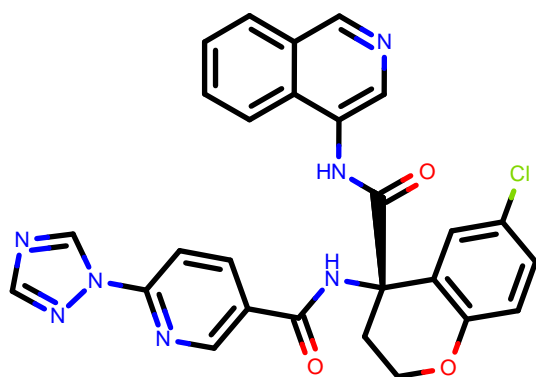
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)C(C)CC(=O)N5CC[C@@H]3[C@H](C5)n6ccn6

RUN: RUN15097

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.27

EN300-27261_1_1



CID: EN300-27261_1_1

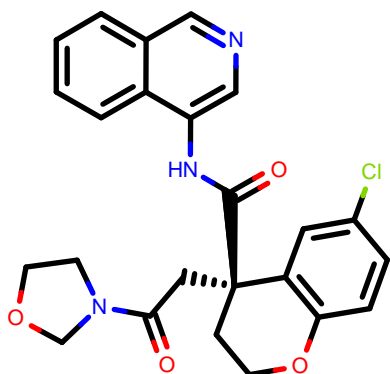
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)C(C)NC(=O)c5ccc(nc5)n6cnc6

RUN: RUN9889

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.21

EN300-211422_1_1



CID: EN300-211422_1_1

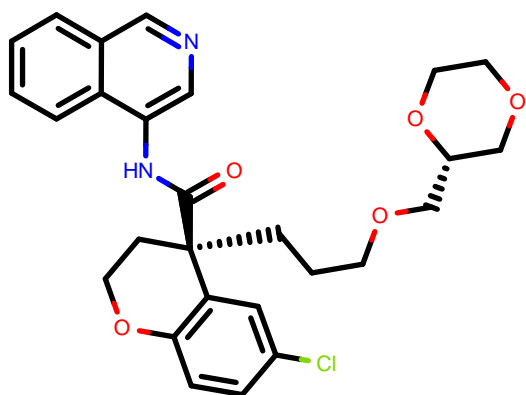
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(C)CCOC4C3cc(cc4)C(C)CC(=O)N5CCOC5

RUN: RUN11593

DDG (kcal/mol): -0.86

dDDG (kcal/mol): 0.19

EN300-139167_4_1



CID: EN300-139167_4_1

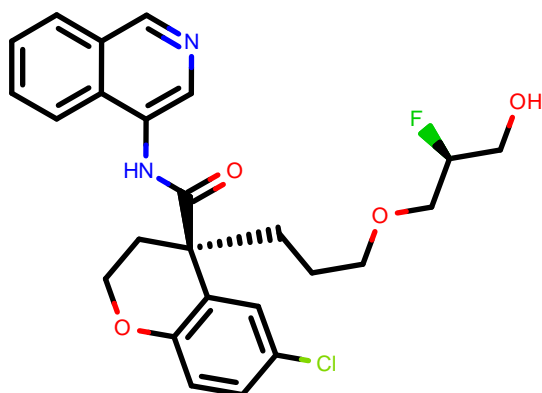
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCOC5

RUN: RUN1946

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.23

EN300-1600517_4_1



CID: EN300-1600517_4_1

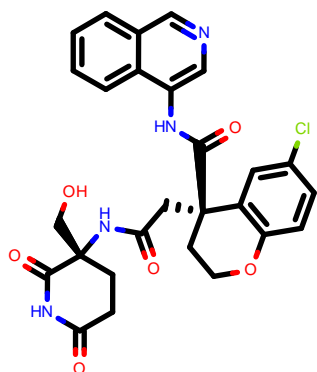
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CO)F

RUN: RUN453

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.22

EN300-7537340_1_1



CID: EN300-7537340_1_1

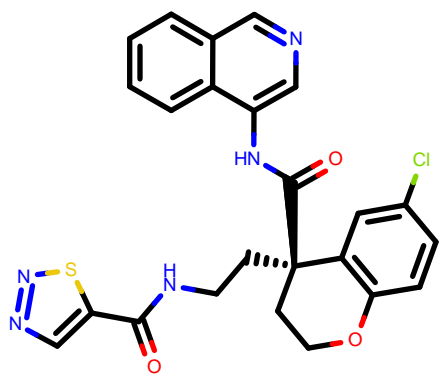
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N[C@@]3(C)CC(=O)N5C(=O)CO

RUN: RUN13588

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.30

EN300-42269_3_1



CID: EN300-42269_3_1

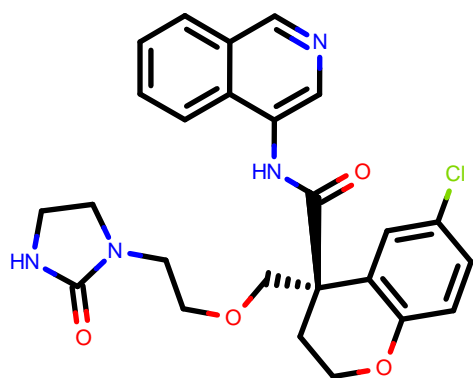
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5nnns5

RUN: RUN15282

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.20

EN300-214800_2_1



CID: EN300-214800_2_1

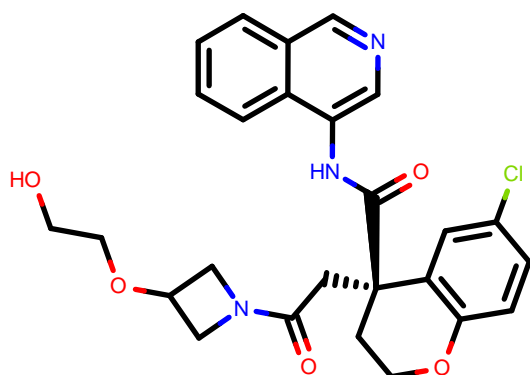
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCN5CCN5=O

RUN: RUN564

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.26

EN300-258081_1_1



CID: EN300-258081_1_1

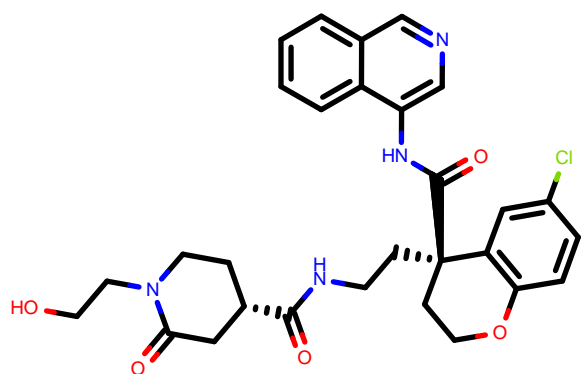
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)OCCO

RUN: RUN10970

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.22

EN300-1723663_3_1



CID: EN300-1723663_3_1

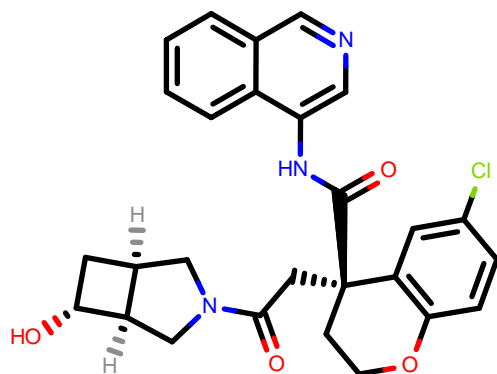
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCN(C(=O)C5)OCCO

RUN: RUN969

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.30

EN300-305294_1_4



CID: EN300-305294_1_4

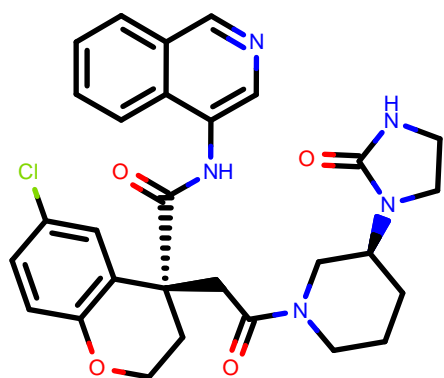
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5[C@H]6[C@@H](C5)C[C@H]6C5=O

RUN: RUN1159

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.18

EN300-55087_1_1



CID: EN300-55087_1_1

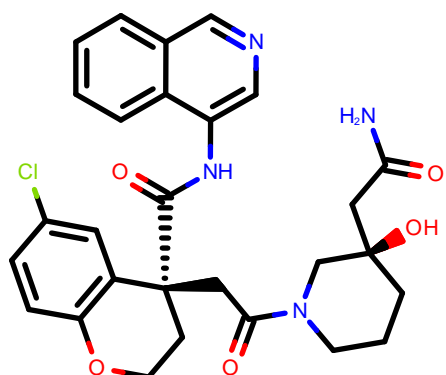
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)N6CCNC6=O

RUN: RUN12562

DDG (kcal/mol): -0.85

dDDG (kcal/mol): 0.26

EN300-259060_1_2



CID: EN300-259060_1_2

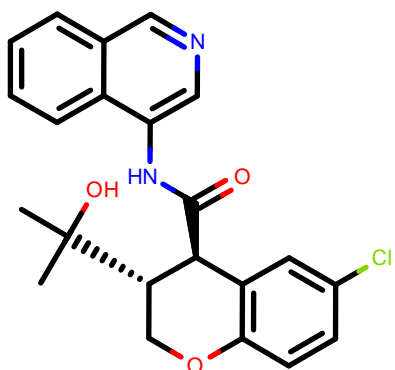
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)(CO)N

RUN: RUN5457

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

BEN-BAS-5c03e89e-1_2



CID: BEN-BAS-5c03e89e-1_2

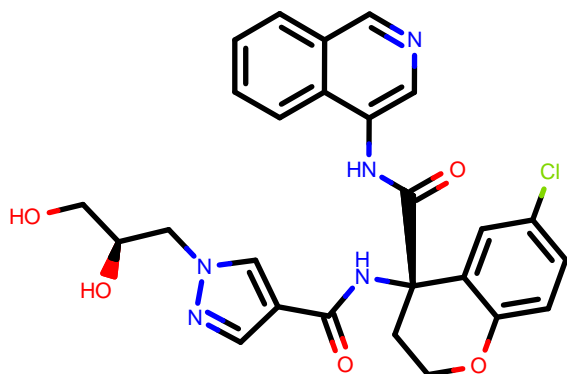
SMILES: CC(C)(C@H)1COc2ccc(cc2[C@@H]1C(=O)Nc3cccc4c3ccc4)Cl)O

RUN: RUN23

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.11

EN300-246178_1_2



CID: EN300-246178_1_2

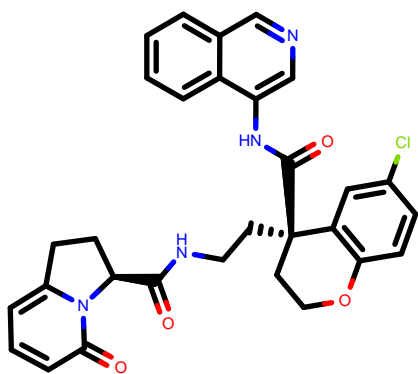
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc(c5)C[C@@H](CO)O

RUN: RUN1249

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.29

EN300-332002_3_1



CID: EN300-332002_3_1

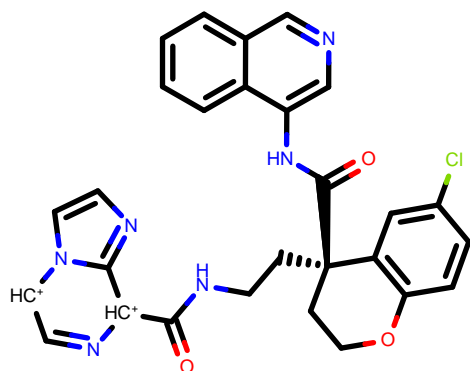
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5C6C6nc6c(-O)c6c6

RUN: RUN15140

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.30

EN300-225012_3_1



CID: EN300-225012_3_1

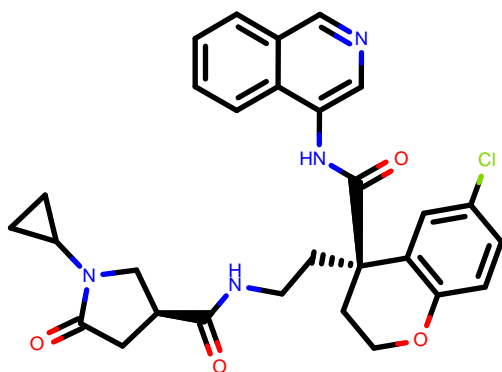
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5c6nc6c6c6c5

RUN: RUN5025

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.24

EN300-12440_3_2



CID: EN300-12440_3_2

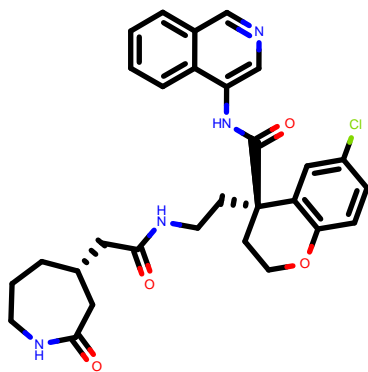
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5C6C6nc6c(-O)c6c6

RUN: RUN15164

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.32

EN300-195590_3_1



CID: EN300-195590_3_1

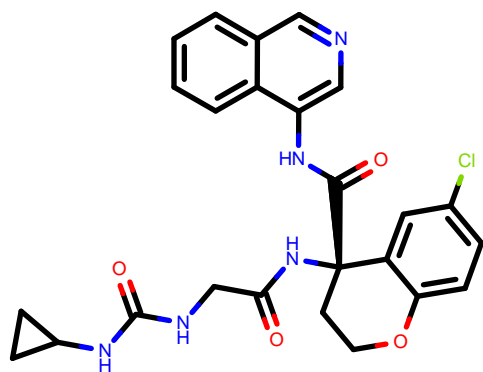
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5C6C6nc6c(-O)c6c5

RUN: RUN8443

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.29

EN300-42591_1_1



CID: EN300-42591_1_1

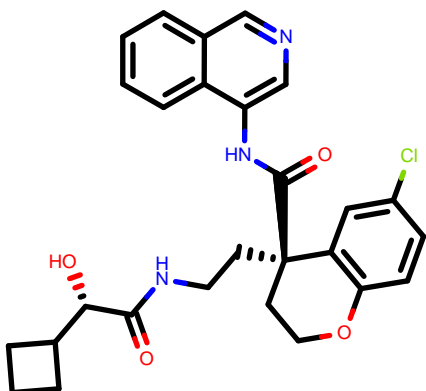
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)NC5CC5

RUN: RUN9189

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-249764_3_2



CID: EN300-249764_3_2

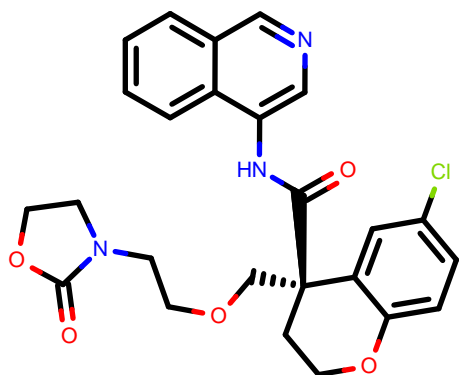
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H](C5CC5)O

RUN: RUN10898

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.28

EN300-370967_2_1



CID: EN300-370967_2_1

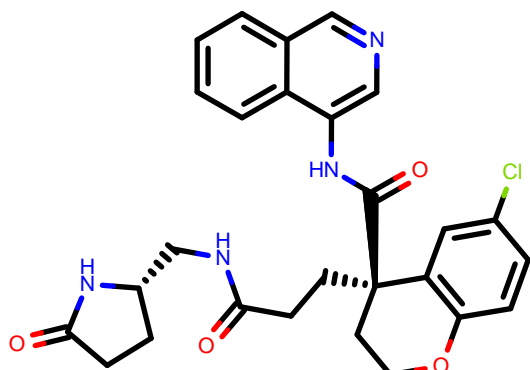
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCCN5CCOC5=O

RUN: RUN1082

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.25

EN300-75030_2_2



CID: EN300-75030_2_2

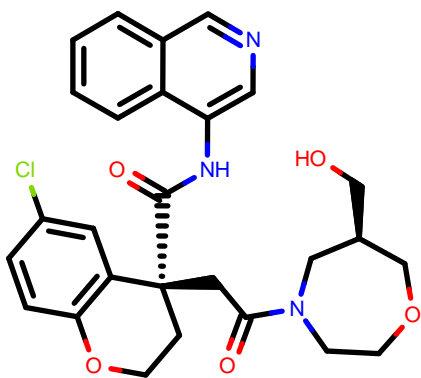
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC[C@@]4H5CCCC(=O)N5

RUN: RUN5008

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.26

EN300-6478054_1_2



CID: EN300-6478054_1_2

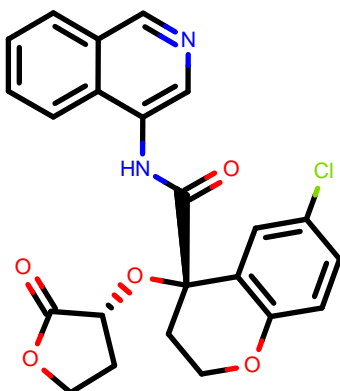
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)CO

RUN: RUN10079

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.27

EN300-20496_1_2



CID: EN300-20496_1_2

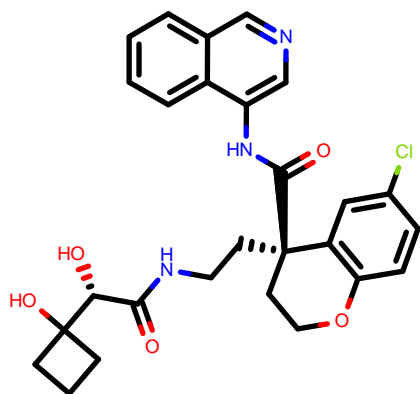
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCOC5=O

RUN: RUN2179

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.17

EN300-1073320_3_2



CID: EN300-1073320_3_2

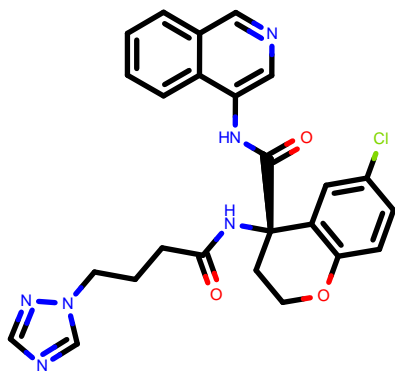
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](C5(CCC5)O)O

RUN: RUN3465

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.31

EN300-316216_1_1



CID: EN300-316216_1_1

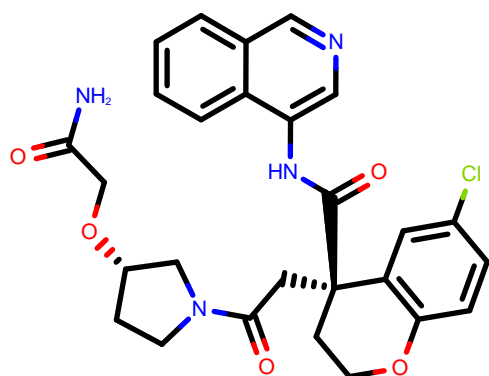
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cnr5

RUN: RUN6680

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.23

EN300-98802_1_1



CID: EN300-98802_1_1

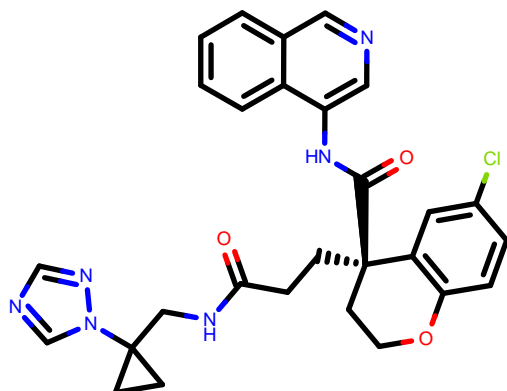
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)OCC(=O)N

RUN: RUN3265

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.23

EN300-6733137_2_1



CID: EN300-6733137_2_1

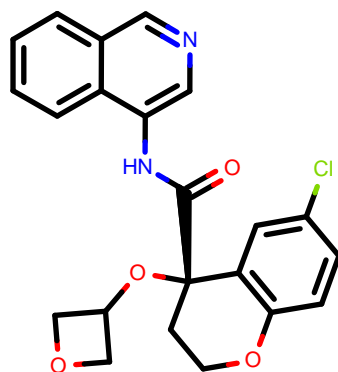
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5(CO5)n6ncn6

RUN: RUN13573

DDG (kcal/mol): -0.84

dDDG (kcal/mol): 0.31

EN300-317082_1_1



CID: EN300-317082_1_1

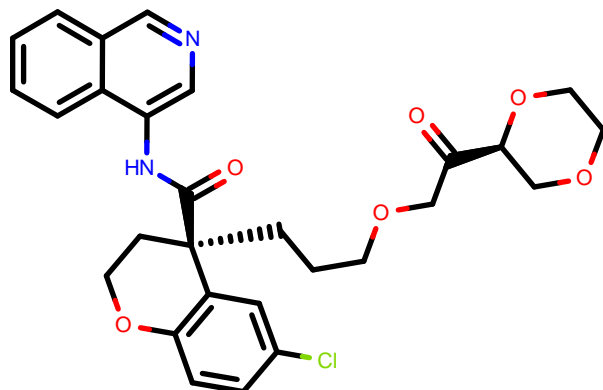
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5OCC5

RUN: RUN2312

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.12

EN300-6238494_4_1



CID: EN300-6238494_4_1

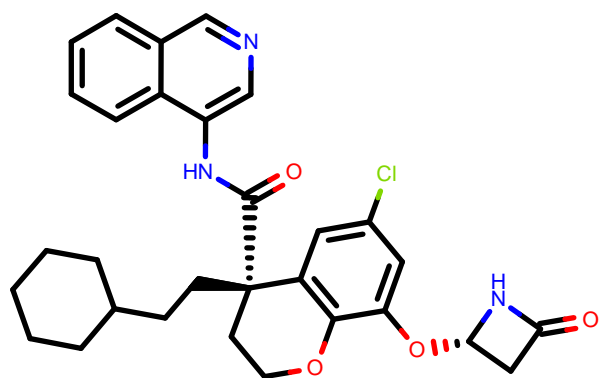
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@H]5COCOC5

RUN: RUN1651

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.26

VLA-UCB-05e51b3f-12_2



CID: VLA-UCB-05e51b3f-12_2

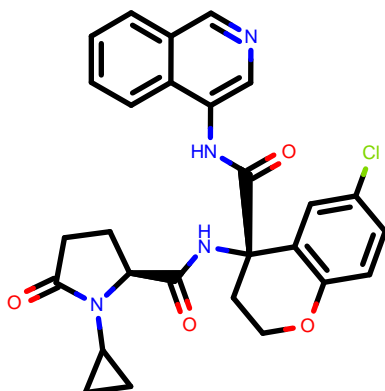
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)[C@H]5CC(=O)N5)C)CCc6CCCC6

RUN: RUN205

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.32

EN300-3044054_1_1



CID: EN300-3044054_1_1

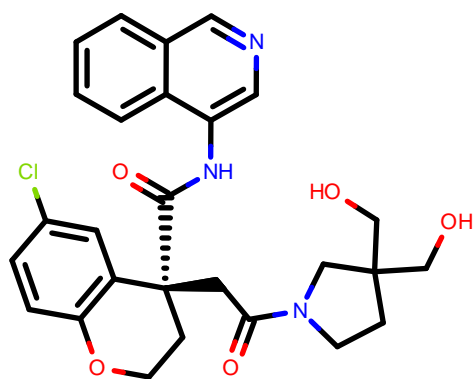
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)NC(=O)[C@H]5CC(=O)N5)C6CC6

RUN: RUN4726

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.20

EN300-306144_1_1



CID: EN300-306144_1_1

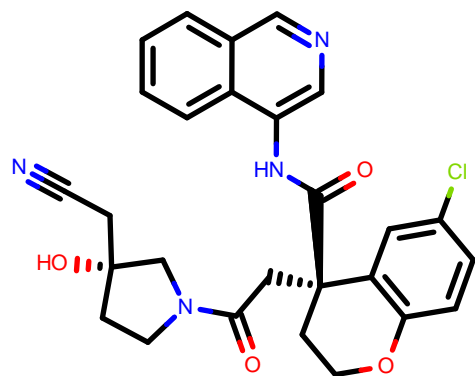
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4O)CC(=O)N5CC(C5)(CO)CO

RUN: RUN3425

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.24

EN300-257405_1_2



CID: EN300-257405_1_2

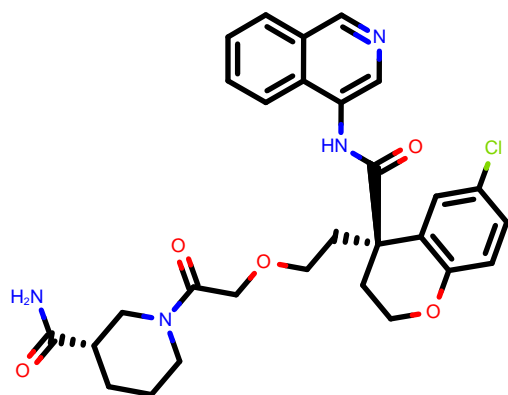
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]1(C5)(CC#N)O

RUN: RUN9894

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.24

EN300-22880_3_1



CID: EN300-22880_3_1

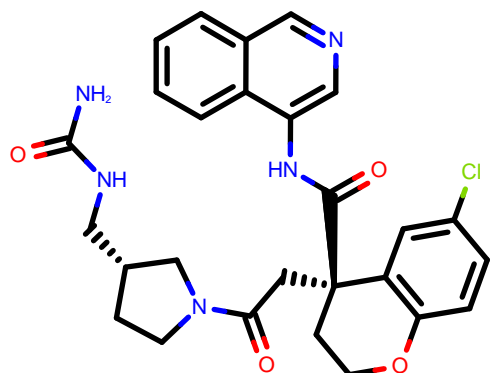
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)Cl=O

RUN: RUN682

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.30

EN300-210256_1_1



CID: EN300-210256_1_1

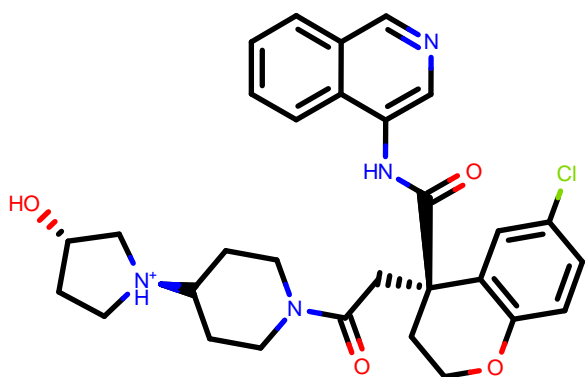
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC[C@@H](C5)CNC(=O)N

RUN: RUN6232

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.25

EN300-241988_1_2



CID: EN300-241988_1_2

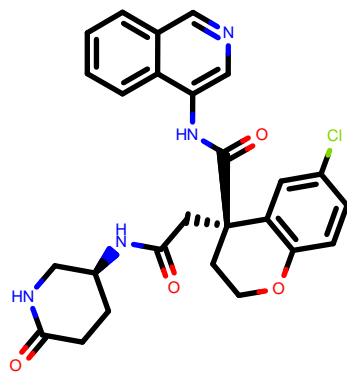
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(C5)[NH+]C6CC[C@@H](C6)O

RUN: RUN10473

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.35

EN300-62191_1_2



CID: EN300-62191_1_2

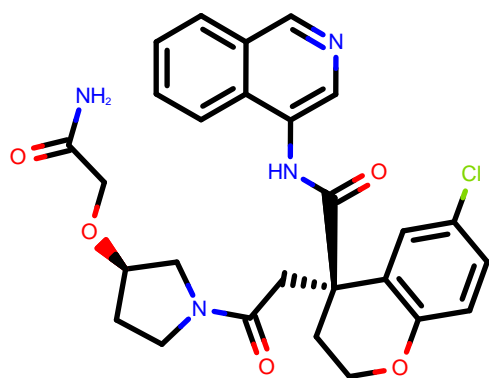
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCCC(=O)N5C5

RUN: RUN11833

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.21

EN300-98802_1_2



CID: EN300-98802_1_2

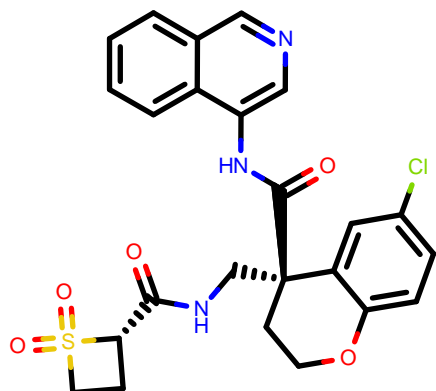
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)OCC(=O)N

RUN: RUN10813

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.24

EN300-1387104_2_1



CID: EN300-1387104_2_1

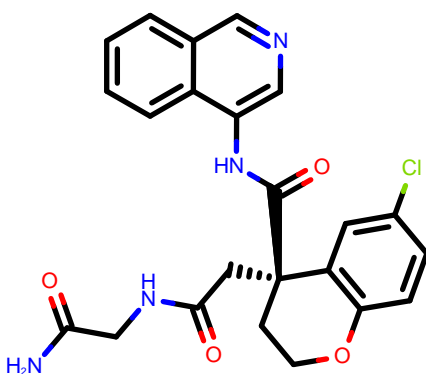
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4H5CCSS(=O)=O

RUN: RUN7773

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.26

EN300-16216_1_1



CID: EN300-16216_1_1

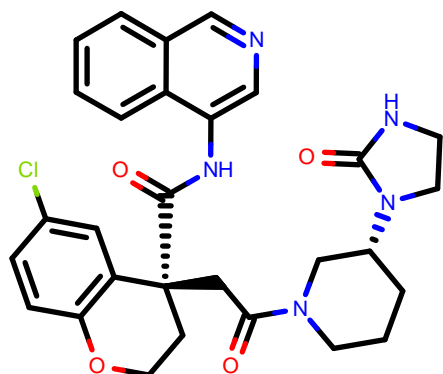
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC(=O)N

RUN: RUN9528

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.18

EN300-55087_1_2



CID: EN300-55087_1_2

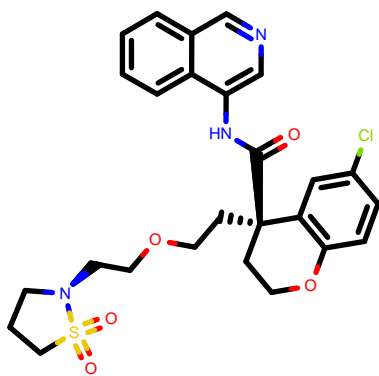
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)N6CCN6=O

RUN: RUN3489

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.22

EN300-114134_3_2



CID: EN300-114134_3_2

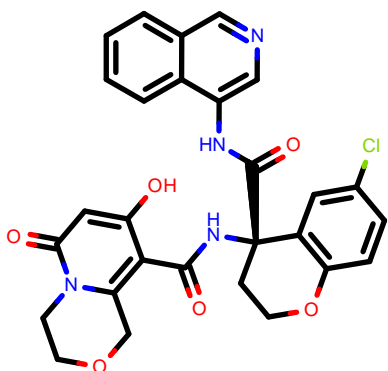
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCOC(N@@)5SCCS5(=O)=O

RUN: RUN2350

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.31

EN300-6479273_1_1



CID: EN300-6479273_1_1

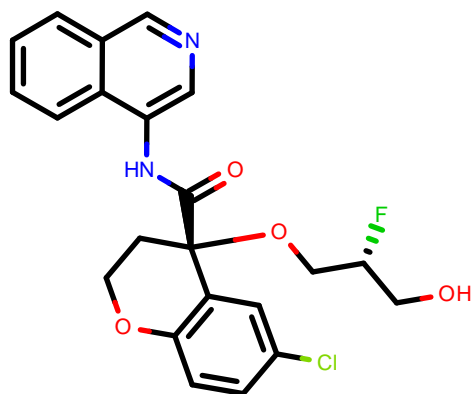
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(cc(=O)n6c5COCC6)[O-]

RUN: RUN5406

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.26

EN300-1600517_1_2



CID: EN300-1600517_1_2

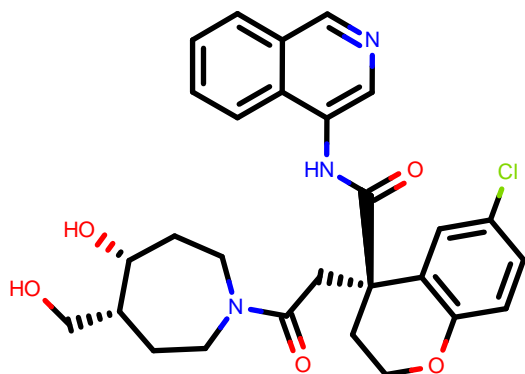
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](CO)F

RUN: RUN1197

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.22

EN300-7353672_1_3



CID: EN300-7353672_1_3

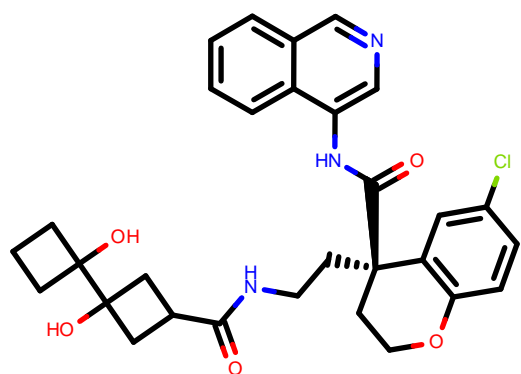
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C@@)CC5(O)CO

RUN: RUN5153

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.28

EN300-7459768_3_1



CID: EN300-7459768_3_1

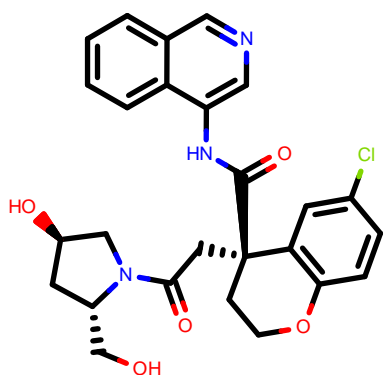
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC(C5)(C6(CCC6)O)O

RUN: RUN2646

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.29

EN300-152756_1_1



CID: EN300-152756_1_1

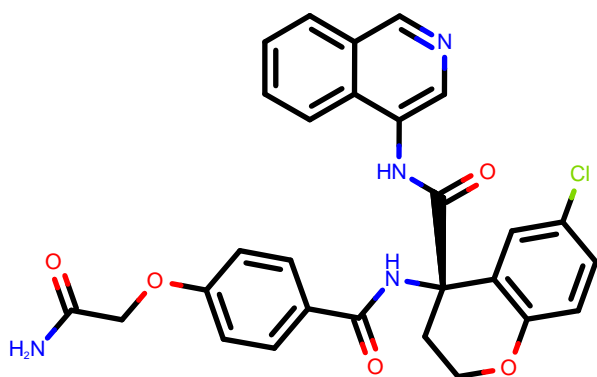
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]@H1C@H5CO)O

RUN: RUN6599

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-14949_1_1



CID: EN300-14949_1_1

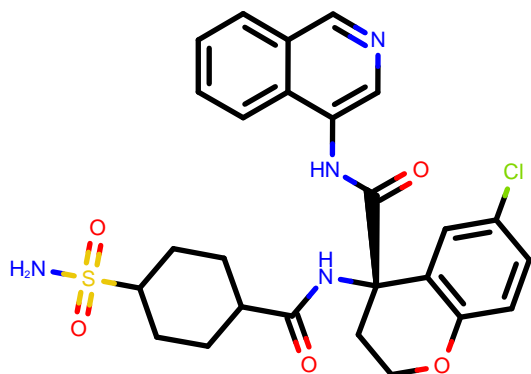
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)OCC(=O)N

RUN: RUN6608

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.27

EN300-83864_1_1



CID: EN300-83864_1_1

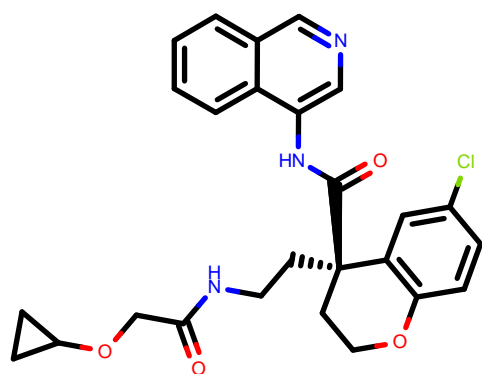
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCCC(C5)S(=O)(=O)N

RUN: RUN8677

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.24

EN300-378373_3_1



CID: EN300-378373_3_1

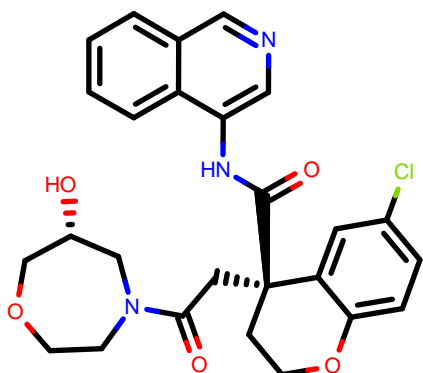
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC(=O)C)CCNC(=O)COC5C5

RUN: RUN8776

DDG (kcal/mol): -0.83

dDDG (kcal/mol): 0.22

EN300-233951_1_2



CID: EN300-233951_1_2

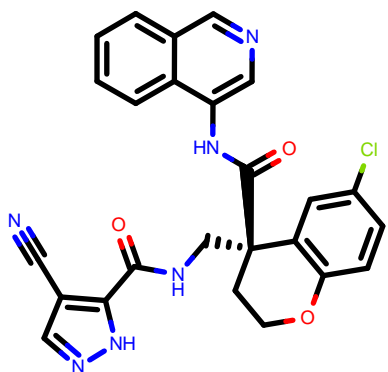
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC(=O)C)CC(=O)N5CCOC[C@@H](C5)O

RUN: RUN1375

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.27

EN300-1267109_2_1



CID: EN300-1267109_2_1

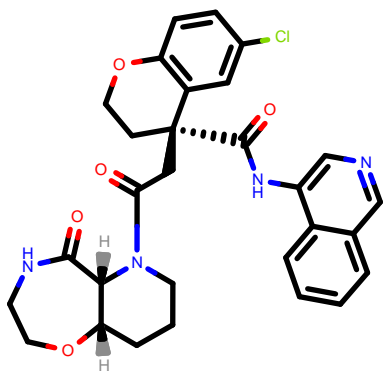
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC(=O)C)CCNC(=O)c5c[nH]5C#N

RUN: RUN8305

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.22

EN300-364612_1_4



CID: EN300-364612_1_4

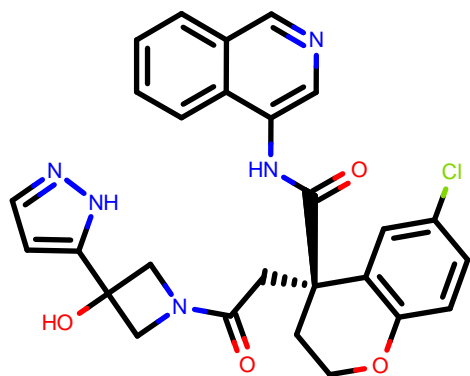
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](COC(=O)C)CC(=O)N5CCOC[C@@H](C5)N6CCO6

RUN: RUN12570

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.28

EN300-1667046_1_1



CID: EN300-1667046_1_1

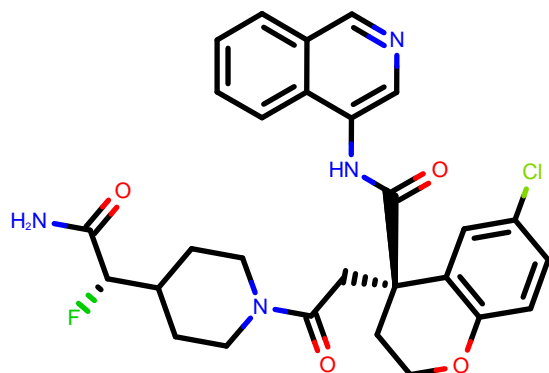
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cc[nH]6)O

RUN: RUN10069

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.29

EN300-318110_1_2



CID: EN300-318110_1_2

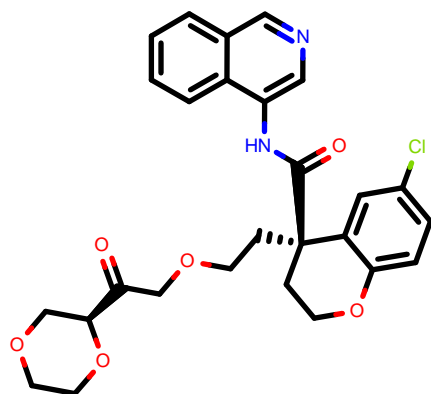
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C)N

RUN: RUN3669

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.28

EN300-6238494_3_1



CID: EN300-6238494_3_1

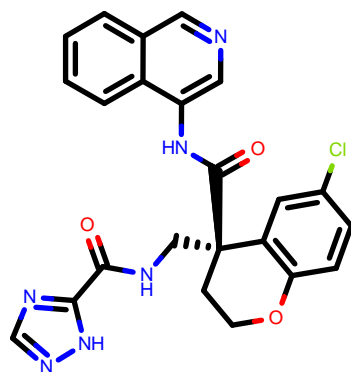
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@@H]5COCOC5

RUN: RUN282

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.26

EN300-100741_2_1



CID: EN300-100741_2_1

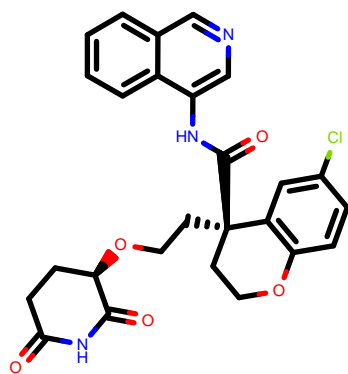
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5[nH]n5

RUN: RUN2556

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-120920_3_2



CID: EN300-120920_3_2

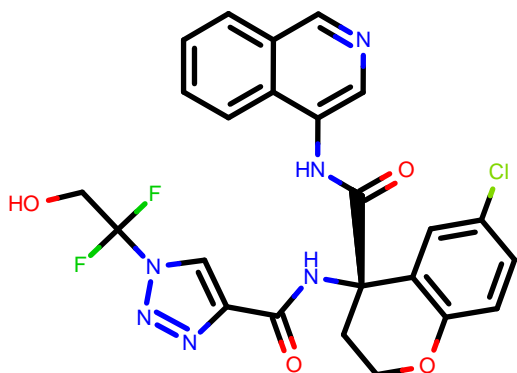
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCO[C@@H]5CCC(=O)NC5=O

RUN: RUN1879

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.19

EN300-716207_1_1



CID: EN300-716207_1_1

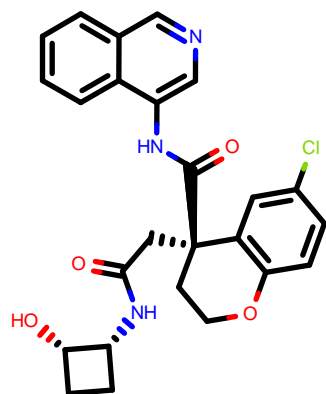
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5n[nH]5C(CO)F

RUN: RUN547

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-257949_1_1



CID: EN300-257949_1_1

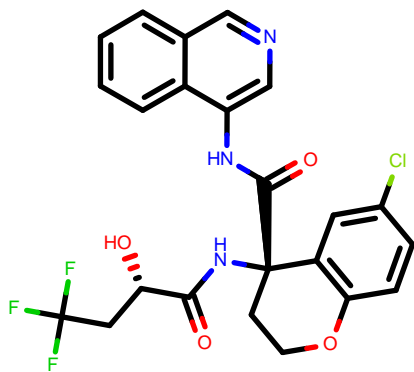
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CC[C@@H]5O

RUN: RUN5165

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.20

EN300-1932013_1_2



CID: EN300-1932013_1_2

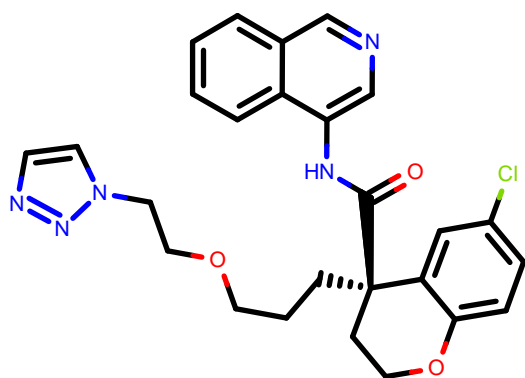
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H](CC(F)(F)F)O

RUN: RUN8080

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.30

EN300-1715993_4_1



CID: EN300-1715993_4_1

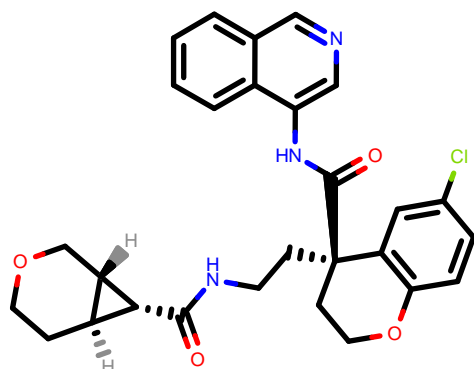
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCCCOCCn5cnn5

RUN: RUN1491

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-1644723_3_1



CID: EN300-1644723_3_1

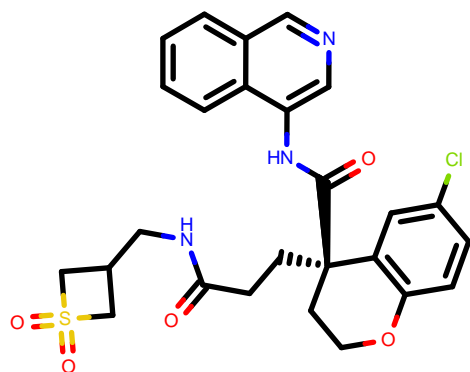
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@]5H5[C@@]6H5[C@@]6H5COCC6

RUN: RUN15349

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.23

EN300-266183_2_1



CID: EN300-266183_2_1

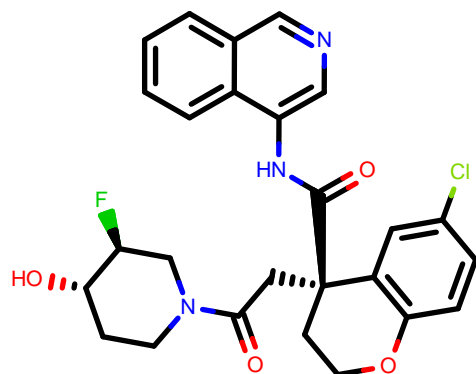
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)NCC5CS(=O)(=O)C5

RUN: RUN8843

DDG (kcal/mol): -0.82

dDDG (kcal/mol): 0.26

EN300-741926_1_1



CID: EN300-741926_1_1

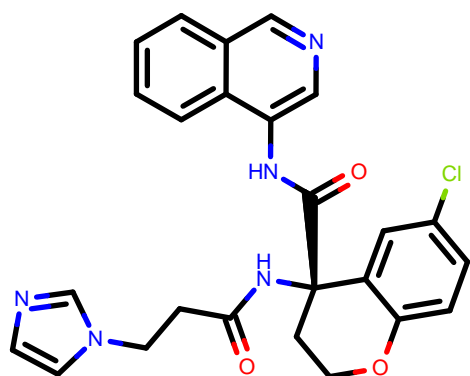
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CC[C@@]H1[C@@]H(C5)F)O

RUN: RUN10559

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.24

EN300-75342_1_1



CID: EN300-75342_1_1

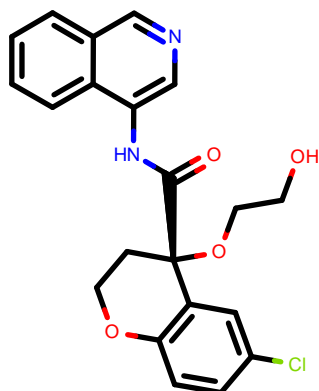
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnc5

RUN: RUN8921

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.23

EN300-21258_1_1



CID: EN300-21258_1_1

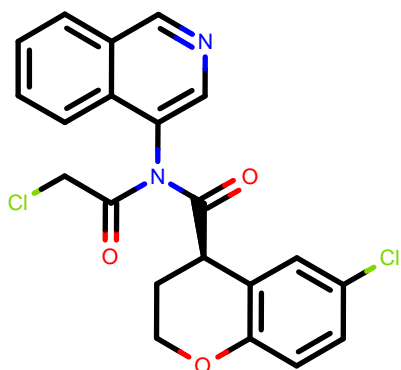
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO

RUN: RUN783

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.14

VLA-UCB-50c39ae8-6_1



CID: VLA-UCB-50c39ae8-6_1

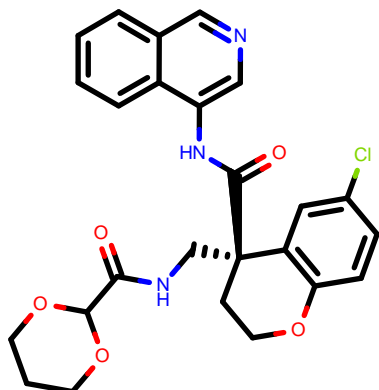
SMILES: c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN149

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.18

EN300-170985_2_1



CID: EN300-170985_2_1

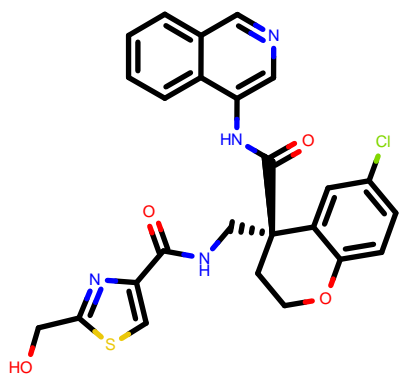
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5OCCCO5

RUN: RUN7425

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.21

EN300-250112_2_1



CID: EN300-250112_2_1

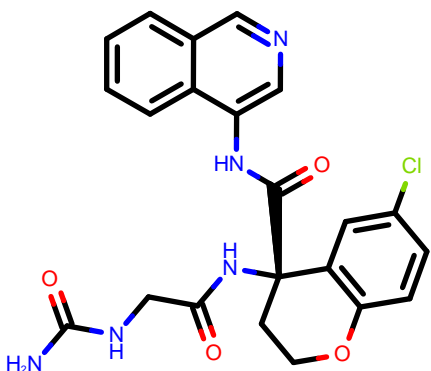
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cscc(n5)CO

RUN: RUN3127

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.24

EN300-10397_1_1



CID: EN300-10397_1_1

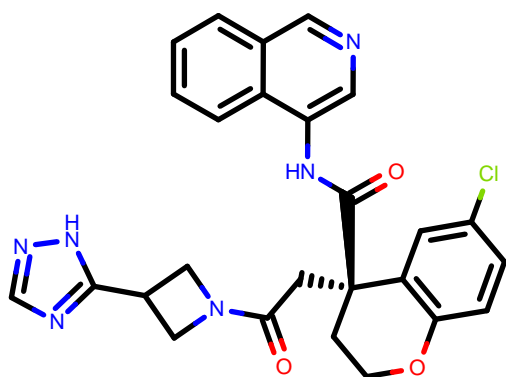
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N

RUN: RUN6668

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.20

EN300-1707980_1_1



CID: EN300-1707980_1_1

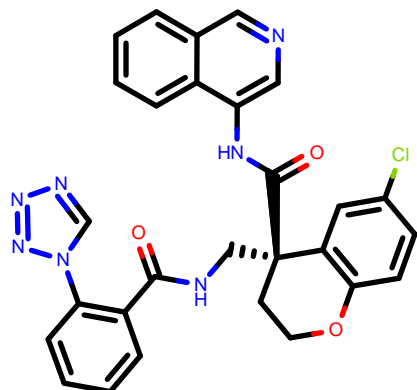
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)c6[nH]ncn6

RUN: RUN9993

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.20

EN300-09325_2_1



CID: EN300-09325_2_1

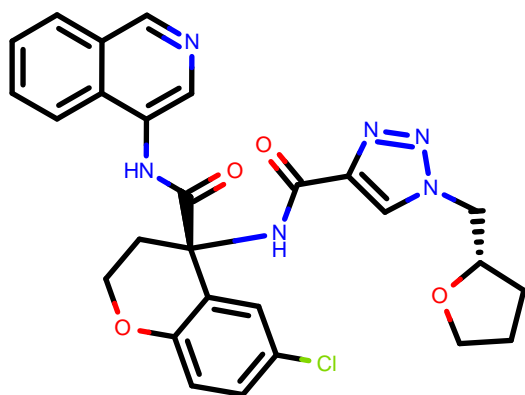
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccccc5n6c7cn[nH]7

RUN: RUN3859

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.28

EN300-368758_1_2



CID: EN300-368758_1_2

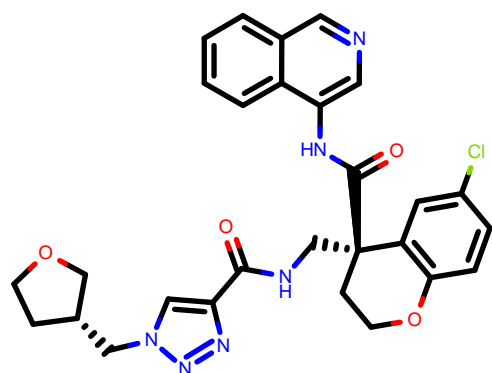
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)C[C@@H]6CCCC6

RUN: RUN1553

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.23

EN300-317272_2_1



CID: EN300-317272_2_1

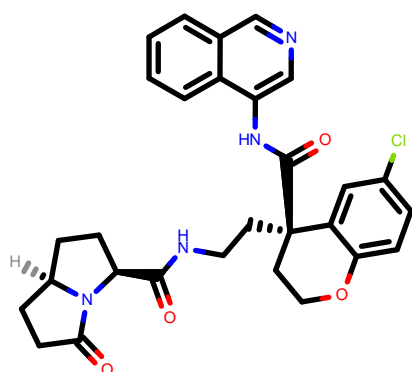
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)C[C@@H]6CCCC6

RUN: RUN9358

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.27

EN300-6479181_3_3



CID: EN300-6479181_3_3

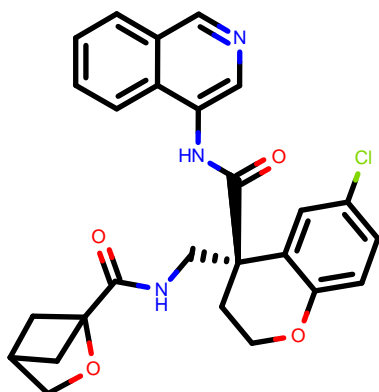
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC[C@@H]6N5C(=O)CC6

RUN: RUN15254

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.26

EN300-2007648_2_1



CID: EN300-2007648_2_1

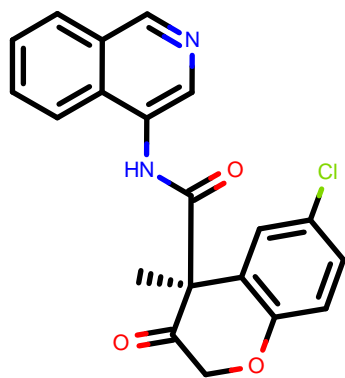
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CC(C5)CC6

RUN: RUN4927

DDG (kcal/mol): -0.81

dDDG (kcal/mol): 0.21

VLA-UCB-1dbca3b4-14_2



CID: VLA-UCB-1dbca3b4-14_2

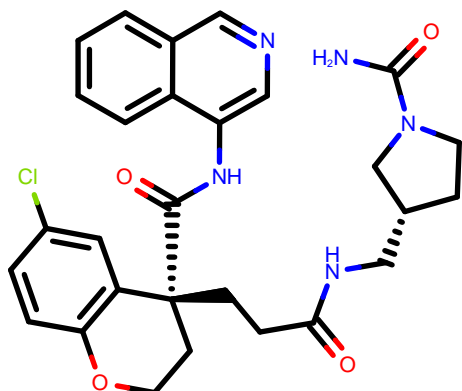
SMILES: C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN70

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.09

EN300-210933_2_2



CID: EN300-210933_2_2

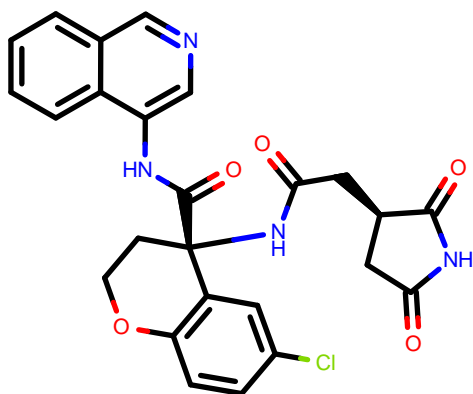
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCN(C5)C(=O)N

RUN: RUN11684

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.26

EN300-227055_1_2



CID: EN300-227055_1_2

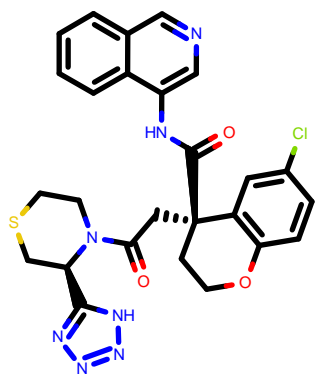
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC(=O)NC5=O

RUN: RUN3850

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.23

EN300-141254_1_2



CID: EN300-141254_1_2

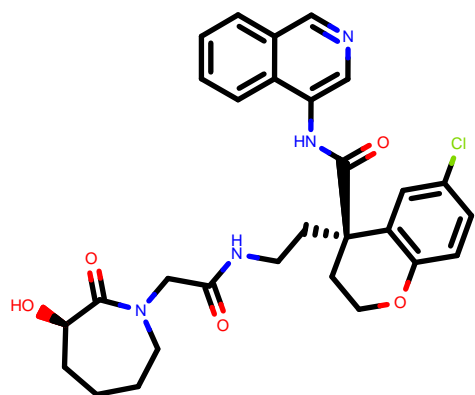
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCSC[C@@H]5c6nfn-}n6

RUN: RUN13092

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.29

EN300-259849_3_1



CID: EN300-259849_3_1

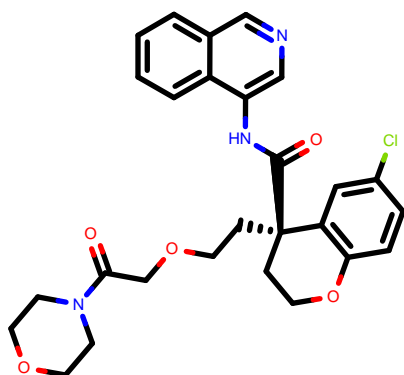
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CN5CCCC[C@H](C5=O)O

RUN: RUN12944

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.29

EN300-1241327_3_1



CID: EN300-1241327_3_1

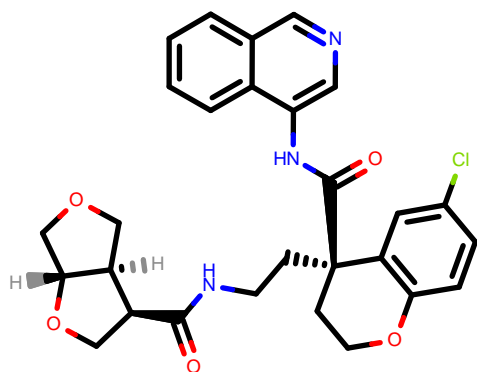
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)N5COCC5

RUN: RUN2262

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.25

EN300-6482296_3_6



CID: EN300-6482296_3_6

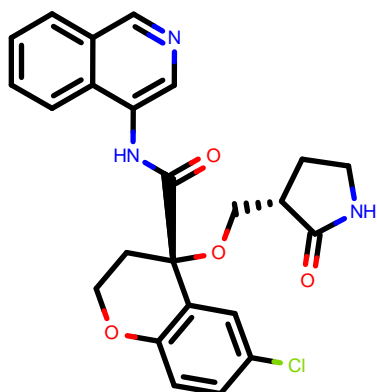
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5COC[C@H]6[C@@H]5COC6

RUN: RUN15112

DDG (kcal/mol): -0.80

dDDG (kcal/mol): 0.23

EN300-246248_1_2



CID: EN300-246248_1_2

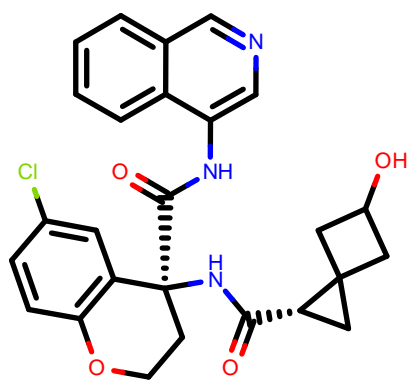
SMILES: c1ccc2c(c1)nc(=O)N[C@@]3(CCOc4c3cc(cc4)C)OC[C@H]5CCNC5=O

RUN: RUN1908

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.24

EN300-1717166_1_2



CID: EN300-1717166_1_2

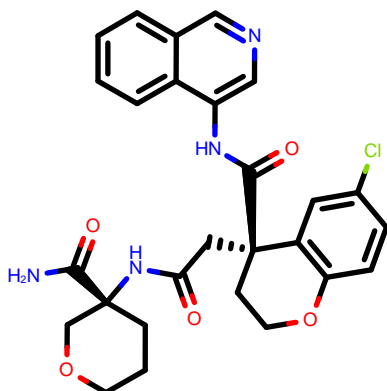
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CC56CC(C6)O

RUN: RUN8809

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.21

EN300-120255_1_2



CID: EN300-120255_1_2

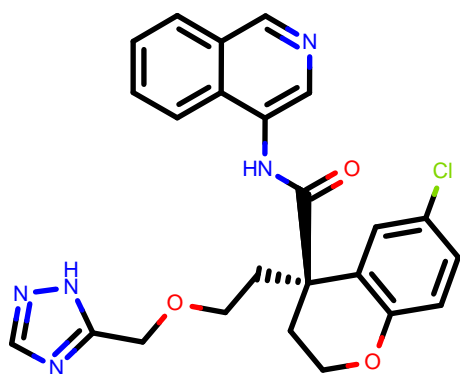
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5(CCCOC5)C(=O)N

RUN: RUN11980

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.28

EN300-306316_3_1



CID: EN300-306316_3_1

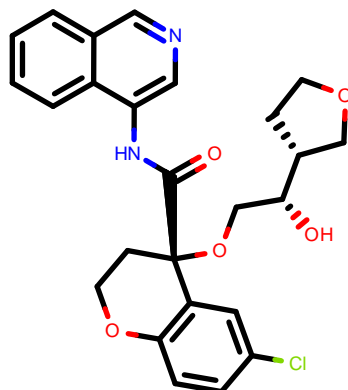
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC5[nH]ncn5

RUN: RUN1632

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.18

EN300-1911992_1_1



CID: EN300-1911992_1_1

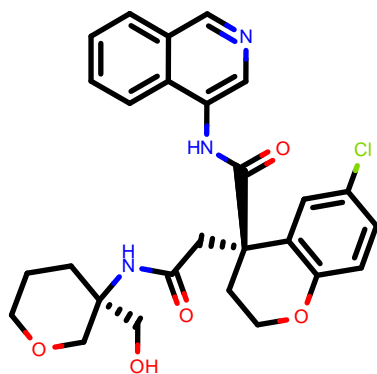
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@H](C@@H)5CCOC5)O

RUN: RUN2107

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.33

EN300-2969289_1_2



CID: EN300-2969289_1_2

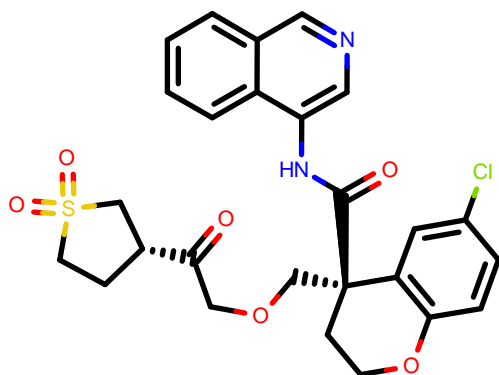
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CCCOC5)CO

RUN: RUN11924

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.36

EN300-226314_2_1



CID: EN300-226314_2_1

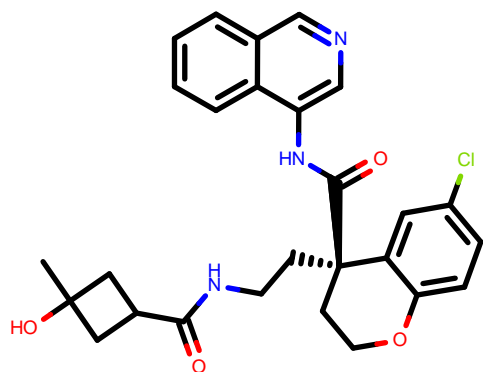
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)[C@@H]5CCS(=O)(=O)C5

RUN: RUN284

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.30

EN300-7183657_3_1



CID: EN300-7183657_3_1

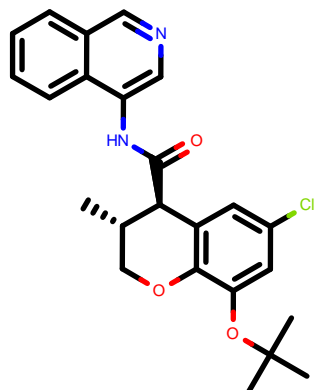
SMILES: C[C@@]1(C[C@@H](C1)C(=O)NCC[C@@]2(c3c(ccc(c3)Cl)OCC2)C(=O)Nc4c5c(nc4)ccc5)O

RUN: RUN14922

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.23

DAR-DIA-0d514e7d-19_1



CID: DAR-DIA-0d514e7d-19_1

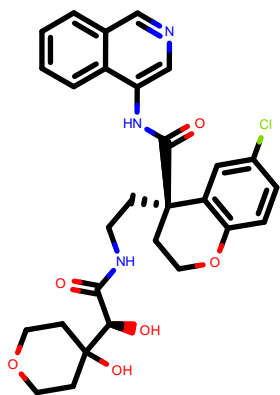
SMILES: C[C@@H]1COc2c(cc2OC(C)C)C1[C@@H]1C(=O)Nc3ncc4c3cccc4

RUN: RUN161

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.17

EN300-749499_3_2



CID: EN300-749499_3_2

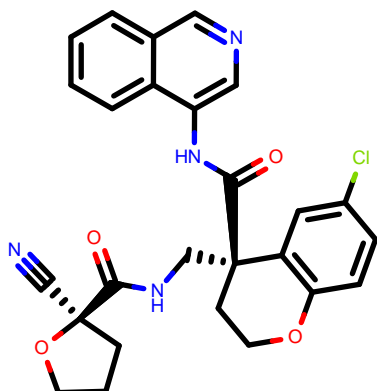
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5(CCCOC5)O)O

RUN: RUN705

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.32

EN300-3710141_2_1



CID: EN300-3710141_2_1

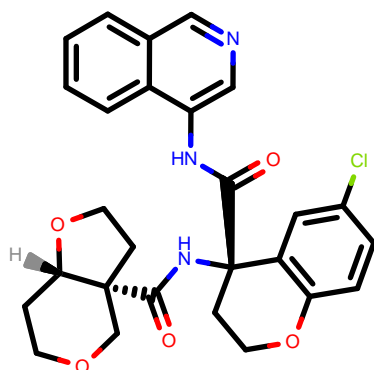
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCCOC5)C#N

RUN: RUN6043

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.22

EN300-341337_1_4



CID: EN300-341337_1_4

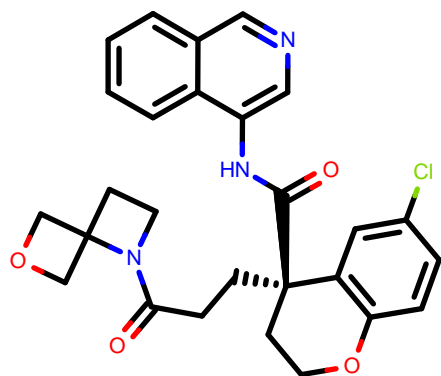
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCO[C@H]5CCOC6

RUN: RUN8172

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.26

EN300-247468_2_1



CID: EN300-247468_2_1

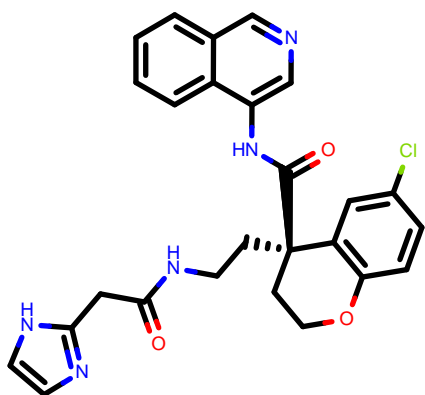
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC5COC6

RUN: RUN10664

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.25

EN300-220527_3_1



CID: EN300-220527_3_1

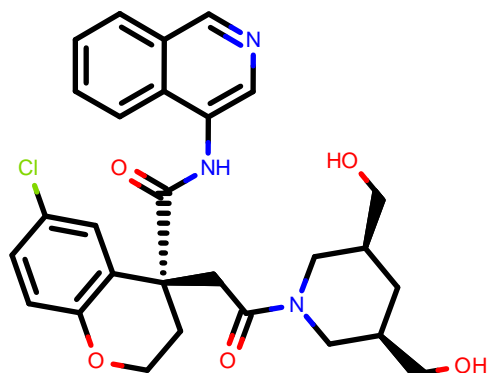
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5[nH]cn5

RUN: RUN15232

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.24

EN300-2007627_1_2



CID: EN300-2007627_1_2

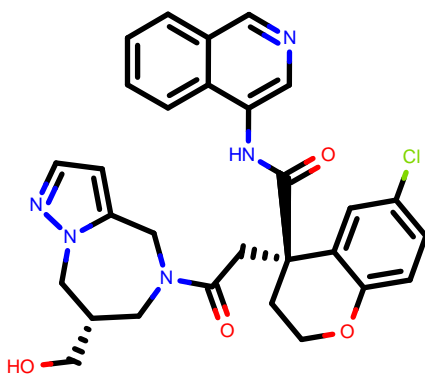
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N5C[C@@H](C)[C@@H](C5)CO

RUN: RUN1151

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.27

EN300-6739414_1_2



CID: EN300-6739414_1_2

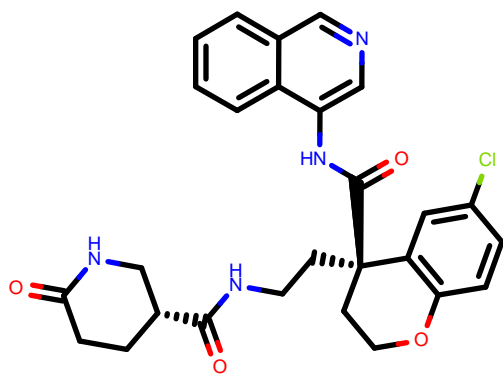
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6c6cnn6[C@H](C5)CO

RUN: RUN3737

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.23

EN300-42819_3_1



CID: EN300-42819_3_1

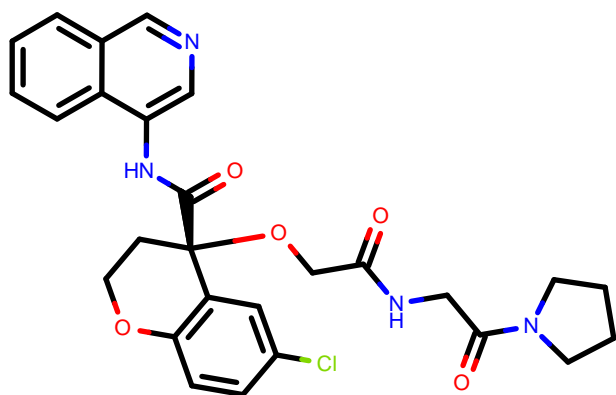
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCC(=O)NCS

RUN: RUN14728

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.31

EN300-28340_1_1



CID: EN300-28340_1_1

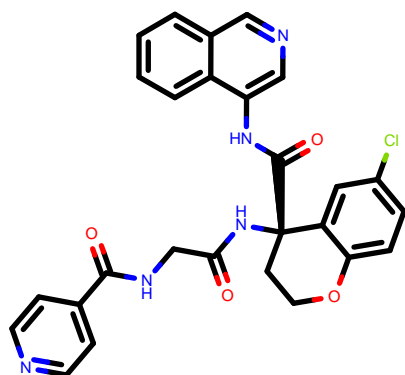
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCC(=O)N5CCCC5

RUN: RUN735

DDG (kcal/mol): -0.79

dDDG (kcal/mol): 0.35

EN300-36089_1_1



CID: EN300-36089_1_1

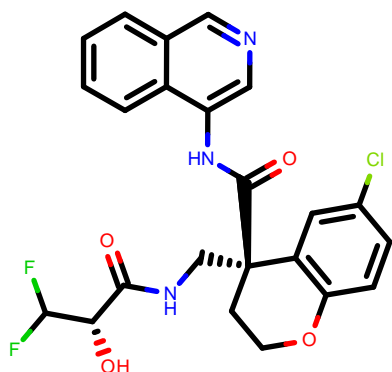
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Nc5ccncc5

RUN: RUN9826

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.24

EN300-1932780_2_1



CID: EN300-1932780_2_1

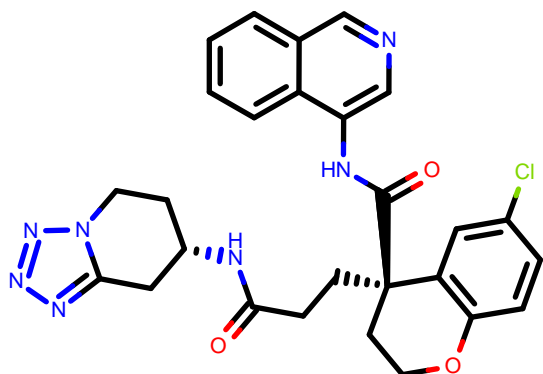
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H(C(F)F)O

RUN: RUN2748

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.25

EN300-7438451_2_1



CID: EN300-7438451_2_1

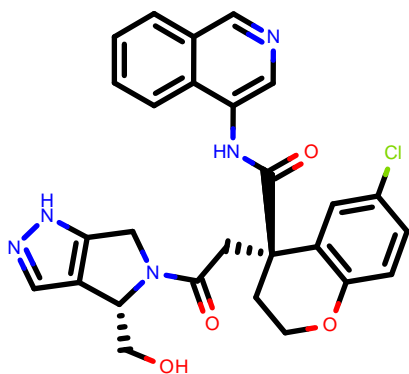
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCn6c(nnn6)C5

RUN: RUN6307

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.23

EN300-1666341_1_2



CID: EN300-1666341_1_2

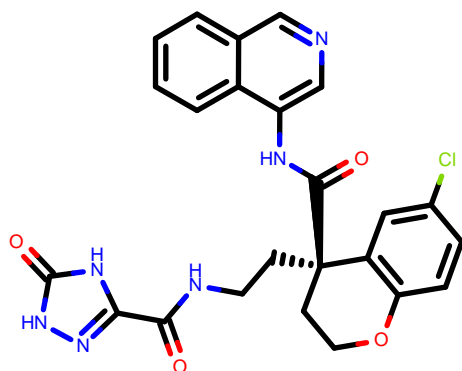
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cc6c(c[nH]6)C@H5CO

RUN: RUN5781

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.31

EN300-35843_3_1



CID: EN300-35843_3_1

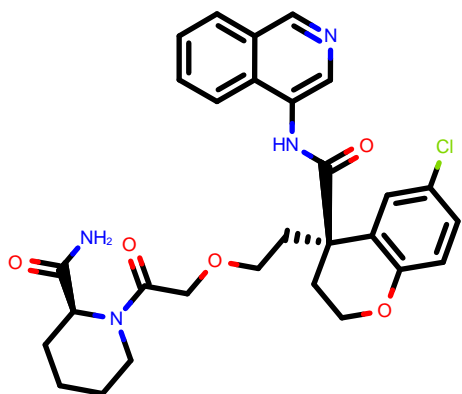
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5[nH]c([nH])n5

RUN: RUN15440

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

EN300-22879_3_1



CID: EN300-22879_3_1

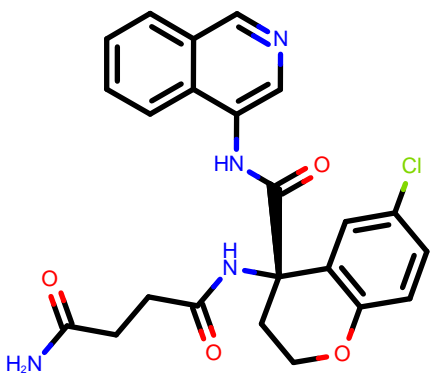
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN674

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.32

EN300-178515_1_1



CID: EN300-178515_1_1

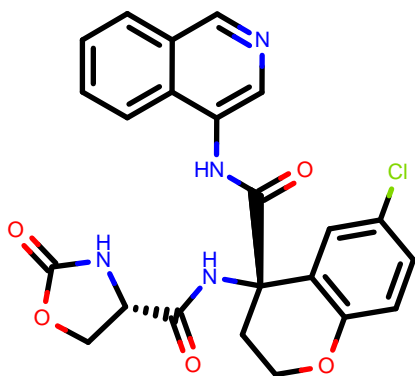
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCC(=O)N

RUN: RUN3610

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.27

EN300-201346_1_1



CID: EN300-201346_1_1

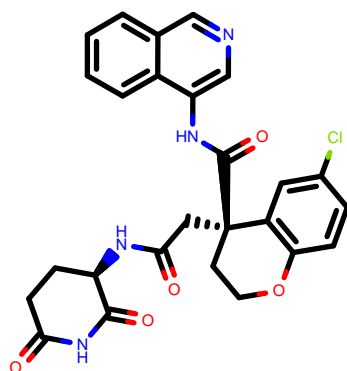
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5COC(=O)N5

RUN: RUN763

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.19

EN300-113633_1_2



CID: EN300-113633_1_2

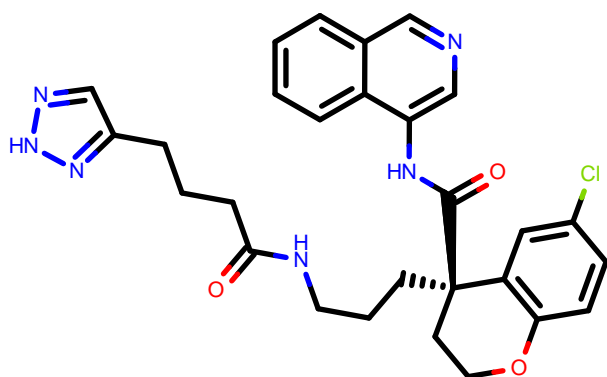
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCCC(=O)NCS=O

RUN: RUN12988

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.19

EN300-156995_4_1



CID: EN300-156995_4_1

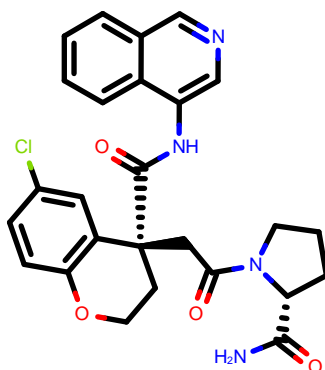
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCCc5en[nH]n5

RUN: RUN11504

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-07127_1_2



CID: EN300-07127_1_2

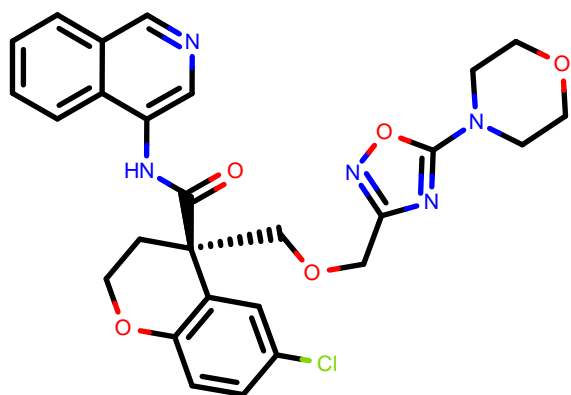
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC[C@@H]5C(=O)N

RUN: RUN5513

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.21

EN300-1608590_2_1



CID: EN300-1608590_2_1

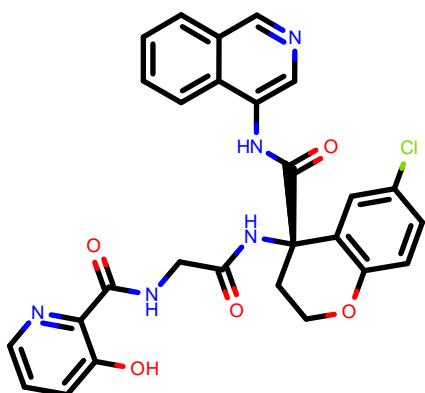
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCc5nc(on5)N6CCOCC6

RUN: RUN2719

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.24

EN300-115421_1_1



CID: EN300-115421_1_1

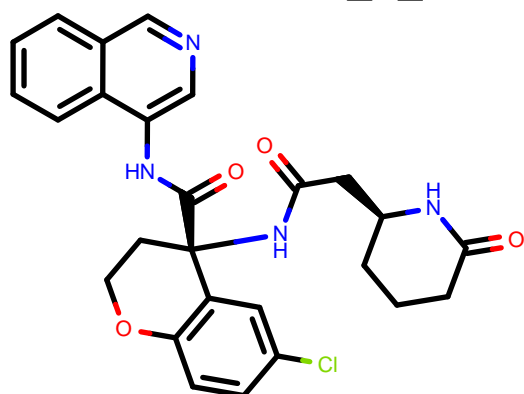
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)c5c(cccn5)O

RUN: RUN9625

DDG (kcal/mol): -0.78

dDDG (kcal/mol): 0.30

EN300-210084_1_2



CID: EN300-210084_1_2

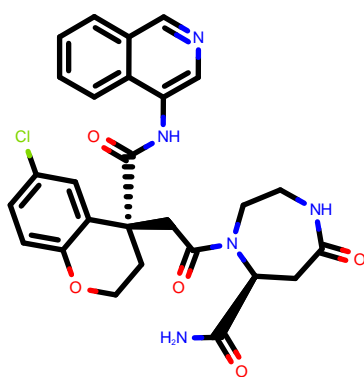
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[C@@]4H5CCCC(=O)N5

RUN: RUN5626

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.30

EN300-7356782_1_1



CID: EN300-7356782_1_1

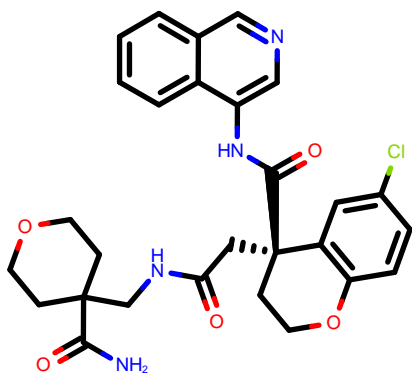
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)C[C@@]4H5C(=O)N4

RUN: RUN10499

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.28

EN300-36931_1_1



CID: EN300-36931_1_1

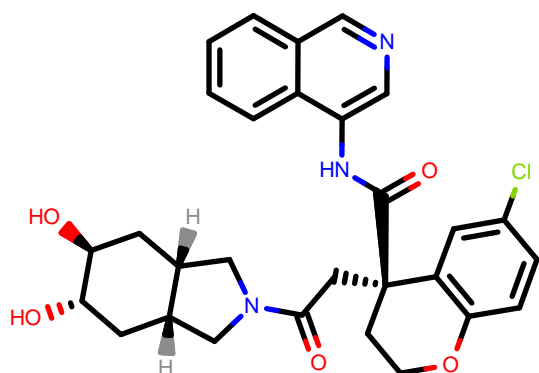
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CC(=O)NCC5(C(COCC5)C(=O)N

RUN: RUN13220

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.26

EN300-7355477_1_2



CID: EN300-7355477_1_2

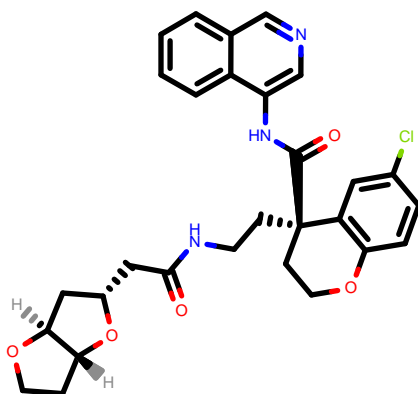
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)O)CC(=O)N5C[C@@H]6C[C@@H]7C[C@@H]6C5O)O

RUN: RUN1471

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.30

EN300-7355519_3_7



CID: EN300-7355519_3_7

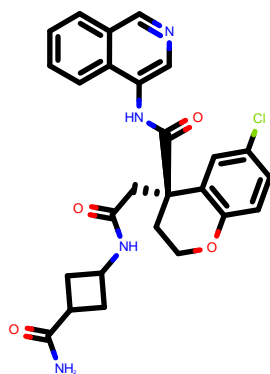
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)O)CC(=O)N5C[C@@H]6C[C@@H]7C[C@@H]6C5O)O

RUN: RUN14724

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.29

EN300-266565_1_1



CID: EN300-266565_1_1

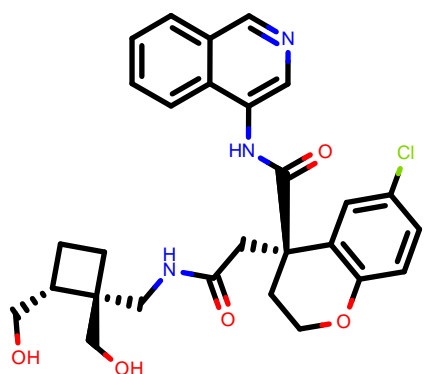
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]4COCc4c3cc(cc4)C)CC(=O)N5C5CC(C5)C(=O)N

RUN: RUN9304

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.21

EN300-1692359_1_2



CID: EN300-1692359_1_2

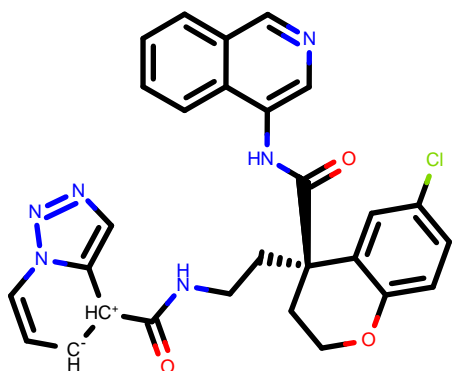
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@]5(C)C[C@H]5CO

RUN: RUN9997

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.27

EN300-1074262_3_1



CID: EN300-1074262_3_1

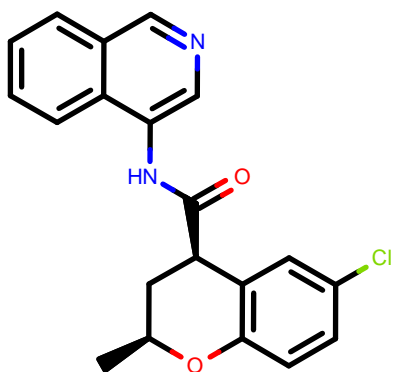
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cccn6c5nn6

RUN: RUN15021

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.24

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

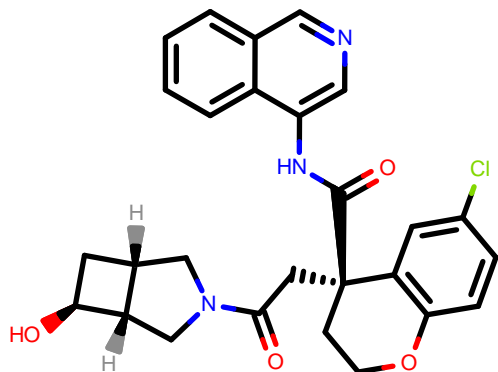
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN83

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.09

EN300-305294_1_5



CID: EN300-305294_1_5

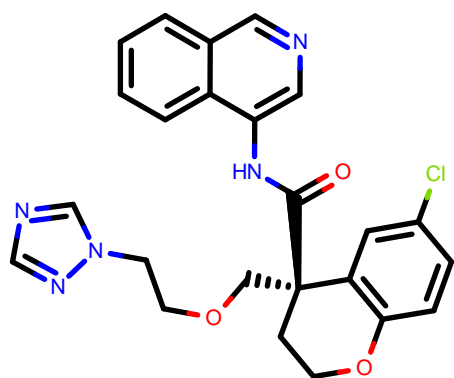
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@]5(C)C[C@H]5CO

RUN: RUN5885

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.22

EN300-6255179_2_1



CID: EN300-6255179_2_1

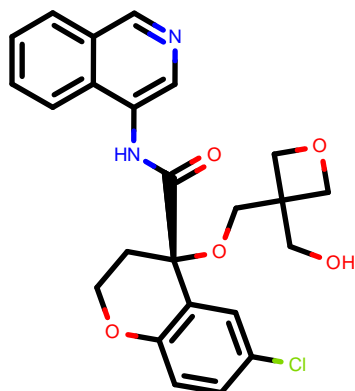
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5ncnc5

RUN: RUN732

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.17

EN300-102347_1_1



CID: EN300-102347_1_1

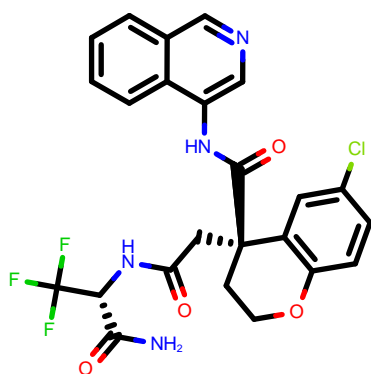
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5(COC5)CO

RUN: RUN943

DDG (kcal/mol): -0.77

dDDG (kcal/mol): 0.21

EN300-6763470_1_2



CID: EN300-6763470_1_2

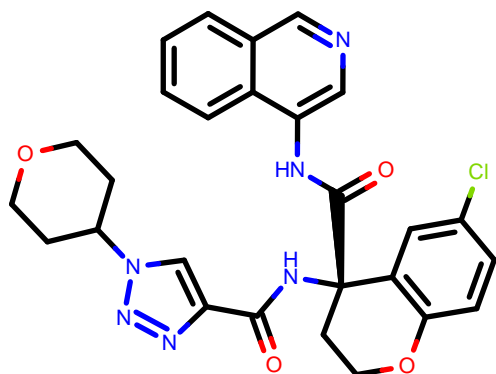
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](C(=O)N)C(F)(F)F

RUN: RUN14158

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-215968_1_1



CID: EN300-215968_1_1

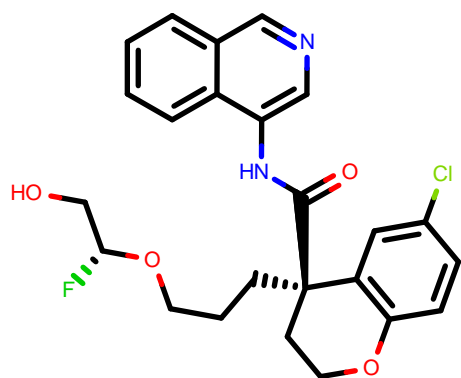
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C6CCOCC6

RUN: RUN3250

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-861925_4_2



CID: EN300-861925_4_2

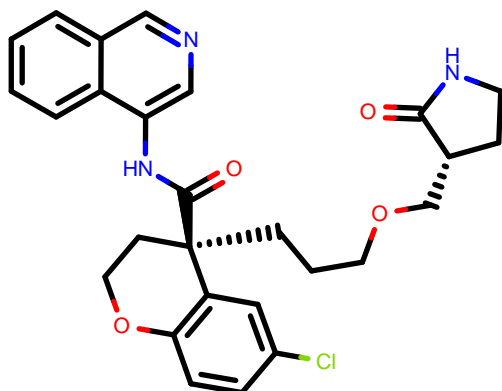
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)C)CCCO[C@@H](CO)F

RUN: RUN1826

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.21

EN300-246248_4_1



CID: EN300-246248_4_1

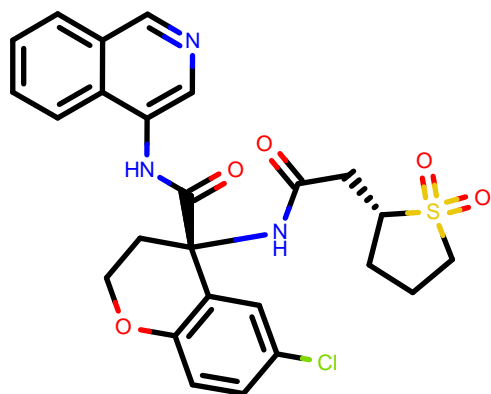
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)C)CCOC[C@@H]5CCNC5=O

RUN: RUN1890

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.25

EN300-155176_1_1



CID: EN300-155176_1_1

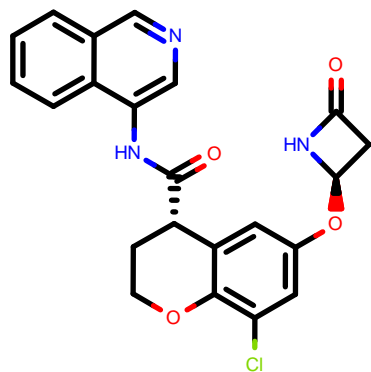
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)C)NC(=O)C[C@@H]5CCCS5(=O)=O

RUN: RUN8192

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.28

FRA-DIA-b66f7109-3_1



CID: FRA-DIA-b66f7109-3_1

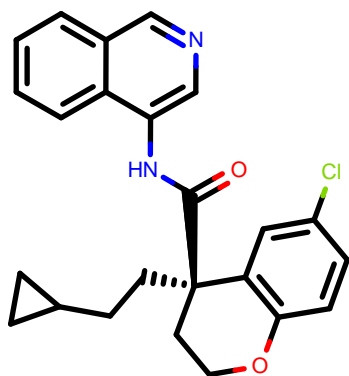
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)O)C[C@@H]5CC(=O)N5

RUN: RUN167

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

ALP-POS-477dc5b7-3_1



CID: ALP-POS-477dc5b7-3_1

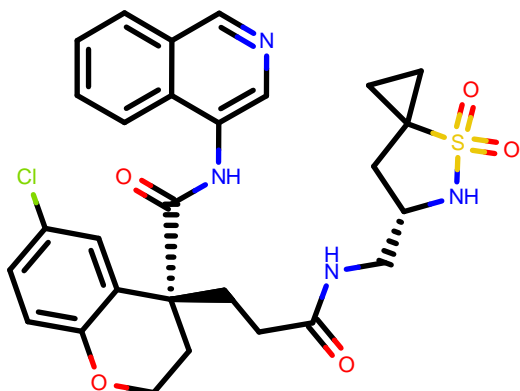
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC5CC5

RUN: RUN37

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.15

EN300-7431620_2_2



CID: EN300-7431620_2_2

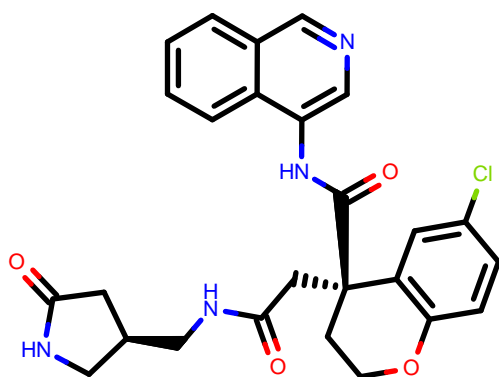
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(C)CC6(S(=O)(=O)N)C65

RUN: RUN13355

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.32

EN300-238405_1_1



CID: EN300-238405_1_1

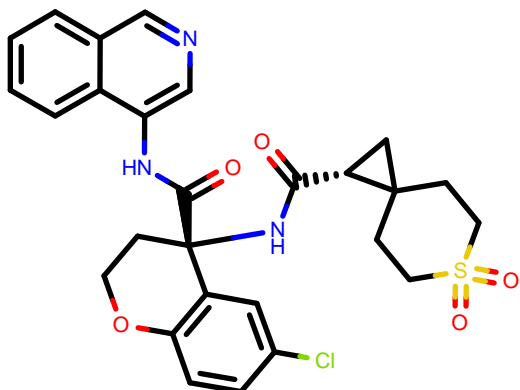
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(C)CC(=O)N5

RUN: RUN10051

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.20

EN300-141809_1_1



CID: EN300-141809_1_1

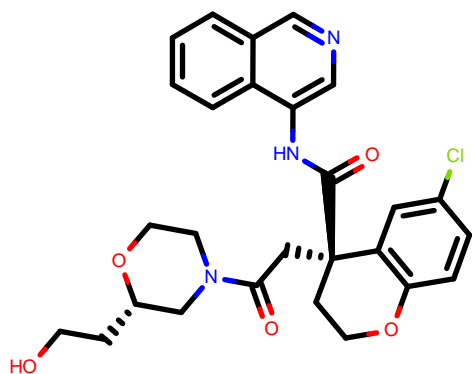
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(C)CC6(S(=O)(=O)N)C65

RUN: RUN9661

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.28

EN300-102007_1_2



CID: EN300-102007_1_2

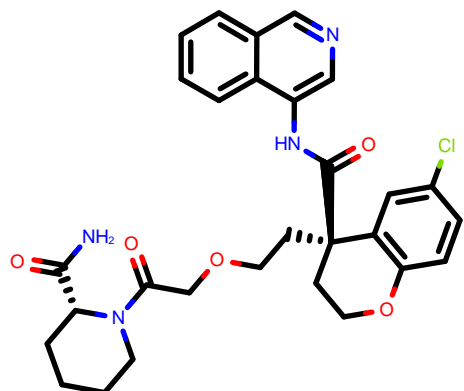
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CCO

RUN: RUN6264

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.22

EN300-22879_3_2



CID: EN300-22879_3_2

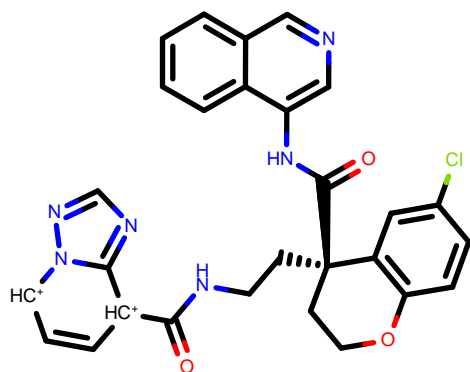
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC[C@H]5Cl=O

RUN: RUN754

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.30

EN300-366857_3_1



CID: EN300-366857_3_1

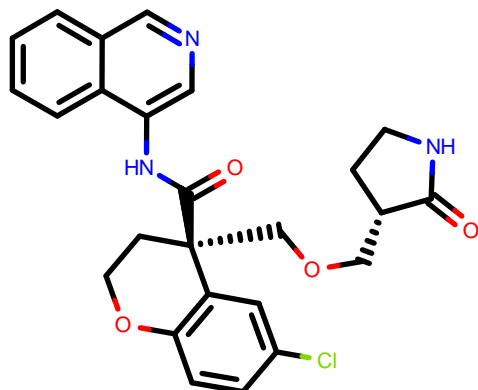
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cccn6c5ncn6

RUN: RUN15185

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.25

EN300-246248_2_2



CID: EN300-246248_2_2

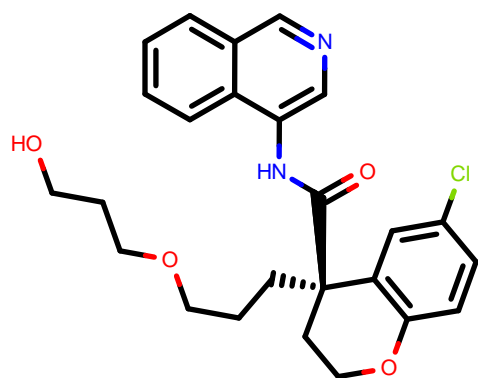
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNC5=O

RUN: RUN620

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.23

EN300-221518_4_1



CID: EN300-221518_4_1

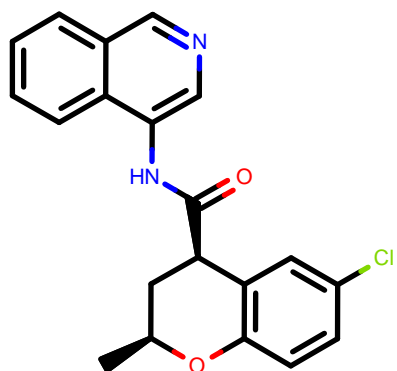
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCCOCCO

RUN: RUN701

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.21

ALP-POS-d3acb8cc-4_1



CID: ALP-POS-d3acb8cc-4_1

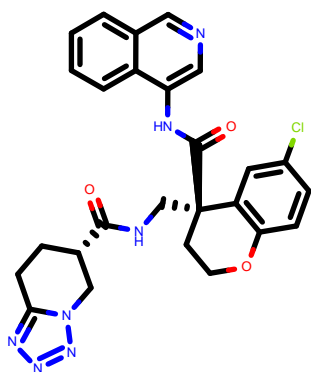
SMILES: C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN82

DDG (kcal/mol): -0.76

dDDG (kcal/mol): 0.08

EN300-269453_2_2



CID: EN300-269453_2_2

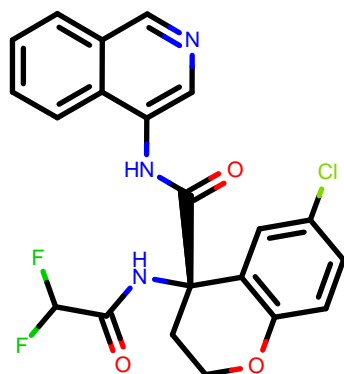
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCc6nnnn6C5

RUN: RUN5947

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.25

EN300-19507_1_1



CID: EN300-19507_1_1

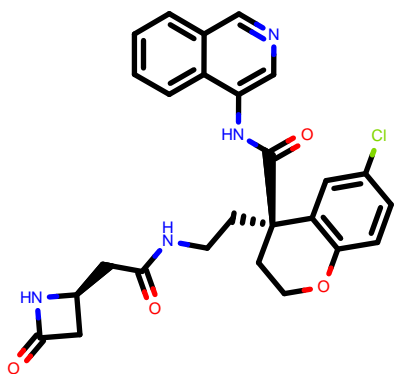
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(F)F

RUN: RUN5402

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.14

EN300-250593_3_1



CID: EN300-250593_3_1

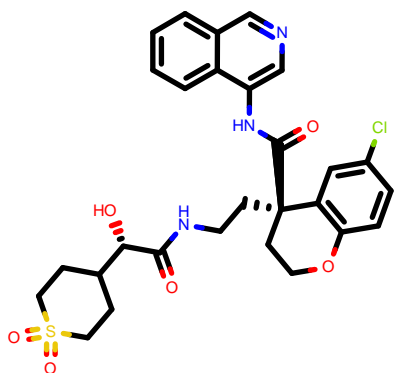
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CC(=O)N5

RUN: RUN15087

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.34

EN300-210907_3_2



CID: EN300-210907_3_2

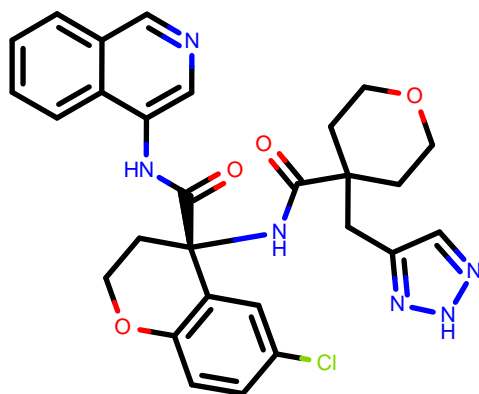
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H](CS(=O)(=O)O)C5O

RUN: RUN2640

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.30

EN300-1716880_1_1



CID: EN300-1716880_1_1

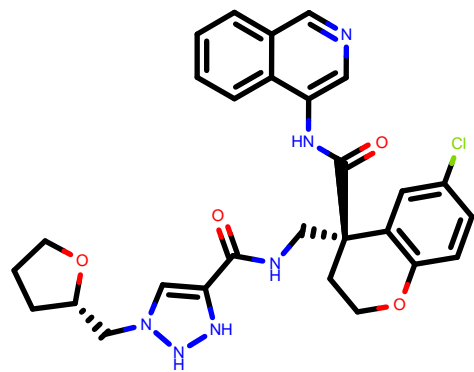
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)C6cn[nH]n6

RUN: RUN8268

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.27

EN300-368758_2_2



CID: EN300-368758_2_2

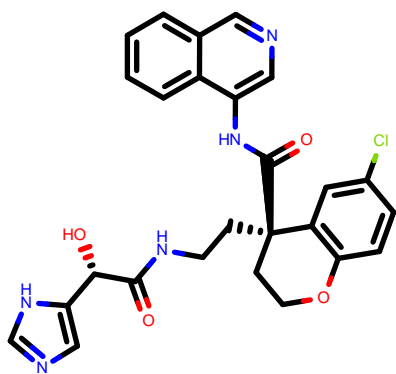
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]n5C[C@H]6CCCO6

RUN: RUN9334

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.28

EN300-254121_3_1



CID: EN300-254121_3_1

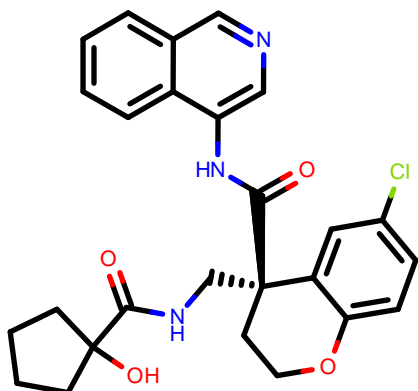
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOC4C3cc(cc4)Cl)CCNC(=O)[C@H](c5cn[nH]5)O

RUN: RUN7583

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.30

EN300-25960_2_1



CID: EN300-25960_2_1

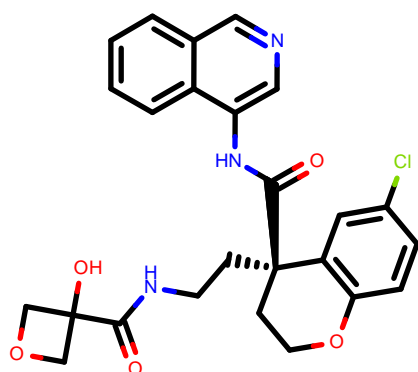
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](COC4C3cc(cc4)Cl)CNC(=O)C5(CCCC5)O

RUN: RUN2528

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.26

EN300-101443_3_1



CID: EN300-101443_3_1

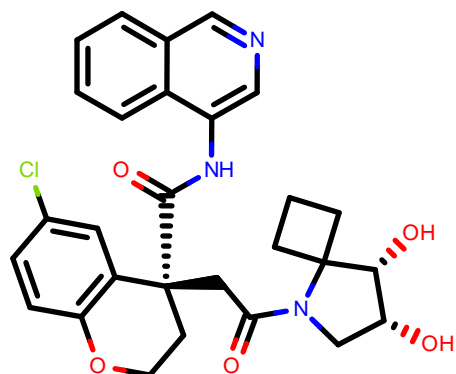
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](COC4C3cc(cc4)Cl)CNC(=O)C5(COC5)O

RUN: RUN9072

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.20

EN300-7444121_1_1



CID: EN300-7444121_1_1

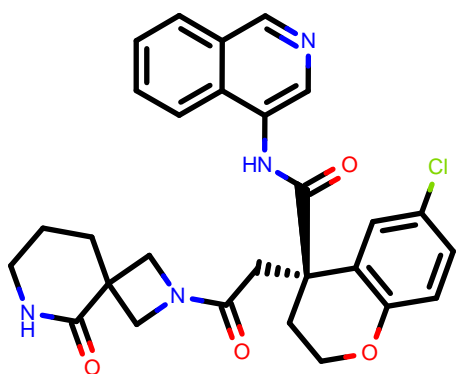
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](COC4C3cc(cc4)Cl)CC(O)N[C@@H](C@H)(C)C5(C)C5O

RUN: RUN4409

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.28

EN300-6763045_1_1



CID: EN300-6763045_1_1

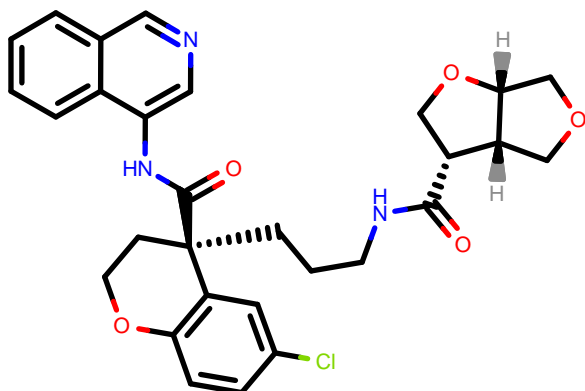
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CCNC6=O

RUN: RUN14092

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.28

EN300-6482296_4_1



CID: EN300-6482296_4_1

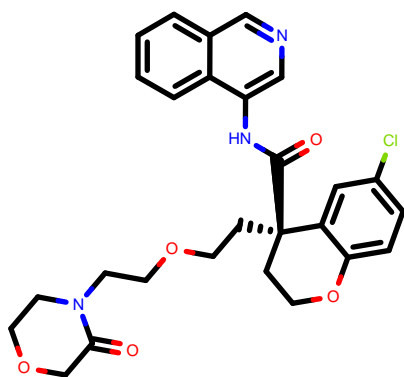
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(C)C[C@@H]6C[C@H]5CO6

RUN: RUN13399

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.30

EN300-219330_3_1



CID: EN300-219330_3_1

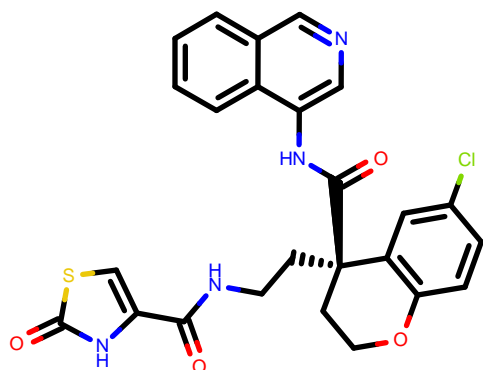
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOCC5=O

RUN: RUN2322

DDG (kcal/mol): -0.75

dDDG (kcal/mol): 0.28

EN300-133915_3_1



CID: EN300-133915_3_1

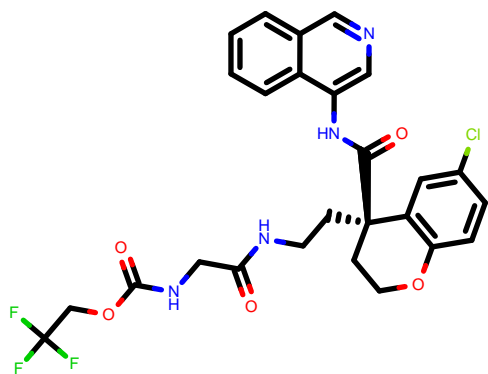
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5csc(=O)[nH]5

RUN: RUN15391

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-50488_3_1



CID: EN300-50488_3_1

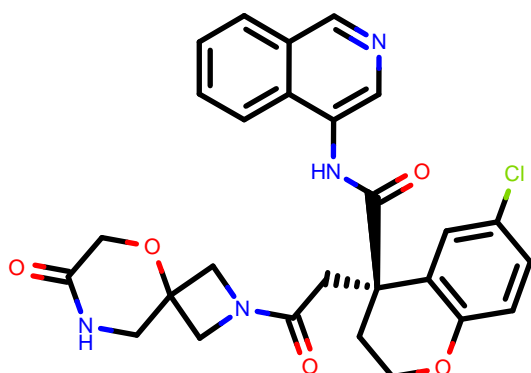
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)OCC(F)(F)F

RUN: RUN11956

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.26

EN300-7430372_1_1



CID: EN300-7430372_1_1

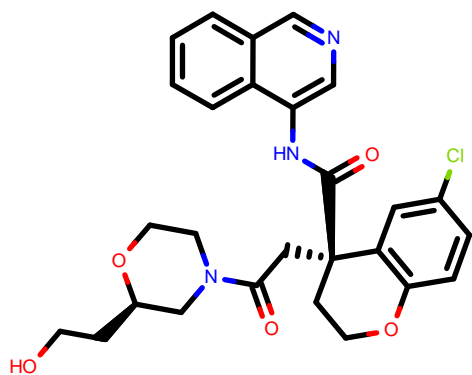
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CNC(=O)CO6

RUN: RUN11269

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-102007_1_1



CID: EN300-102007_1_1

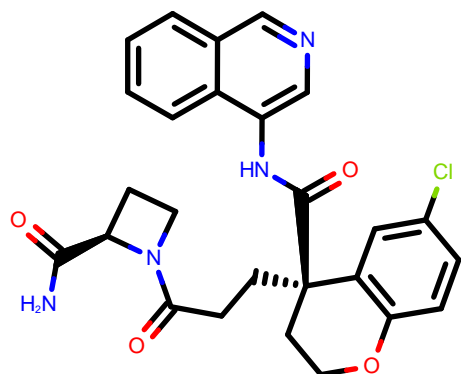
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CO

RUN: RUN11491

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-862094_2_2



CID: EN300-862094_2_2

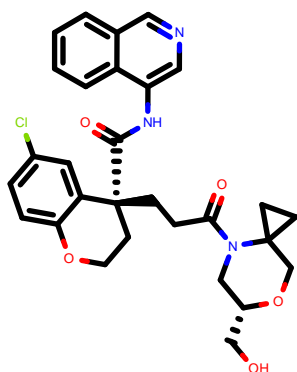
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](C5)C(=O)N

RUN: RUN6630

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.24

EN300-7493255_2_1



CID: EN300-7493255_2_1

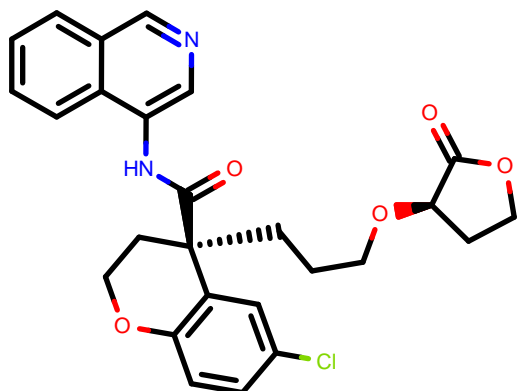
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](O)COC3C(=O)N5C[C@H](OCC56C6)CO

RUN: RUN3028

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.35

EN300-20496_4_2



CID: EN300-20496_4_2

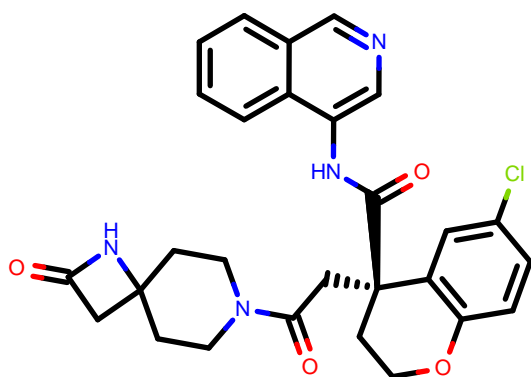
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](O)COC3C(=O)N5C[C@H](O)CC5=O

RUN: RUN1771

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.22

EN300-52210_1_1



CID: EN300-52210_1_1

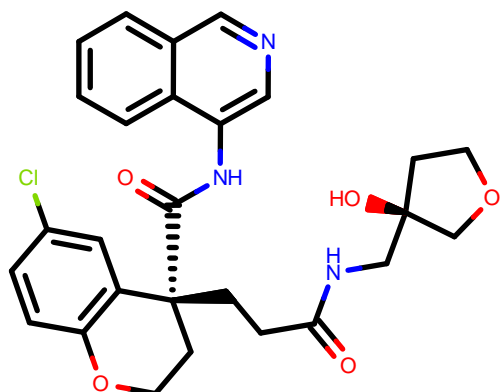
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](O)COC3C(=O)N5C[C@H](O)CC5=O

RUN: RUN10507

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.25

EN300-200699_2_1



CID: EN300-200699_2_1

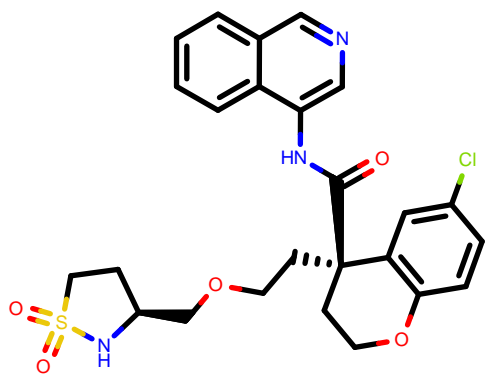
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@H](O)COC3C(=O)N5C[C@H](O)CC5=O

RUN: RUN1174

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.32

EN300-1699871_3_2



CID: EN300-1699871_3_2

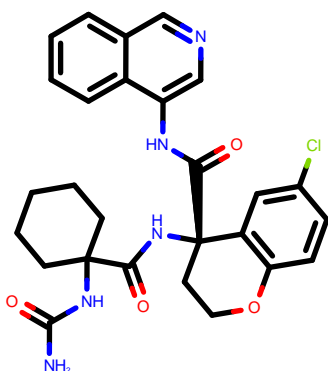
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)N5

RUN: RUN2190

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.26

EN300-78368_1_1



CID: EN300-78368_1_1

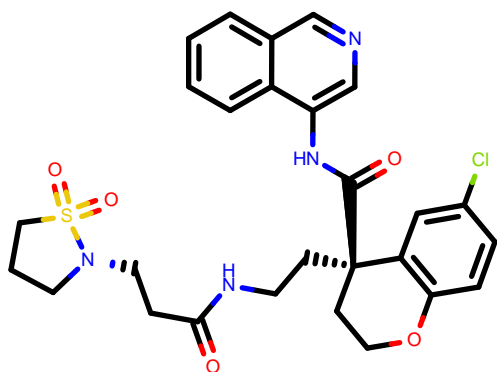
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCC5)NC(=O)N

RUN: RUN8008

DDG (kcal/mol): -0.74

dDDG (kcal/mol): 0.25

EN300-44873_3_1



CID: EN300-44873_3_1

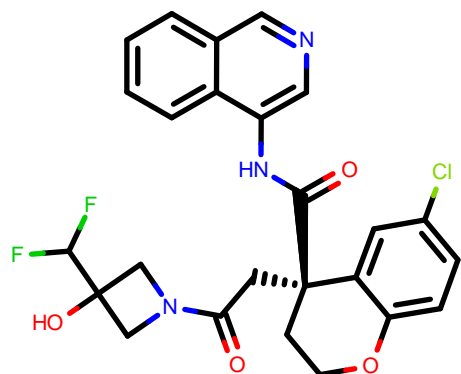
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[N@]5CCCS(=O)=O

RUN: RUN12006

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.42

EN300-249245_1_1



CID: EN300-249245_1_1

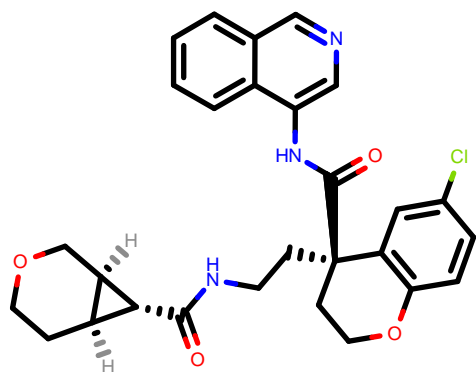
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C(F)F)O

RUN: RUN10649

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.25

EN300-1644723_3_5



CID: EN300-1644723_3_5

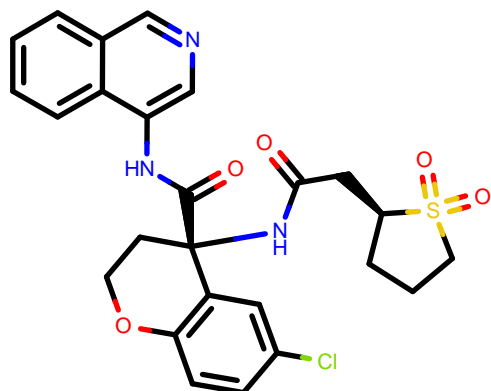
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3(C)CCOC4C3CC(=O)C(C)CCNC(=O)C@H5[C@@H]6C@H5COCC6

RUN: RUN14226

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.23

EN300-155176_1_2



CID: EN300-155176_1_2

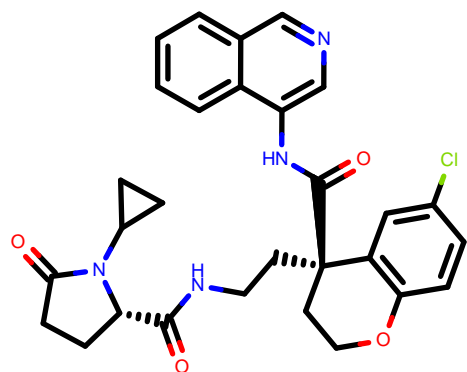
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3(C)CCOC4C3CC(=O)C(C)CCNC(=O)C@H5[C@@H]6C@H5COCC6(=O)=O

RUN: RUN5478

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.36

EN300-3044054_3_1



CID: EN300-3044054_3_1

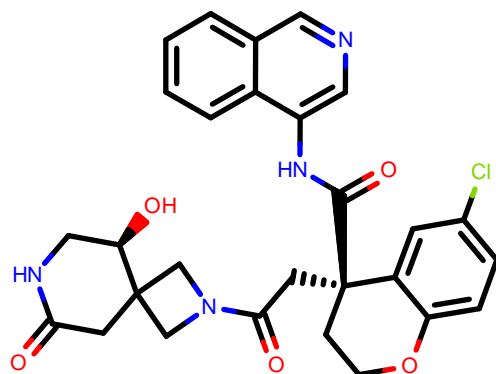
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3(C)CCOC4C3CC(=O)C(C)CCNC(=O)C@H5[C@@H]6C@H5COCC6

RUN: RUN9100

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.27

EN300-821316_1_1



CID: EN300-821316_1_1

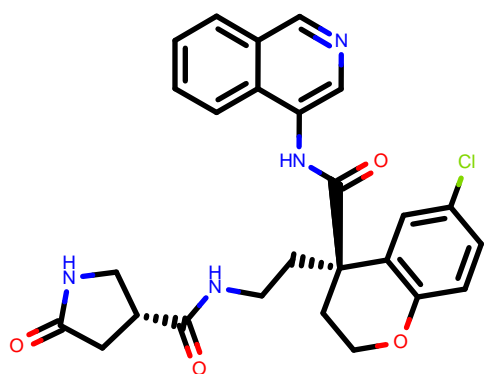
SMILES: c1ccc2c(c1)ncnc2NC(=O)C@3(C)CCOC4C3CC(=O)C(C)CC(=O)N5CC(=O)C(C)C(=O)N5C@H]6O

RUN: RUN13414

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.29

EN300-59487_3_1



CID: EN300-59487_3_1

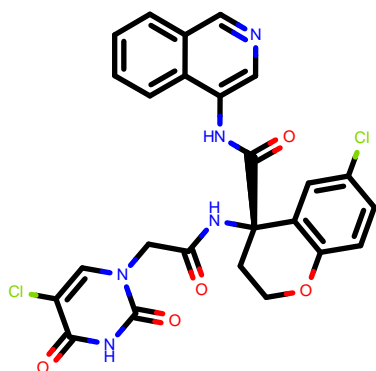
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)NC5

RUN: RUN441

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.23

EN300-6494606_1_1



CID: EN300-6494606_1_1

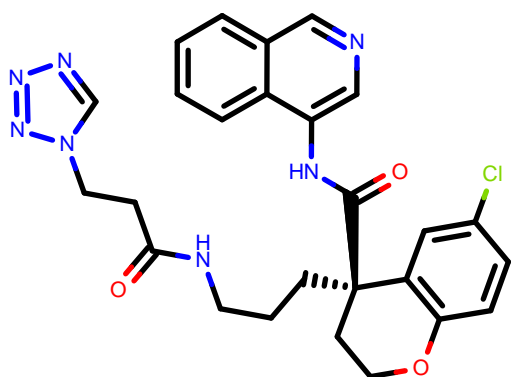
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(c(=O)[nH]5=O)Cl

RUN: RUN9820

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.23

EN300-191904_4_1



CID: EN300-191904_4_1

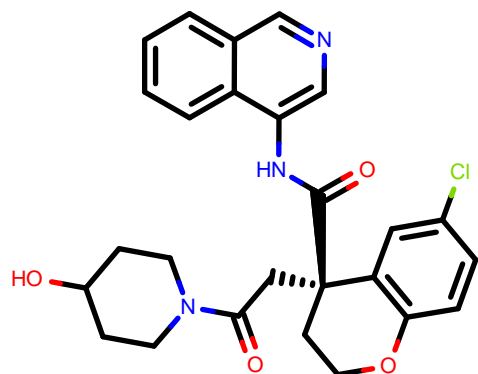
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5nnn5

RUN: RUN10588

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.27

EN300-379533_1_1



CID: EN300-379533_1_1

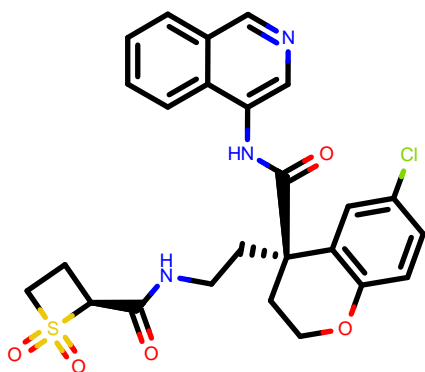
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)O

RUN: RUN5141

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.22

EN300-1387104_3_1



CID: EN300-1387104_3_1

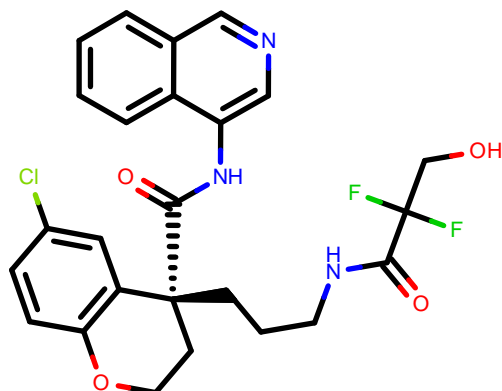
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCS5(=O)=O

RUN: RUN2865

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.25

EN300-123489_4_1



CID: EN300-123489_4_1

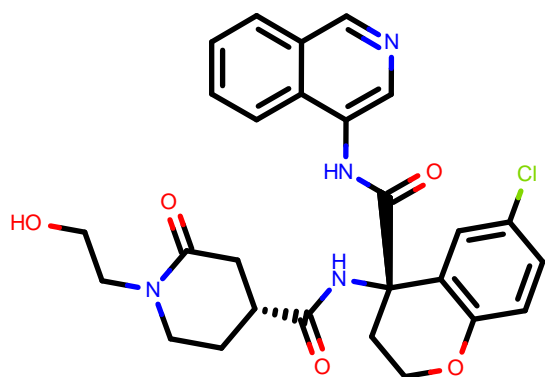
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(CO)(F)F

RUN: RUN7870

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.27

EN300-1723663_1_2



CID: EN300-1723663_1_2

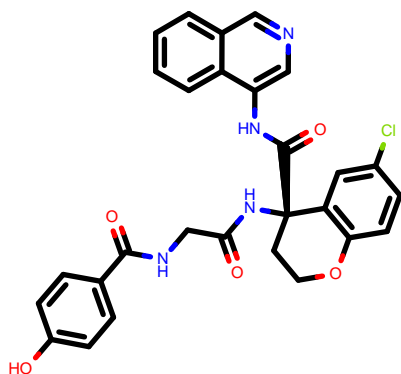
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCN(C(=O)C5)CCO

RUN: RUN8480

DDG (kcal/mol): -0.73

dDDG (kcal/mol): 0.29

EN300-66800_1_1



CID: EN300-66800_1_1

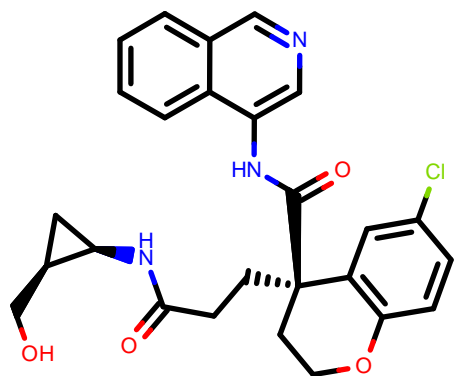
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5ccc(cc5)O

RUN: RUN9835

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.27

EN300-196962_2_1



CID: EN300-196962_2_1

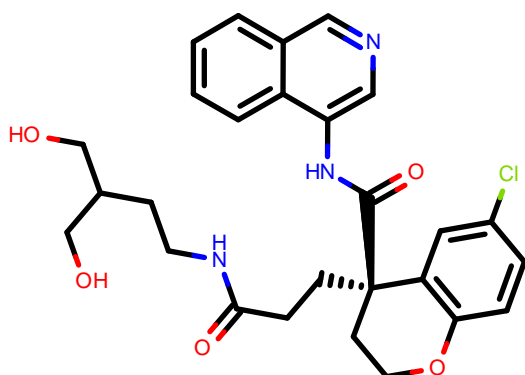
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]5H5C[C@@]5H5CO

RUN: RUN2446

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.25

EN300-1600613_2_1



CID: EN300-1600613_2_1

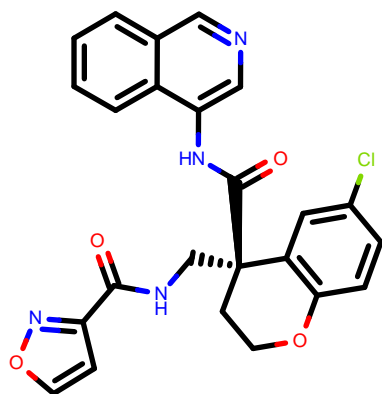
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCC(O)CO

RUN: RUN1110

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.26

EN300-22245_2_1



CID: EN300-22245_2_1

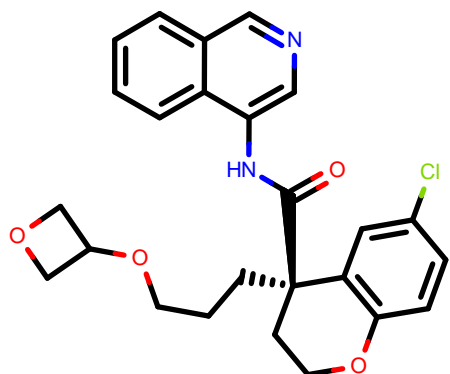
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccon5

RUN: RUN8165

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.20

EN300-317082_4_1



CID: EN300-317082_4_1

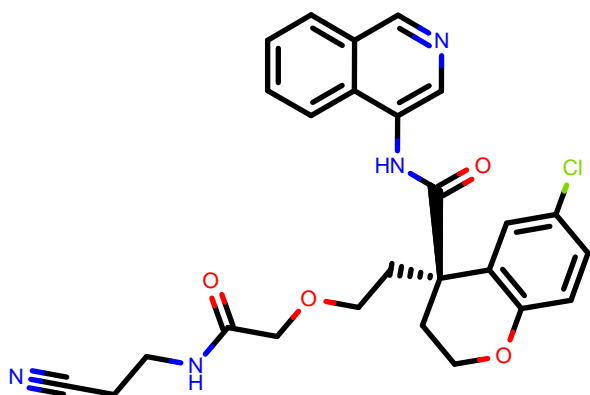
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC5COC5

RUN: RUN765

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.19

EN300-10895_3_1



CID: EN300-10895_3_1

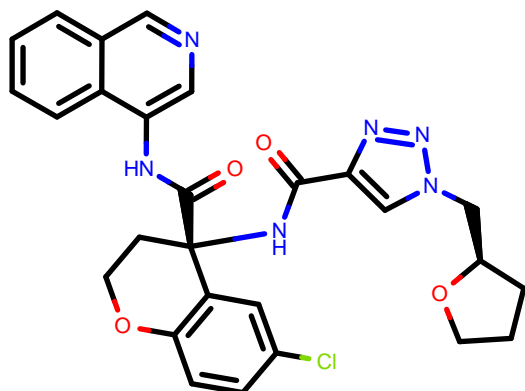
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCCC#N

RUN: RUN410

DDG (kcal/mol): -0.72

dDDG (kcal/mol): 0.26

EN300-368758_1_1



CID: EN300-368758_1_1

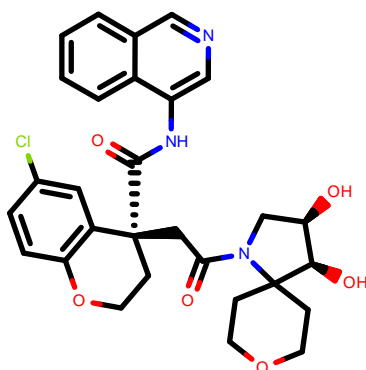
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn[nH]5C[C@H]6CCCC6

RUN: RUN3098

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.22

EN300-7456317_1_1



CID: EN300-7456317_1_1

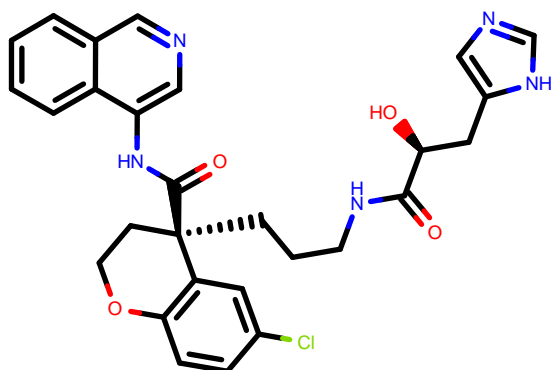
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C1=CN1)C(=O)N5C[C@H]6C56CCCC6O

RUN: RUN13038

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.36

EN300-6503811_4_1



CID: EN300-6503811_4_1

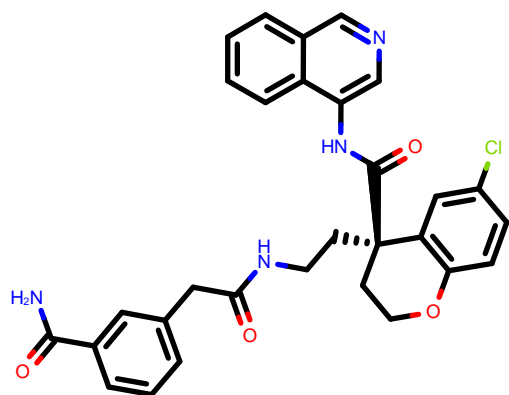
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(C=O)C[C@H]5C5cnc[nH]5O

RUN: RUN10604

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.27

EN300-1179673_3_1



CID: EN300-1179673_3_1

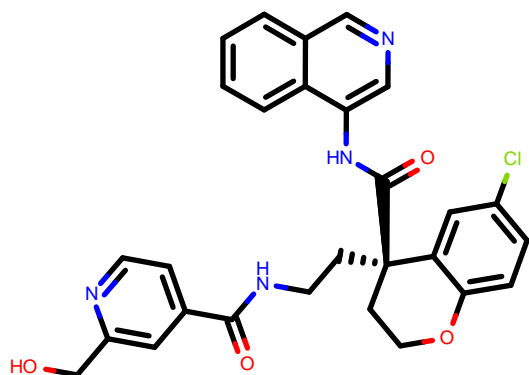
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccccc5C(=O)N

RUN: RUN14946

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.28

EN300-396748_3_1



CID: EN300-396748_3_1

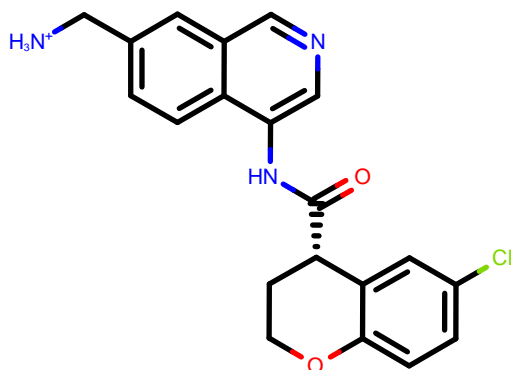
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnc(c5)CO

RUN: RUN14284

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.25

MAK-UNK-8be7dca9-5_2



CID: MAK-UNK-8be7dca9-5_2

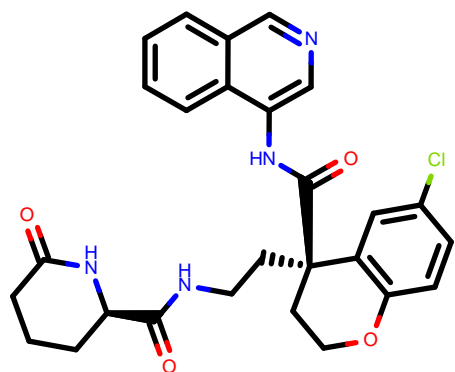
SMILES: c1cc2c(cc1C[NH3+])ncnc2NC(=O)[C@H]3CCOC4c3cc(cc4)Cl

RUN: RUN130

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.18

EN300-146491_3_1



CID: EN300-146491_3_1

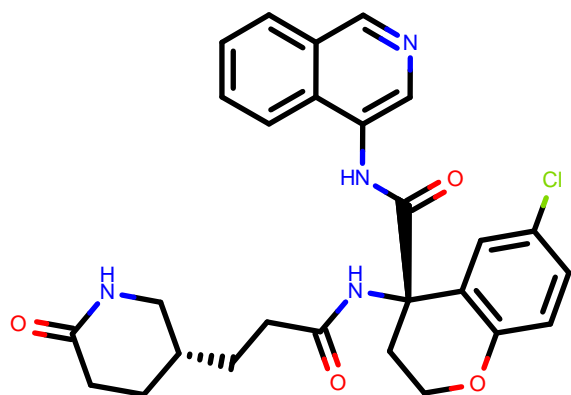
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)N5

RUN: RUN4761

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.26

EN300-1215738_1_1



CID: EN300-1215738_1_1

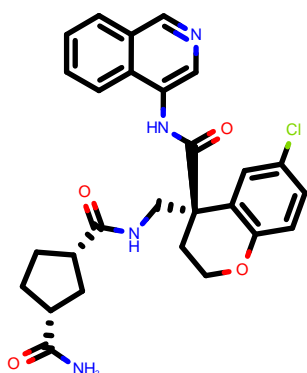
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@@H]5CCCC(=O)NCS

RUN: RUN9317

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.29

EN300-370753_2_1



CID: EN300-370753_2_1

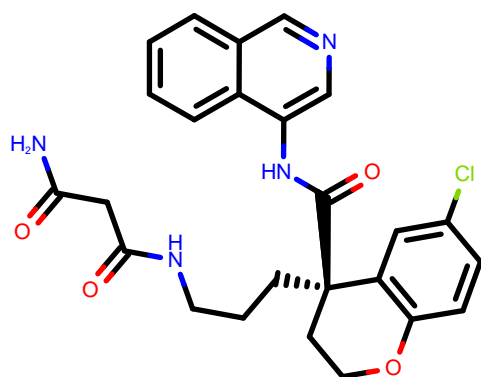
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC[C@@H](C5)C(=O)N

RUN: RUN6921

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.34

EN300-82179_4_1



CID: EN300-82179_4_1

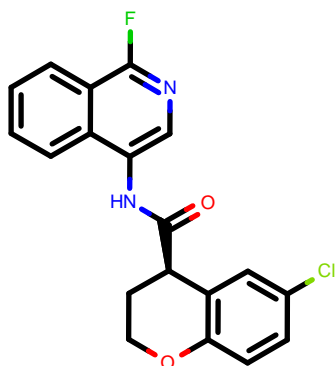
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)N

RUN: RUN7154

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.18

JOH-SUS-a69c159d-2_1



CID: JOH-SUS-a69c159d-2_1

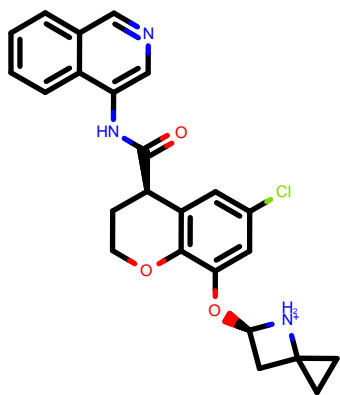
SMILES: c1ccc2c(c1)c(cnc2F)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN10

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.06

DAR-DIA-23e5a6a0-5_1



CID: DAR-DIA-23e5a6a0-5_1

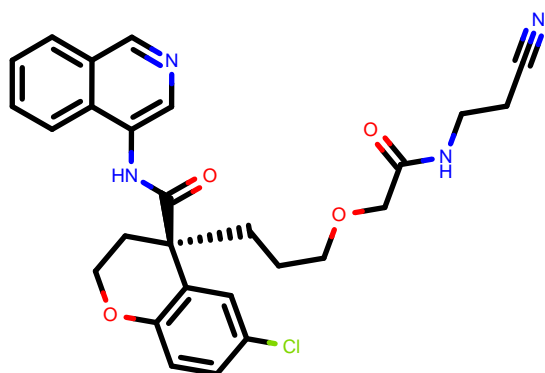
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOCc4c3cc(cc4O)[C@@H]5CC6([NH2+][5]CC6)Cl

RUN: RUN7

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.32

EN300-10895_4_1



CID: EN300-10895_4_1

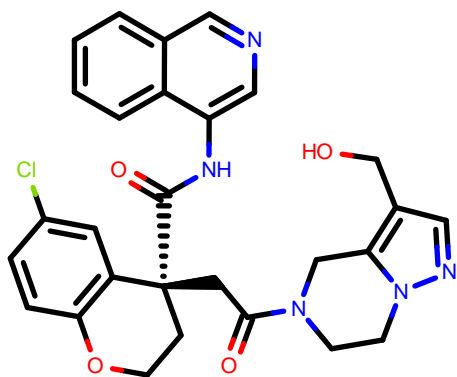
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCOCC(=O)NCCC#N

RUN: RUN1235

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.25

EN300-259251_1_1



CID: EN300-259251_1_1

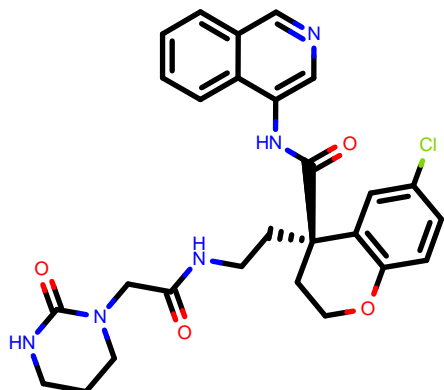
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CC(=O)N5Cn6c(c(en6)CO)C5

RUN: RUN1583

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.24

EN300-36096_3_1



CID: EN300-36096_3_1

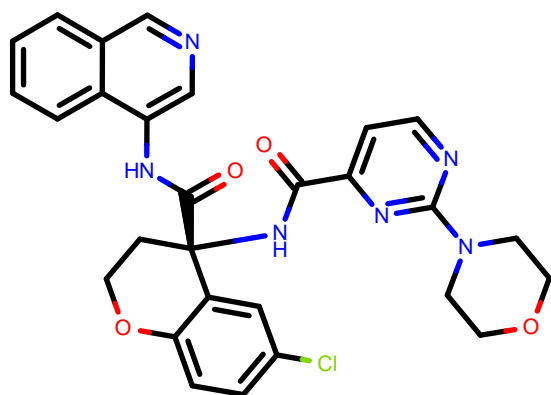
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CCN(=O)C5CCNC5=O

RUN: RUN10892

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.28

EN300-312450_1_1



CID: EN300-312450_1_1

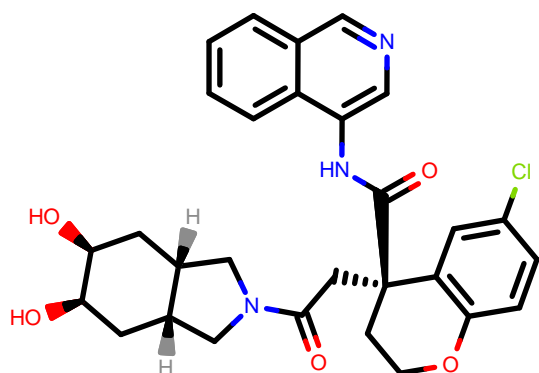
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5ccnc(n5)N6CCOCC6

RUN: RUN4378

DDG (kcal/mol): -0.71

dDDG (kcal/mol): 0.23

EN300-7355477_1_10



CID: EN300-7355477_1_10

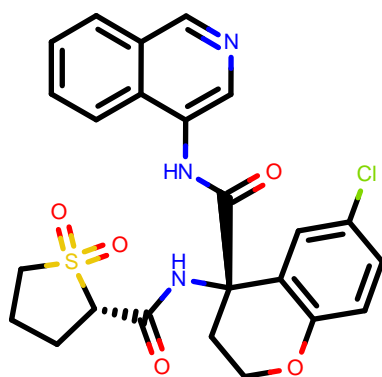
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(C)C(=O)N5C[C@@H]6C[C@@H]7C[C@@H]8C[C@@H]6C5=O

RUN: RUN1639

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.23

EN300-88656_1_1



CID: EN300-88656_1_1

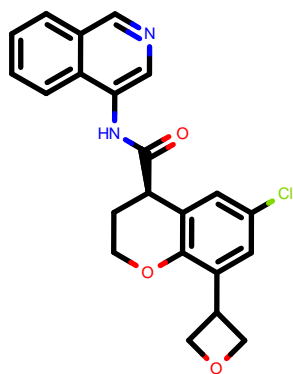
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4C[C@@H]5CCCS(=O)=O

RUN: RUN7448

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EDJ-MED-e4b030d8-5_1



CID: EDJ-MED-e4b030d8-5_1

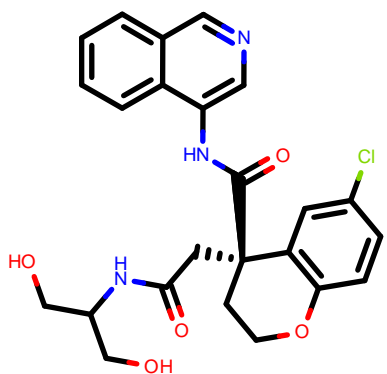
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C1=CC=C(C=C1)C2=O

RUN: RUN163

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.15

EN300-84186_1_1



CID: EN300-84186_1_1

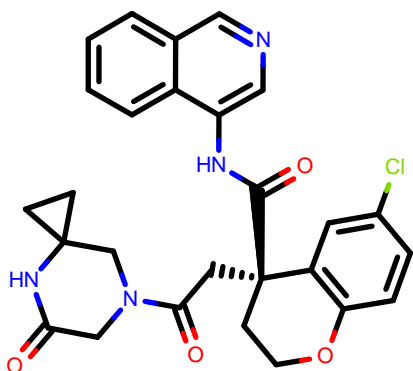
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC(CO)CO

RUN: RUN9816

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.34

EN300-6472573_1_1



CID: EN300-6472573_1_1

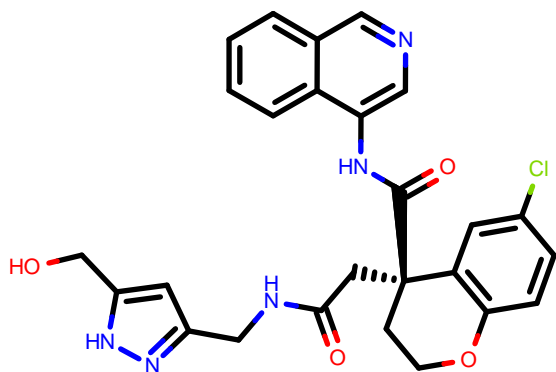
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)N6(C5)CC6

RUN: RUN6384

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.20

EN300-7439043_1_1



CID: EN300-7439043_1_1

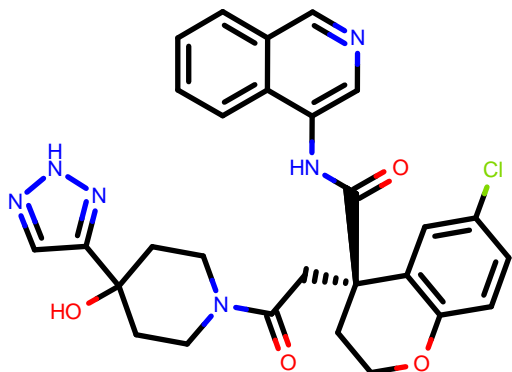
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5csc([nH]5)CO

RUN: RUN3869

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-1588753_1_1



CID: EN300-1588753_1_1

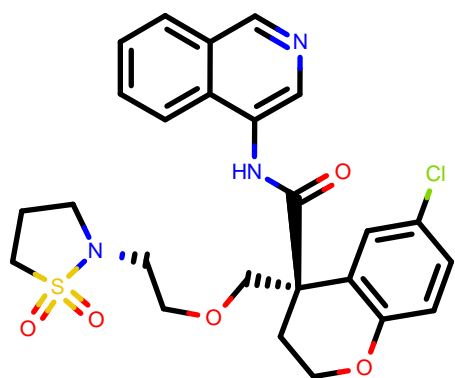
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)(c6cn[nH]6)O

RUN: RUN15075

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.29

EN300-114134_2_1



CID: EN300-114134_2_1

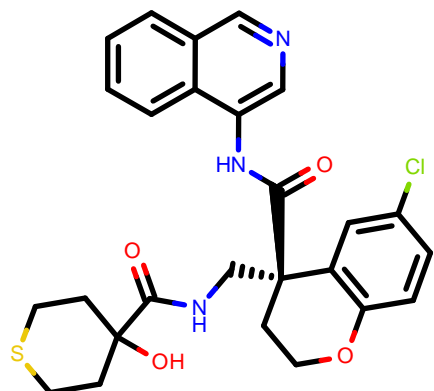
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CCSCS5(=O)=O

RUN: RUN1043

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.30

EN300-122340_2_1



CID: EN300-122340_2_1

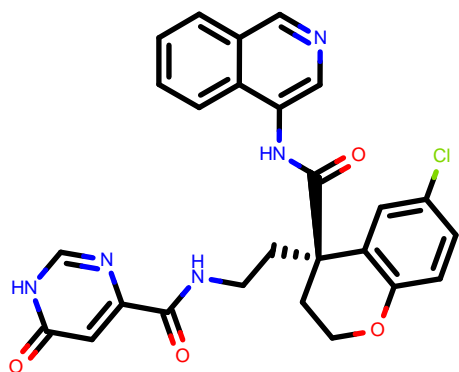
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCS(=O)O)S

RUN: RUN5551

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.25

EN300-817811_3_1



CID: EN300-817811_3_1

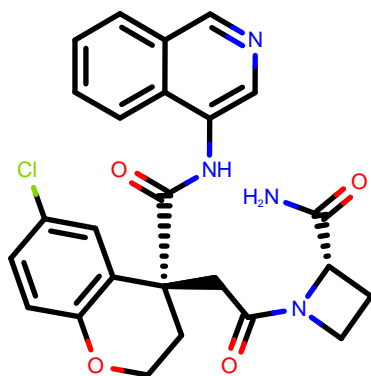
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc(=O)[nH]cn5

RUN: RUN14452

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-862094_1_1



CID: EN300-862094_1_1

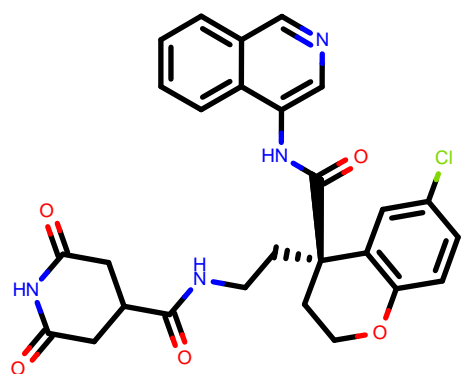
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5C(=O)N

RUN: RUN11767

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.18

EN300-62192_3_1



CID: EN300-62192_3_1

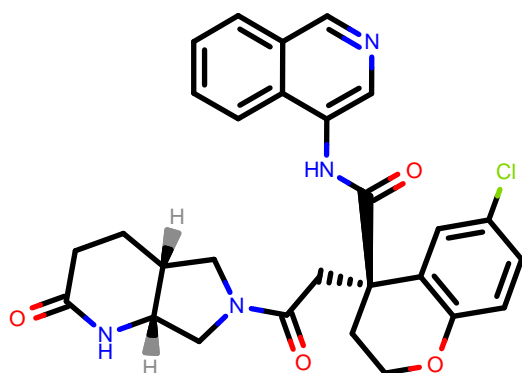
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC(=O)NC(=O)C5

RUN: RUN15234

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.23

EN300-1087187_1_3



CID: EN300-1087187_1_3

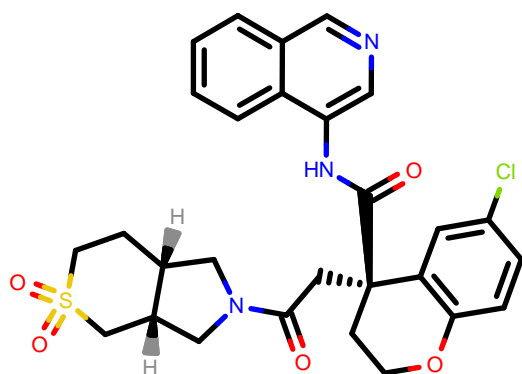
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6CC(=O)NC(=O)C6

RUN: RUN11050

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.25

EN300-1081929_1_1



CID: EN300-1081929_1_1

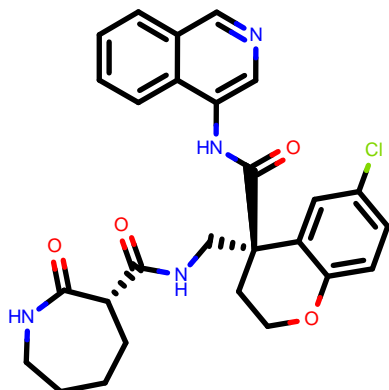
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6CC(=O)NC(=O)C6

RUN: RUN10583

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.28

EN300-6737762_2_1



CID: EN300-6737762_2_1

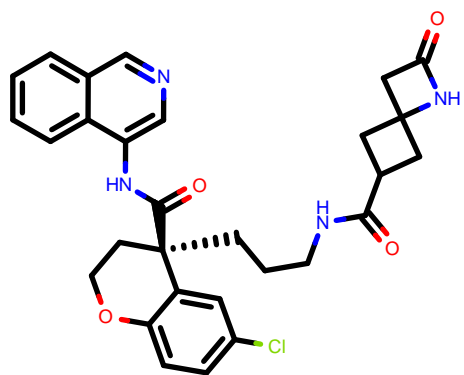
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC(=O)[C@@]4H5CCCCNC5=O

RUN: RUN7757

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-1700760_4_1



CID: EN300-1700760_4_1

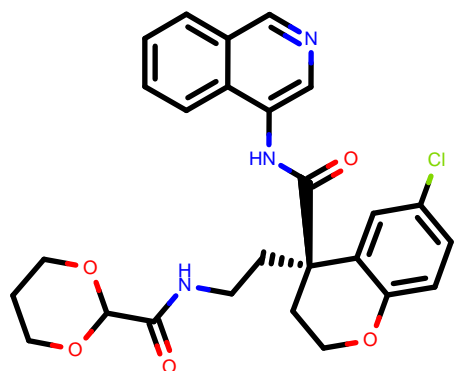
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN11919

DDG (kcal/mol): -0.70

dDDG (kcal/mol): 0.24

EN300-170985_3_1



CID: EN300-170985_3_1

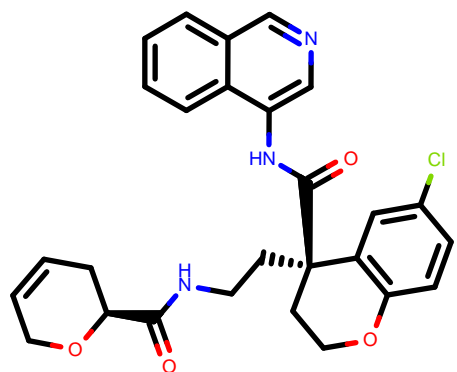
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5OCCO5

RUN: RUN4933

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.22

EN300-378044_3_1



CID: EN300-378044_3_1

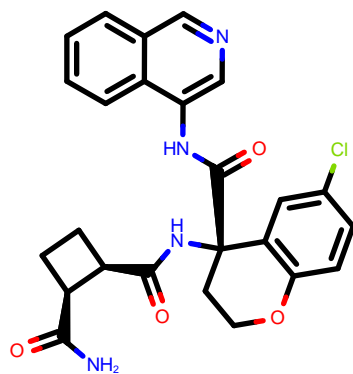
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5H5CC=CCO5

RUN: RUN9120

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.24

EN300-217107_1_3



CID: EN300-217107_1_3

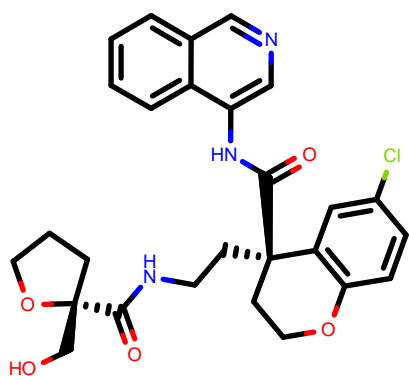
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5H5CC[C@@]5H5C(=O)N

RUN: RUN7576

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.23

EN300-1425677_3_1



CID: EN300-1425677_3_1

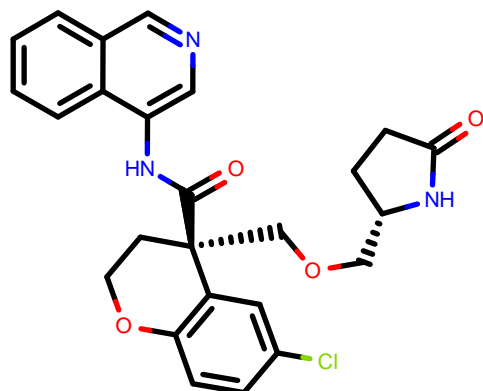
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCCO5)CO

RUN: RUN4485

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.36

EN300-195756_2_2



CID: EN300-195756_2_2

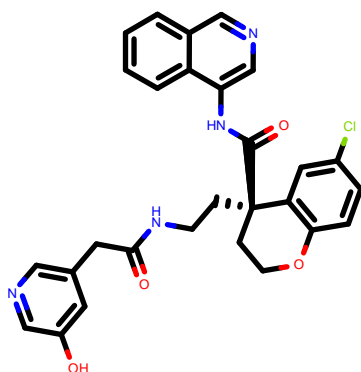
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]5(CCCO5)N

RUN: RUN1945

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.23

EN300-222620_3_1



CID: EN300-222620_3_1

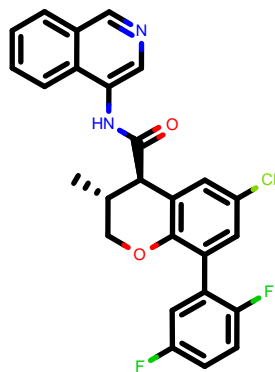
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cc(nc5)O

RUN: RUN15151

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

DAR-DIA-0d514e7d-15_1



CID: DAR-DIA-0d514e7d-15_1

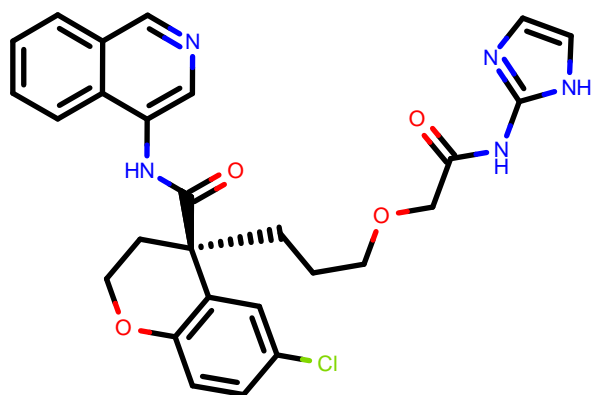
SMILES: C[C@H]1COc2c(cc(cc2[C@@]3(CCOc4c3cc(cc4)Cl)Nc3ncoc4c3ccc4)Cl)c5cc(ccc5)F

RUN: RUN223

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.20

EN300-331993_4_1



CID: EN300-331993_4_1

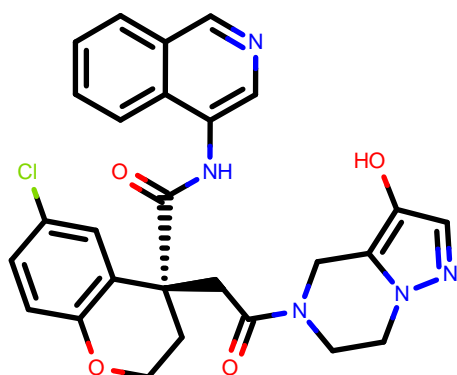
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)Nc5[nH]cn5

RUN: RUN1611

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.22

EN300-7355835_1_1



CID: EN300-7355835_1_1

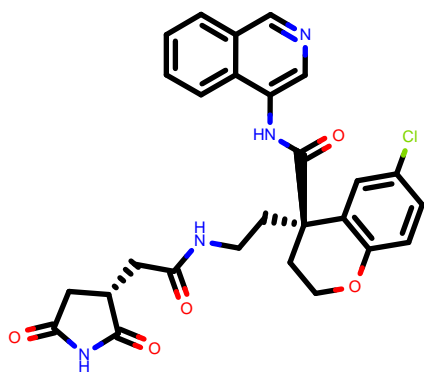
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN6c(c1cn6)O)C5

RUN: RUN3217

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

EN300-227055_3_1



CID: EN300-227055_3_1

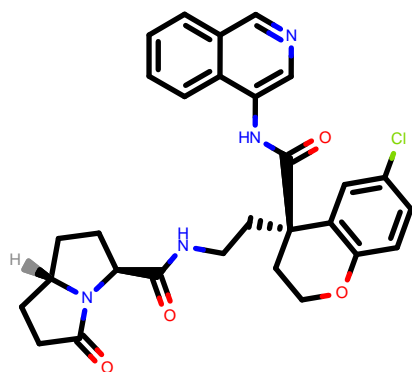
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@H]5CC(=O)NC5=O

RUN: RUN13162

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.25

EN300-6479181_3_1



CID: EN300-6479181_3_1

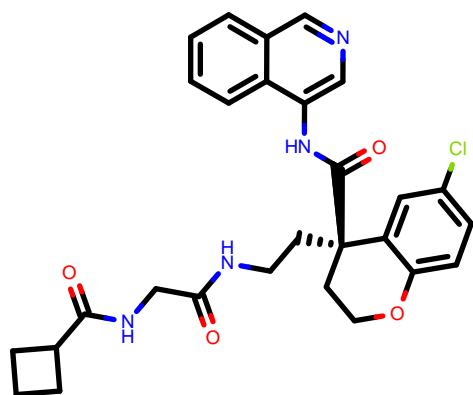
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@H]5CC[C@@H]N5C(=O)OC6

RUN: RUN2961

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

EN300-62448_3_1



CID: EN300-62448_3_1

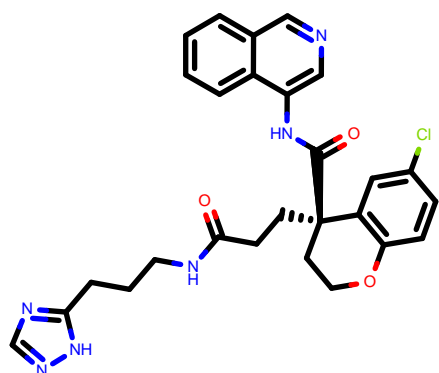
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CNC(=O)C5CC5

RUN: RUN11134

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.29

EN300-196614_2_1



CID: EN300-196614_2_1

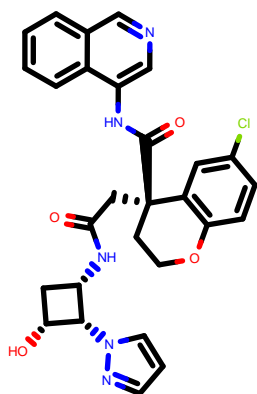
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCCc5[nH]nnc5

RUN: RUN1989

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.25

EN300-260696_1_8



CID: EN300-260696_1_8

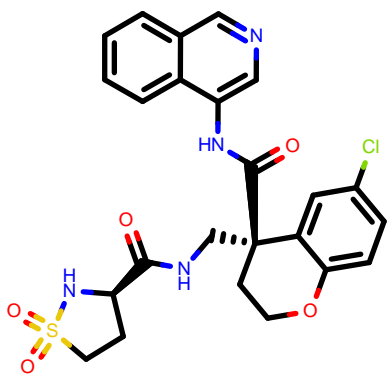
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5[C@@H](C@H)5Nc6ccccc6O

RUN: RUN4233

DDG (kcal/mol): -0.69

dDDG (kcal/mol): 0.25

EN300-45049_2_2



CID: EN300-45049_2_2

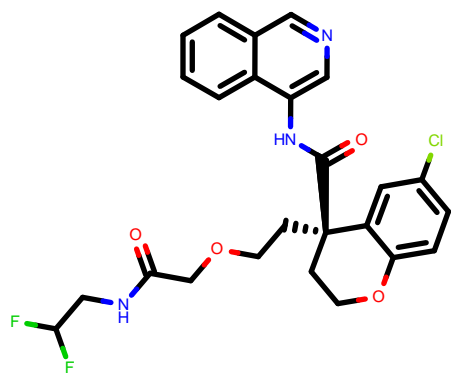
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5[C@@H]5SCCS(=O)(=O)N5

RUN: RUN7073

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.24

EN300-120586_3_1



CID: EN300-120586_3_1

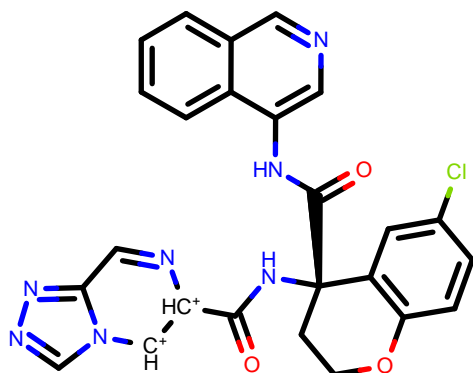
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCOC(=O)NCC(F)F

RUN: RUN402

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.24

EN300-309106_1_1



CID: EN300-309106_1_1

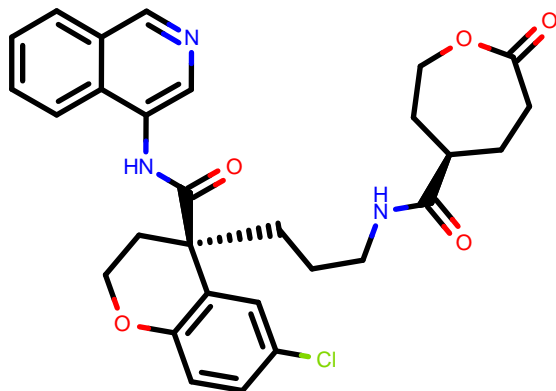
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn6nnc6n5

RUN: RUN6050

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.19

EN300-2011083_4_1



CID: EN300-2011083_4_1

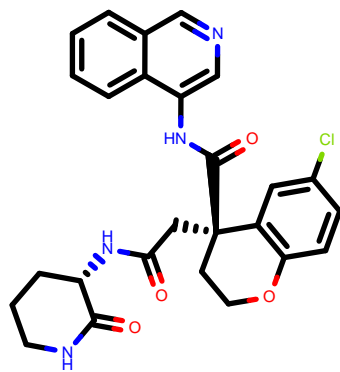
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]3[C@@]3(H)5CCC(=O)OCC5

RUN: RUN11832

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.24

EN300-60035_1_1



CID: EN300-60035_1_1

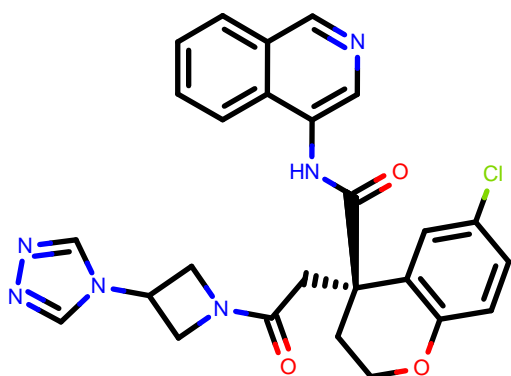
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]3[C@@]3H5CCNC(=O)O

RUN: RUN10861

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.20

EN300-7427921_1_1



CID: EN300-7427921_1_1

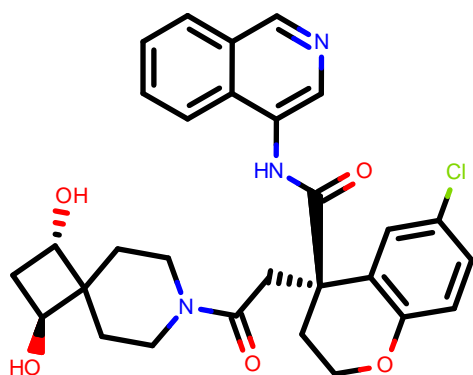
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6cnc6

RUN: RUN3617

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.23

EN300-7448078_1_3



CID: EN300-7448078_1_3

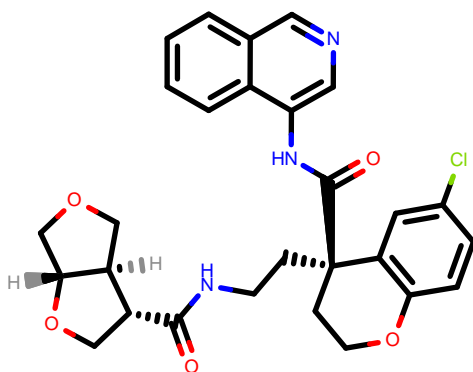
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CCCC(C5)C#H)C)C#H5CO)C#H5CO

RUN: RUN10835

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.30

EN300-6482296_3_5



CID: EN300-6482296_3_5

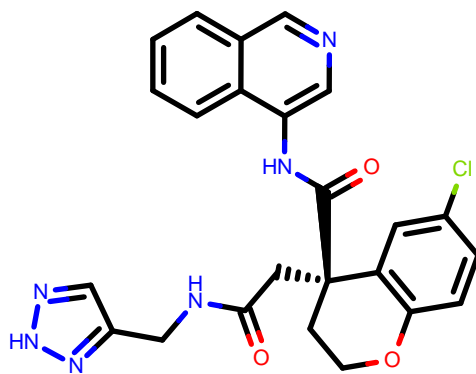
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)[C@@]5(C)C#H5CO)C#H5CO)C#H5CO

RUN: RUN9216

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.22

EN300-98429_1_1



CID: EN300-98429_1_1

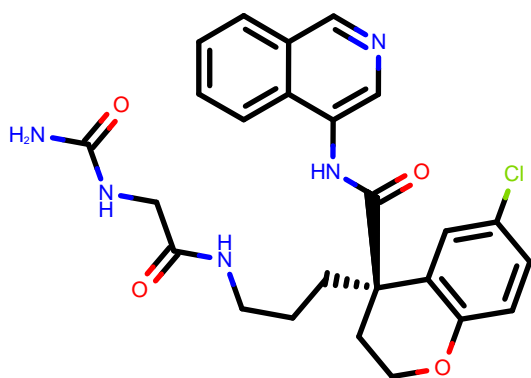
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)NC5c[nH]n5

RUN: RUN9328

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.21

EN300-10397_4_1



CID: EN300-10397_4_1

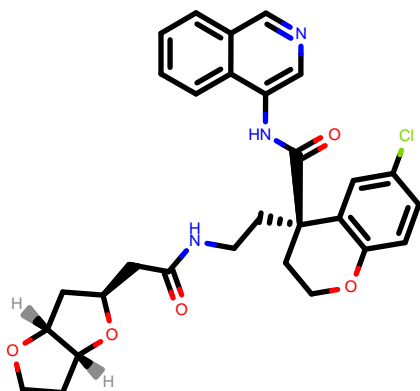
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(c4)Cl)CCNC(=O)CNC(=O)N

RUN: RUN12157

DDG (kcal/mol): -0.68

dDDG (kcal/mol): 0.24

EN300-7355519_3_6



CID: EN300-7355519_3_6

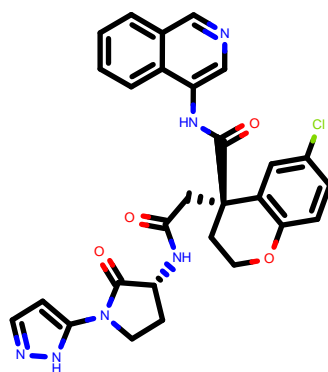
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(c4)Cl)CCNC(=O)C[C@@]5[C@@]([C@@H]6[C@@]([C@H]7[C@@]([C@H]6)O)CCO6

RUN: RUN13882

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.31

EN300-7547467_1_2



CID: EN300-7547467_1_2

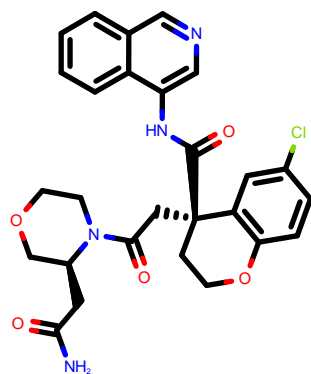
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(c4)Cl)CC(=O)N[C@@]5[C@@]([C@@H]6[C@@]([C@H]7[C@@]([C@H]6)O)CCO7)CNC(=O)N5

RUN: RUN15032

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.23

EN300-249093_1_1



CID: EN300-249093_1_1

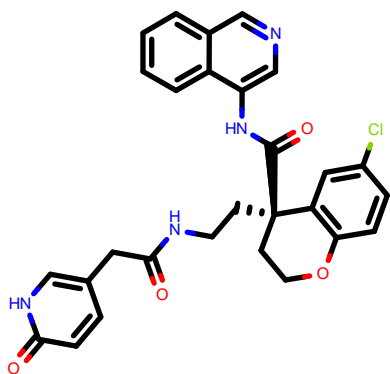
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(c4)Cl)CC(=O)N5CCOC[C@@]5[C@@]([C@@H]6[C@@]([C@H]7[C@@]([C@H]6)O)CCO7)CNC(=O)N

RUN: RUN9300

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.42

EN300-189672_3_1



CID: EN300-189672_3_1

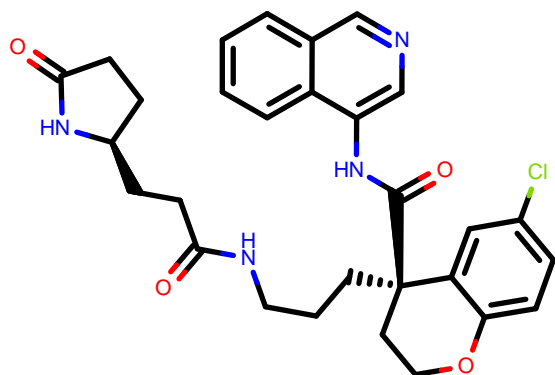
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(=O)[nH]c5

RUN: RUN9188

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.25

EN300-104592_4_2



CID: EN300-104592_4_2

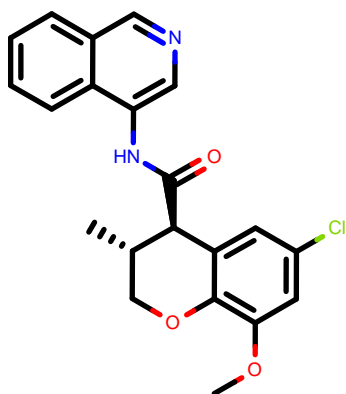
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[C@@]4H5CCC(=O)N5

RUN: RUN8374

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

DAR-DIA-0d514e7d-1_1



CID: DAR-DIA-0d514e7d-1_1

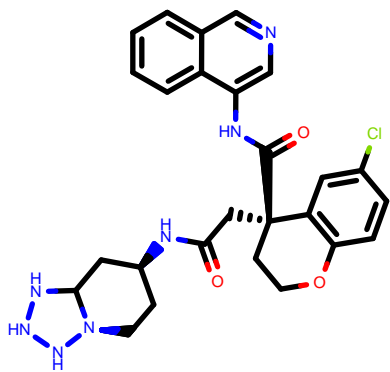
SMILES: C[C@@H]1COc2c(cc2OC)Cl][C@@]1C(=O)Nc3ccc4c3ccc4

RUN: RUN145

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.12

EN300-7438451_1_1



CID: EN300-7438451_1_1

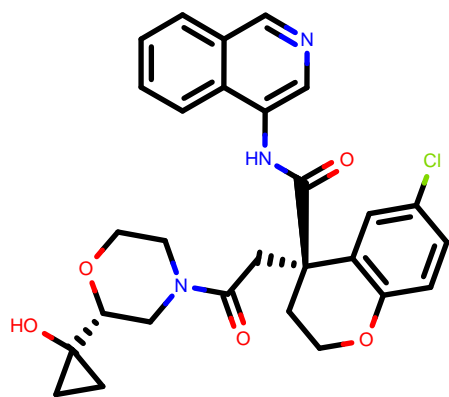
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CNc6c(nnn6)C5

RUN: RUN8596

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.27

EN300-6482801_1_2



CID: EN300-6482801_1_2

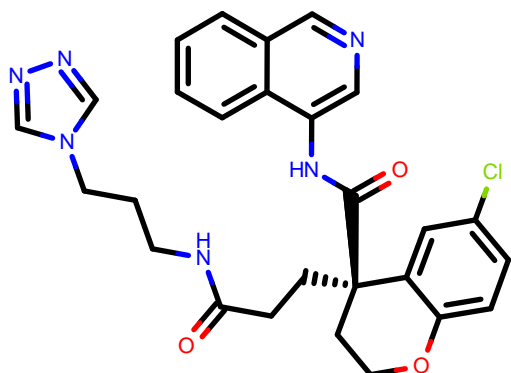
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)C6(C6)O

RUN: RUN7131

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.32

EN300-257315_2_1



CID: EN300-257315_2_1

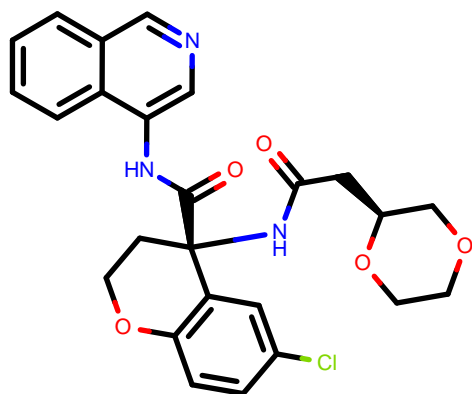
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCn5nnnc5

RUN: RUN8166

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-731622_1_1



CID: EN300-731622_1_1

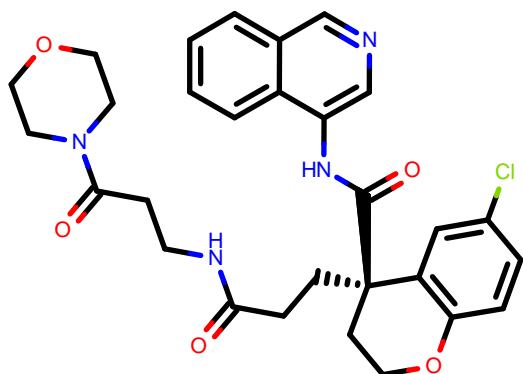
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5COCOC5

RUN: RUN3606

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.21

EN300-27314_2_1



CID: EN300-27314_2_1

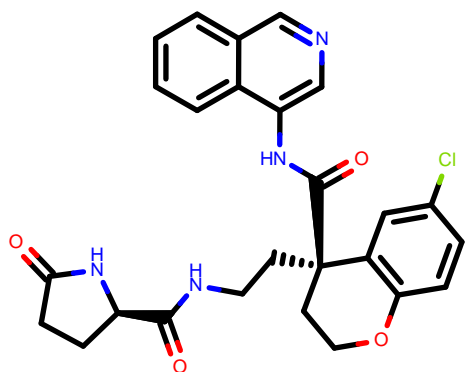
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCC(=O)N5CCOC5

RUN: RUN9974

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.39

EN300-54541_3_1



CID: EN300-54541_3_1

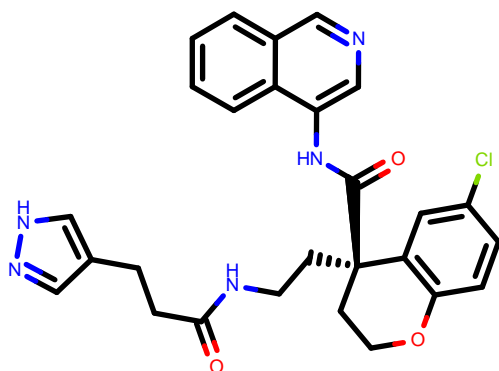
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)N5

RUN: RUN857

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.22

EN300-250836_3_1



CID: EN300-250836_3_1

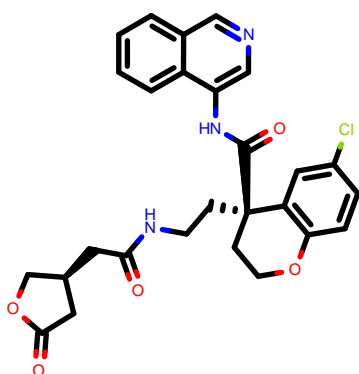
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5c[nH]n5

RUN: RUN9116

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.26

EN300-109535_3_2



CID: EN300-109535_3_2

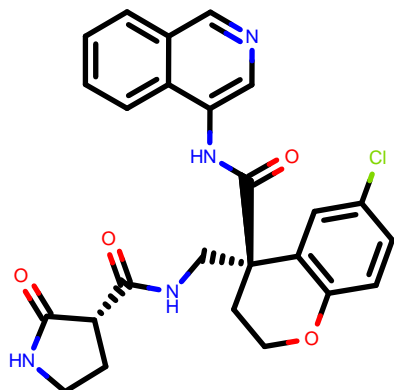
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CC(=O)OC5

RUN: RUN14996

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-94945_2_1



CID: EN300-94945_2_1

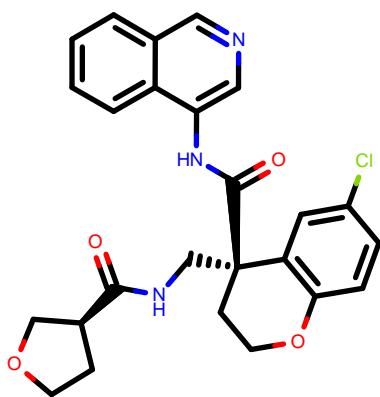
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCNC5=O

RUN: RUN5151

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.24

EN300-53423_2_2



CID: EN300-53423_2_2

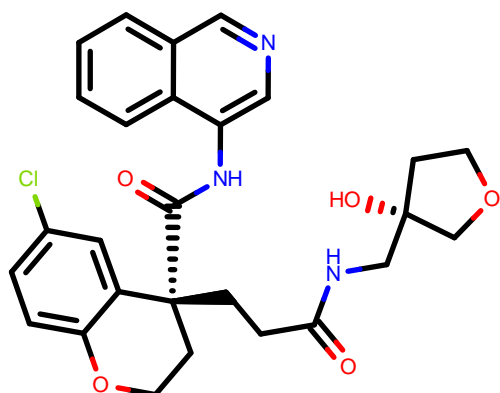
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCOC5

RUN: RUN5747

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.21

EN300-200699_2_2



CID: EN300-200699_2_2

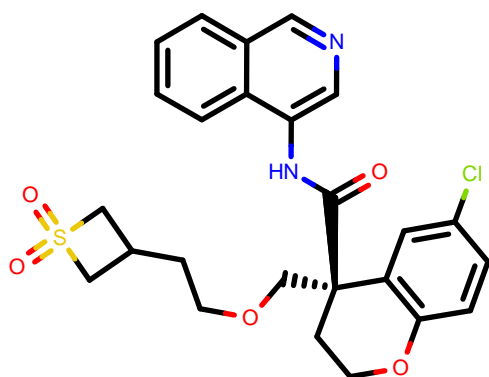
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@H]5(CCOCS)O

RUN: RUN4392

DDG (kcal/mol): -0.67

dDDG (kcal/mol): 0.32

EN300-189563_2_1



CID: EN300-189563_2_1

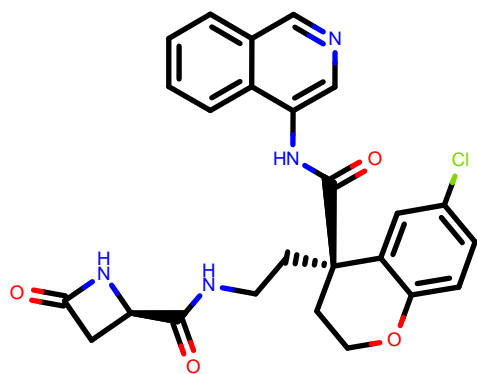
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCS(=O)(=O)CS

RUN: RUN1162

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.25

EN300-101505_3_2



CID: EN300-101505_3_2

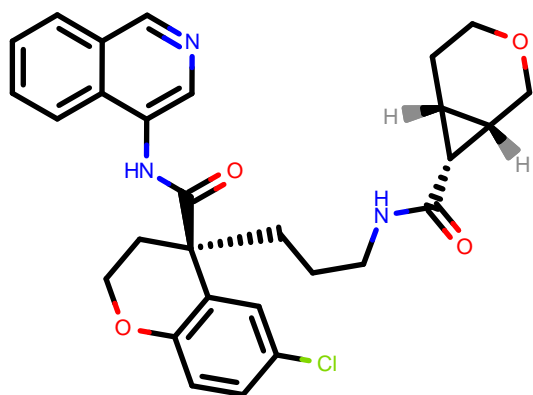
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)N5

RUN: RUN15155

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.19

EN300-1644723_4_3



CID: EN300-1644723_4_3

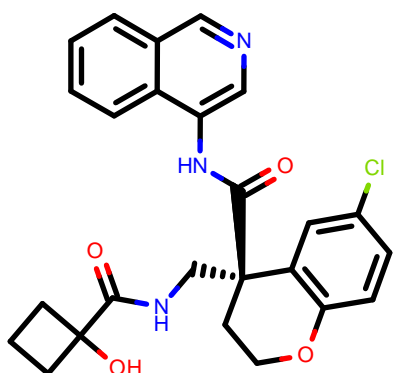
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CCNC(=O)[C@@H]5[C@@H]6[C@@H]5COC6

RUN: RUN11241

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.23

EN300-52009_2_1



CID: EN300-52009_2_1

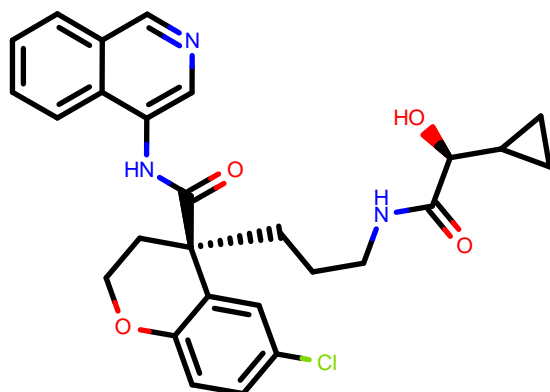
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CNC(=O)C5(CCC5)O

RUN: RUN4203

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.23

EN300-72211_4_2



CID: EN300-72211_4_2

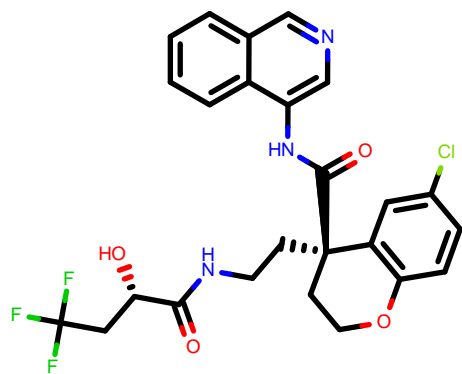
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CCNC(=O)[C@@H]5(C5CC5)O

RUN: RUN10678

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.21

EN300-1932013_3_2



CID: EN300-1932013_3_2

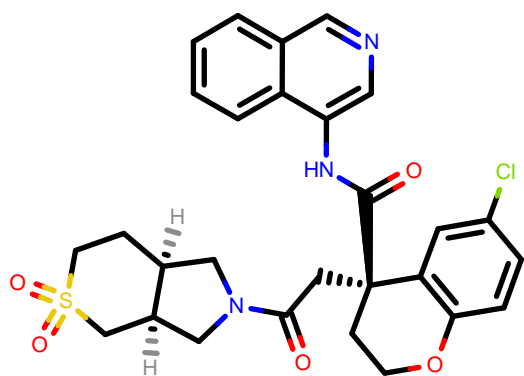
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4ccc(cc4)C)CCNC(=O)[C@@H]5(C5C(F)F)O

RUN: RUN6787

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.29

EN300-1081929_1_4



CID: EN300-1081929_1_4

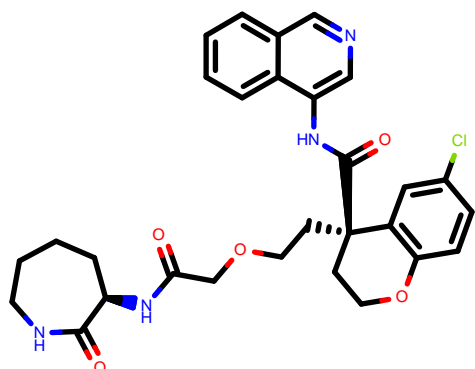
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@]H6CCS(=O)(=O)C[C@@]H6C5

RUN: RUN5753

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.25

EN300-37195_3_2



CID: EN300-37195_3_2

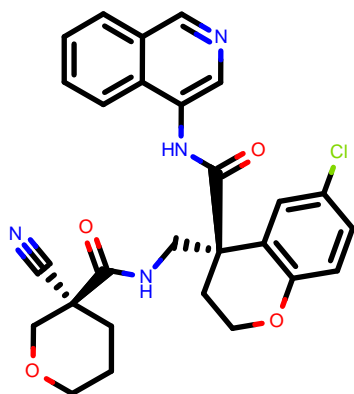
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)COC(=O)N[C@@]H5CCCCNC5=O

RUN: RUN594

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.27

EN300-301925_2_1



CID: EN300-301925_2_1

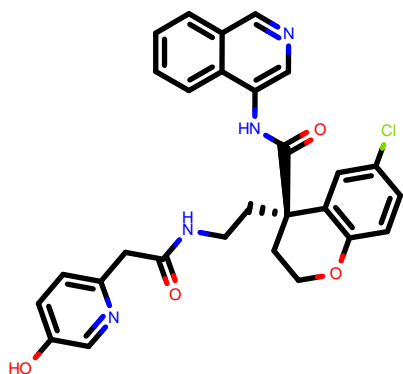
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN4527

DDG (kcal/mol): -0.66

dDDG (kcal/mol): 0.23

EN300-188341_3_1



CID: EN300-188341_3_1

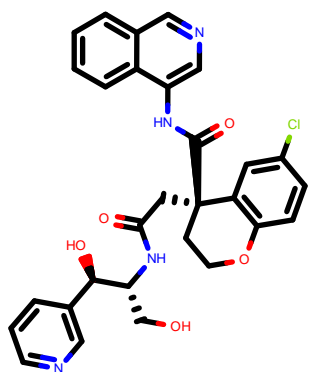
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5ccc(O)cn5

RUN: RUN15211

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.27

EN300-332453_1_4



CID: EN300-332453_1_4

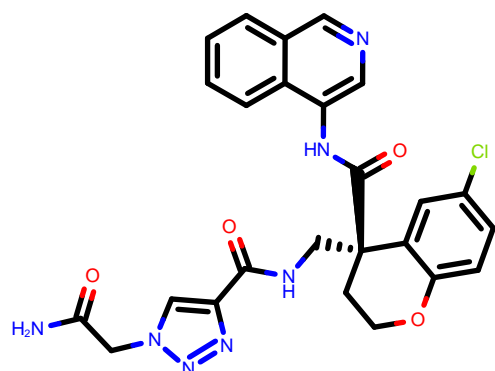
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)O)C[C@H](C)C(=O)C[C@H](c5ccccc5)O

RUN: RUN1351

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.38

EN300-52380_2_1



CID: EN300-52380_2_1

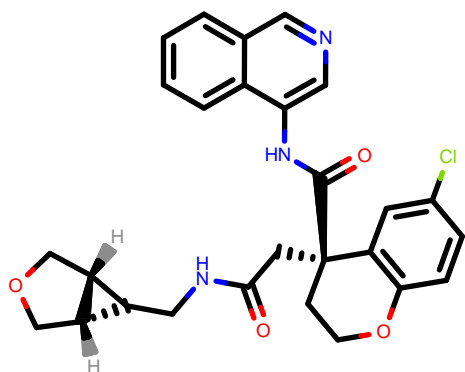
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)O)C[C@H](C)C(=O)C[C@H](c5ccccc5)O

RUN: RUN9126

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.27

EN300-210089_1_2



CID: EN300-210089_1_2

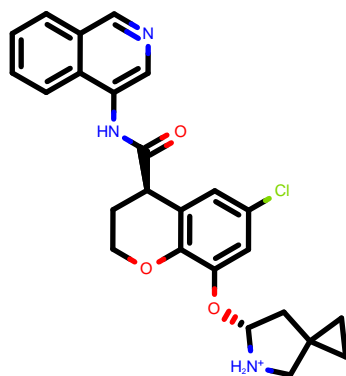
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)O)C[C@H](C)C(=O)C[C@H](c5ccccc5)O

RUN: RUN1575

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.23

DAR-DIA-23e5a6a0-4_1



CID: DAR-DIA-23e5a6a0-4_1

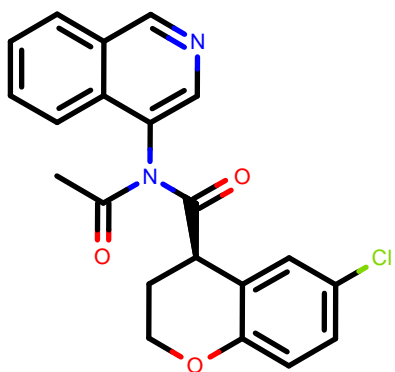
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3[C@@H](COC4=CC=C(C=C4)O)C[C@H](C)C(=O)C[C@H](c5ccccc5)O

RUN: RUN176

DDG (kcal/mol): -0.65

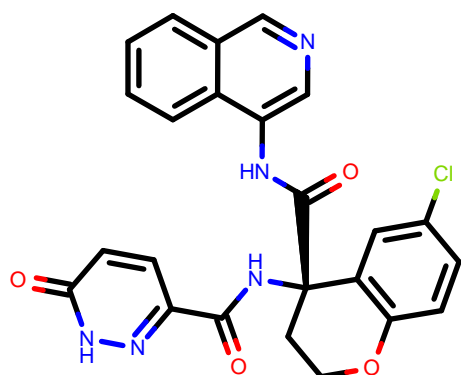
dDDG (kcal/mol): 0.37

VLA-UCB-50c39ae8-1_1



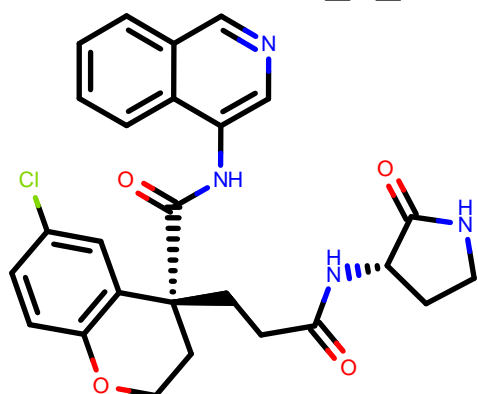
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	<chem>CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOC4c3cc(cc4)Cl</chem>
RUN:	RUN104
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.16

EN300-04614_1_1



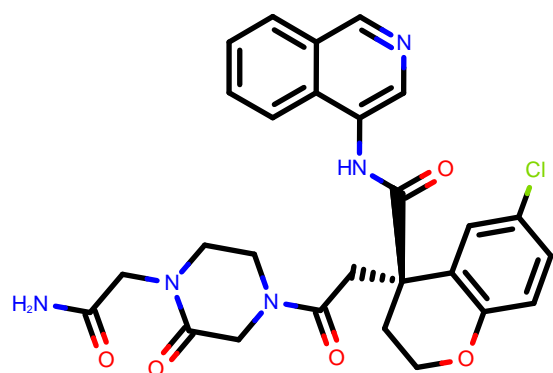
CID:	EN300-04614_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(O)[nH]5</chem>
RUN:	RUN5554
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.19

EN300-298184_2_1



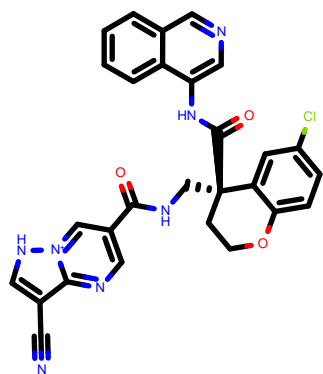
CID:	EN300-298184_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCNC5=O</chem>
RUN:	RUN3044
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.25

EN300-251571_1_1



CID:	EN300-251571_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(C(=O)C5)CC(=O)N</chem>
RUN:	RUN9292
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.26

EN300-1697480_2_1



CID: EN300-1697480_2_1

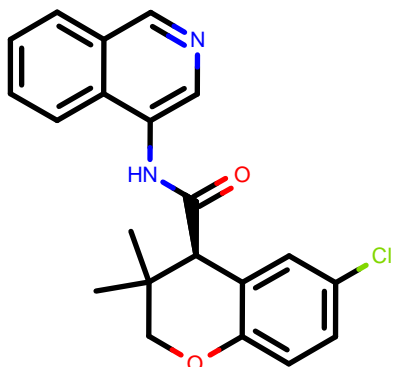
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5nc6c(cnn6c5)C#N

RUN: RUN9494

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-3_1



CID: DAR-DIA-0d514e7d-3_1

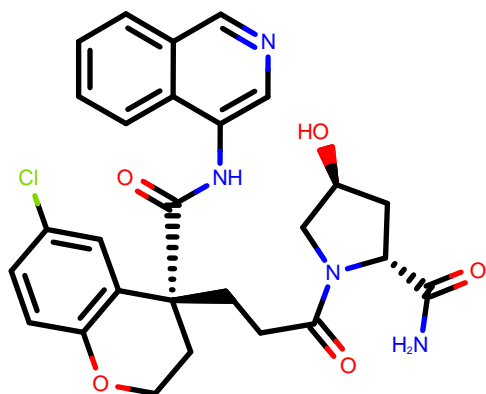
SMILES: CC1(COc2ccc(cc2[C@@]3(C)C(=O)Nc3cnc4c3cccc4)C)C1

RUN: RUN74

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.08

EN300-07752_2_3



CID: EN300-07752_2_3

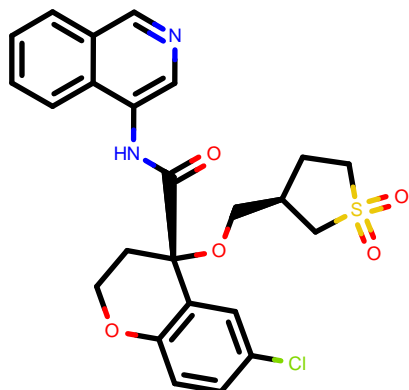
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(C)C(=O)N5C[C@@H](C)C[C@@H]5C(=O)N

RUN: RUN1933

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.28

EN300-1448603_1_2



CID: EN300-1448603_1_2

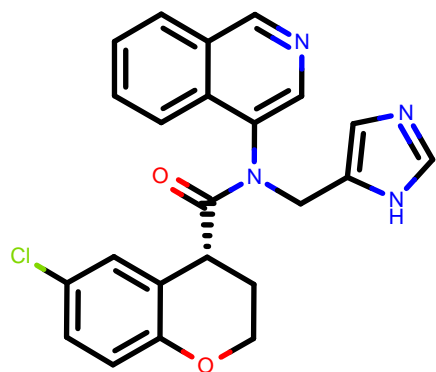
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN1014

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.25

ALP-UNI-44c99a80-2_1



CID: ALP-UNI-44c99a80-2_1

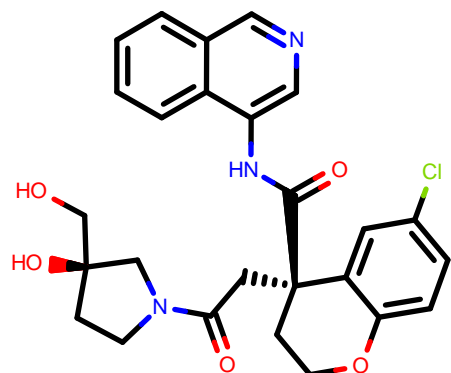
SMILES: c1ccc2c(c1)ncnc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOC5c4cc(cc5)Cl

RUN: RUN185

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.19

EN300-781107_1_1



CID: EN300-781107_1_1

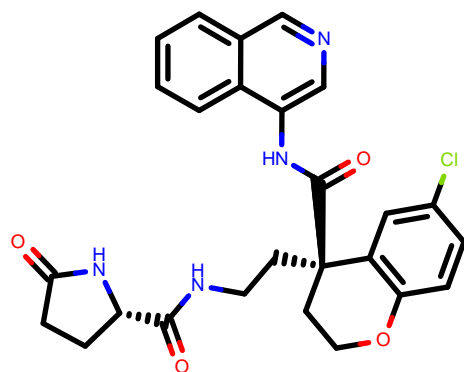
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO

RUN: RUN1247

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.34

EN300-72896_3_1



CID: EN300-72896_3_1

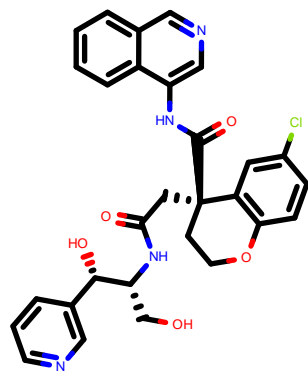
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCC(=O)N5

RUN: RUN14446

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.20

EN300-332453_1_2



CID: EN300-332453_1_2

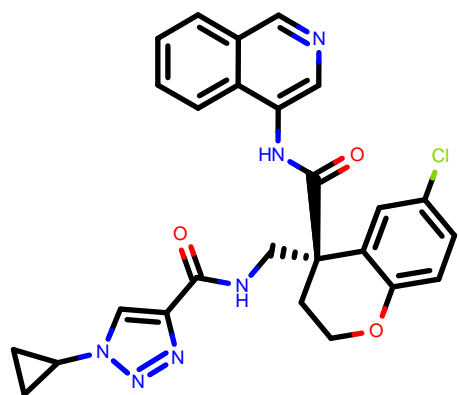
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H](c5ccccc5)O

RUN: RUN297

DDG (kcal/mol): -0.65

dDDG (kcal/mol): 0.39

EN300-210110_2_1



CID: EN300-210110_2_1

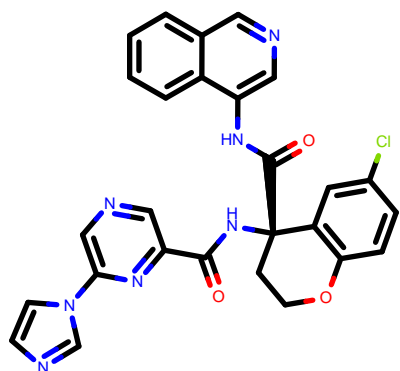
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn(n5)C6CC6

RUN: RUN3243

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.23

EN300-2666482_1_1



CID: EN300-2666482_1_1

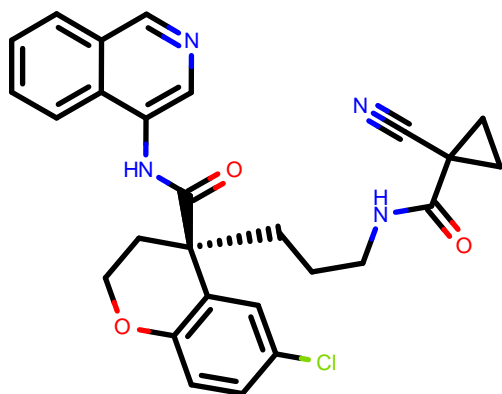
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nccn5n6ccn6

RUN: RUN8508

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.21

EN300-114082_4_1



CID: EN300-114082_4_1

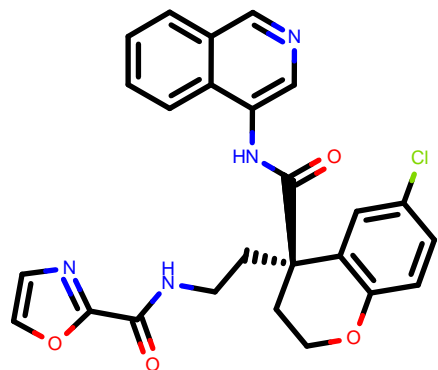
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCNC(=O)C5(C5)C#N

RUN: RUN12181

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.22

EN300-318344_3_1



CID: EN300-318344_3_1

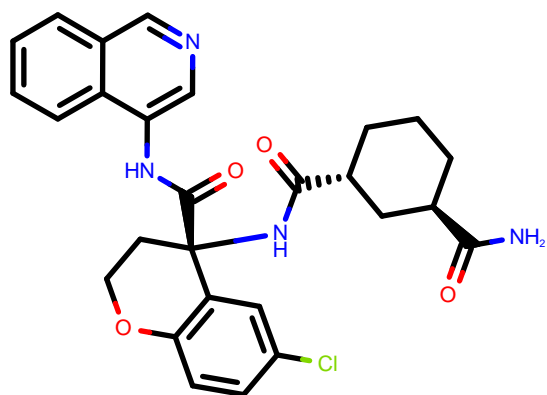
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5nccoc5

RUN: RUN15278

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.19

EN300-90142_1_3



CID: EN300-90142_1_3

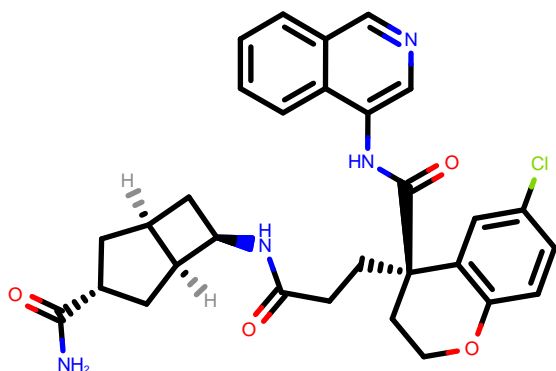
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)[C@@]5(C)C(C)C1=O

RUN: RUN7896

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.25

EN300-1268016_2_15



CID: EN300-1268016_2_15

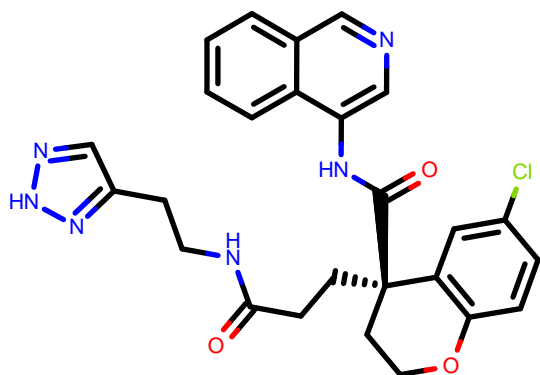
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)N[C@@]5(C)C(C)C1=O

RUN: RUN6239

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.33

EN300-1178209_2_1



CID: EN300-1178209_2_1

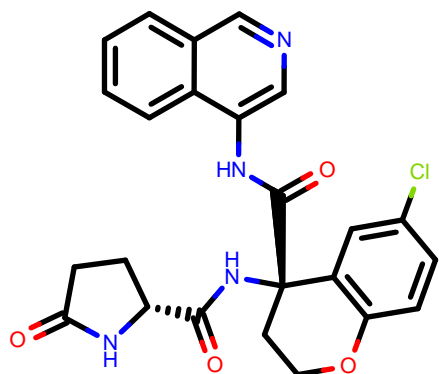
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C(=O)NCC5c5cn[nH]5

RUN: RUN4808

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.23

EN300-54541_1_1



CID: EN300-54541_1_1

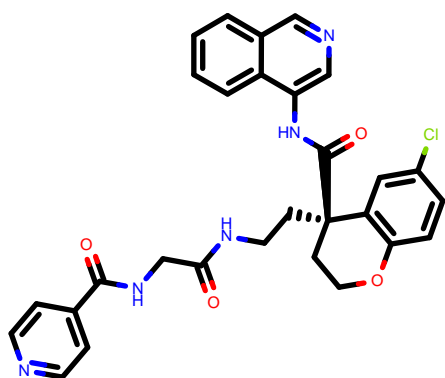
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)N(C=O)[C@@]5(C)C(C)C1=O

RUN: RUN7916

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.21

EN300-36089_3_1



CID: EN300-36089_3_1

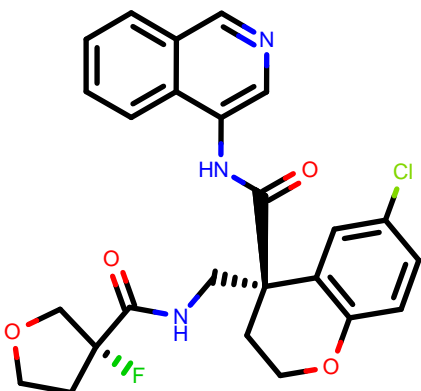
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CNC(=O)c5ccncc5

RUN: RUN11863

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.24

EN300-188356_2_2



CID: EN300-188356_2_2

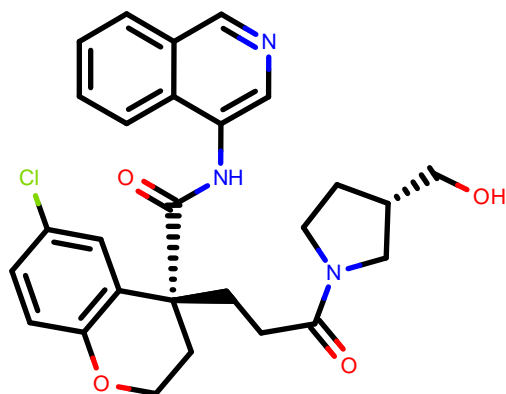
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@@]5(CCOc5)F

RUN: RUN4271

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.28

EN300-88131_2_1



CID: EN300-88131_2_1

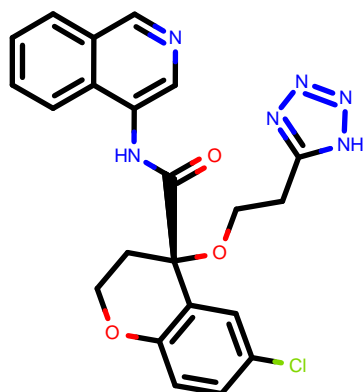
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](C5)CO

RUN: RUN11272

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.27

EN300-183231_1_1



CID: EN300-183231_1_1

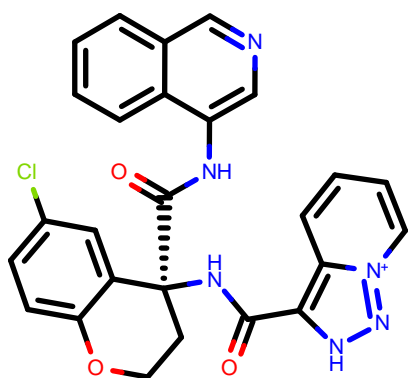
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5n[n-]nn5

RUN: RUN1421

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.26

EN300-325737_1_1



CID: EN300-325737_1_1

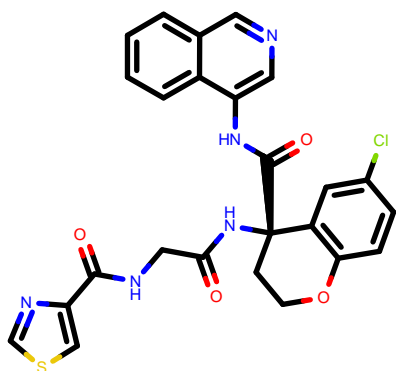
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6ccccc6n5

RUN: RUN4902

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.19

EN300-182084_1_1



CID: EN300-182084_1_1

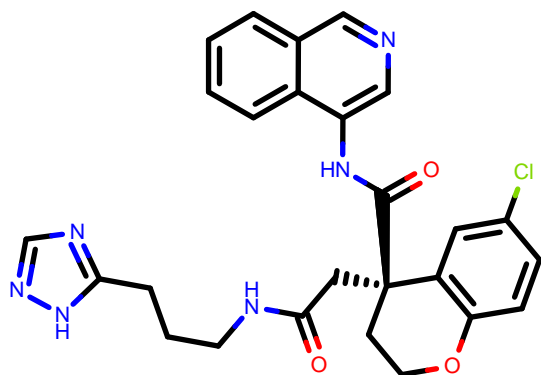
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CNC(=O)c5csn5

RUN: RUN9281

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.24

EN300-196614_1_1



CID: EN300-196614_1_1

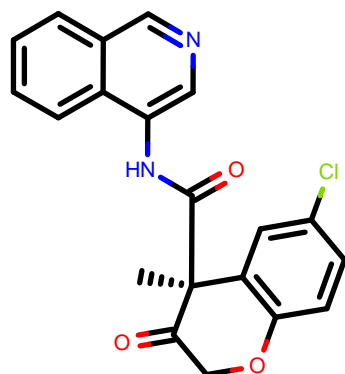
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCC5([NH])n5

RUN: RUN12066

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.26

VLA-UCB-1dbca3b4-14_2



CID: VLA-UCB-1dbca3b4-14_2

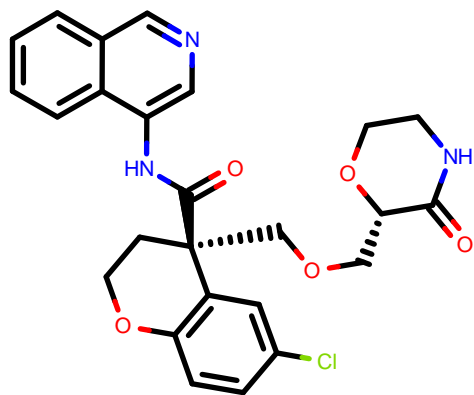
SMILES: C[C@@]1(c2cc(ccc2OCC1=O)C)C(=O)Nc3ncc4c3cccc4

RUN: RUN71

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.09

EN300-1706036_2_1



CID: EN300-1706036_2_1

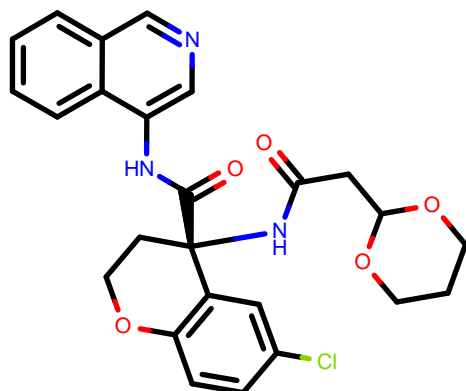
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C(=O)NCCO5

RUN: RUN644

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.24

EN300-157502_1_1



CID: EN300-157502_1_1

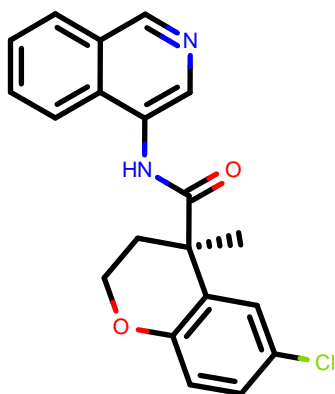
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5OCCCCO5

RUN: RUN2215

DDG (kcal/mol): -0.64

dDDG (kcal/mol): 0.21

DAR-DIA-6a508060-10_1



CID: DAR-DIA-6a508060-10_1

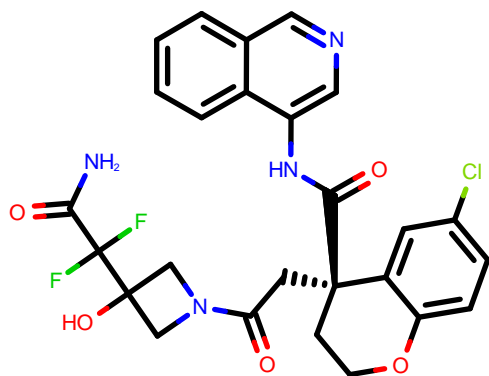
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccccc4

RUN: RUN68

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.09

EN300-1720923_1_1



CID: EN300-1720923_1_1

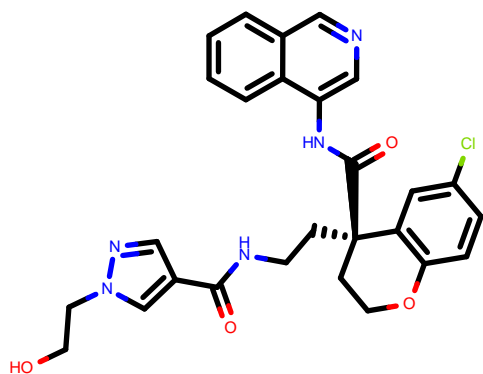
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C(C(=O)N)(F)F)O

RUN: RUN3153

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.25

EN300-761209_3_1



CID: EN300-761209_3_1

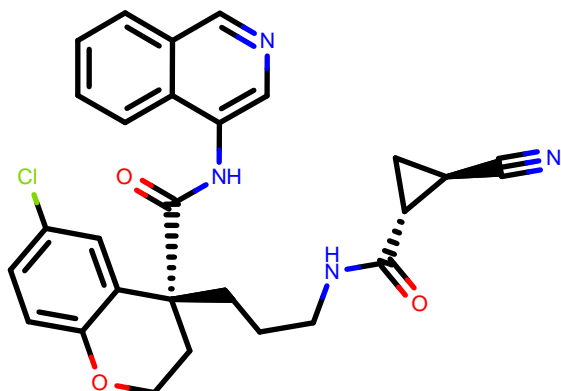
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5enn(c5)CCO

RUN: RUN15339

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.23

EN300-1588617_4_1



CID: EN300-1588617_4_1

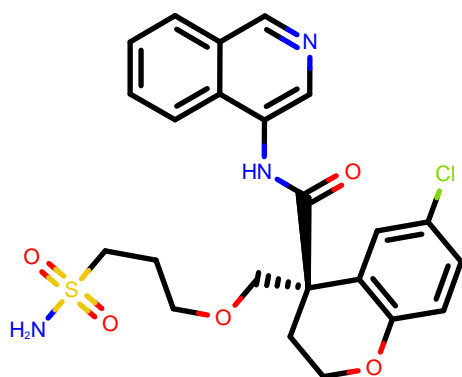
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5C[C@H]5C#N

RUN: RUN14067

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.22

EN300-79588_2_1



CID: EN300-79588_2_1

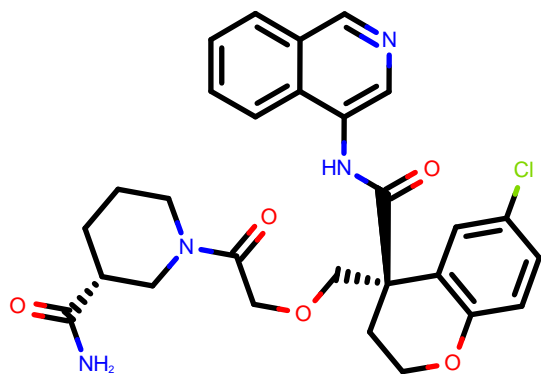
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NS(=O)(=O)N

RUN: RUN1210

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.26

EN300-22880_2_2



CID: EN300-22880_2_2

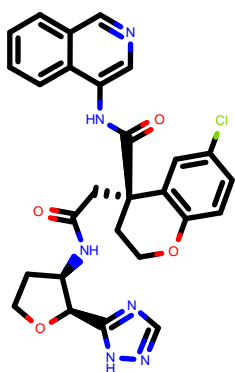
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN2200

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.23

EN300-1272704_1_1



CID: EN300-1272704_1_1

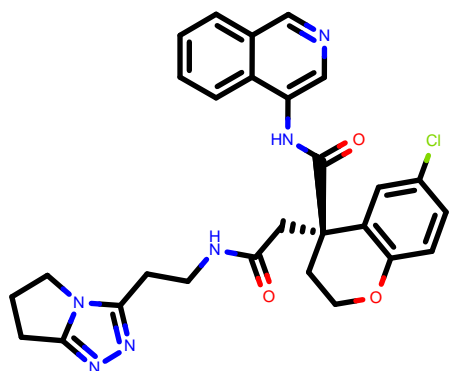
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC@@H5CCOC@@H5d6(H)on6

RUN: RUN12596

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.27

EN300-175300_1_1



CID: EN300-175300_1_1

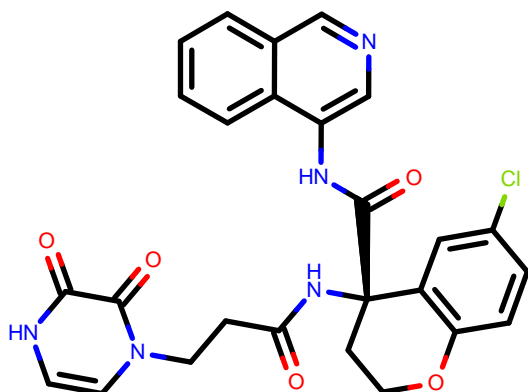
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5nnc6n5CC6

RUN: RUN10529

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-65383_1_1



CID: EN300-65383_1_1

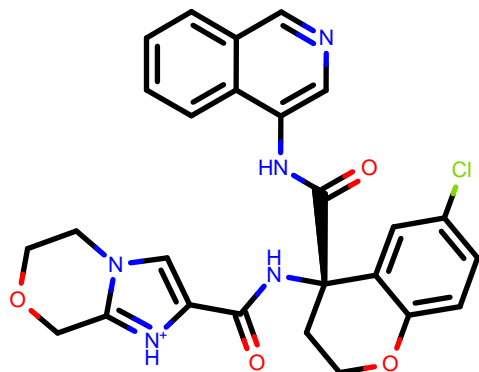
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cc[nH]5(=O)c5=O

RUN: RUN5522

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.26

EN300-321960_1_1



CID: EN300-321960_1_1

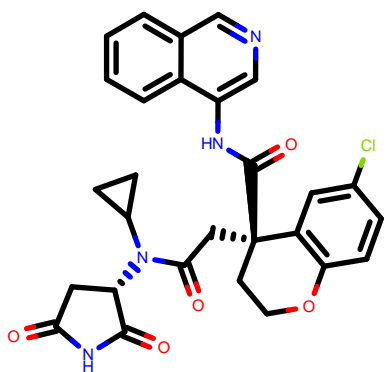
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5n6c([nH]5)COC6

RUN: RUN4854

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.23

EN300-61086_1_1



CID: EN300-61086_1_1

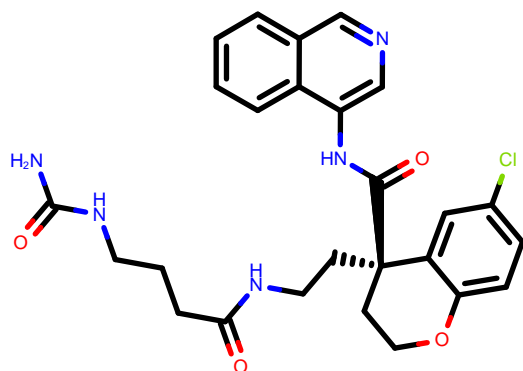
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(Oc4cc3cc4)C(C)OC[C@H]5C(=O)NC5=O/C6CC6

RUN: RUN6400

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.30

EN300-05620_3_1



CID: EN300-05620_3_1

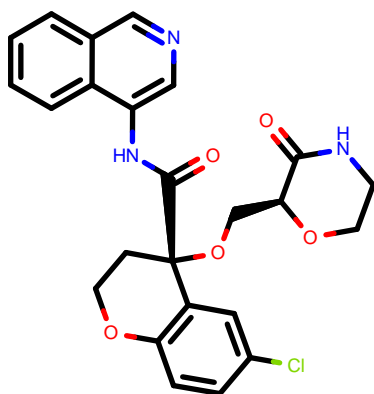
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(Oc4cc3cc4)C(C)OC(=O)CCNC(=O)N

RUN: RUN7875

DDG (kcal/mol): -0.63

dDDG (kcal/mol): 0.22

EN300-1706036_1_1



CID: EN300-1706036_1_1

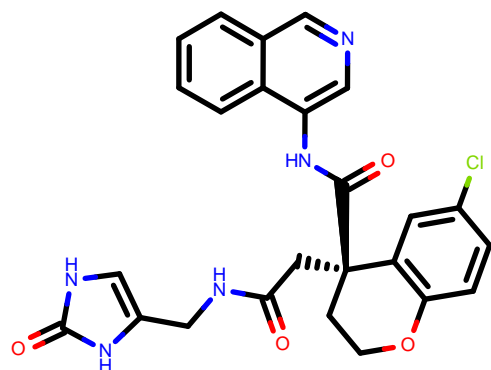
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(Oc4cc3cc4)C(C)OC[C@H]5C(=O)NCCO5

RUN: RUN863

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.21

EN300-260603_1_1



CID: EN300-260603_1_1

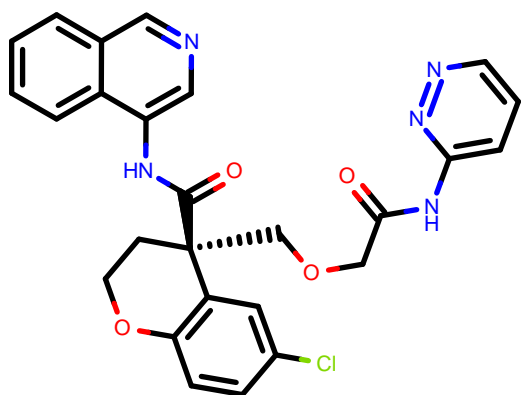
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(Oc4cc3cc4)C(C)OC(=O)NC5c[nH]c(=O)[nH]5

RUN: RUN12296

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.21

EN300-761618_2_1



CID: EN300-761618_2_1

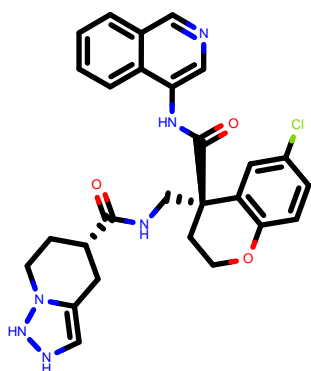
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)Nc5ccnnc5

RUN: RUN2648

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.24

EN300-7430501_2_1



CID: EN300-7430501_2_1

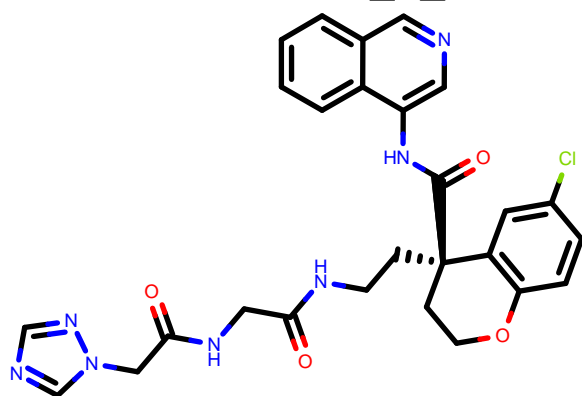
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CNC6c(cnn6)C5

RUN: RUN7305

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.25

EN300-52383_3_1



CID: EN300-52383_3_1

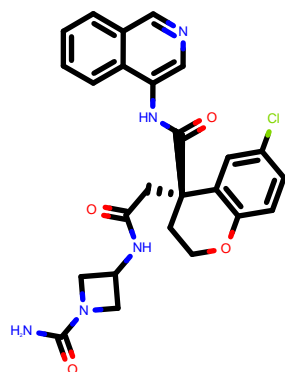
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CNC(=O)Cn5cnnc5

RUN: RUN14472

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.31

EN300-6472847_1_1



CID: EN300-6472847_1_1

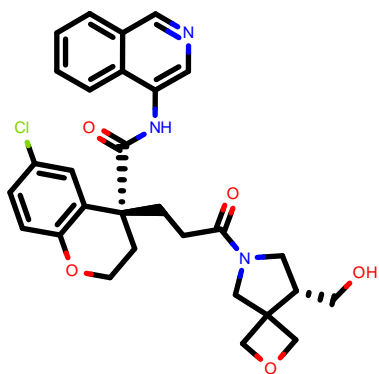
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5CN(C5)C(=O)N

RUN: RUN12714

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.21

EN300-395654_2_1



CID: EN300-395654_2_1

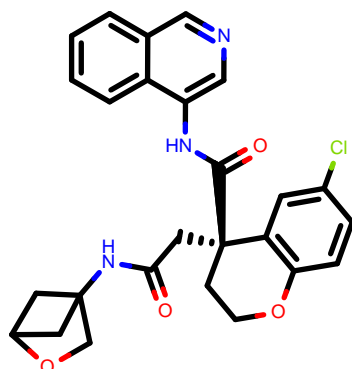
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCC(=O)N5C[C@@H](C6(C)C5)OC6

RUN: RUN14031

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.25

EN300-6734977_1_1



CID: EN300-6734977_1_1

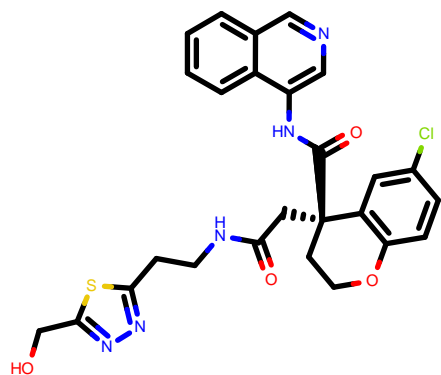
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCC(=O)N5C6CC(C5)OC6

RUN: RUN8604

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.23

EN300-7549247_1_1



CID: EN300-7549247_1_1

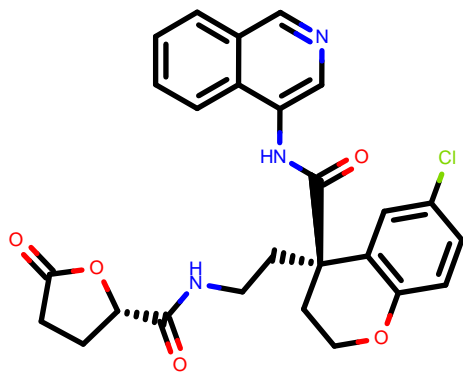
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCC(=O)N5C6C(S)N(C5)CO

RUN: RUN10879

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.28

EN300-359750_3_1



CID: EN300-359750_3_1

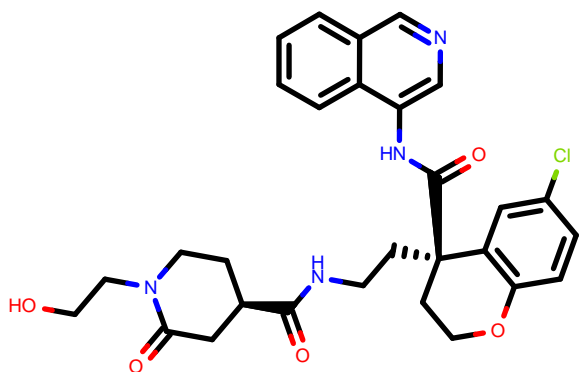
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)C(CO)C4=CC=CC=C4C1CCNC(=O)[C@@H]5CCC(=O)O5

RUN: RUN14904

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.21

EN300-1723663_3_2



CID: EN300-1723663_3_2

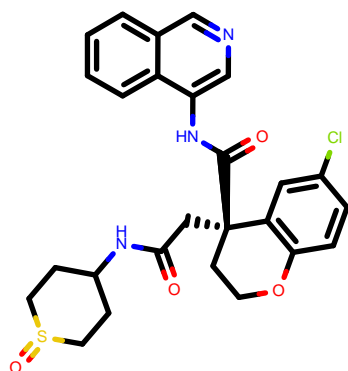
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCNC(=O)C5CCO

RUN: RUN4097

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.32

EN300-124964_1_1



CID: EN300-124964_1_1

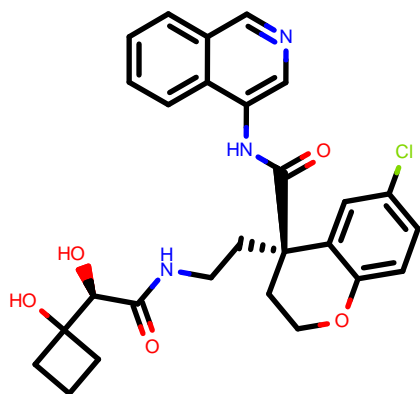
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5CCS(=O)C5

RUN: RUN13246

DDG (kcal/mol): -0.62

dDDG (kcal/mol): 0.17

EN300-1073320_3_1



CID: EN300-1073320_3_1

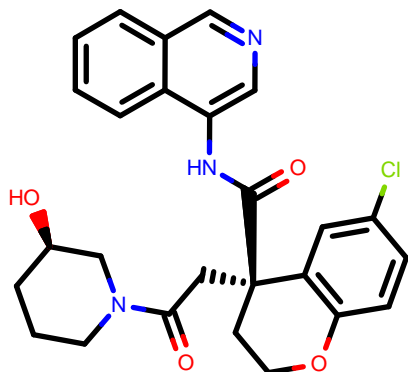
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5(C5(CCC5)O)O

RUN: RUN4269

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.27

EN300-266117_1_1



CID: EN300-266117_1_1

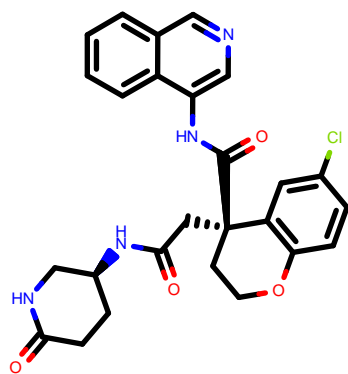
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC[C@H]5O

RUN: RUN5281

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.20

EN300-62191_1_2



CID: EN300-62191_1_2

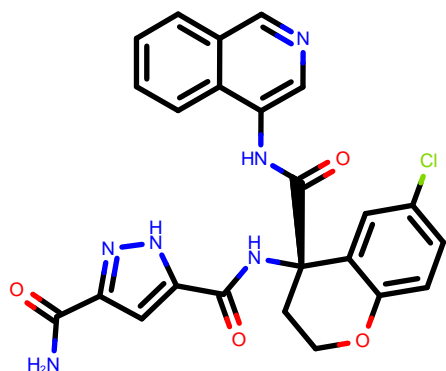
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCC(=O)NCS

RUN: RUN11835

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.22

EN300-1689158_1_1



CID: EN300-1689158_1_1

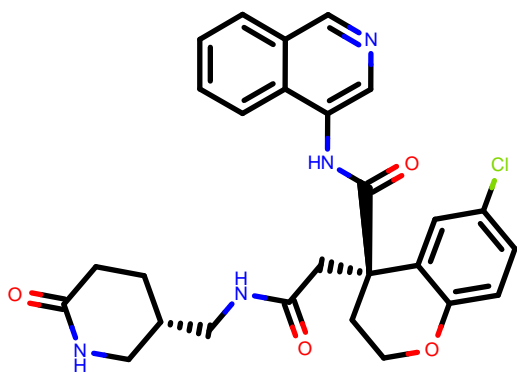
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(n[nH]5)C(=O)N

RUN: RUN6536

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.18

EN300-6746326_1_2



CID: EN300-6746326_1_2

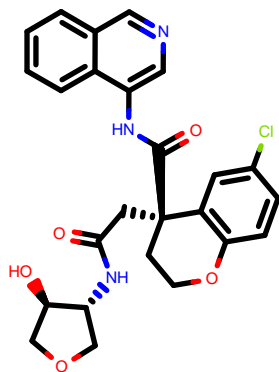
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCC(=O)NCS

RUN: RUN8195

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.21

EN300-331476_1_1



CID: EN300-331476_1_1

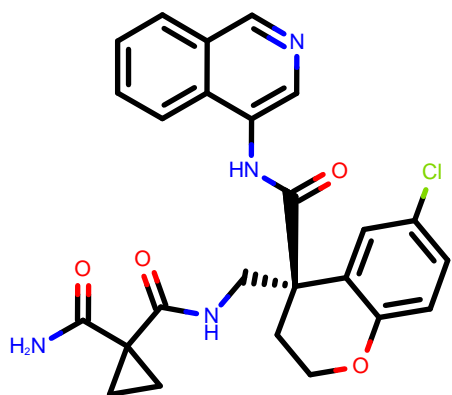
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5O

RUN: RUN6923

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.19

EN300-69070_2_1



CID: EN300-69070_2_1

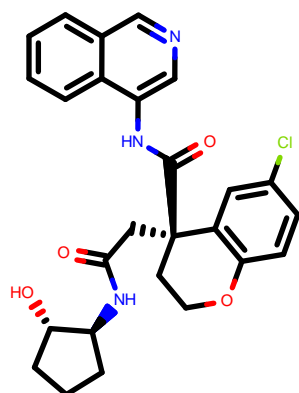
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(C)C(=O)N

RUN: RUN4615

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

EN300-344121_1_1



CID: EN300-344121_1_1

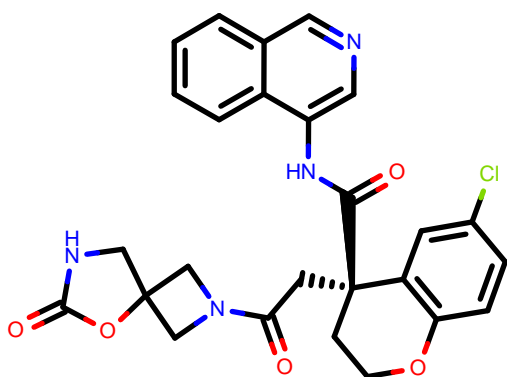
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@H]5O

RUN: RUN4489

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.25

EN300-6494361_1_1



CID: EN300-6494361_1_1

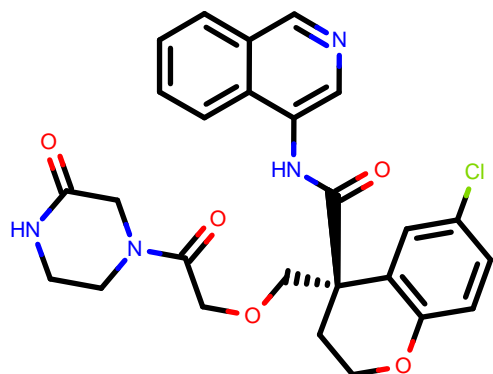
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CNC(=O)O6

RUN: RUN3605

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.20

EN300-22884_2_1



CID: EN300-22884_2_1

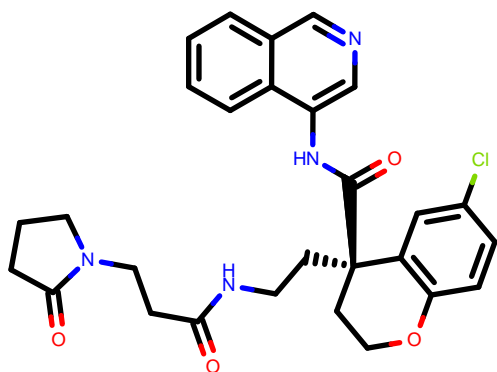
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCNC(=O)C5

RUN: RUN1770

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.22

EN300-67191_3_1



CID: EN300-67191_3_1

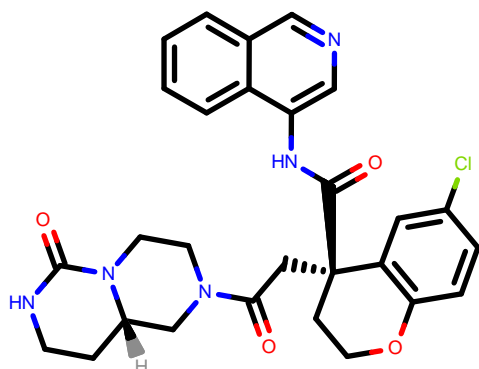
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCC5=O

RUN: RUN14002

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.31

EN300-6474647_1_1



CID: EN300-6474647_1_1

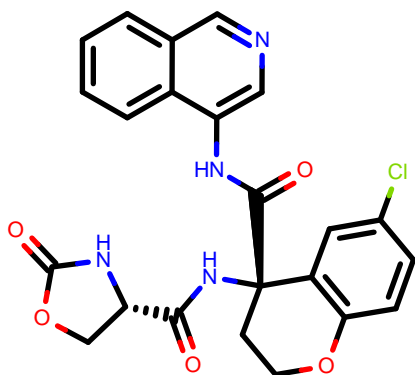
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@H](C5)CCNC6=O

RUN: RUN4285

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

EN300-201346_1_1



CID: EN300-201346_1_1

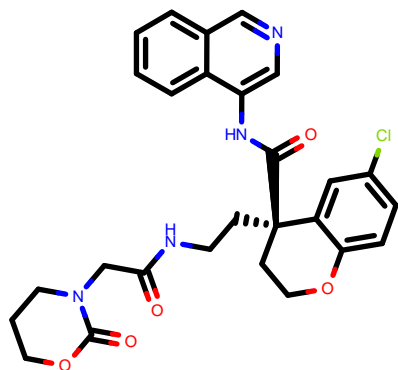
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]4H5COC(=O)N5

RUN: RUN755

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.19

EN300-103638_3_1



CID: EN300-103638_3_1

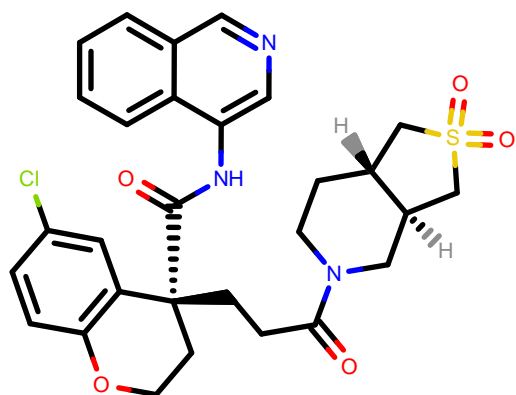
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCC5=O

RUN: RUN10885

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.24

EN300-365993_2_1



CID: EN300-365993_2_1

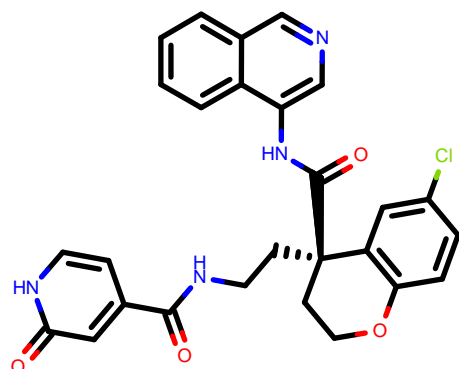
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC[C@]@H6CS(=O)(=O)C[C@]@H5C5

RUN: RUN14699

DDG (kcal/mol): -0.61

dDDG (kcal/mol): 0.28

EN300-97661_3_1



CID: EN300-97661_3_1

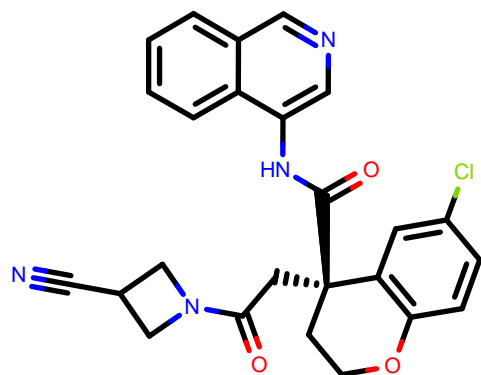
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)c5cc[nH]c(=O)c5

RUN: RUN3005

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.21

EN300-206282_1_1



CID: EN300-206282_1_1

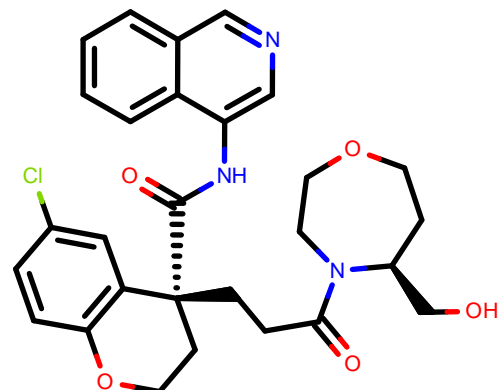
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)C#N

RUN: RUN12972

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.18

EN300-6732376_2_2



CID: EN300-6732376_2_2

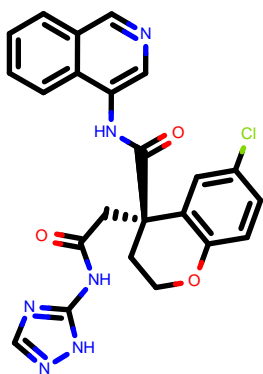
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCOCC[C@]@H5CO

RUN: RUN5660

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.29

EN300-17045_1_1



CID: EN300-17045_1_1

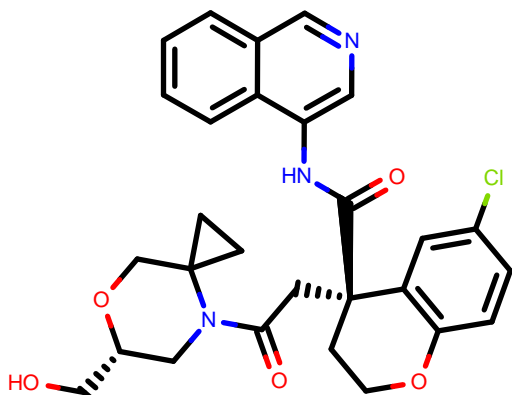
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5[nH]nnc5

RUN: RUN12056

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.17

EN300-7493255_1_2



CID: EN300-7493255_1_2

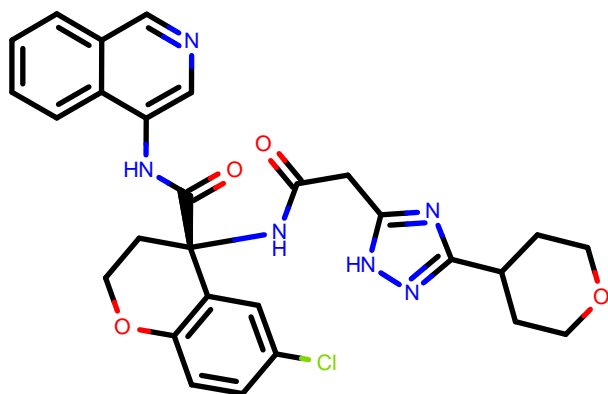
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](OCC56C06)CO

RUN: RUN3397

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.33

EN300-385132_1_1



CID: EN300-385132_1_1

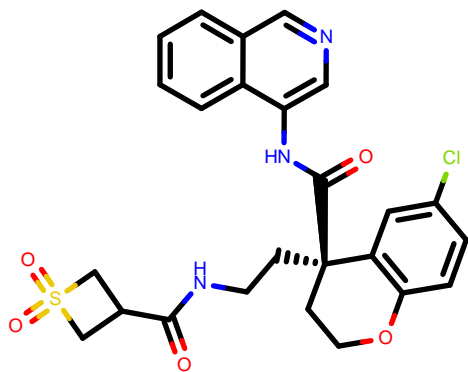
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]nc(n5)C6CCOCC6

RUN: RUN5994

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.31

EN300-261365_3_1



CID: EN300-261365_3_1

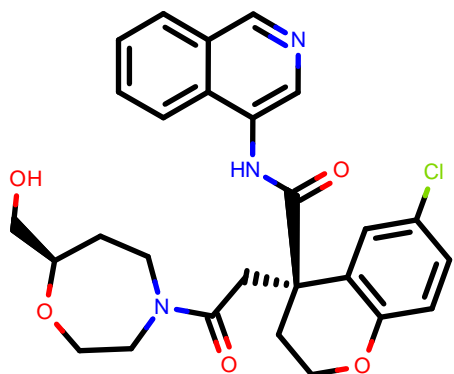
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CS(=O)(=O)C5

RUN: RUN14984

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.26

EN300-2007620_1_2



CID: EN300-2007620_1_2

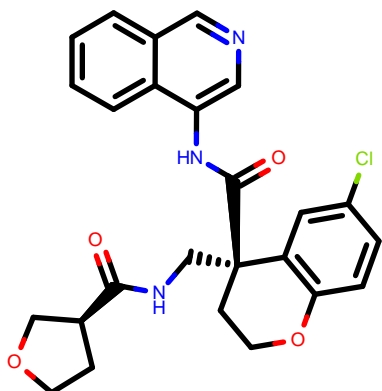
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](OCC5)CO

RUN: RUN9368

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.29

EN300-53423_2_2



CID: EN300-53423_2_2

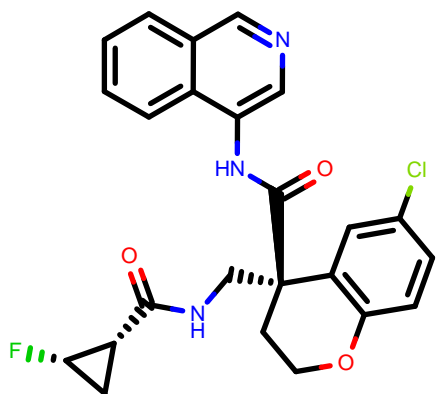
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCOC5

RUN: RUN5751

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.22

EN300-4698402_2_1



CID: EN300-4698402_2_1

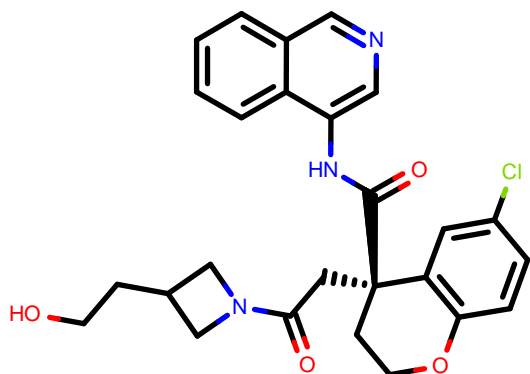
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5H5C[C@@H]5F

RUN: RUN4963

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.18

EN300-7413100_1_1



CID: EN300-7413100_1_1

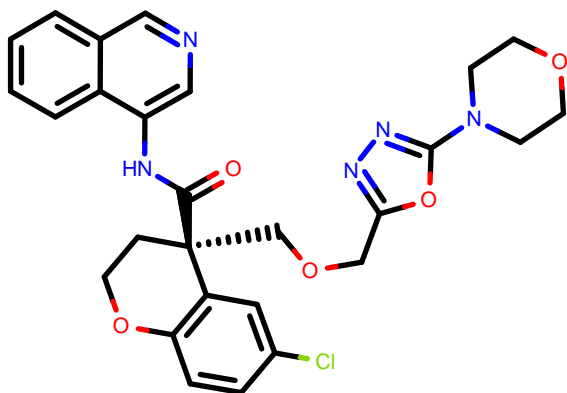
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CCO

RUN: RUN5977

DDG (kcal/mol): -0.60

dDDG (kcal/mol): 0.21

EN300-6486576_2_1



CID: EN300-6486576_2_1

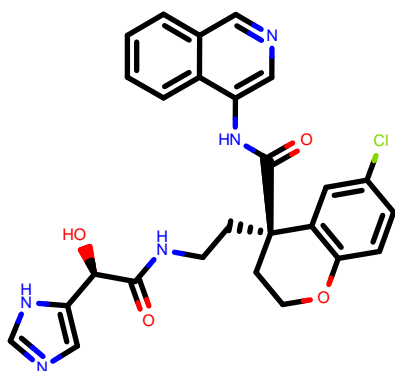
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nnc(o5)N6CCOCC6

RUN: RUN2707

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.24

EN300-254121_3_2



CID: EN300-254121_3_2

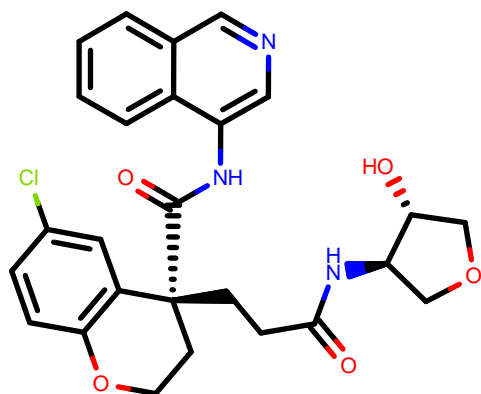
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H(c5ncc[nH]5)O

RUN: RUN9520

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.30

EN300-331476_2_1



CID: EN300-331476_2_1

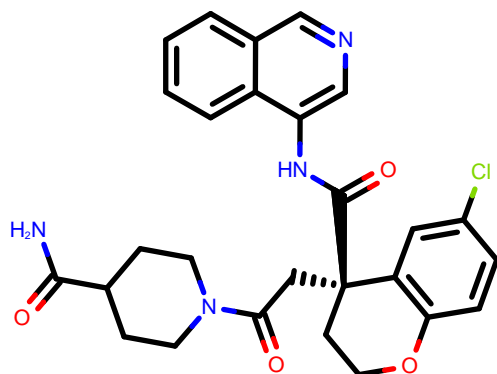
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]H5OCC[C@@]H5O

RUN: RUN3860

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.25

EN300-1265946_1_1



CID: EN300-1265946_1_1

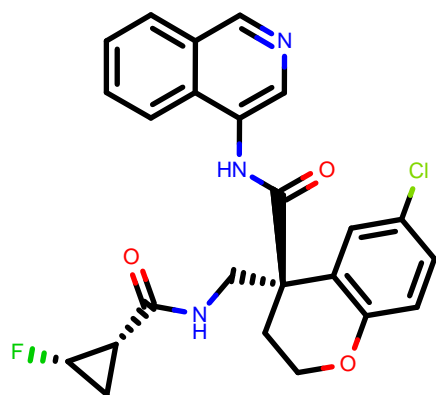
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)C(=O)N

RUN: RUN5337

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.24

EN300-4698402_2_1



CID: EN300-4698402_2_1

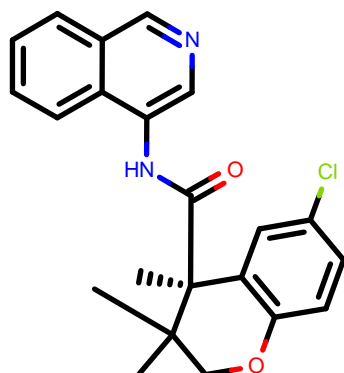
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN4959

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.19

DAR-DIA-0d514e7d-30_1



CID: DAR-DIA-0d514e7d-30_1

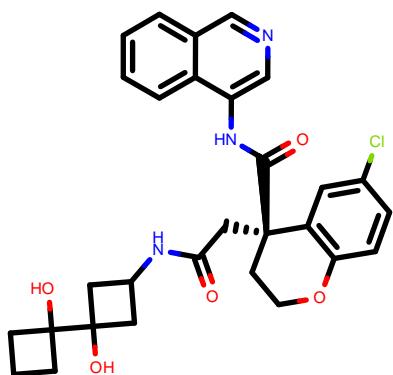
SMILES: C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3ncnc4c3cccc4

RUN: RUN65

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.10

EN300-7465104_1_1



CID: EN300-7465104_1_1

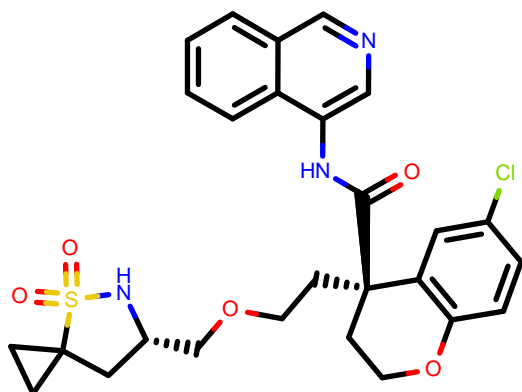
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)(C6(CCC6)O)O

RUN: RUN7515

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.28

EN300-6504697_3_2



CID: EN300-6504697_3_2

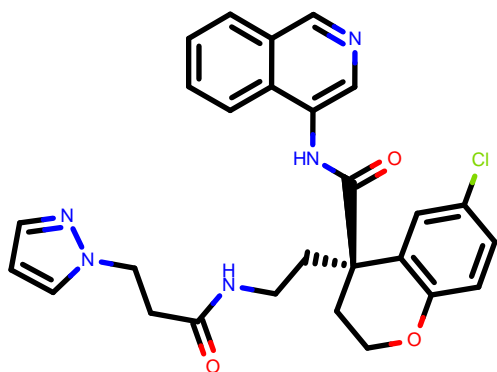
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C6(C6)S(=O)(=O)N5

RUN: RUN2518

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.33

EN300-25986_3_1



CID: EN300-25986_3_1

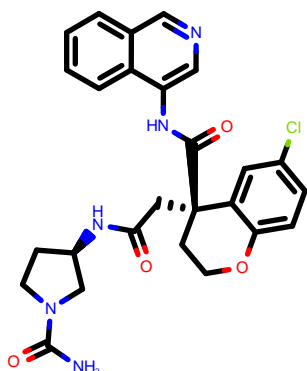
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cccn5

RUN: RUN7435

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.23

EN300-75402_1_1



CID: EN300-75402_1_1

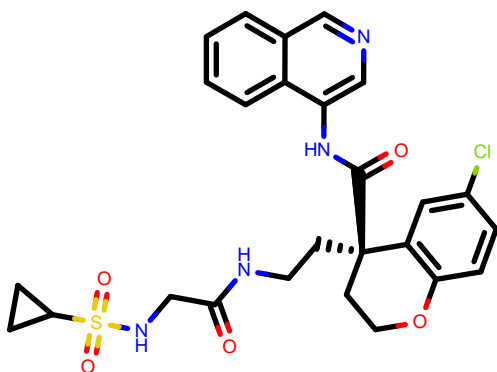
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5CCCN(C5)C(=O)N

RUN: RUN10803

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.21

EN300-203853_3_1



CID: EN300-203853_3_1

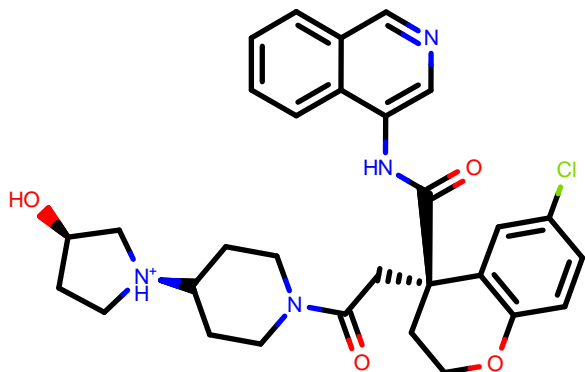
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CCNC(=O)CNS(=O)(=O)C5CC5

RUN: RUN13872

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.33

EN300-241988_1_4



CID: EN300-241988_1_4

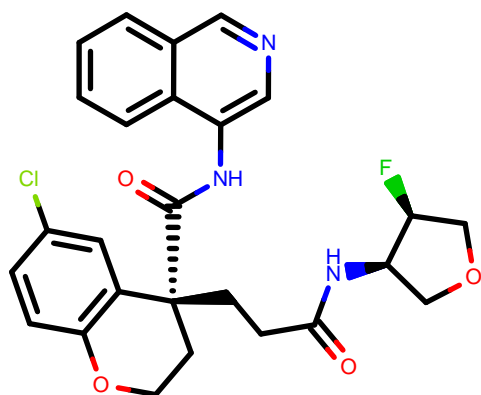
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(C5)N@H]6CC[C@H]6O

RUN: RUN2269

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.26

EN300-7549621_2_1



CID: EN300-7549621_2_1

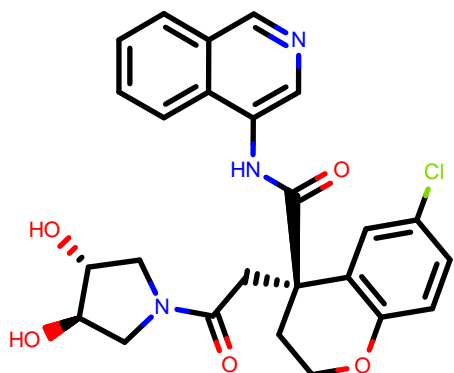
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5COC(C@@H)5F

RUN: RUN4268

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.23

EN300-97938_1_1



CID: EN300-97938_1_1

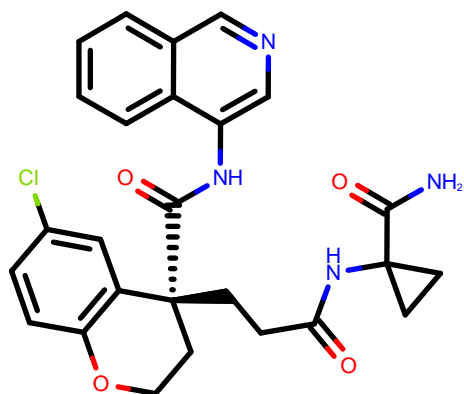
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C@@H)(C5)O

RUN: RUN6831

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.21

EN300-106988_2_1



CID: EN300-106988_2_1

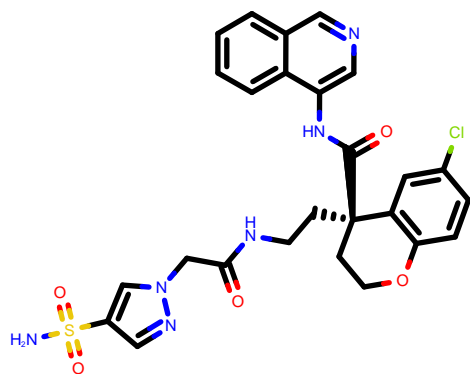
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N(C5)C5)C(=O)N

RUN: RUN12581

DDG (kcal/mol): -0.59

dDDG (kcal/mol): 0.27

EN300-60514_3_1



CID: EN300-60514_3_1

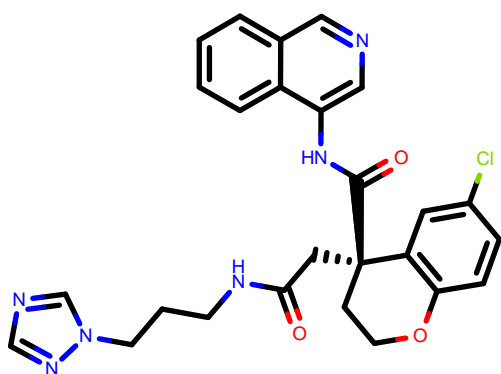
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccn(S(=O)(=O)N)5

RUN: RUN7263

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.33

EN300-270328_1_1



CID: EN300-270328_1_1

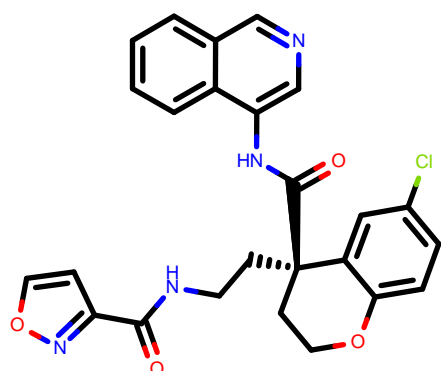
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCCn5cnns5

RUN: RUN5277

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.29

EN300-22245_3_1



CID: EN300-22245_3_1

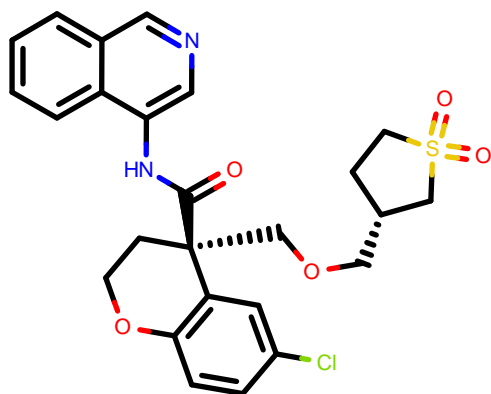
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccon5

RUN: RUN15266

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.19

EN300-1448603_2_1



CID: EN300-1448603_2_1

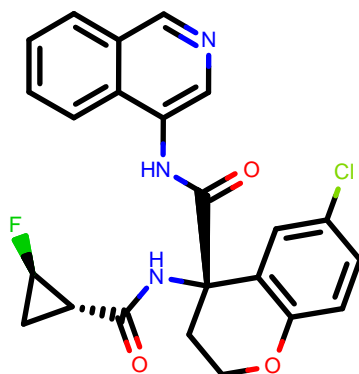
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COC[C@@]5H5CCS(=O)(=O)C5

RUN: RUN652

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.24

EN300-1654606_1_1



CID: EN300-1654606_1_1

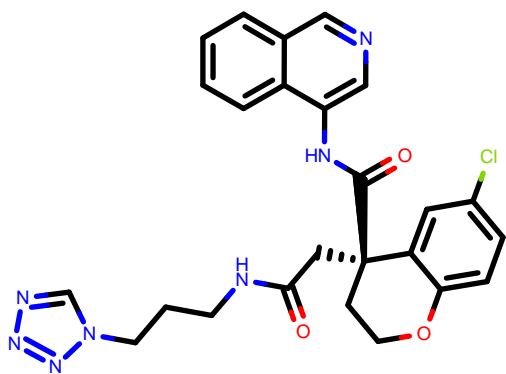
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]5H5C[C@@]5F

RUN: RUN5846

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.21

EN300-1698571_1_1



CID: EN300-1698571_1_1

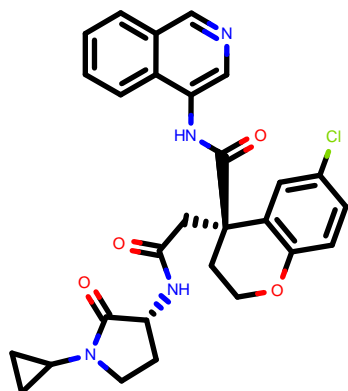
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCn5nnn5

RUN: RUN12096

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.25

EN300-77438_1_2



CID: EN300-77438_1_2

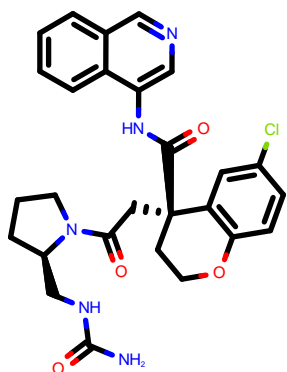
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5H5CCN(C5=O)C6CC6

RUN: RUN12418

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.24

EN300-212795_1_1



CID: EN300-212795_1_1

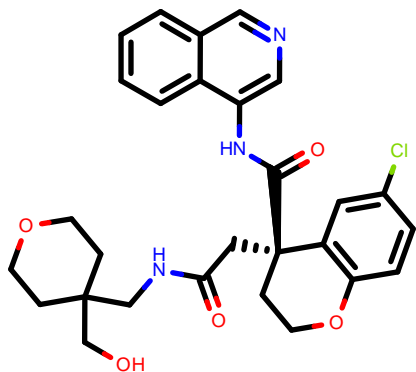
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]C@H5CNC(=O)N

RUN: RUN5289

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.23

EN300-115011_1_1



CID: EN300-115011_1_1

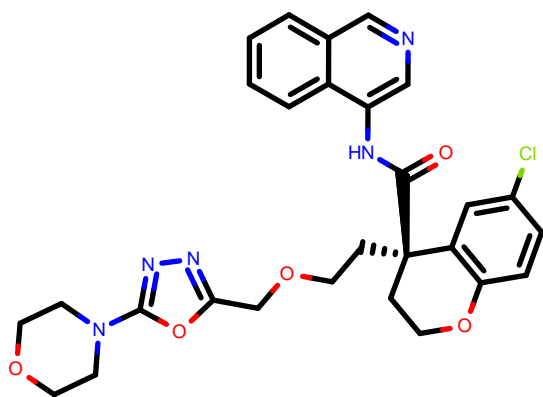
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CCOCC5)CO

RUN: RUN10671

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.25

EN300-6486576_3_1



CID: EN300-6486576_3_1

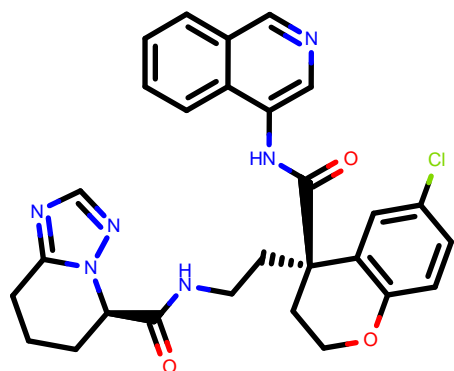
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nn(c5)N6CCOCC6

RUN: RUN1009

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.26

EN300-1273016_3_2



CID: EN300-1273016_3_2

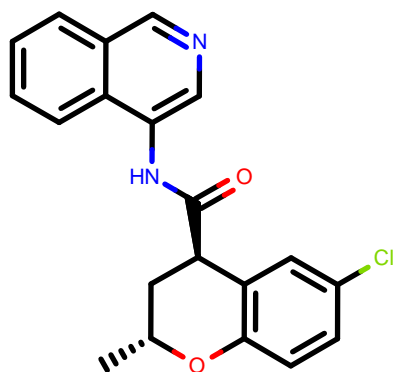
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCc6n5n6

RUN: RUN15220

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.28

ALP-POS-d3acb8cc-1_1



CID: ALP-POS-d3acb8cc-1_1

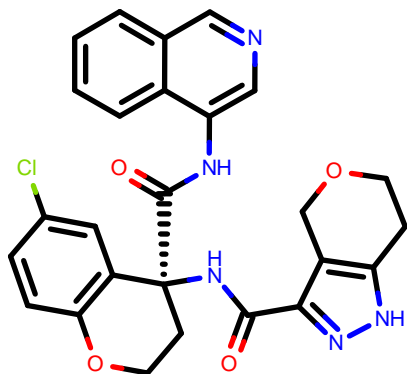
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cnc4c3cccc4

RUN: RUN42

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.06

EN300-103031_1_1



CID: EN300-103031_1_1

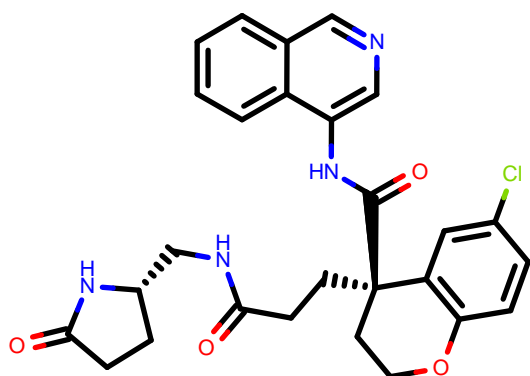
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c([nH]n5)CCOC6

RUN: RUN3230

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.19

EN300-75030_2_2



CID: EN300-75030_2_2

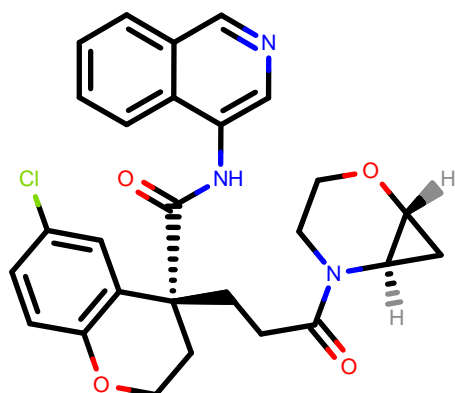
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@]H5CCCC(=O)N5

RUN: RUN5012

DDG (kcal/mol): -0.58

dDDG (kcal/mol): 0.29

EN300-91609_2_1



CID: EN300-91609_2_1

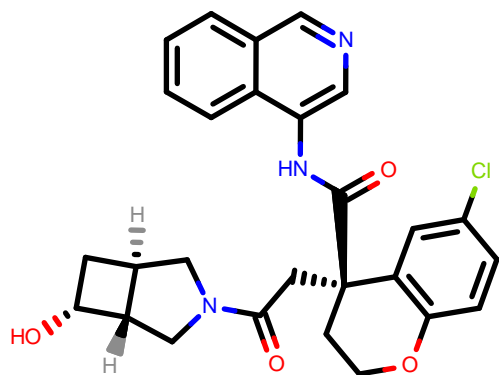
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCO[C@@]H6[C@@]H5C6

RUN: RUN7458

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

EN300-305294_1_8



CID: EN300-305294_1_8

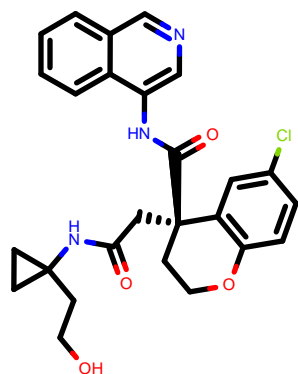
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C[C@@]H6[C@@]H[C@@]H5C5O

RUN: RUN6145

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

EN300-121078_1_1



CID: EN300-121078_1_1

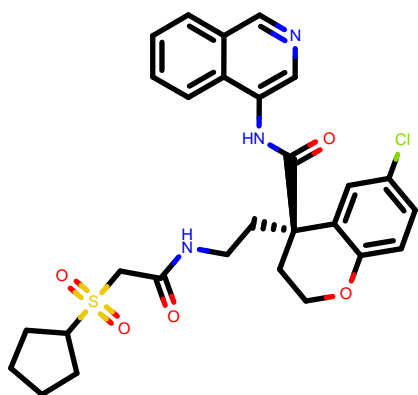
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(C)CCO

RUN: RUN12622

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

EN300-42154_3_1



CID: EN300-42154_3_1

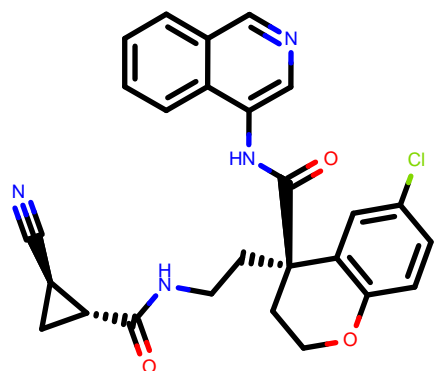
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)C5CCCC5

RUN: RUN14344

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.33

EN300-1588617_3_1



CID: EN300-1588617_3_1

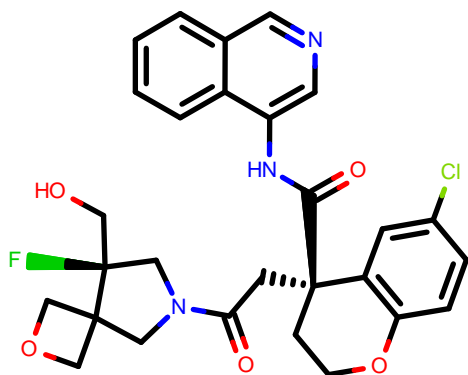
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5C[C@H]5C#N

RUN: RUN15174

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.20

EN300-1719075_1_2



CID: EN300-1719075_1_2

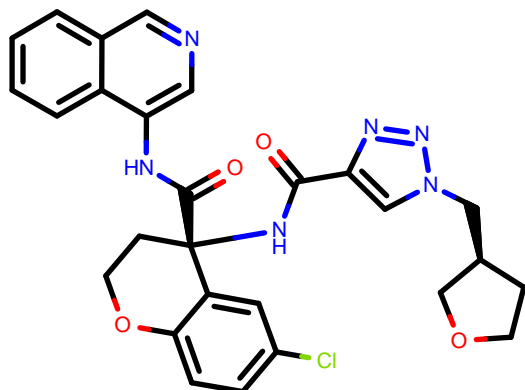
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@](C6(C5)COC6)(CO)F

RUN: RUN12698

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.31

EN300-317272_1_2



CID: EN300-317272_1_2

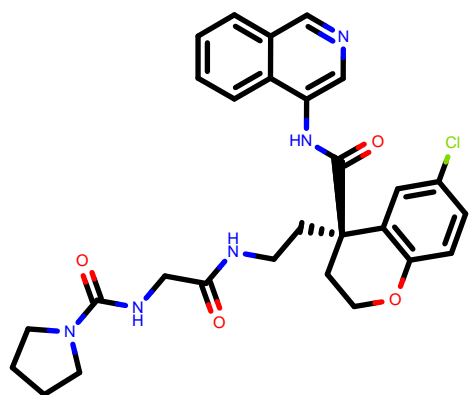
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@H]6CCOC6

RUN: RUN635

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.23

EN300-383906_3_1



CID: EN300-383906_3_1

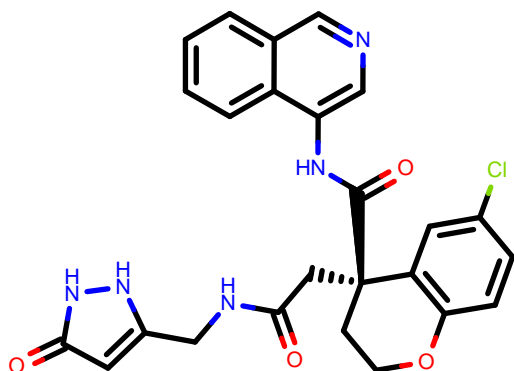
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)N5CCCC5

RUN: RUN633

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.24

EN300-260760_1_1



CID: EN300-260760_1_1

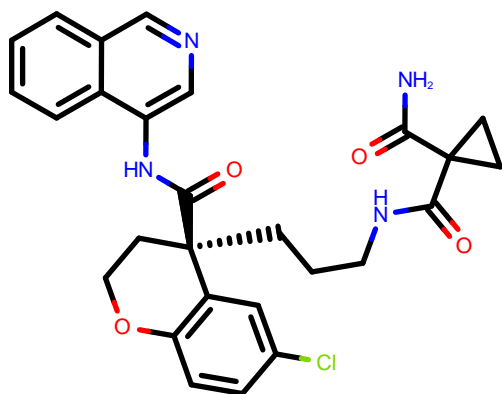
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5c5c([nH][nH]5)

RUN: RUN3013

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.20

EN300-69070_4_1



CID: EN300-69070_4_1

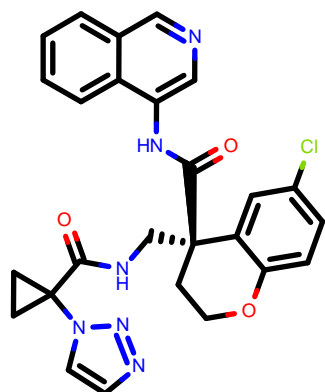
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C5(C)C5Cl(=O)N

RUN: RUN10941

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.22

EN300-658559_2_1



CID: EN300-658559_2_1

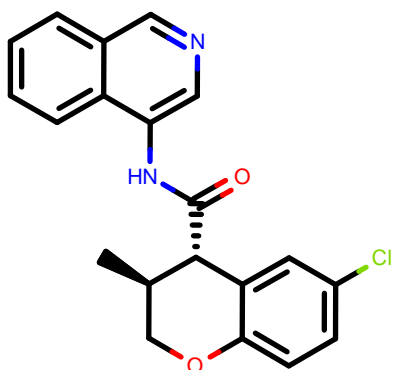
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(C)C5n6cnm6

RUN: RUN3955

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.25

ADA-UCB-dc2b944c-13_1



CID: ADA-UCB-dc2b944c-13_1

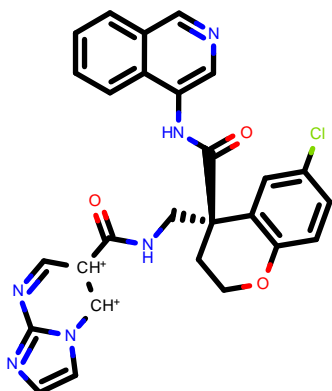
SMILES: C[C@@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl

RUN: RUN112

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.14

EN300-147397_2_1



CID: EN300-147397_2_1

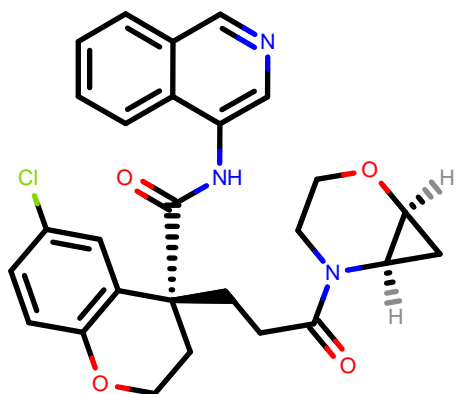
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncc6nccn6c5

RUN: RUN9030

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.25

EN300-91609_2_2



CID: EN300-91609_2_2

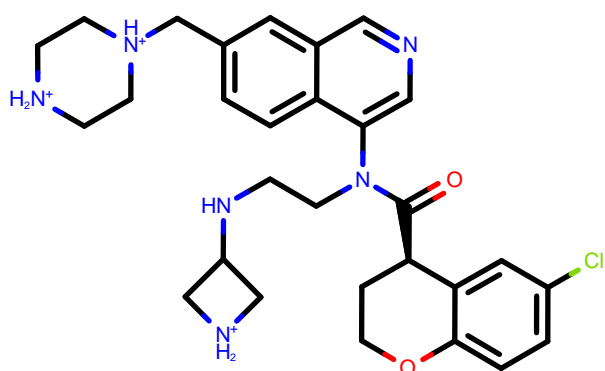
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCO[C@@H]6[C@H]5C6

RUN: RUN14429

DDG (kcal/mol): -0.57

dDDG (kcal/mol): 0.26

MAK-UNK-83e0a0b4-2_1



CID: MAK-UNK-83e0a0b4-2_1

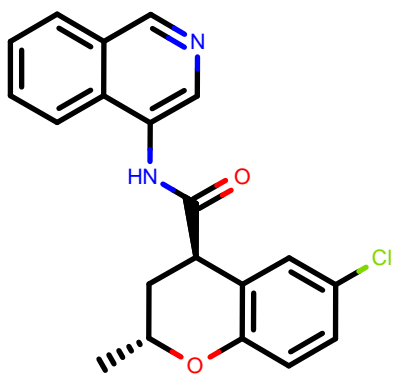
SMILES: c1cc2cc1CN3CC[NH2+]CC3)cncc2N(CCN4CQ[NH2+]C4)C(=O)[C@@]5(H)SCCOc6c5ccc6)Cl

RUN: RUN197

DDG (kcal/mol): -0.57

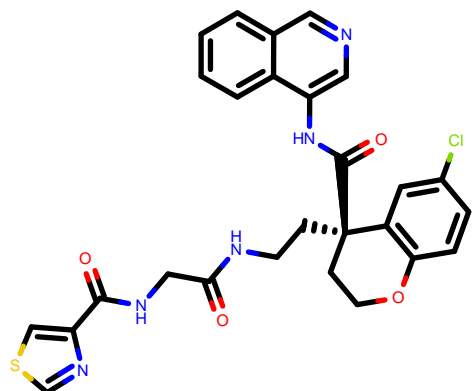
dDDG (kcal/mol): 0.40

ALP-POS-d3acb8cc-1_1



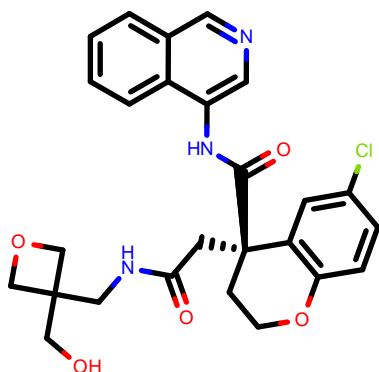
CID:	ALP-POS-d3acb8cc-1_1
SMILES:	<chem>C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4</chem>
RUN:	RUN43
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.06

EN300-182084_3_1



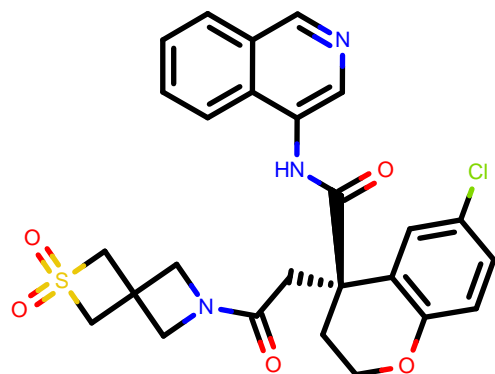
CID:	EN300-182084_3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)CSc5cn5</chem>
RUN:	RUN11918
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.26

EN300-105482_1_1



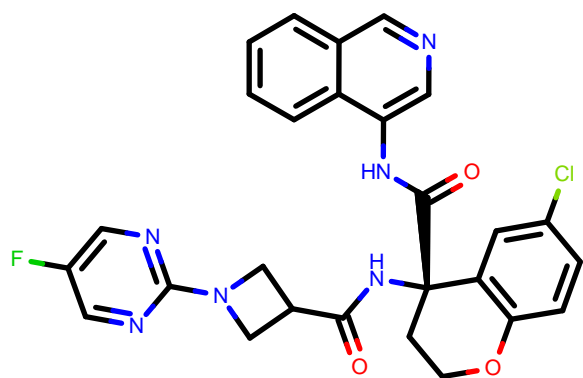
CID:	EN300-105482_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(COC5)CO</chem>
RUN:	RUN8059
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.21

EN300-255498_1_1



CID:	EN300-255498_1_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CS(=O)(=O)C6</chem>
RUN:	RUN10035
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.21

EN300-905492_1_1



CID: EN300-905492_1_1

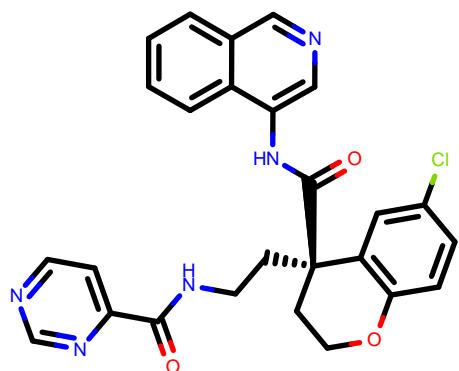
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CSCN(C5)c6ncc(en6)F

RUN: RUN9796

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.26

EN300-111006_3_1



CID: EN300-111006_3_1

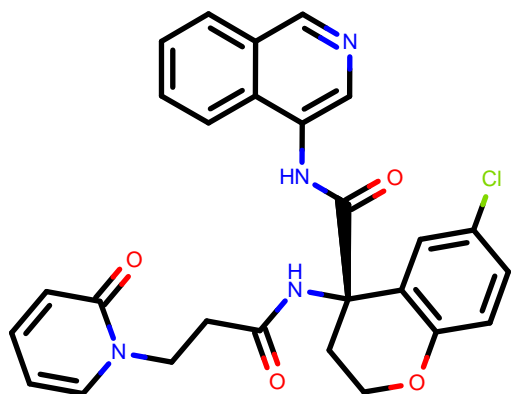
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccncc5

RUN: RUN15422

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.22

EN300-36622_1_1



CID: EN300-36622_1_1

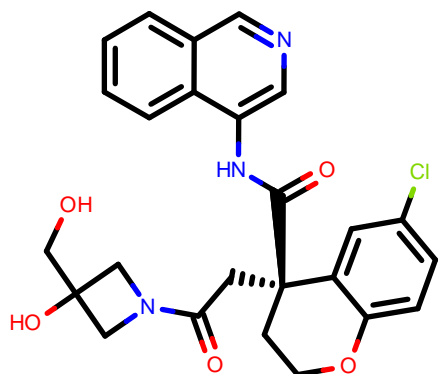
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CCn5ccccc5=O

RUN: RUN5426

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-226776_1_1



CID: EN300-226776_1_1

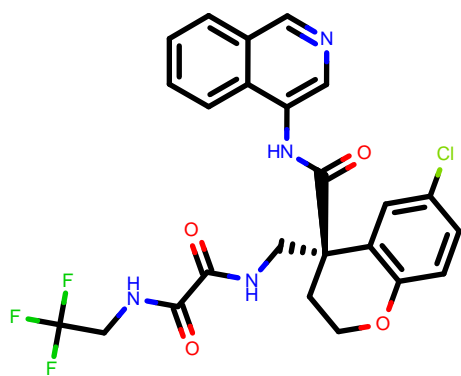
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)(CO)O

RUN: RUN6691

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.25

EN300-139268_2_1



CID: EN300-139268_2_1

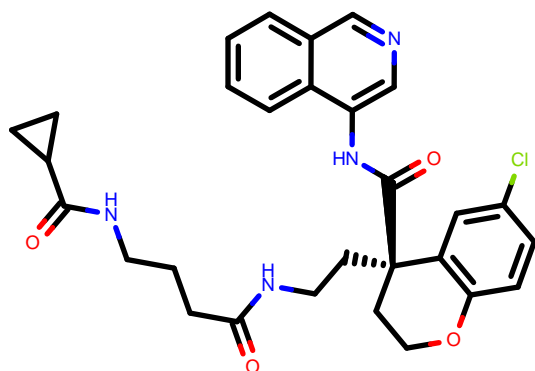
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CNC(=O)C(=O)NCC(F)(F)F

RUN: RUN8017

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-36850_3_1



CID: EN300-36850_3_1

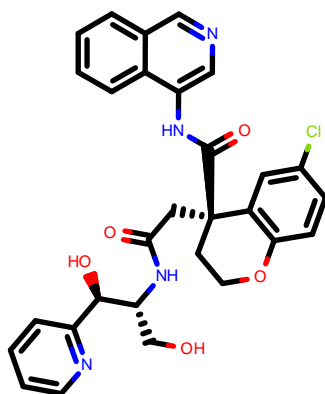
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCNC(=O)CCCCC3

RUN: RUN14618

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.28

EN300-332714_1_4



CID: EN300-332714_1_4

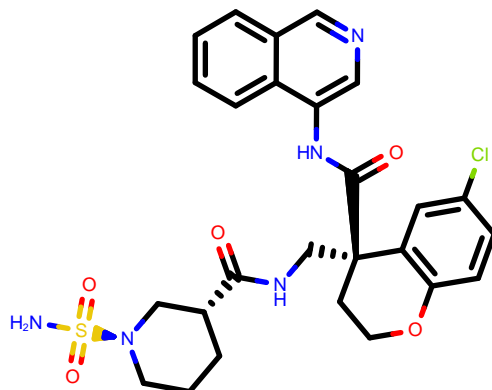
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CC(O)Nc5ccncc5O

RUN: RUN3789

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.39

EN300-219496_2_3



CID: EN300-219496_2_3

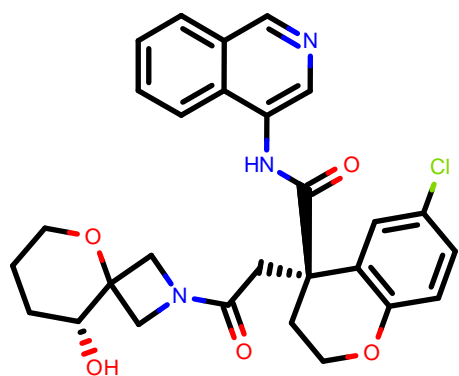
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)Cl)CCNC(=O)C4CCN(C4)S(=O)(=O)N

RUN: RUN5435

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.63

EN300-7434114_1_2



CID: EN300-7434114_1_2

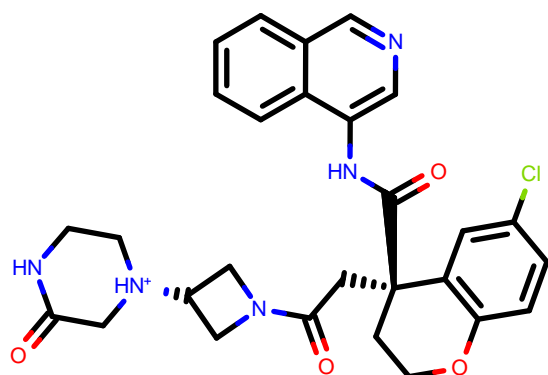
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(COCC4c3cc(cc4)Cl)C(=O)N5CC6(C5)C@H](CCOC6)O

RUN: RUN5369

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.23

EN300-6489476_1_1



CID: EN300-6489476_1_1

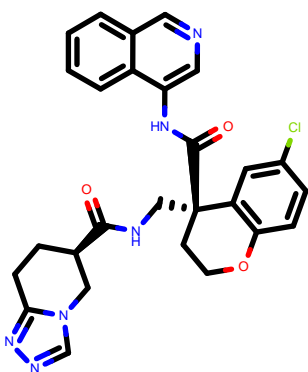
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(COCC4c3cc(cc4)Cl)C(=O)N5C(C5)(N#H)CCNCl=O)O

RUN: RUN13568

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.26

EN300-51350_2_1



CID: EN300-51350_2_1

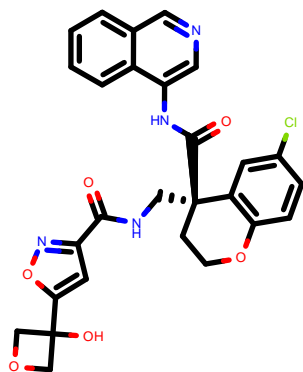
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(COCC4c3cc(cc4)Cl)C(=O)N(C)C@H]5CC6nncn6C5

RUN: RUN7237

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.29

EN300-365017_2_1



CID: EN300-365017_2_1

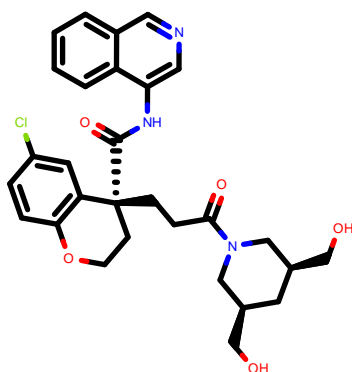
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(COCC4c3cc(cc4)Cl)C(=O)N(C)C@H]5CC6nncn6C5

RUN: RUN3419

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.28

EN300-2007627_2_2



CID: EN300-2007627_2_2

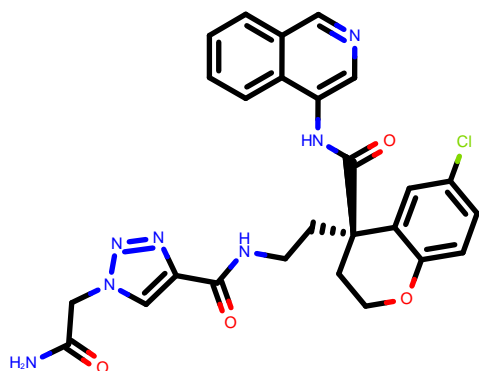
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CC(=O)N6C[C@@H](C)[C@@H](C5)CO5CO

RUN: RUN2606

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.36

EN300-52380_3_1



CID: EN300-52380_3_1

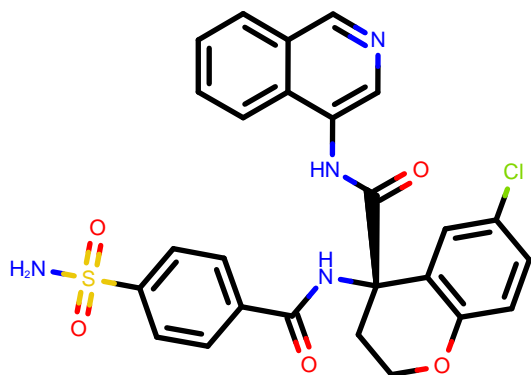
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CCNC(=O)c5nncn5)CC(=O)N

RUN: RUN15291

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.23

EN300-16248_1_1



CID: EN300-16248_1_1

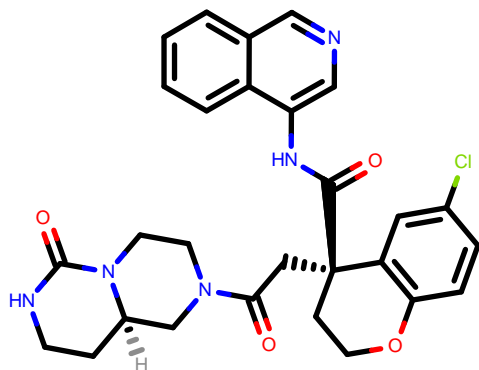
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)NC(=O)c5ccc(cc5)S(=O)(=O)N

RUN: RUN7004

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-6474647_1_2



CID: EN300-6474647_1_2

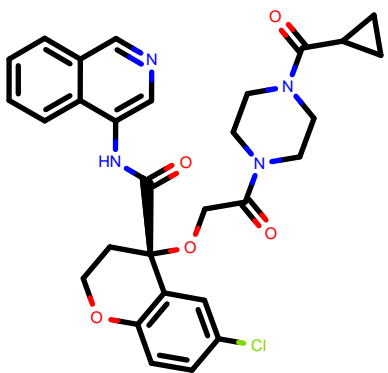
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(c4)C)CC(=O)N5CCN6C[C@@H](C5)CCN6=O

RUN: RUN4241

DDG (kcal/mol): -0.56

dDDG (kcal/mol): 0.24

EN300-47046_1_1



CID: EN300-47046_1_1

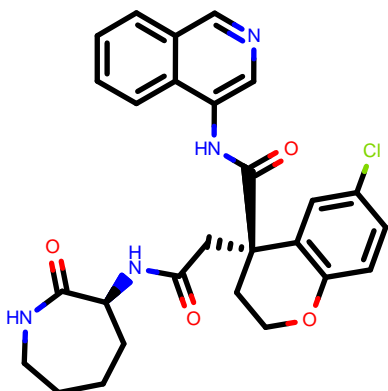
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)OCC(=O)N5CCN(CC5)C(=O)C6CC6

RUN: RUN679

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.30

EN300-129384_1_1



CID: EN300-129384_1_1

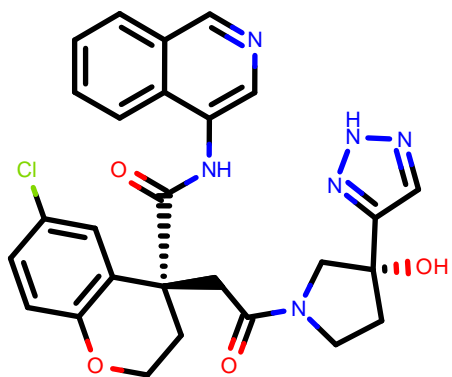
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@H]5CCCCN5=O

RUN: RUN13958

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.23

EN300-221122_1_1



CID: EN300-221122_1_1

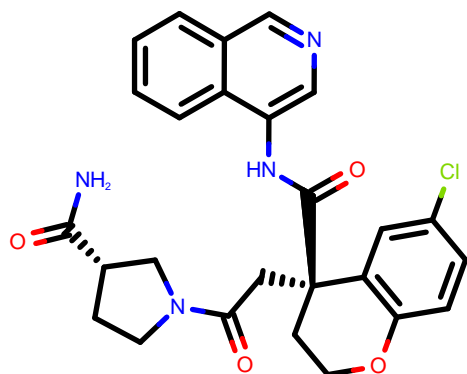
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]3(C)C5(c6cc[nH]6)O

RUN: RUN6459

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.33

EN300-70092_1_1



CID: EN300-70092_1_1

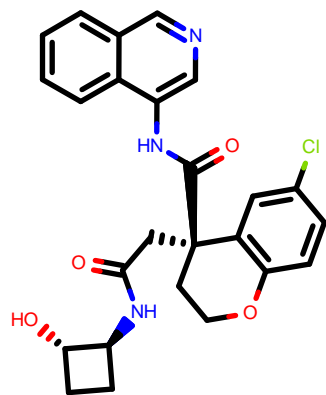
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]3(C)C5(C)C(=O)N

RUN: RUN12444

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.22

EN300-129424_1_4



CID: EN300-129424_1_4

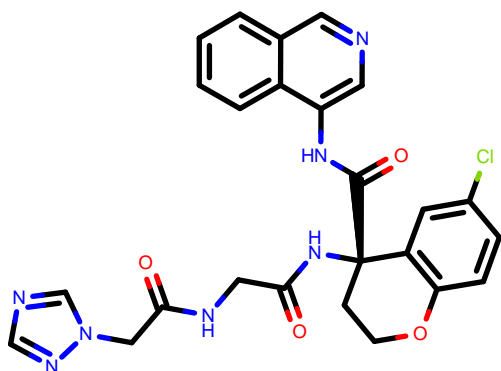
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@@]3H5O

RUN: RUN6699

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.24

EN300-52383_1_1



CID: EN300-52383_1_1

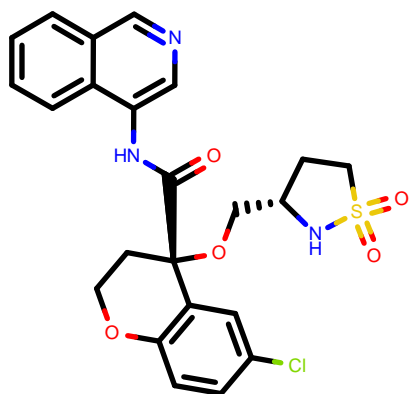
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnns5

RUN: RUN4690

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.28

EN300-1699871_1_2



CID: EN300-1699871_1_2

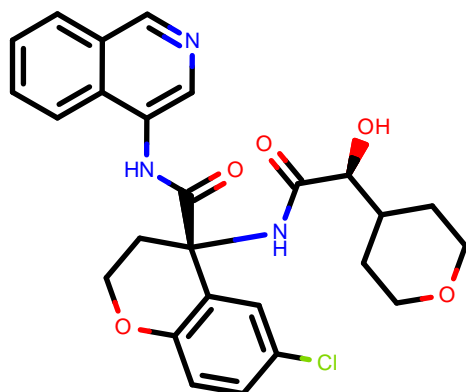
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]3H5S(=O)(=O)N5

RUN: RUN1661

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.27

EN300-6792206_1_1



CID: EN300-6792206_1_1

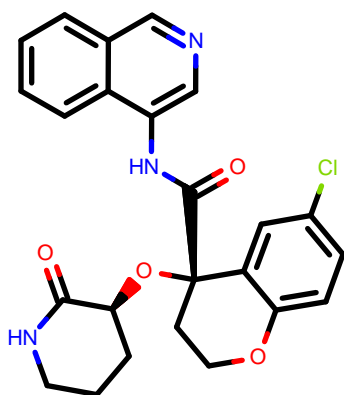
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5CCOCC5)O

RUN: RUN7188

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.34

EN300-107267_1_1



CID: EN300-107267_1_1

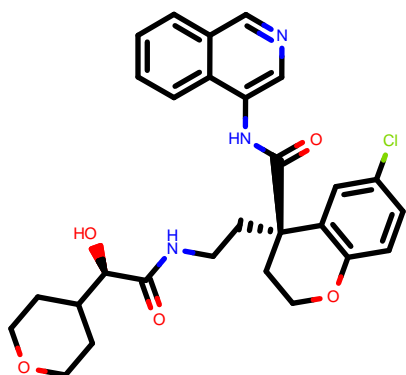
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(Cc4cc3cc(c4)Cl)O[C@H]5C(C)CNC5=O

RUN: RUN2739

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.18

EN300-79180_3_1



CID: EN300-79180_3_1

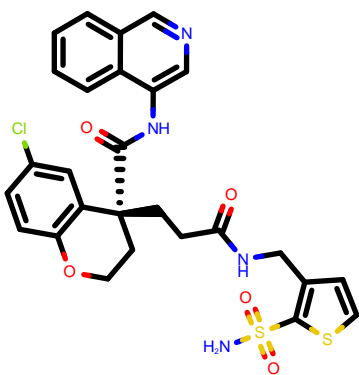
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(Cc4cc3cc(c4)Cl)CCNC(=O)[C@H]5C5C(C)CNC5=O

RUN: RUN15039

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.28

EN300-1268512_2_1



CID: EN300-1268512_2_1

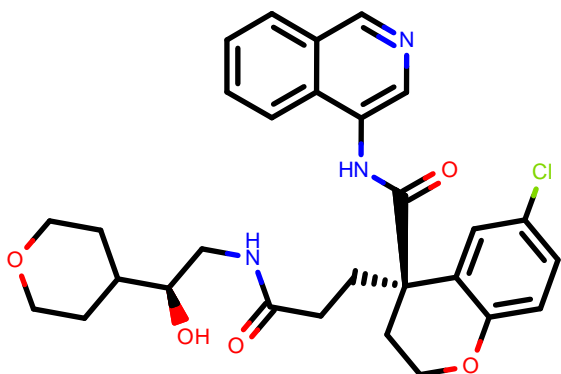
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(Cc4cc3cc(c4)Cl)CCC(=O)NC5C5C(C)S(=O)(=O)N

RUN: RUN13311

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.28

EN300-80481_2_1



CID: EN300-80481_2_1

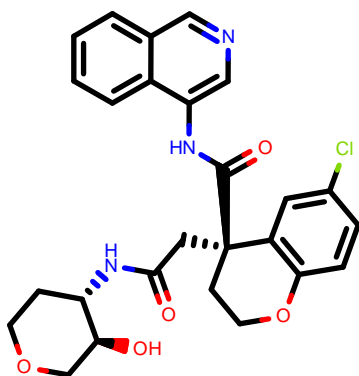
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(C)C(Cc4cc3cc(c4)Cl)CCC(=O)NC[C@H]5C5C(C)CNC5=O

RUN: RUN6072

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.34

EN300-321053_1_4



CID: EN300-321053_1_4

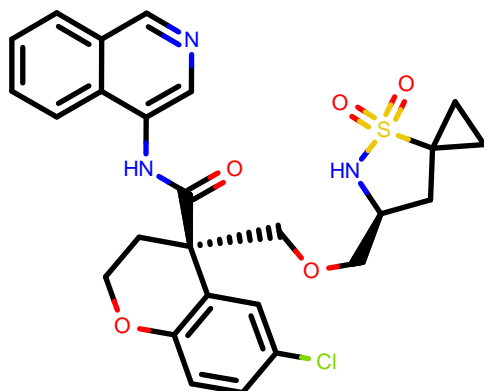
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC[C@@]3H5O

RUN: RUN11954

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.20

EN300-6504697_2_2



CID: EN300-6504697_2_2

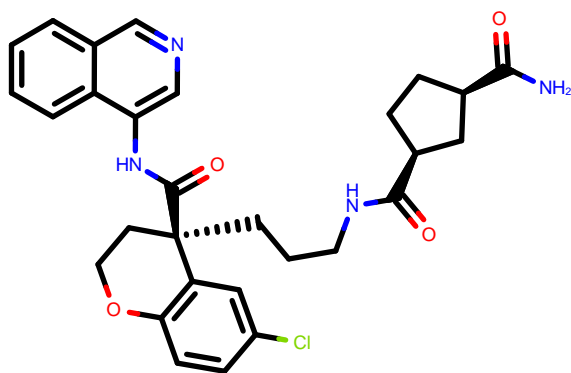
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@]3H5CC6(CO6)S(=O)(=O)N5

RUN: RUN540

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.26

EN300-370753_4_1



CID: EN300-370753_4_1

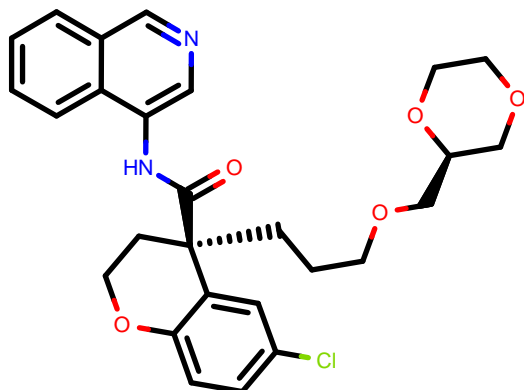
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5(C)C[C@@H]5N

RUN: RUN11650

DDG (kcal/mol): -0.55

dDDG (kcal/mol): 0.24

EN300-139167_4_2



CID: EN300-139167_4_2

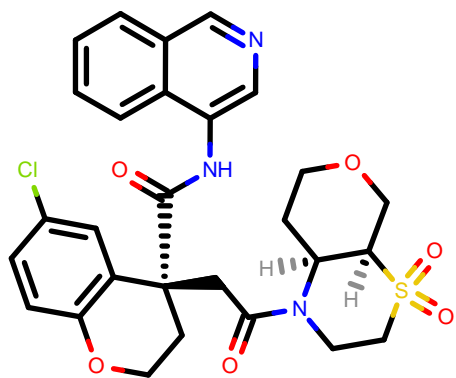
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]3H5CCOCCO5

RUN: RUN1123

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.24

EN300-252113_1_3



CID: EN300-252113_1_3

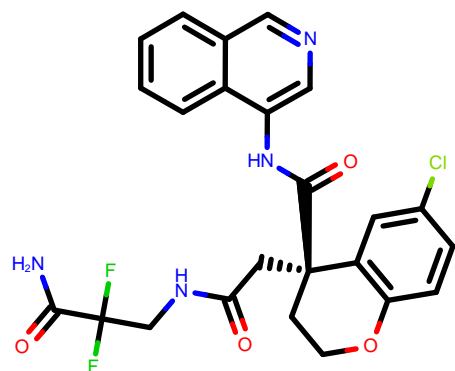
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)NCCS(=O)(=O)[C@H](C)C@H5CCCC5

RUN: RUN13462

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.35

EN300-1179690_1_1



CID: EN300-1179690_1_1

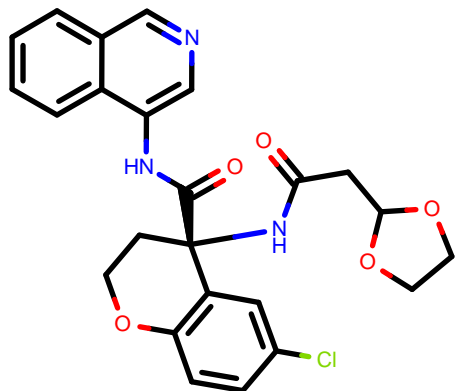
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)NCC(C(=O)N)(F)F

RUN: RUN10185

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.28

EN300-154944_1_1



CID: EN300-154944_1_1

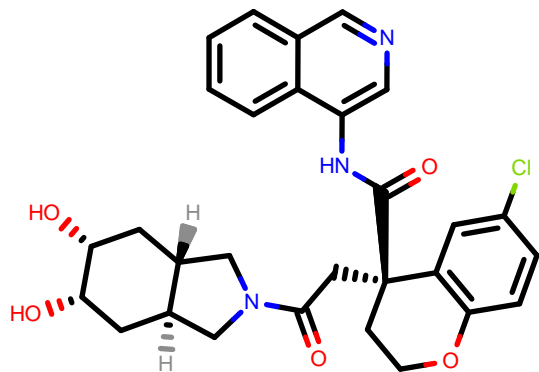
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)NC(=O)CC5OCCO5

RUN: RUN3514

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.22

EN300-7355477_1_5



CID: EN300-7355477_1_5

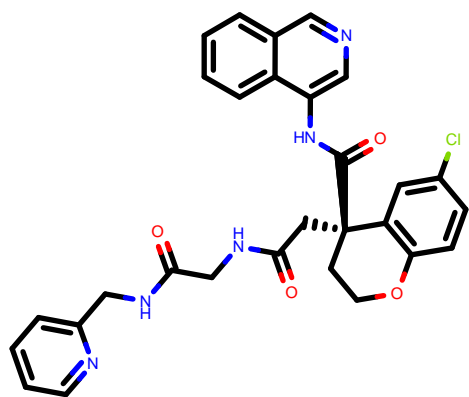
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@@H](C)C[C@@H]6C5)O

RUN: RUN12950

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.28

EN300-57949_1_1



CID: EN300-57949_1_1

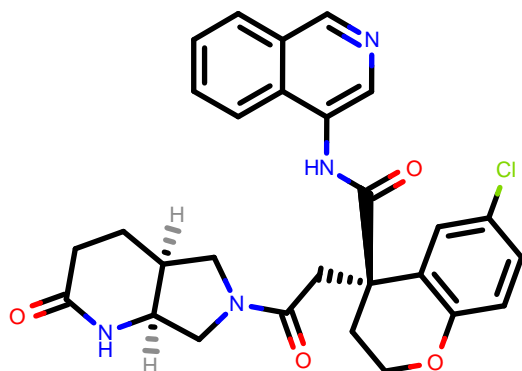
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC(=O)NCc5ccccc5

RUN: RUN10007

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.27

EN300-1087187_1_2



CID: EN300-1087187_1_2

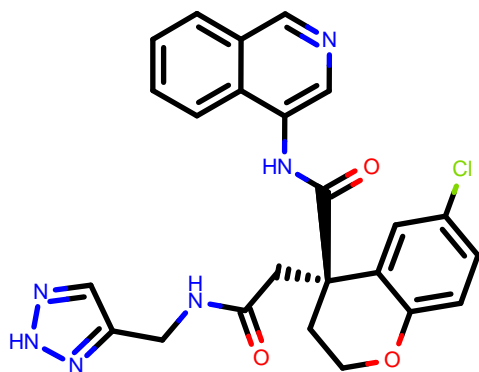
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CC[C@@H]5C6

RUN: RUN13606

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.20

EN300-98429_1_1



CID: EN300-98429_1_1

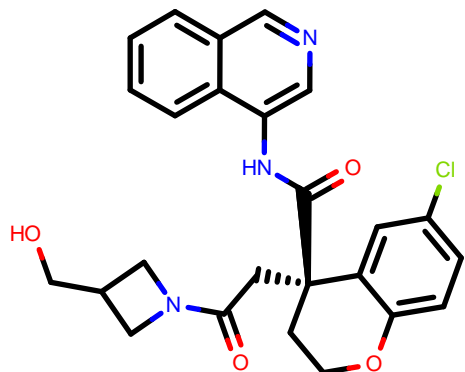
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5cn[nH]n5

RUN: RUN9332

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.22

EN300-7370063_1_1



CID: EN300-7370063_1_1

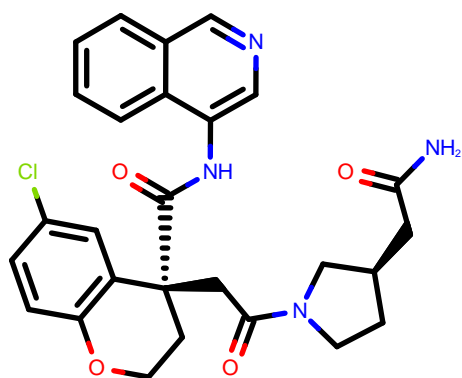
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CO

RUN: RUN6336

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.18

EN300-304381_1_1



CID: EN300-304381_1_1

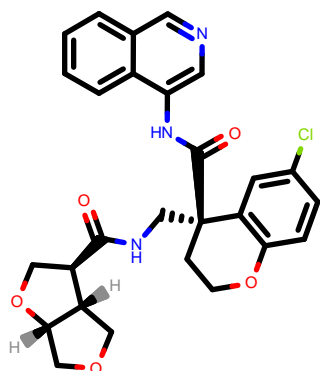
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CC(=O)N5CC[C@@H](C5)CC(=O)N

RUN: RUN6499

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.25

EN300-6482296_2_7



CID: EN300-6482296_2_7

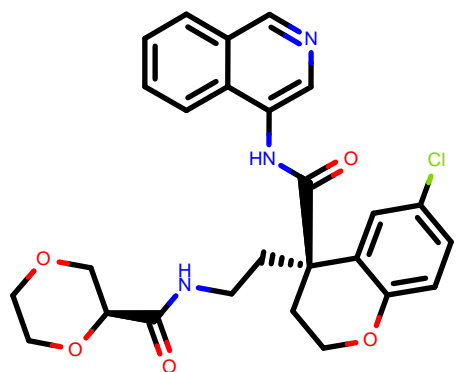
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CNC(=O)[C@@H]5CO[C@@H]5COC6

RUN: RUN7765

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.26

EN300-36158_3_1



CID: EN300-36158_3_1

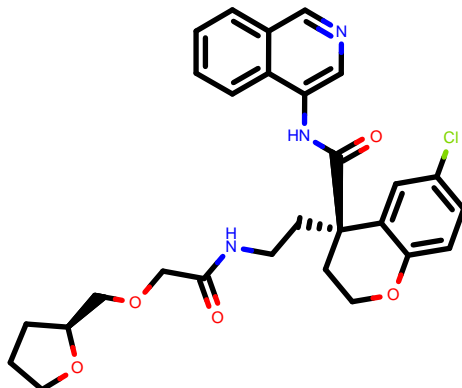
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CCNC(=O)[C@@H]5COCOC5

RUN: RUN11295

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.21

EN300-60033_3_2



CID: EN300-60033_3_2

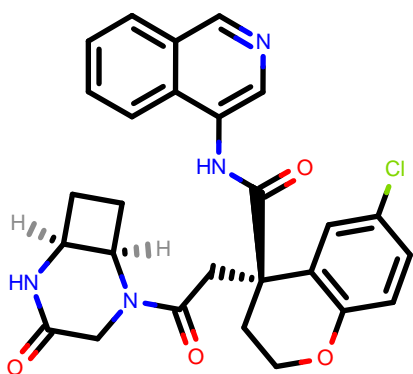
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CCNC(=O)COC[C@@H]5COCOC5

RUN: RUN11238

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.32

EN300-6499164_1_2



CID: EN300-6499164_1_2

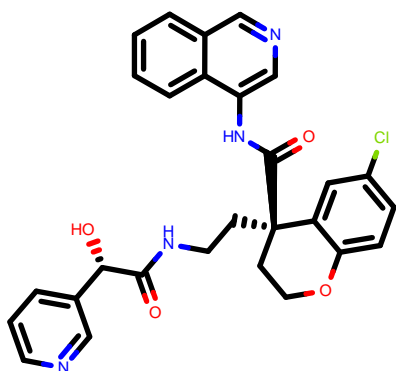
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CC(=O)N5CC1=O)N[C@@]H[C@@]H5CO6

RUN: RUN5785

DDG (kcal/mol): -0.54

dDDG (kcal/mol): 0.21

EN300-134855_3_1



CID: EN300-134855_3_1

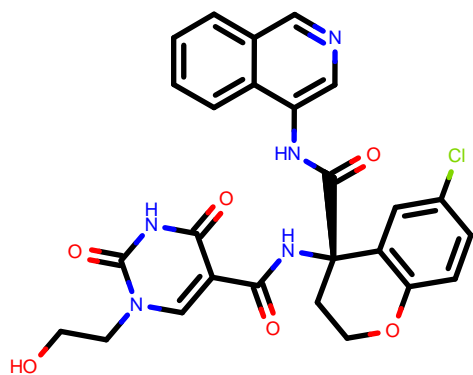
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)CCNC(=O)[C@@]H[C@@]H5COc5O

RUN: RUN3949

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.31

EN300-101291_1_1



CID: EN300-101291_1_1

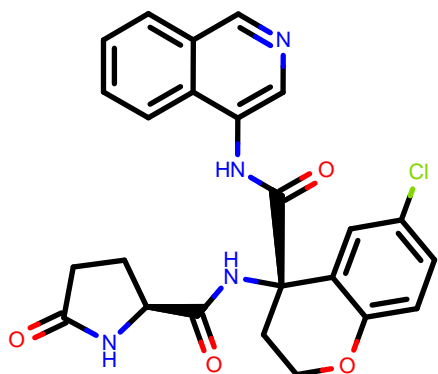
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)NC(=O)c5en(c(=O)[nH]c5=O)CCO

RUN: RUN243

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.29

EN300-72896_1_1



CID: EN300-72896_1_1

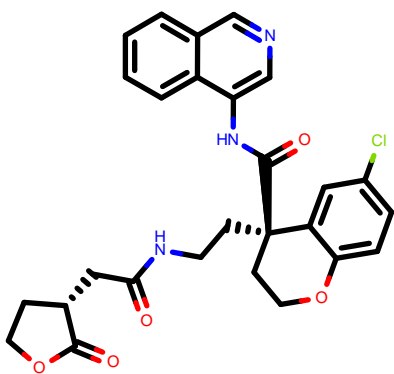
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4C)NC(=O)[C@@]H[C@@]H5CC1=O)N5

RUN: RUN1777

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.21

EN300-1072972_3_1



CID: EN300-1072972_3_1

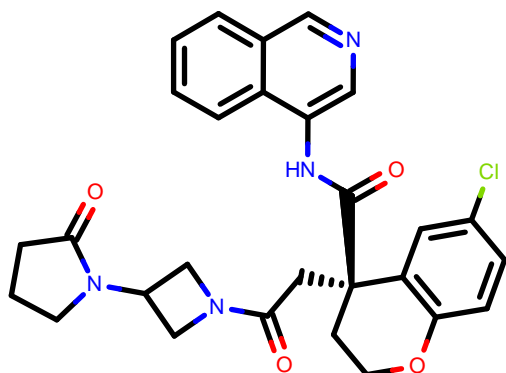
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@H]5CCOC5=O

RUN: RUN2806

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.31

EN300-370951_1_1



CID: EN300-370951_1_1

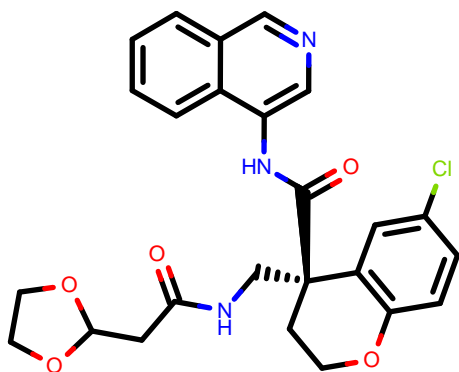
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)N6CCCC6=O

RUN: RUN7479

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.22

EN300-154944_2_1



CID: EN300-154944_2_1

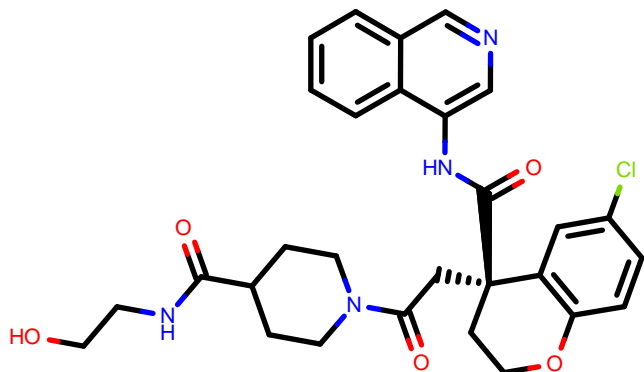
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CC5OCCO5

RUN: RUN1867

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.27

EN300-344753_1_1



CID: EN300-344753_1_1

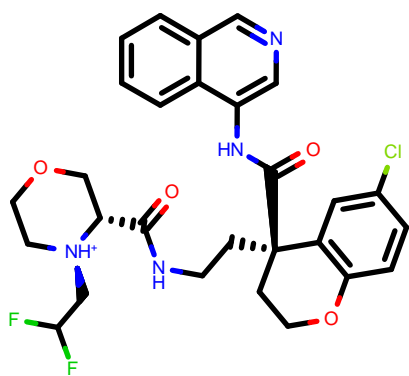
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCC(C5)C(=O)NCCO

RUN: RUN10755

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.36

EN300-140582_3_4



CID: EN300-140582_3_4

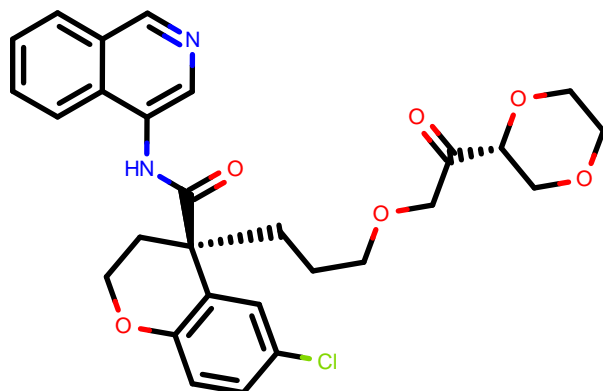
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCN(C=O)[C@@H]5COC(N@@)5C(F)F

RUN: RUN11383

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.28

EN300-6238494_4_2



CID: EN300-6238494_4_2

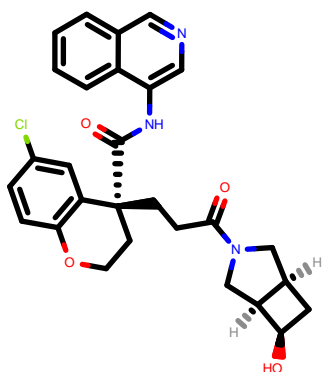
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC(=O)[C@@H]5COCOC5

RUN: RUN621

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.24

EN300-305294_2_7



CID: EN300-305294_2_7

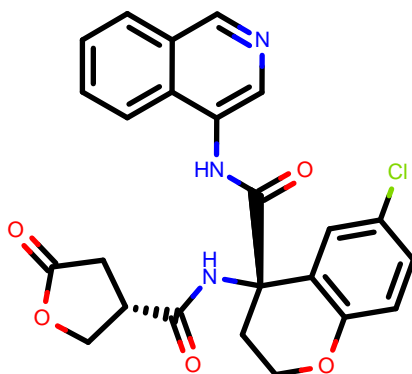
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@@H]6[C@@H](C)H5C5O

RUN: RUN13947

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.24

EN300-113234_1_2



CID: EN300-113234_1_2

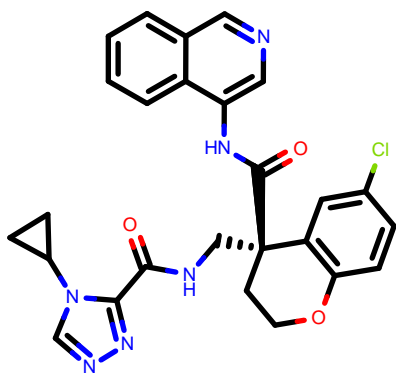
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5C(=O)OC5

RUN: RUN4826

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.17

EN300-6745581_2_1



CID: EN300-6745581_2_1

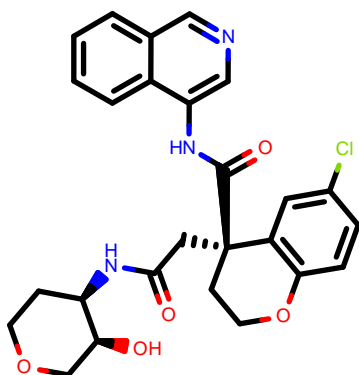
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5nnnc5O6C06

RUN: RUN1827

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.26

EN300-366540_1_1



CID: EN300-366540_1_1

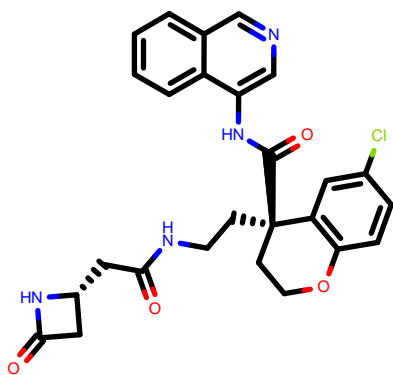
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5COC[C@@]H5O

RUN: RUN8483

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.24

EN300-250593_3_2



CID: EN300-250593_3_2

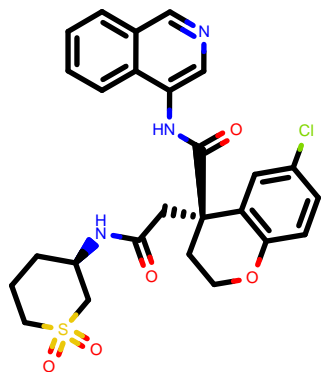
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]H5CC(=O)N5

RUN: RUN9172

DDG (kcal/mol): -0.53

dDDG (kcal/mol): 0.35

EN300-74856_1_1



CID: EN300-74856_1_1

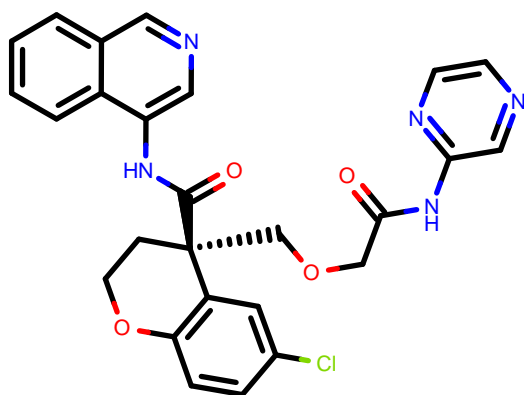
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5SCCS(=O)(=O)C5

RUN: RUN4593

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.30

EN300-105267_2_1



CID: EN300-105267_2_1

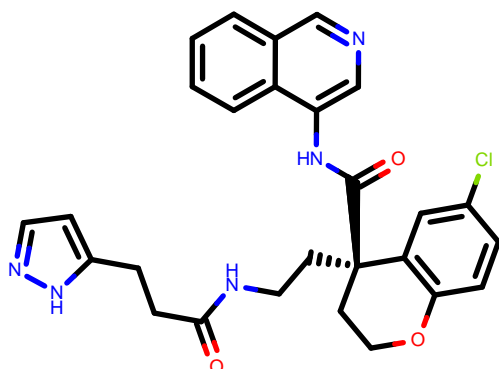
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5nccn5

RUN: RUN2642

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.33

EN300-1664603_3_1



CID: EN300-1664603_3_1

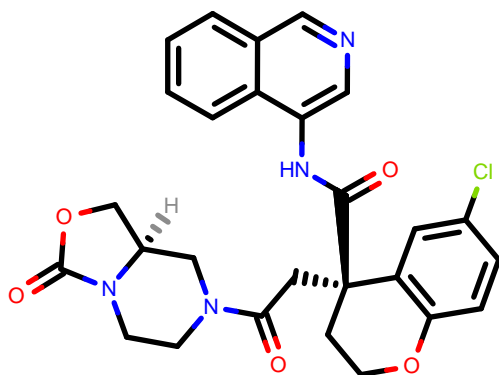
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5cn[nH]5

RUN: RUN2699

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

EN300-109827_1_2



CID: EN300-109827_1_2

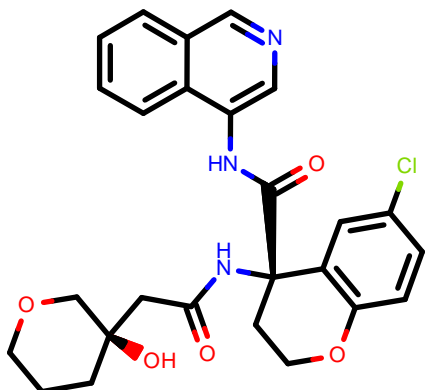
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@H](C5)COC6=O

RUN: RUN8079

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.23

EN300-1071940_1_1



CID: EN300-1071940_1_1

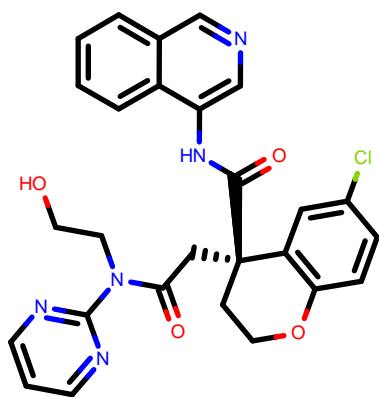
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCCOC5)O

RUN: RUN8000

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.22

EN300-65352_1_1



CID: EN300-65352_1_1

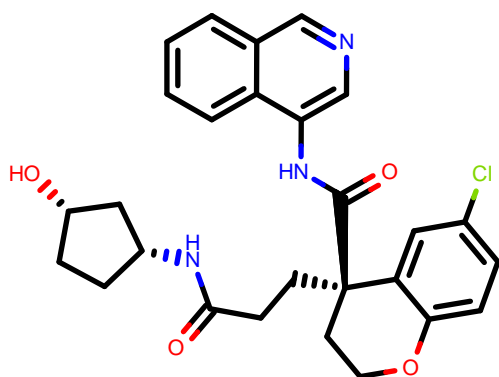
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5ncccc5

RUN: RUN8235

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.39

EN300-266299_2_1



CID: EN300-266299_2_1

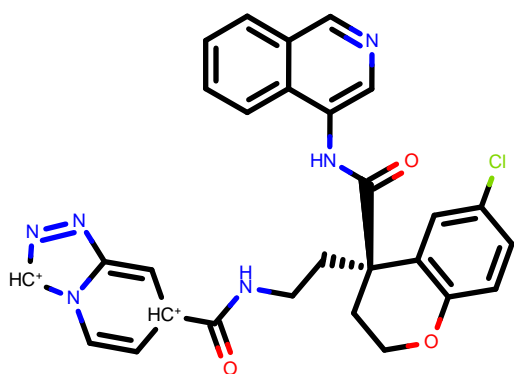
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]5HJ5CC[C@@]5HJ(C5)O

RUN: RUN8030

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

EN300-7537194_3_1



CID: EN300-7537194_3_1

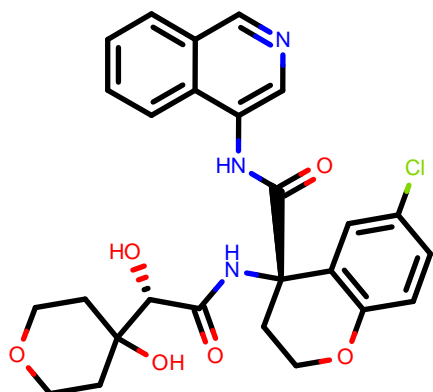
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CCNC(=O)c5ccn6cnn6c5

RUN: RUN15369

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

EN300-749499_1_2



CID: EN300-749499_1_2

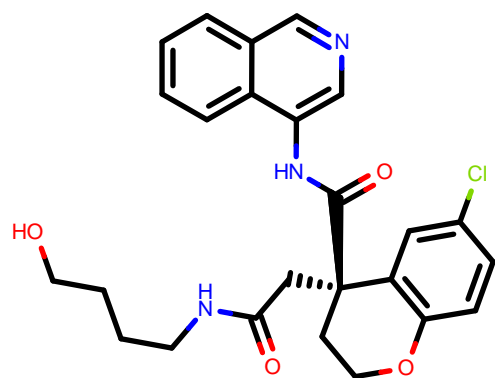
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)NC(=O)[C@@]5HJ(C5(CCOC(C5)O)O

RUN: RUN1018

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.26

EN300-66126_1_1



CID: EN300-66126_1_1

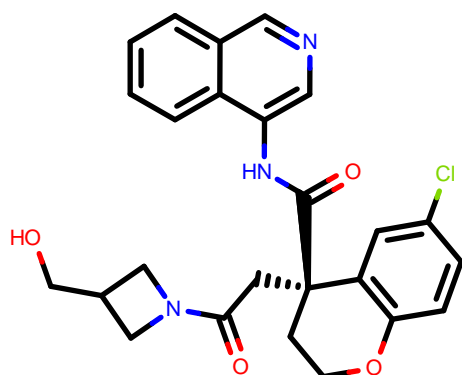
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCCO

RUN: RUN5549

DDG (kcal/mol): -0.52

dDDG (kcal/mol): 0.24

EN300-7370063_1_1



CID: EN300-7370063_1_1

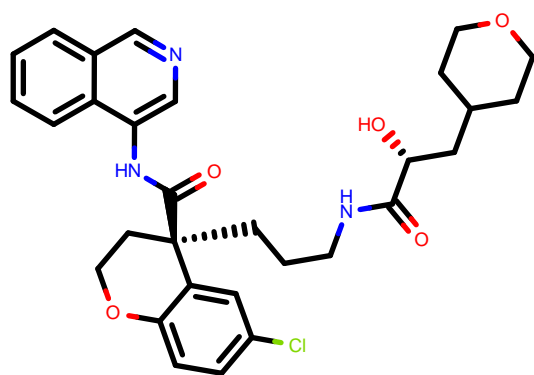
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CC(=O)N5CCNC5CO

RUN: RUN6332

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.17

EN300-1452069_4_1



CID: EN300-1452069_4_1

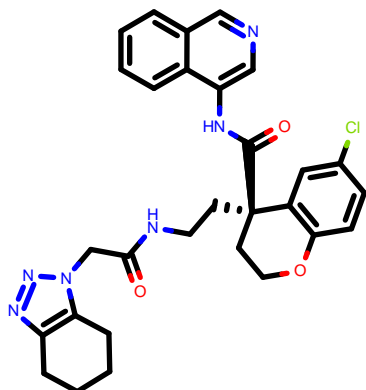
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5H(CC5COCCO5)O

RUN: RUN8931

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.35

EN300-223187_3_1



CID: EN300-223187_3_1

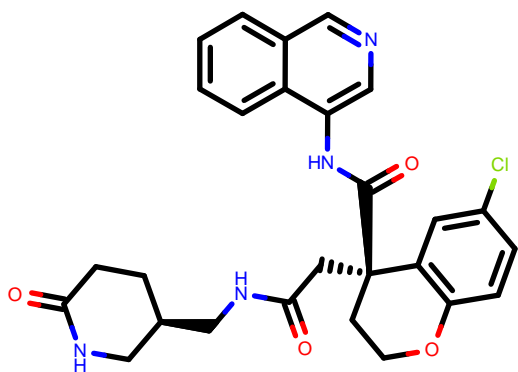
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5c6c(n5)CCCC6

RUN: RUN12014

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.26

EN300-6746326_1_1



CID: EN300-6746326_1_1

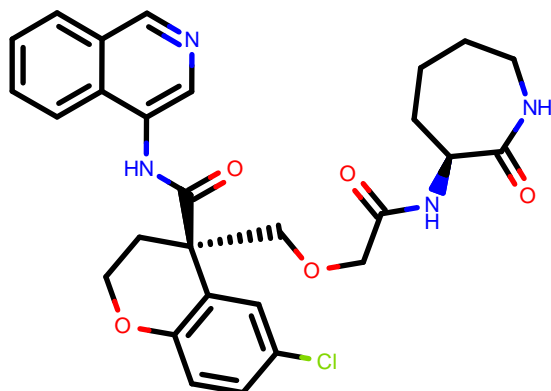
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCCC(=O)NCS

RUN: RUN5725

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.21

EN300-37195_2_1



CID: EN300-37195_2_1

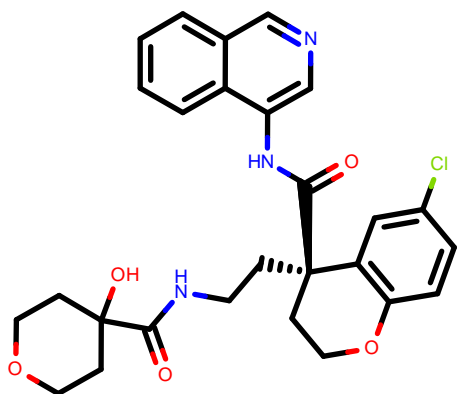
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN2562

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.27

EN300-69368_3_1



CID: EN300-69368_3_1

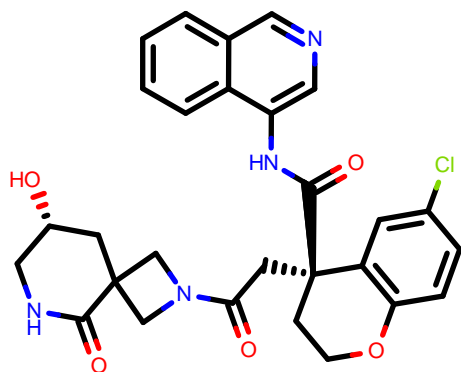
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(COCC5)O

RUN: RUN721

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.26

EN300-396372_1_2



CID: EN300-396372_1_2

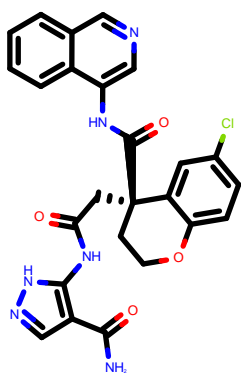
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)C[C@@H](CN6)=O

RUN: RUN14304

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.31

EN300-30536_1_1



CID: EN300-30536_1_1

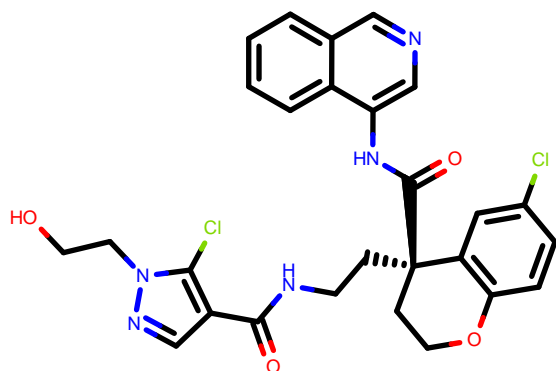
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5c(en[nH]5)C(=O)N

RUN: RUN11443

DDG (kcal/mol): -0.51

dDDG (kcal/mol): 0.20

EN300-333468_3_1



CID: EN300-333468_3_1

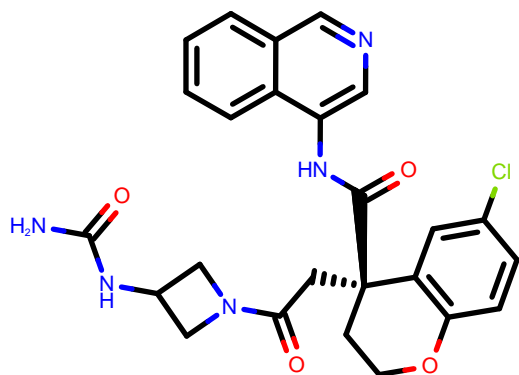
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5=NN(C5)CO

RUN: RUN15258

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.28

EN300-6746622_1_1



CID: EN300-6746622_1_1

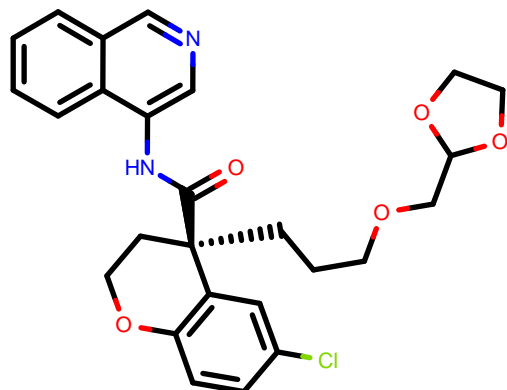
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)NC(=O)N

RUN: RUN8207

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.22

EN300-77092_4_1



CID: EN300-77092_4_1

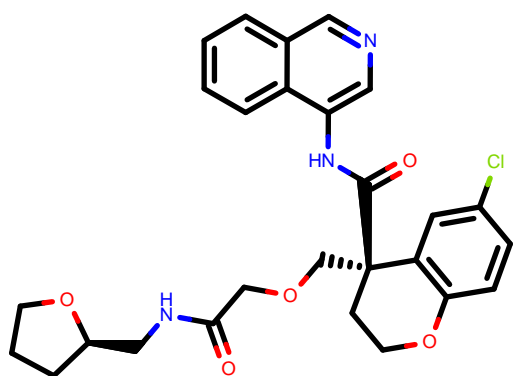
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5

RUN: RUN996

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.24

EN300-01527_2_1



CID: EN300-01527_2_1

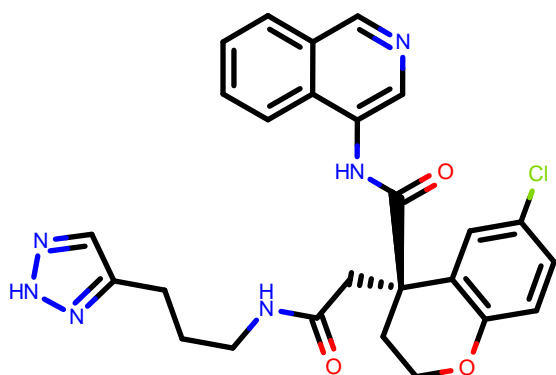
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@H]5CCCCO5

RUN: RUN2104

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.34

EN300-6493892_1_1



CID: EN300-6493892_1_1

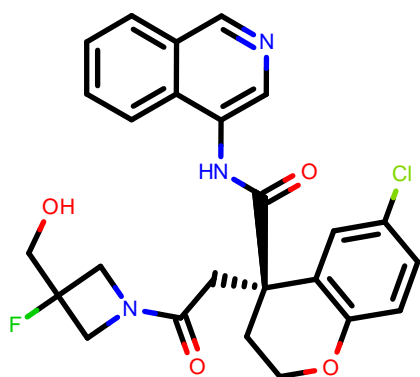
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCc5cn[nH]5

RUN: RUN3077

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.24

EN300-204507_1_1



CID: EN300-204507_1_1

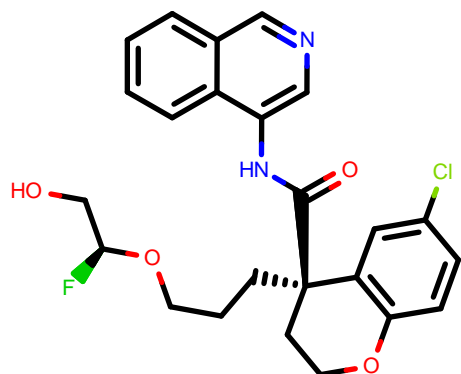
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F

RUN: RUN11751

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.25

EN300-861925_4_1



CID: EN300-861925_4_1

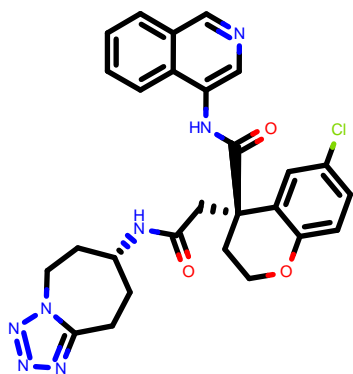
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H](CO)F

RUN: RUN741

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.23

EN300-256798_1_1



CID: EN300-256798_1_1

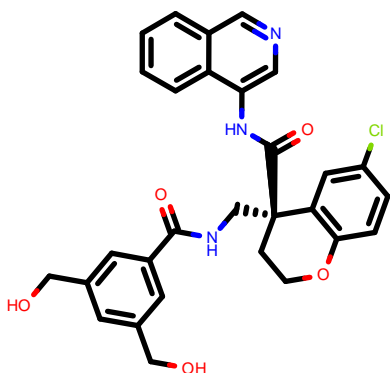
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCc6nnnc6CC5

RUN: RUN2426

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.25

EN300-211158_2_1



CID: EN300-211158_2_1

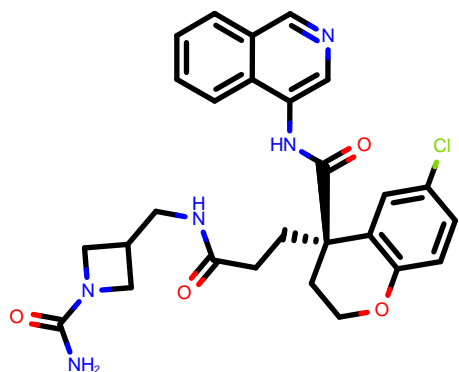
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(O)c(O)c5CO

RUN: RUN3447

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.33

EN300-7431964_2_1



CID: EN300-7431964_2_1

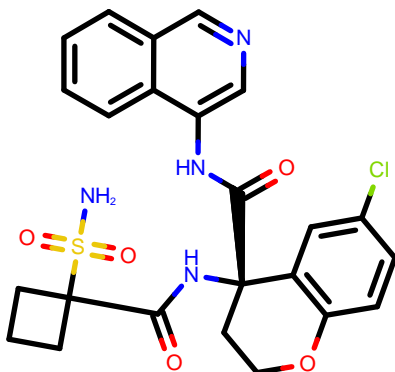
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5CN(C5)C(=O)N

RUN: RUN11073

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.23

EN300-1440321_1_1



CID: EN300-1440321_1_1

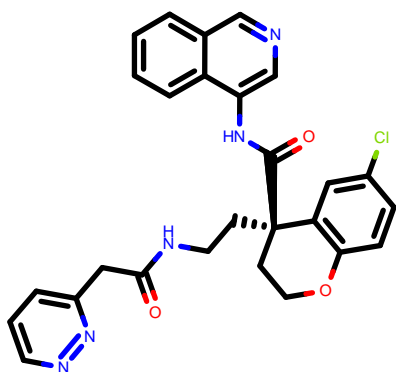
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCS(=O)(=O)N)S(=O)(=O)N

RUN: RUN6341

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.27

EN300-7456948_3_1



CID: EN300-7456948_3_1

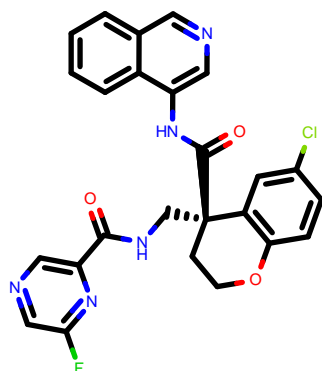
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cccn5

RUN: RUN15238

DDG (kcal/mol): -0.50

dDDG (kcal/mol): 0.26

EN300-373552_2_1



CID: EN300-373552_2_1

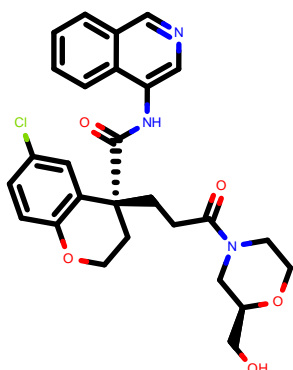
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncc(n5)F

RUN: RUN2833

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.21

EN300-101373_2_2



CID: EN300-101373_2_2

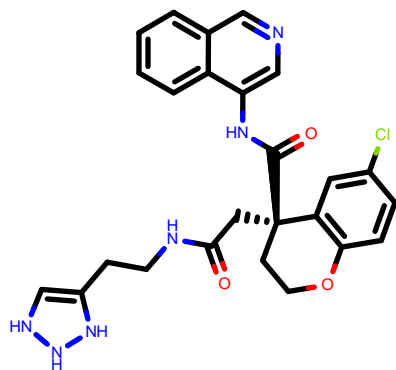
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCO[C@H](C5)CO

RUN: RUN8663

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.25

EN300-1178209_1_1



CID: EN300-1178209_1_1

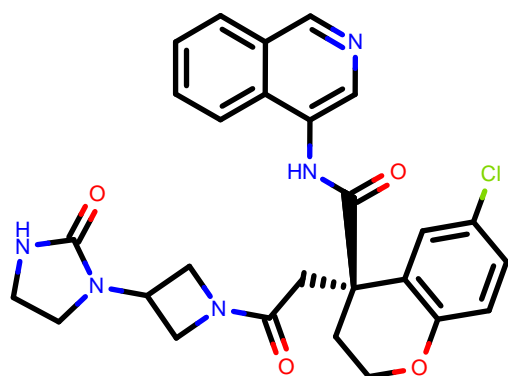
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5cnc(nH)5

RUN: RUN9296

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.25

EN300-208993_1_1



CID: EN300-208993_1_1

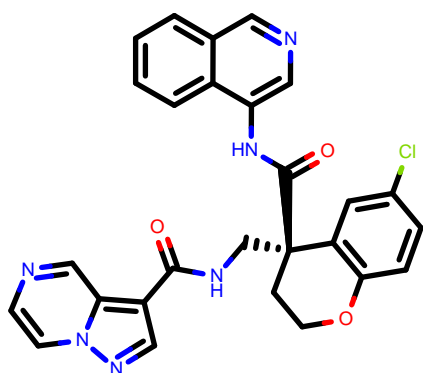
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N5CC(C5)N6CCNC6=O

RUN: RUN14682

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.26

EN300-131572_2_1



CID: EN300-131572_2_1

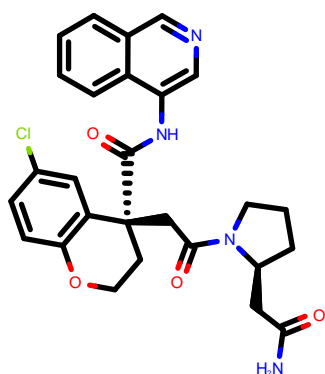
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CNC(=O)c5cnn6c5cnc6

RUN: RUN7489

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.23

EN300-124652_1_2



CID: EN300-124652_1_2

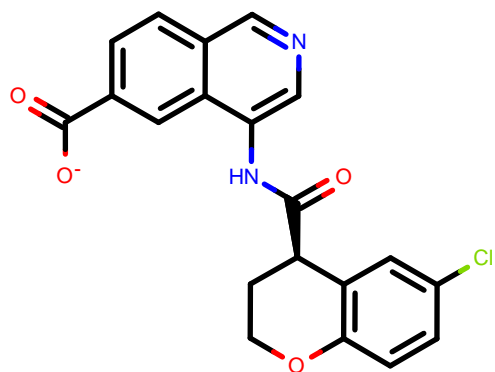
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOC4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5CC(=O)N

RUN: RUN6272

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

MAK-UNK-8be7dca9-7_1



CID: MAK-UNK-8be7dca9-7_1

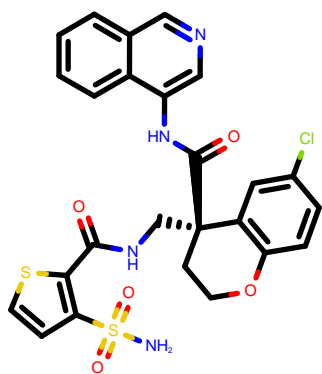
SMILES: c1cc2cnc(c2cc1C(=O)[O-])NC(=O)[C@@H]3CCOC4c3cc(cc4)Cl

RUN: RUN90

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.11

EN300-24419_2_1



CID: EN300-24419_2_1

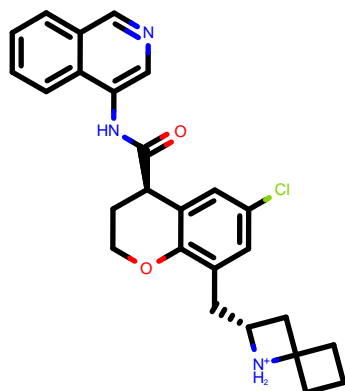
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)c5c(ccs5)S(=O)(=O)N

RUN: RUN7853

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.28

DAR-DIA-23e5a6a0-7_2



CID: DAR-DIA-23e5a6a0-7_2

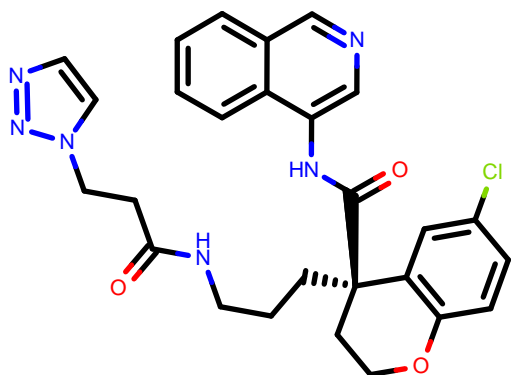
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[NH2+][5]COC6)Cl

RUN: RUN172

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.35

EN300-28871_4_1



CID: EN300-28871_4_1

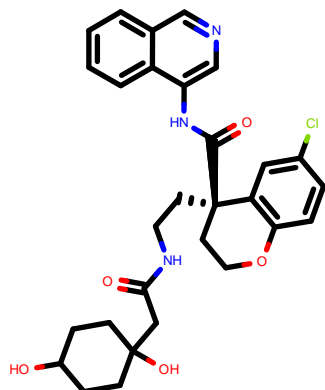
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CCn5ccnn5

RUN: RUN10580

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.23

EN300-181558_3_1



CID: EN300-181558_3_1

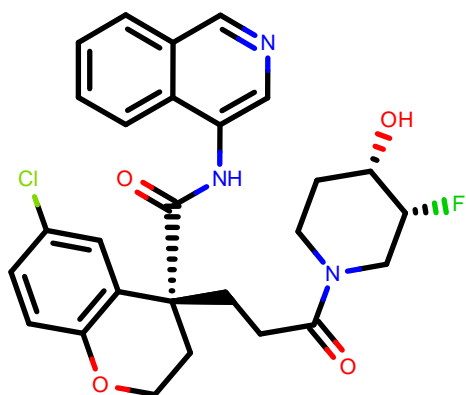
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)CC(C(C)O)O

RUN: RUN8527

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.28

EN300-741926_2_3



CID: EN300-741926_2_3

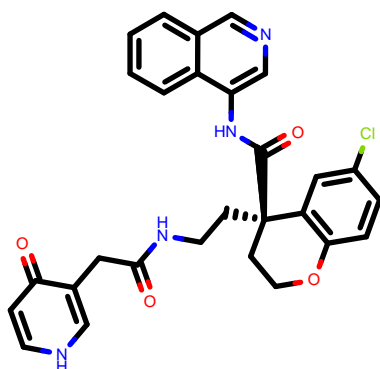
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC@HC5F

RUN: RUN3648

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.26

EN300-205486_3_1



CID: EN300-205486_3_1

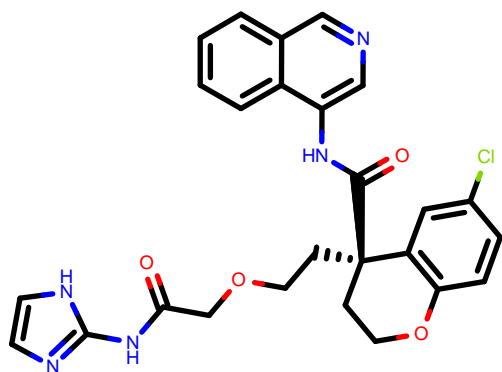
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cc5c[nH]ccc5=O

RUN: RUN4109

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.27

EN300-331993_3_1



CID: EN300-331993_3_1

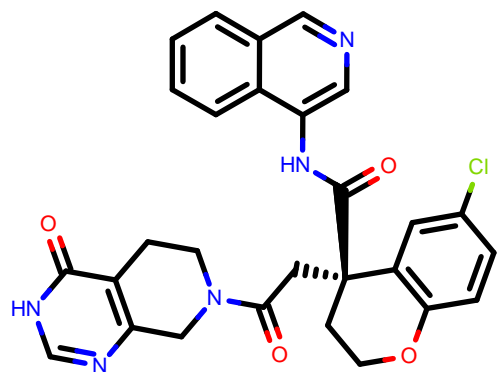
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)Nc5[nH]ccc5

RUN: RUN2434

DDG (kcal/mol): -0.49

dDDG (kcal/mol): 0.23

EN300-132141_1_1



CID: EN300-132141_1_1

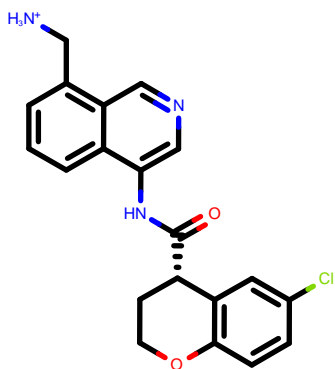
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCc6c(nc[nH]c6=O)C5

RUN: RUN14258

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.25

MAK-UNK-8be7dca9-6_2



CID: MAK-UNK-8be7dca9-6_2

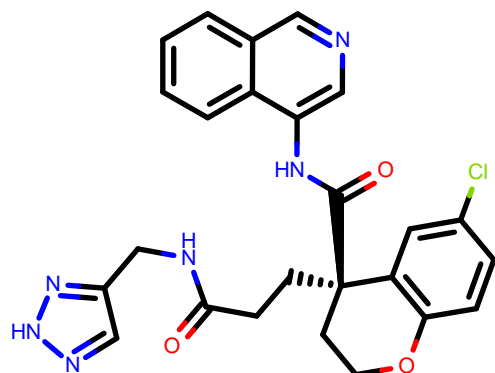
SMILES: c1cc(c2cncc(c2c1)NC(=O)[C@H]3CCOCc4c3cc(cc4)Cl)C[NH3+]

RUN: RUN165

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.18

EN300-98429_2_1



CID: EN300-98429_2_1

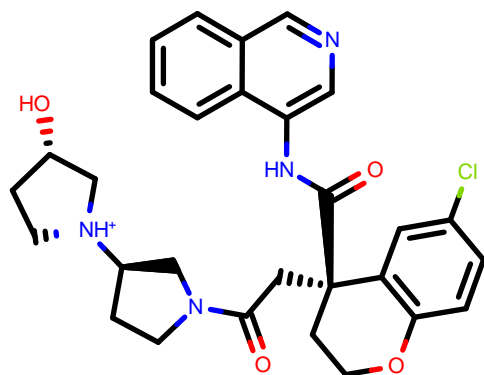
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5n[nH]n5

RUN: RUN3848

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.25

EN300-213215_1_2



CID: EN300-213215_1_2

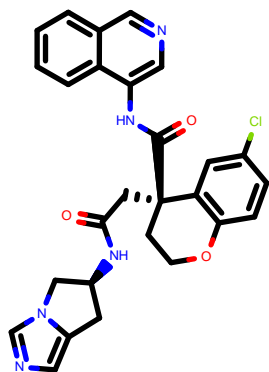
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](C5)N[+]([H])C6C[C@@H](O)C6

RUN: RUN13720

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.31

EN300-244100_1_2



CID: EN300-244100_1_2

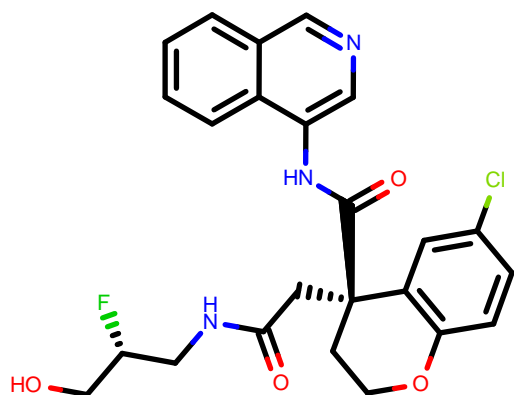
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C6c6nnc65

RUN: RUN10930

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.21

EN300-7353973_1_2



CID: EN300-7353973_1_2

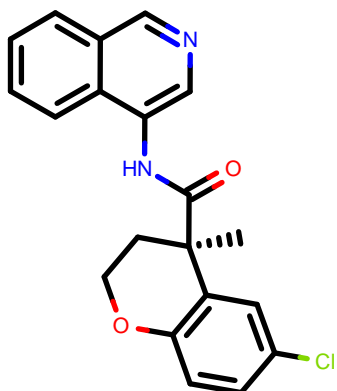
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H](CO)F

RUN: RUN3101

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.26

DAR-DIA-6a508060-10_1



CID: DAR-DIA-6a508060-10_1

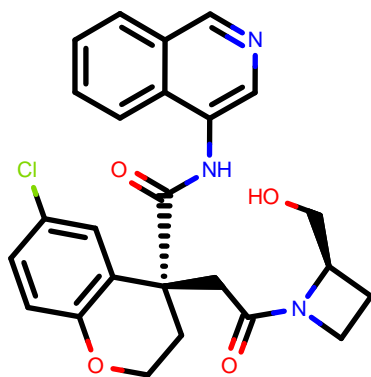
SMILES: C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN69

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.09

EN300-154332_1_1



CID: EN300-154332_1_1

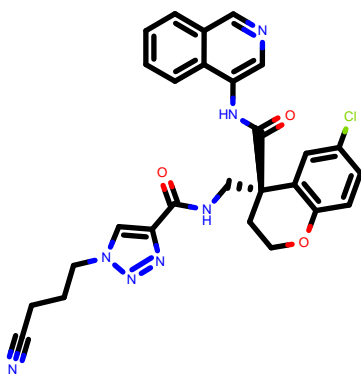
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5CO

RUN: RUN5449

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.24

EN300-120569_2_1



CID: EN300-120569_2_1

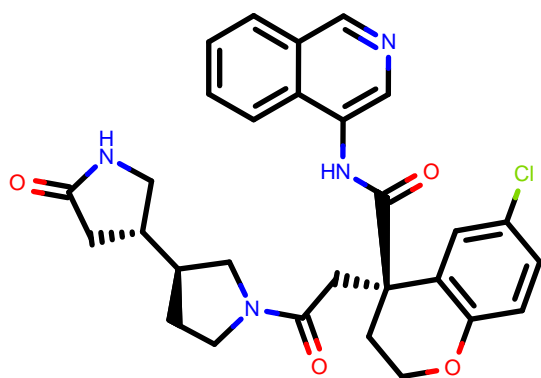
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(n5)CCCC#N

RUN: RUN9190

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.28

EN300-6480951_1_2



CID: EN300-6480951_1_2

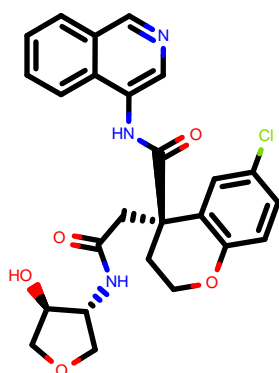
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)[C@@H]6CC(=O)N6

RUN: RUN11649

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.24

EN300-331476_1_1



CID: EN300-331476_1_1

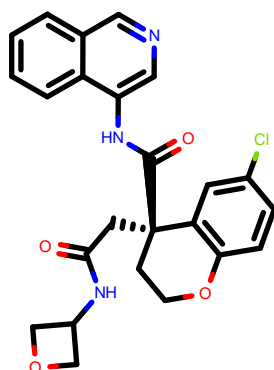
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5COC[C@H]5O

RUN: RUN6919

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.20

EN300-49064_1_1



CID: EN300-49064_1_1

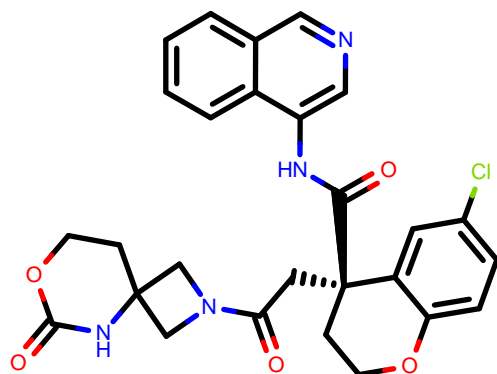
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)NC5COC5

RUN: RUN11545

DDG (kcal/mol): -0.48

dDDG (kcal/mol): 0.18

EN300-264318_1_1



CID: EN300-264318_1_1

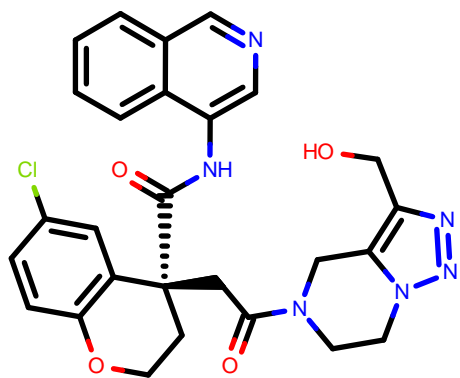
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)N5CC6(C5)CCOC(=O)N6

RUN: RUN6181

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.26

EN300-219427_1_1



CID: EN300-219427_1_1

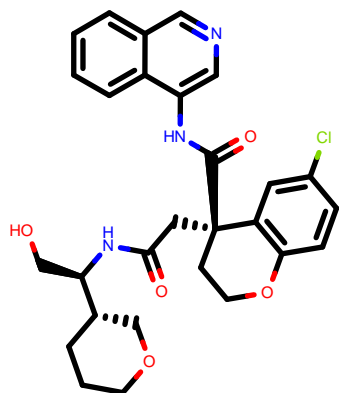
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCn6c(c(nn6)CO)C5

RUN: RUN13054

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.30

EN300-254105_1_3



CID: EN300-254105_1_3

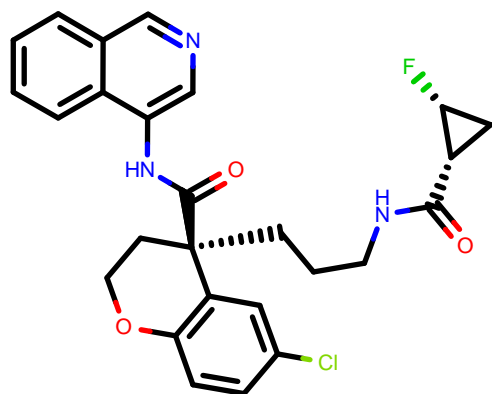
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@H](CO)[C@H]5CCCCO5

RUN: RUN4305

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.29

EN300-97300_4_2



CID: EN300-97300_4_2

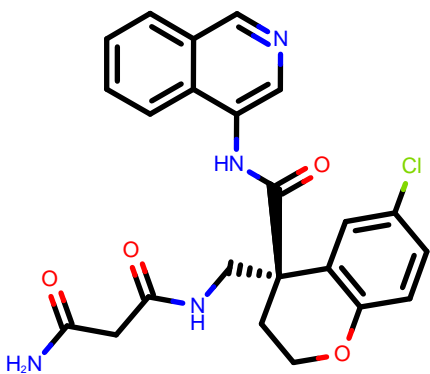
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5C[C@H]5F

RUN: RUN7710

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.18

EN300-82179_2_1



CID: EN300-82179_2_1

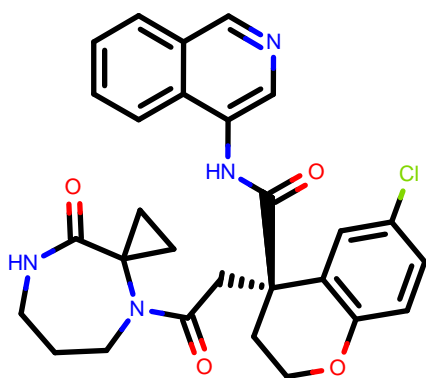
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CC(=O)N

RUN: RUN4347

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.23

EN300-716218_1_1



CID: EN300-716218_1_1

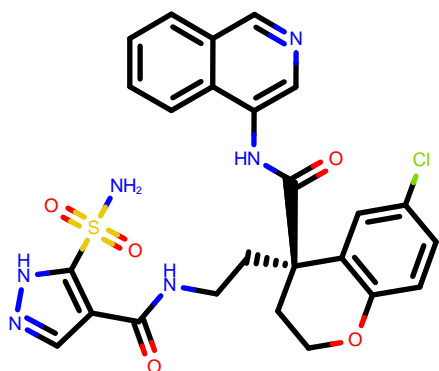
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN(C=O)C56CC6

RUN: RUN11775

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.26

EN300-144606_3_1



CID: EN300-144606_3_1

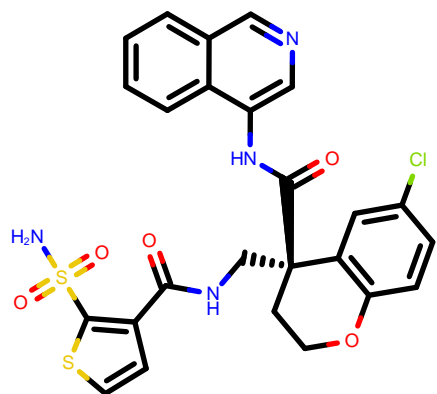
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5n[nH]c5S(=O)(=O)N

RUN: RUN14468

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-294602_2_1



CID: EN300-294602_2_1

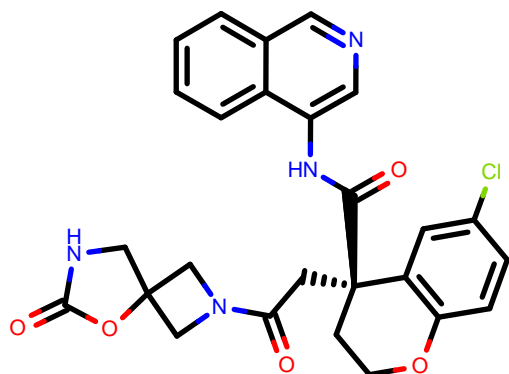
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccsc5S(=O)(=O)N

RUN: RUN7385

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.35

EN300-6494361_1_1



CID: EN300-6494361_1_1

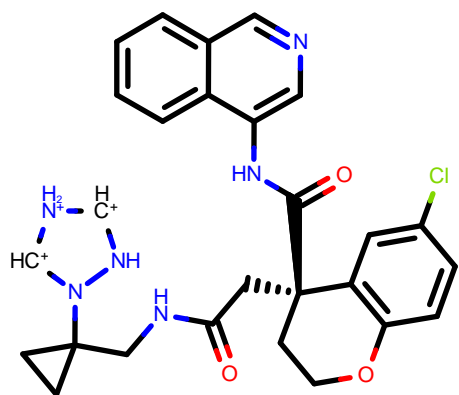
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CNC(=O)O6

RUN: RUN3609

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.20

EN300-6733137_1_1



CID: EN300-6733137_1_1

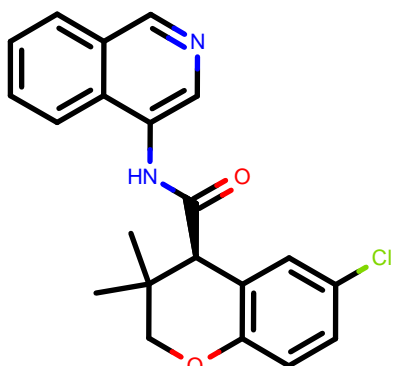
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(C)C5n6cn6

RUN: RUN8451

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.27

DAR-DIA-0d514e7d-3_1



CID: DAR-DIA-0d514e7d-3_1

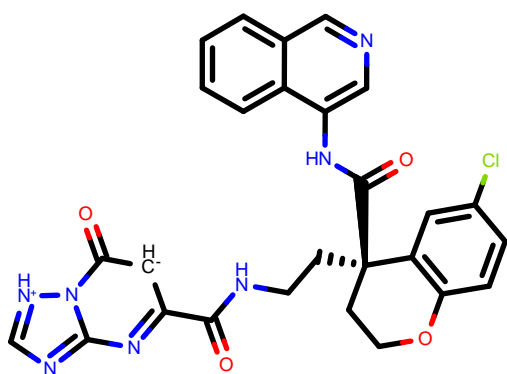
SMILES: CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C

RUN: RUN73

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.08

EN300-135182_3_1



CID: EN300-135182_3_1

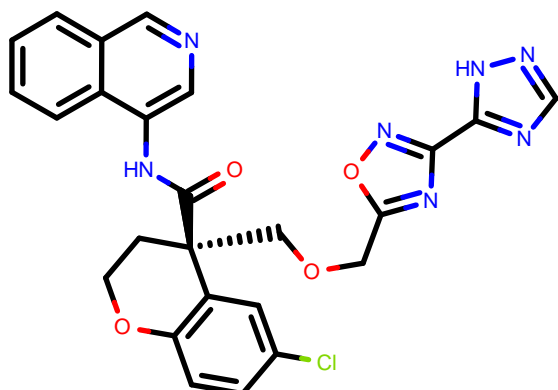
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc(=O)n6c(n6)[nH]6

RUN: RUN15113

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.28

EN300-92031_2_1



CID: EN300-92031_2_1

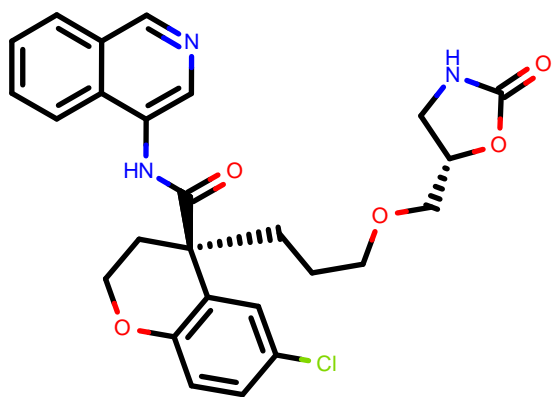
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nc(n6)c6[nH]n6

RUN: RUN1634

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.21

EN300-203293_4_2



CID: EN300-203293_4_2

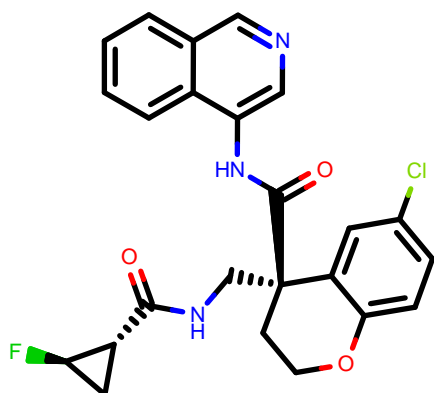
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCCCO[C@@H]5CNC(=O)O5

RUN: RUN1371

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.23

EN300-1654606_2_1



CID: EN300-1654606_2_1

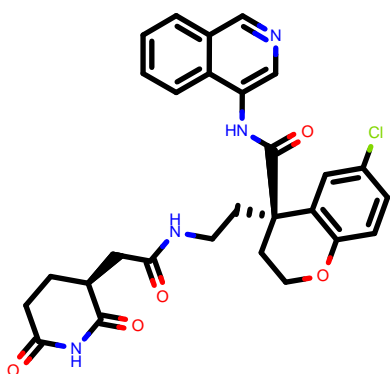
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@@H]5C[C@H]5F

RUN: RUN5791

DDG (kcal/mol): -0.47

dDDG (kcal/mol): 0.19

EN300-3451857_3_2



CID: EN300-3451857_3_2

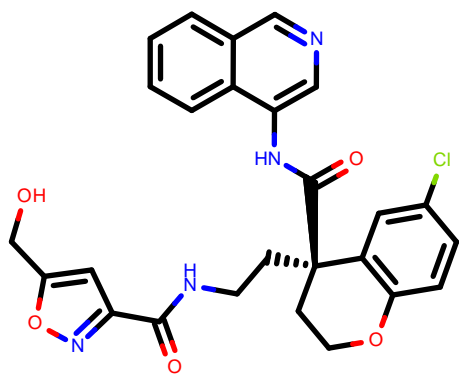
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C[C@@H]5CC(=O)NC5=O

RUN: RUN8856

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.29

EN300-95507_3_1



CID: EN300-95507_3_1

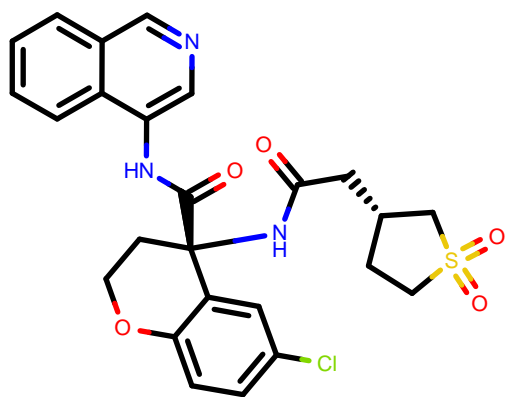
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)c5cc(on5)CO

RUN: RUN15524

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.22

EN300-14006_1_2



CID: EN300-14006_1_2

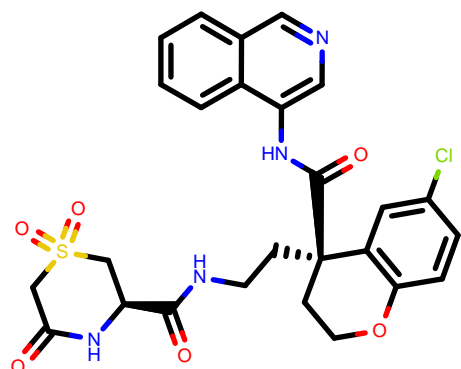
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCS(=O)(=O)C5

RUN: RUN915

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.33

EN300-702756_3_1



CID: EN300-702756_3_1

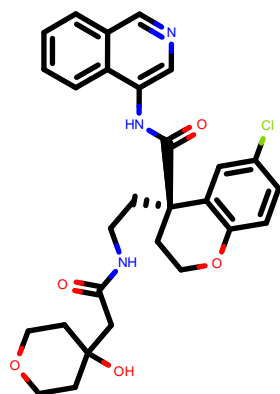
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CNC(=O)[C@H]5CCS(=O)(=O)C5

RUN: RUN15162

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.32

EN300-151423_3_1



CID: EN300-151423_3_1

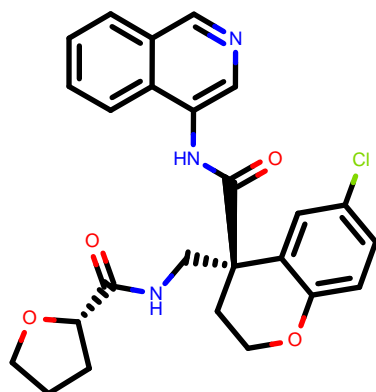
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CC5(O)CCOCC5O

RUN: RUN8411

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

EN300-104395_2_1



CID: EN300-104395_2_1

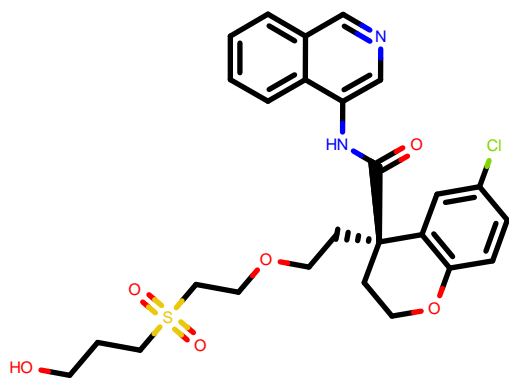
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCOCC5

RUN: RUN5259

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.21

EN300-7456499_3_1



CID: EN300-7456499_3_1

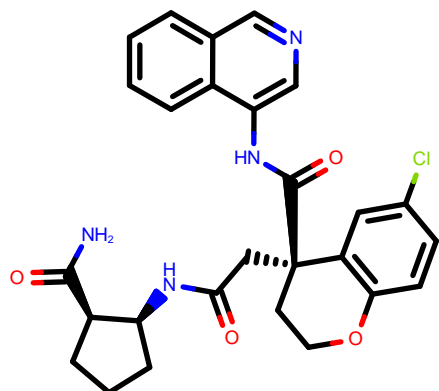
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)CCCCO

RUN: RUN762

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.36

EN300-90531_1_2



CID: EN300-90531_1_2

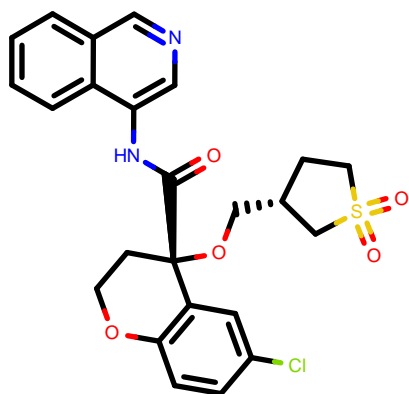
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCC[C@H]5C(=O)N

RUN: RUN11343

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.30

EN300-1448603_1_1



CID: EN300-1448603_1_1

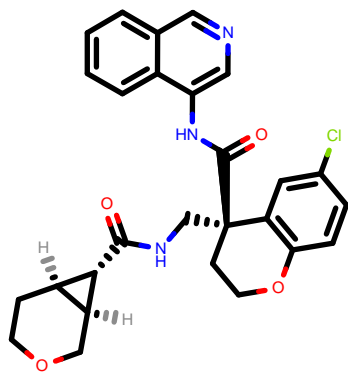
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCS(=O)(=O)C5

RUN: RUN2333

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.28

EN300-1644723_2_4



CID: EN300-1644723_2_4

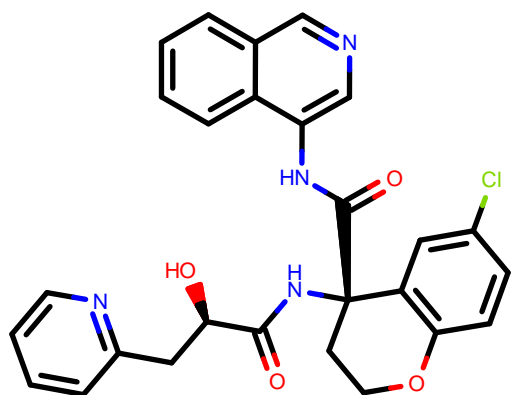
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@H]6C[C@@H]6C5

RUN: RUN3091

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.22

EN300-6762327_1_1



CID: EN300-6762327_1_1

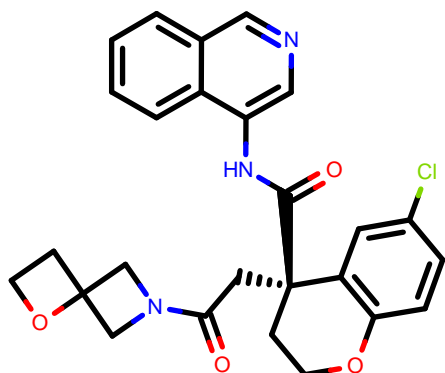
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5H(Cc5ccccc5)O

RUN: RUN2337

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.27

EN300-189729_1_1



CID: EN300-189729_1_1

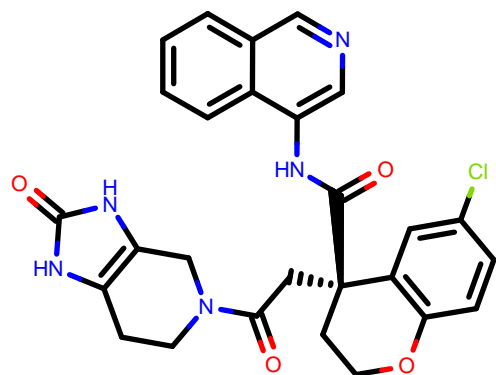
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C)CCO6

RUN: RUN12716

DDG (kcal/mol): -0.46

dDDG (kcal/mol): 0.19

EN300-7237143_1_1



CID: EN300-7237143_1_1

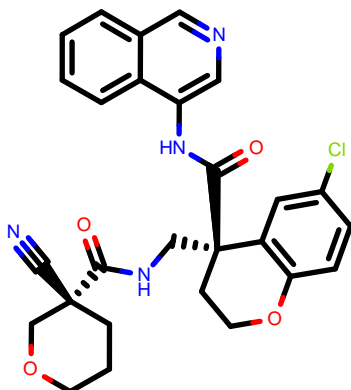
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6c6([nH]c(=O)[nH]6)C5

RUN: RUN15463

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.22

EN300-301925_2_2



CID: EN300-301925_2_2

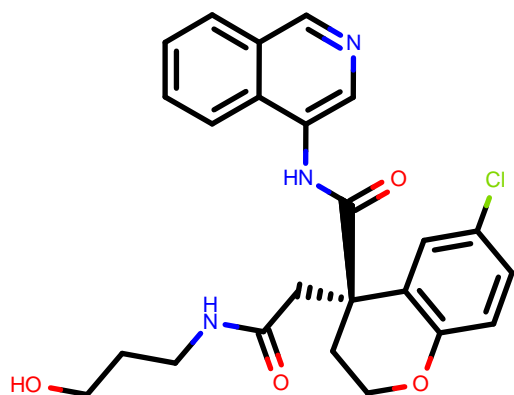
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCCOC5)C#N

RUN: RUN2858

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-16772_1_1



CID: EN300-16772_1_1

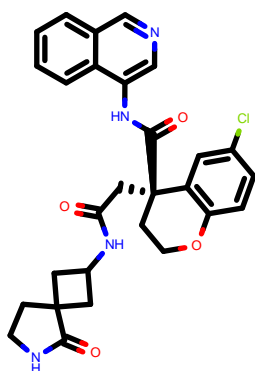
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCCO

RUN: RUN5617

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.20

EN300-743350_1_1



CID: EN300-743350_1_1

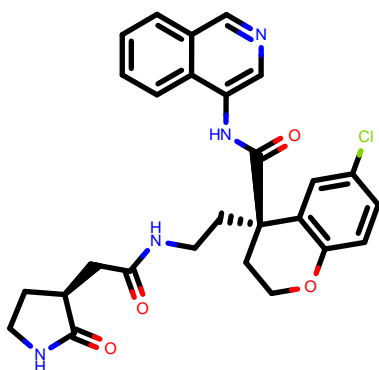
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6C(C5)CCN6C=O

RUN: RUN12734

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.26

EN300-343474_3_2



CID: EN300-343474_3_2

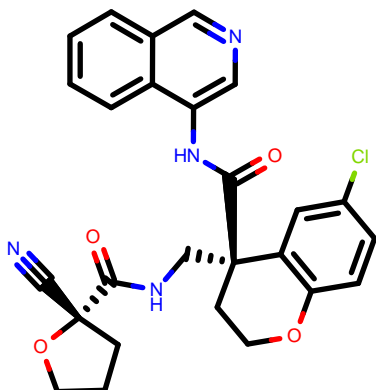
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5(H)CCN6C5=O

RUN: RUN13724

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-3710141_2_2



CID: EN300-3710141_2_2

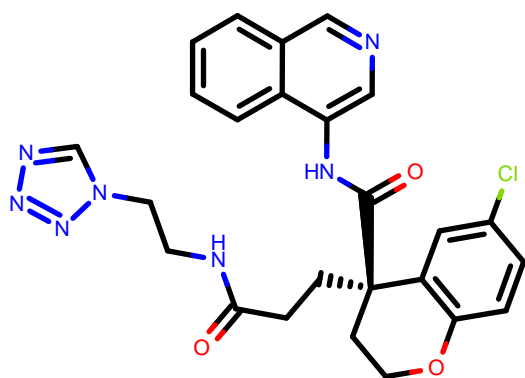
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCCO5)C#N

RUN: RUN2959

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.23

EN300-108022_2_1



CID: EN300-108022_2_1

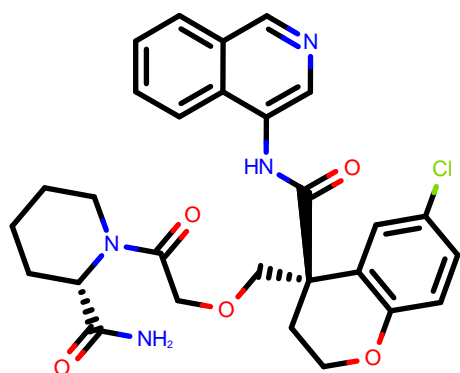
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOC4C3cc(cc4)Cl)CCC(=O)NCCn5nnn5

RUN: RUN12603

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.25

EN300-22879_2_1



CID: EN300-22879_2_1

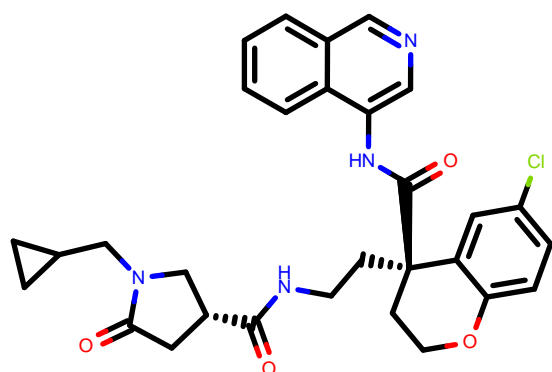
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOC4C3cc(cc4)Cl)COC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN1562

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-31969_3_1



CID: EN300-31969_3_1

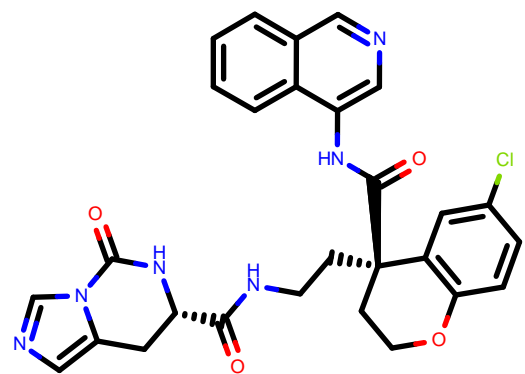
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOC4C3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@H](O)C5

RUN: RUN10906

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-1428805_3_1



CID: EN300-1428805_3_1

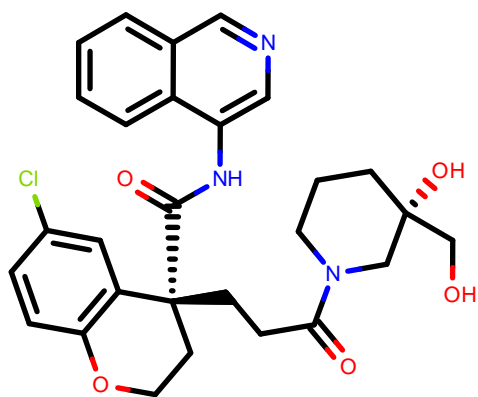
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H](CCOC4C3cc(cc4)Cl)CCNC(=O)[C@@H]5C6C=CN6C1=O)N5

RUN: RUN15318

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.28

EN300-251396_2_2



CID: EN300-251396_2_2

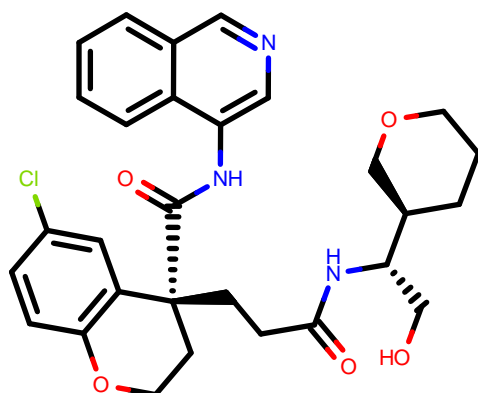
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@](C5)(CO)O

RUN: RUN2355

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.36

EN300-254105_2_2



CID: EN300-254105_2_2

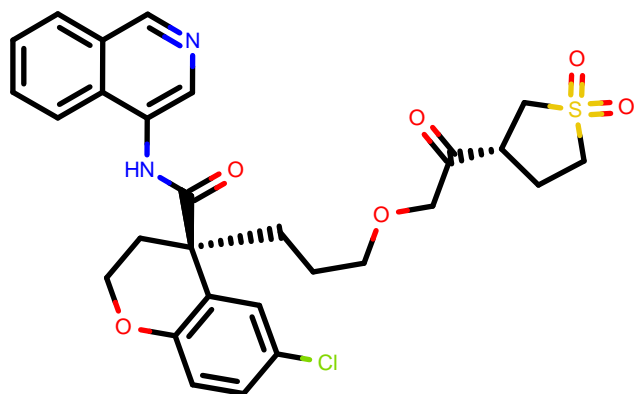
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]5(CO)C[C@H]5CCCCO5

RUN: RUN1662

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.31

EN300-226314_4_2



CID: EN300-226314_4_2

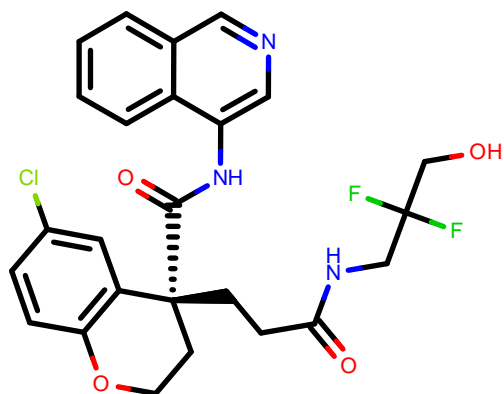
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)[C@H]5CCS(=O)(=O)C5

RUN: RUN1587

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.34

EN300-139846_2_1



CID: EN300-139846_2_1

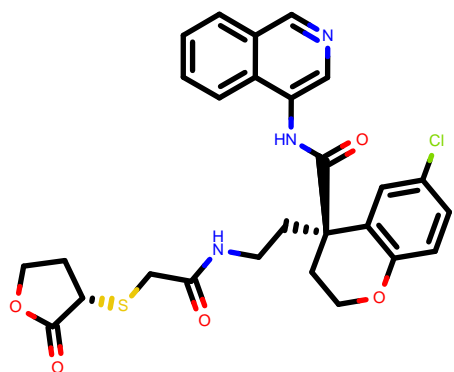
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(CO)(F)F

RUN: RUN4296

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.26

EN300-113218_3_1



CID: EN300-113218_3_1

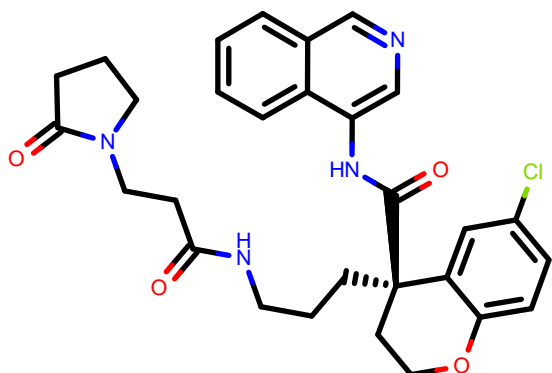
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5CCOC5=O

RUN: RUN14294

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.31

EN300-67191_4_1



CID: EN300-67191_4_1

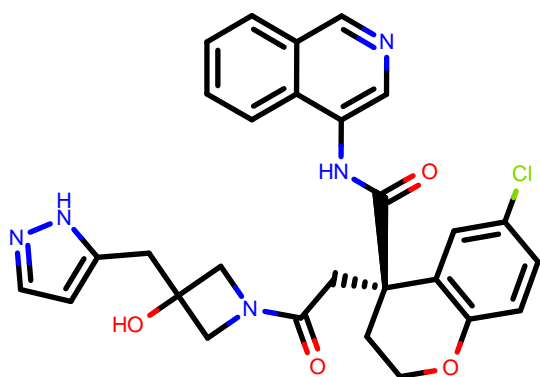
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCN5CCOC5=O

RUN: RUN9656

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.30

EN300-6489696_1_1



CID: EN300-6489696_1_1

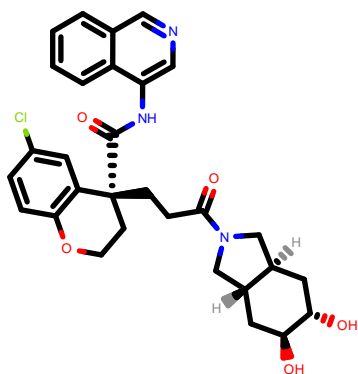
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C6c6cn[nH]6)O

RUN: RUN5317

DDG (kcal/mol): -0.45

dDDG (kcal/mol): 0.31

EN300-7355477_2_1



CID: EN300-7355477_2_1

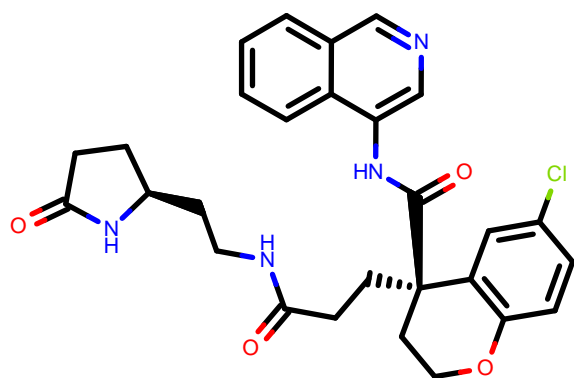
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C6C[C@@H](C6)C[C@@H]6C5)O

RUN: RUN11734

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.28

EN300-205779_2_2



CID: EN300-205779_2_2

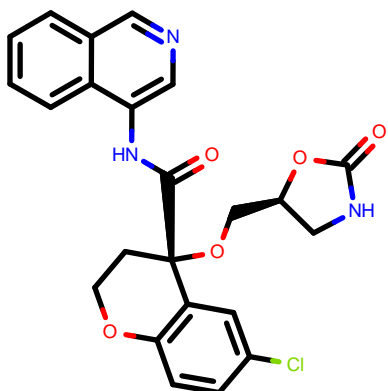
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC[C@@]H5CCCC(=O)N5

RUN: RUN9187

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.25

EN300-203293_1_2



CID: EN300-203293_1_2

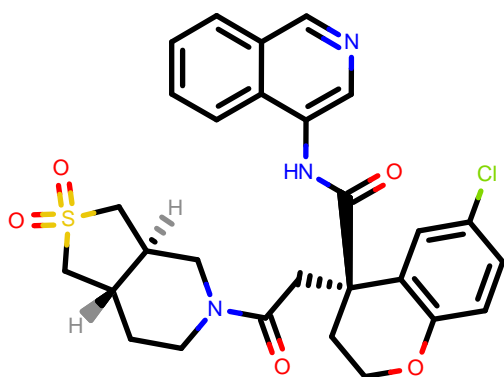
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]H5CNC(=O)O5

RUN: RUN1876

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.26

EN300-365993_1_1



CID: EN300-365993_1_1

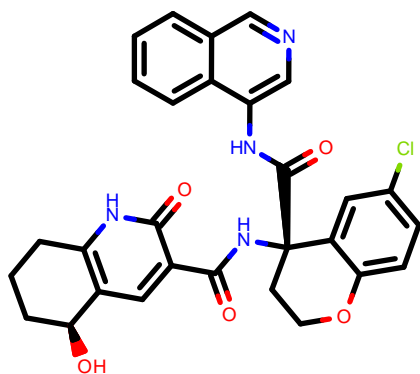
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]H6CS(=O)(=O)C[C@@]H7C

RUN: RUN10449

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.22

EN300-238234_1_1



CID: EN300-238234_1_1

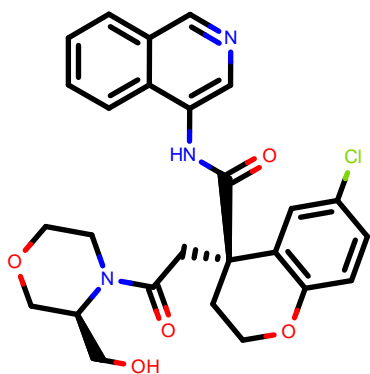
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c([H]5)C(=O)CCC[C@@]H6O

RUN: RUN7148

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.30

EN300-154201_1_1



CID: EN300-154201_1_1

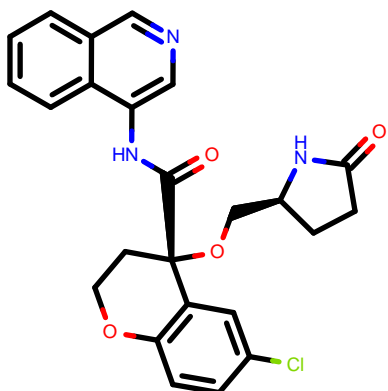
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO

RUN: RUN11463

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.26

EN300-195756_1_2



CID: EN300-195756_1_2

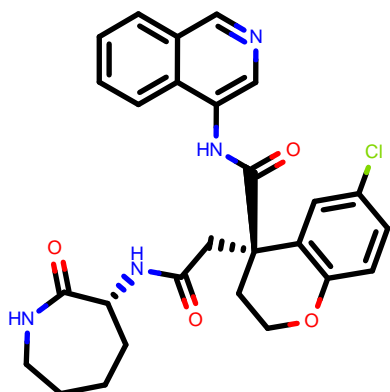
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCCC(=O)N5

RUN: RUN1948

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.25

EN300-129384_1_2



CID: EN300-129384_1_2

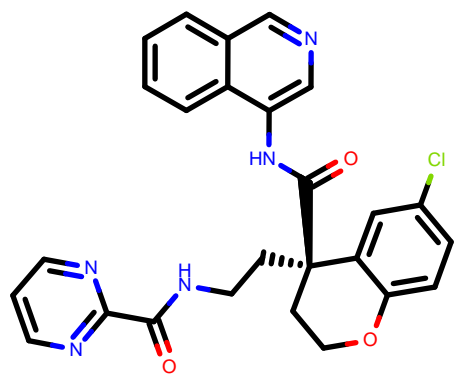
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCCN5=O

RUN: RUN13476

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.23

EN300-80230_3_1



CID: EN300-80230_3_1

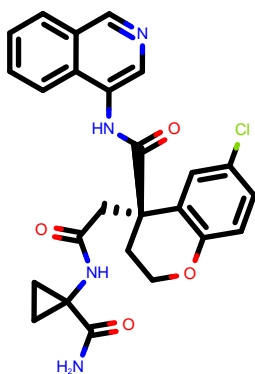
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(C(=O)c5ncccn5)

RUN: RUN15423

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.19

EN300-106988_1_1



CID: EN300-106988_1_1

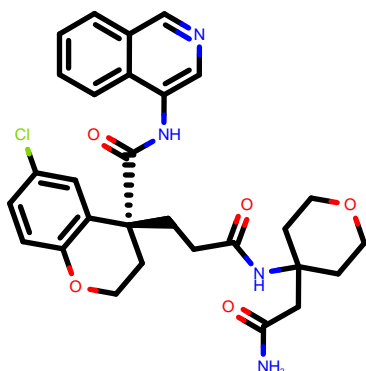
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(CCS)C(=O)N

RUN: RUN13340

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.21

EN300-99653_2_1



CID: EN300-99653_2_1

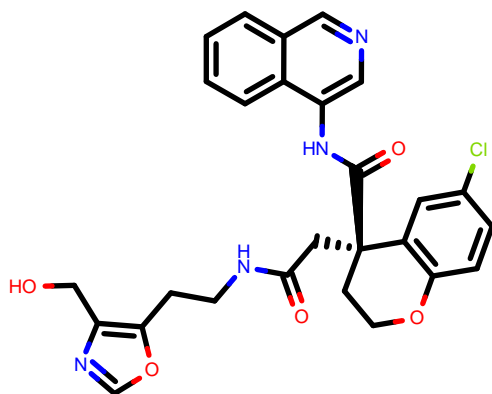
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(CCOCC5)CC(=O)N

RUN: RUN256

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.29

EN300-7470948_1_1



CID: EN300-7470948_1_1

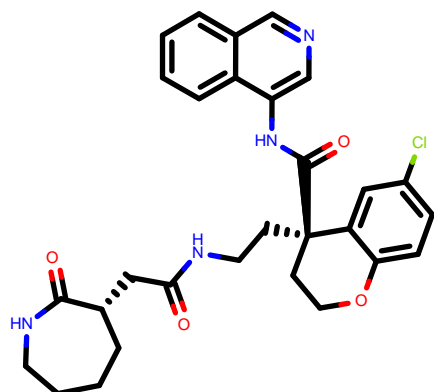
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCc5c(ncs5)CO

RUN: RUN9804

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.33

EN300-198633_3_2



CID: EN300-198633_3_2

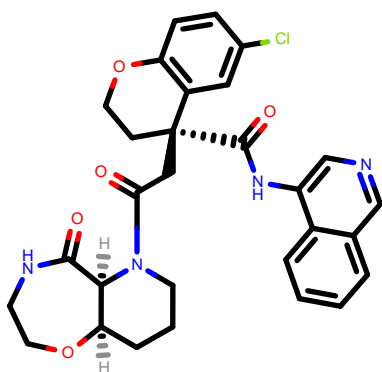
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5(C)CCCCNC5=O

RUN: RUN13188

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.33

EN300-364612_1_1



CID: EN300-364612_1_1

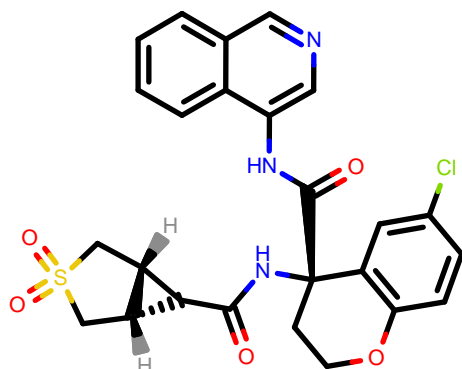
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(C)CCOc4c3ccc(c4)C)C(=O)N5CCCC[C@@H](C@H)5C(=O)NCCO6

RUN: RUN4073

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.30

EN300-6779469_1_2



CID: EN300-6779469_1_2

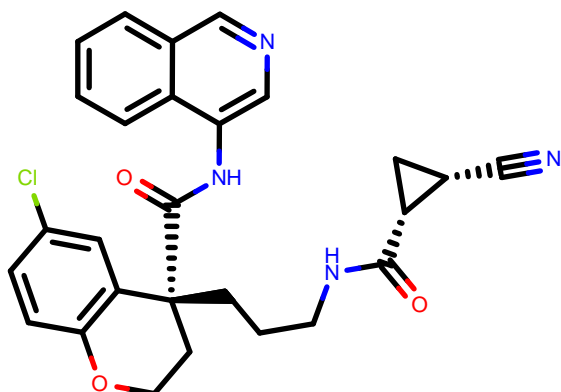
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(C)CCOc4c3ccc(c4)C)NC(=O)C5(C)C@H](C@H)5C(=O)N(=O)C6

RUN: RUN4982

DDG (kcal/mol): -0.44

dDDG (kcal/mol): 0.23

EN300-1600363_4_1



CID: EN300-1600363_4_1

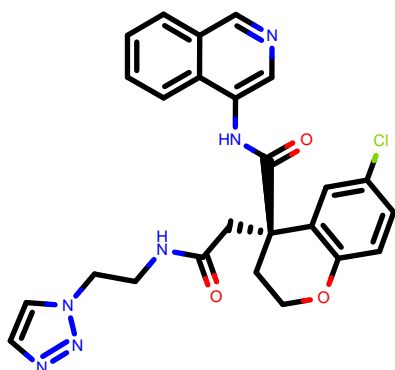
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(C)CCOc4c3ccc(c4)C)C(=O)N(=O)C@H]5C(=O)N(=O)C@H]5#N

RUN: RUN12657

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.21

EN300-295372_1_1



CID: EN300-295372_1_1

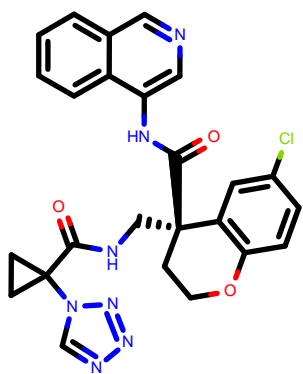
SMILES: c1ccc2c(c1)ncnc2NC(=O)C[C@@]3(C)CCOc4c3ccc(c4)C)CC(=O)N(C)C5c6cn5

RUN: RUN9654

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EN300-263085_2_1



CID: EN300-263085_2_1

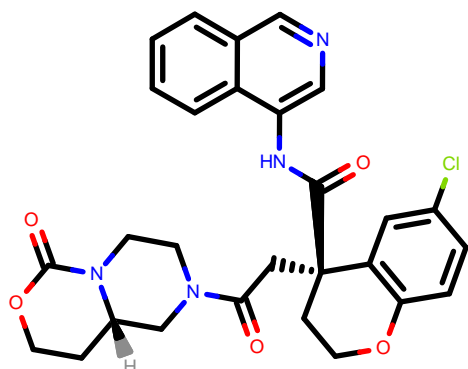
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)n6cnn6

RUN: RUN4115

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.22

EN300-121939_1_1



CID: EN300-121939_1_1

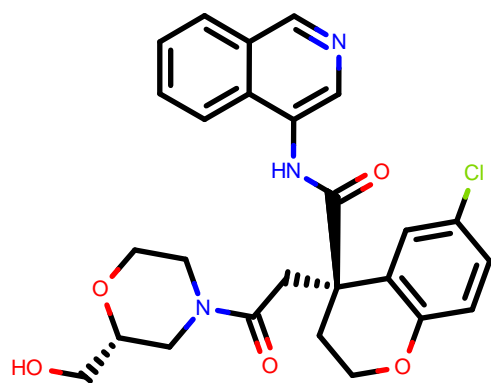
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@H](C5)CCOC6=O

RUN: RUN12884

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.26

EN300-175485_1_1



CID: EN300-175485_1_1

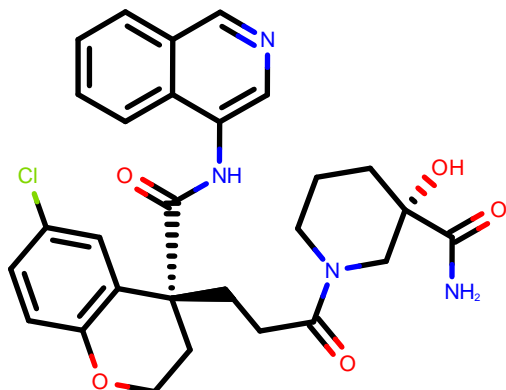
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CO

RUN: RUN9798

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EN300-210553_2_2



CID: EN300-210553_2_2

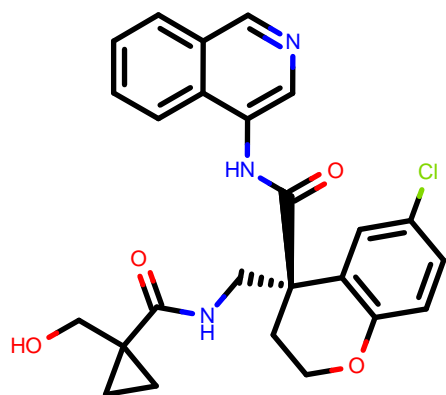
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@H](C5)(C(=O)N)O

RUN: RUN6722

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.36

EN300-146174_2_1



CID: EN300-146174_2_1

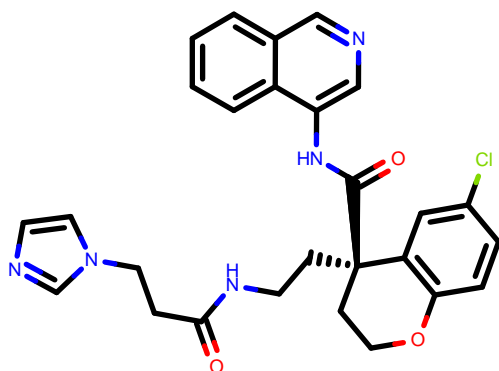
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(CC5)CO

RUN: RUN3699

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.28

EN300-75342_3_1



CID: EN300-75342_3_1

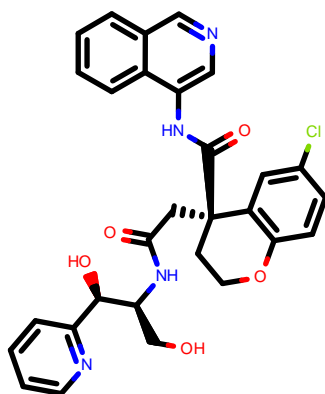
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5ccnc5

RUN: RUN8099

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.28

EN300-332714_1_3



CID: EN300-332714_1_3

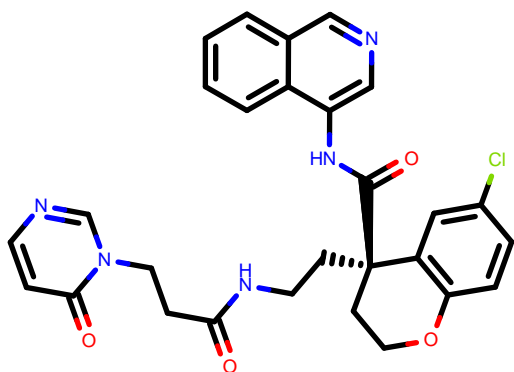
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C[C@@H](CO)[C@@H](c5ccncc5)O

RUN: RUN673

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.43

EN300-219609_3_1



CID: EN300-219609_3_1

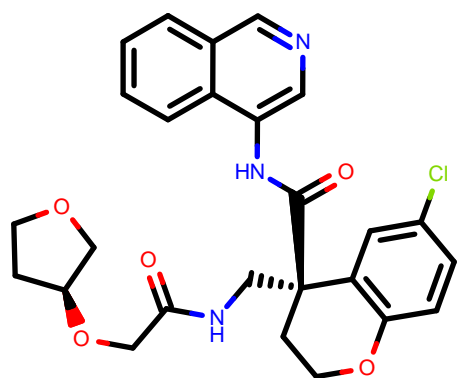
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5cnc(=O)c5

RUN: RUN14496

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.31

EN300-99391_2_2



CID: EN300-99391_2_2

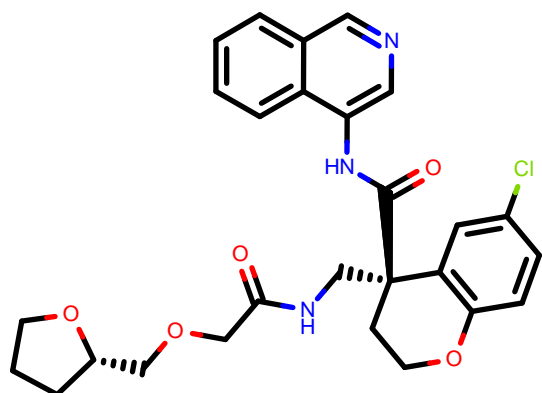
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COC[C@@H]5CCOC5

RUN: RUN5927

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.24

EN300-60033_2_2



CID: EN300-60033_2_2

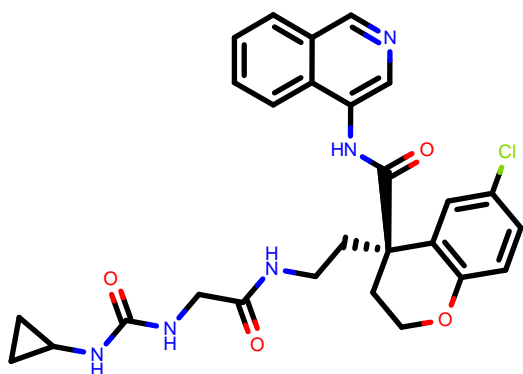
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COC[C@@H]5CCOC5

RUN: RUN7433

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.25

EN300-42591_3_1



CID: EN300-42591_3_1

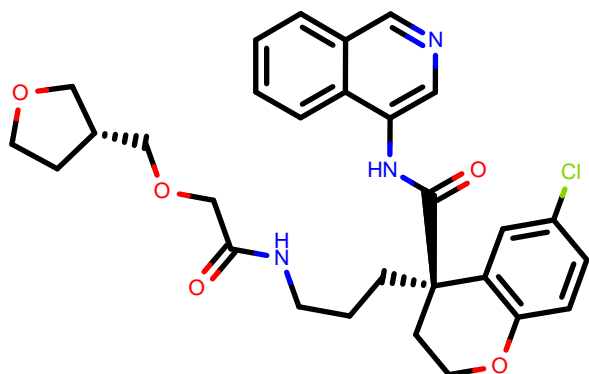
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)NC5CC5

RUN: RUN11753

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.24

EN300-80522_4_1



CID: EN300-80522_4_1

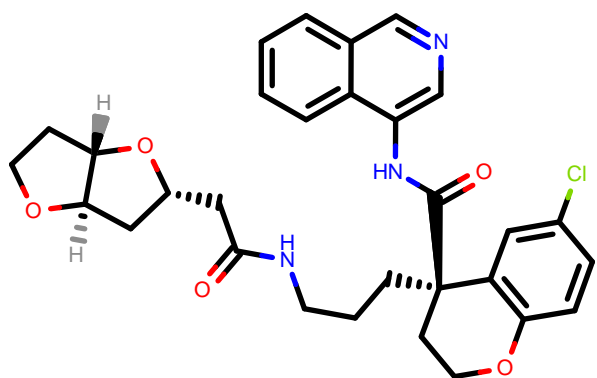
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@@H]5CCOC5

RUN: RUN8178

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.24

EN300-7355519_4_2



CID: EN300-7355519_4_2

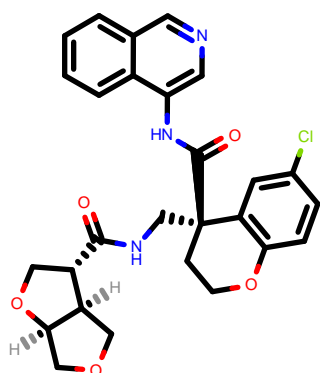
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@H](COc4cc3cc4O)CCN(C=O)C[C@@H]5C[C@@H]6O5CCO6

RUN: RUN11019

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.27

EN300-6482296_2_2



CID: EN300-6482296_2_2

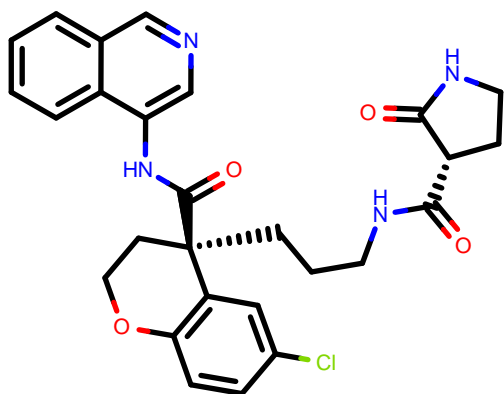
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@H](COc4cc3cc4O)CNC(=O)C[C@@H]5C[C@@H]6O5CCO6

RUN: RUN7441

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.25

EN300-94945_4_2



CID: EN300-94945_4_2

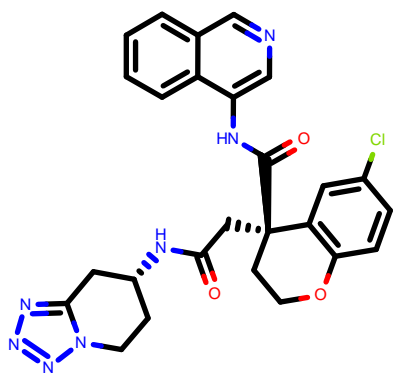
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@H](COc4cc3cc4O)CCN(C=O)C[C@@H]5C[C@@H]6O5=O

RUN: RUN11268

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.22

EN300-7438451_1_2



CID: EN300-7438451_1_2

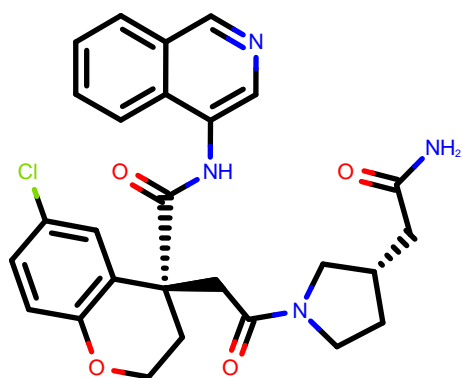
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3[C@@H](COc4cc3cc4O)CC(=O)N[C@@]4[C@@H]5C[C@@H]6O5C5

RUN: RUN4577

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.27

EN300-304381_1_2



CID: EN300-304381_1_2

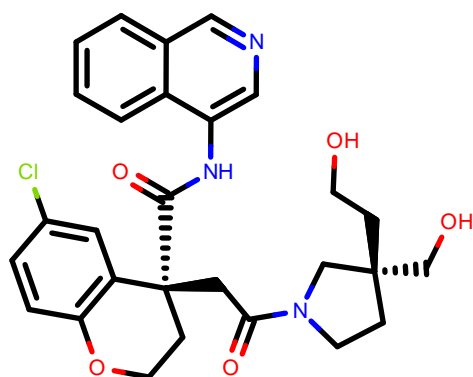
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CC(=O)N

RUN: RUN10065

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.26

EN300-1707870_1_1



CID: EN300-1707870_1_1

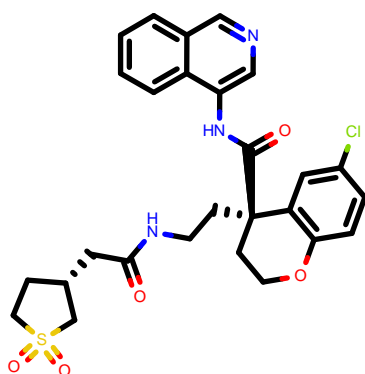
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)(CO)CO

RUN: RUN3545

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.25

EN300-14006_3_2



CID: EN300-14006_3_2

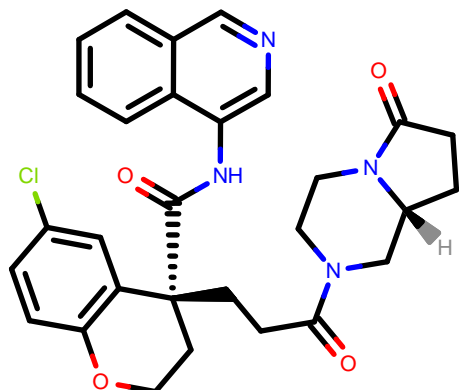
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5SCCS(=O)(=O)C5

RUN: RUN8696

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.34

EN300-60330_2_2



CID: EN300-60330_2_2

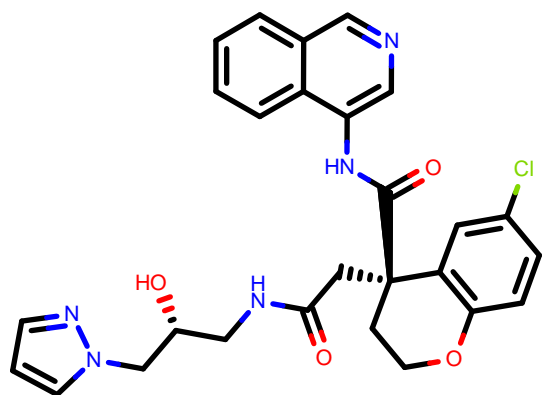
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN[C@@H](C5)CCC6=O

RUN: RUN13637

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.23

EN300-1233032_1_1



CID: EN300-1233032_1_1

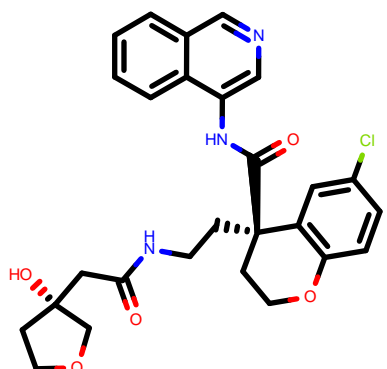
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@H](Cn5cccn5)O

RUN: RUN7455

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.28

EN300-360157_3_1



CID: EN300-360157_3_1

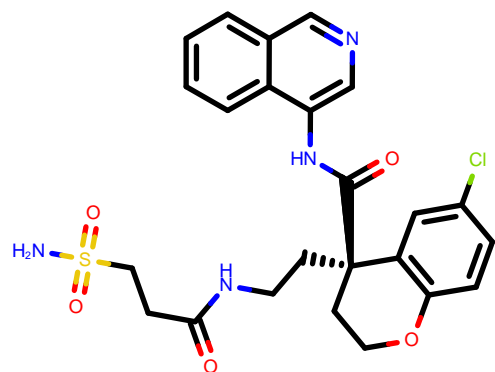
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5(CCOc5)O

RUN: RUN4249

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.26

EN300-31553_3_1



CID: EN300-31553_3_1

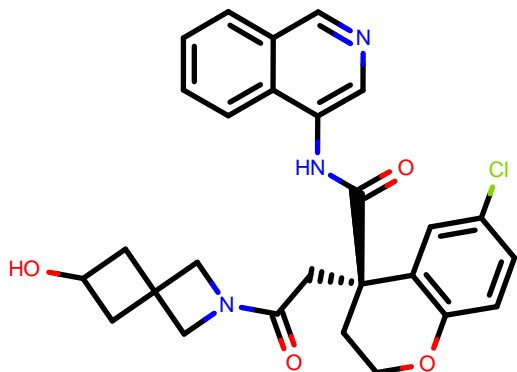
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCS(=O)(=O)N

RUN: RUN11032

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.36

EN300-317210_1_1



CID: EN300-317210_1_1

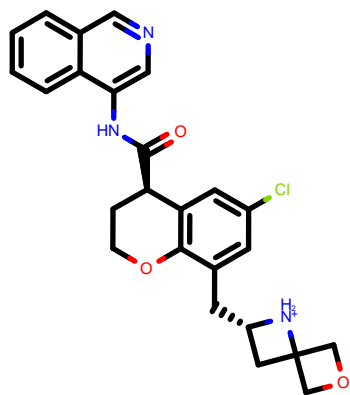
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CC(C6)O

RUN: RUN13330

DDG (kcal/mol): -0.43

dDDG (kcal/mol): 0.22

DAR-DIA-23e5a6a0-8_1



CID: DAR-DIA-23e5a6a0-8_1

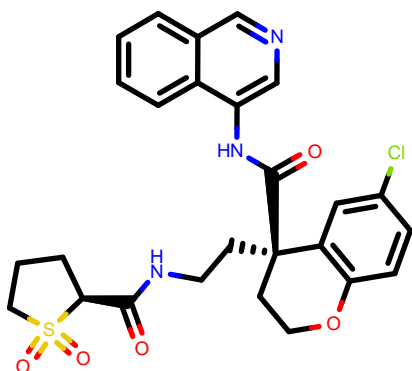
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3CCOCc4ccc(cc4C)[C@H]5CC6([NH2+][5])COC6)Cl

RUN: RUN198

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.34

EN300-88656_3_1



CID: EN300-88656_3_1

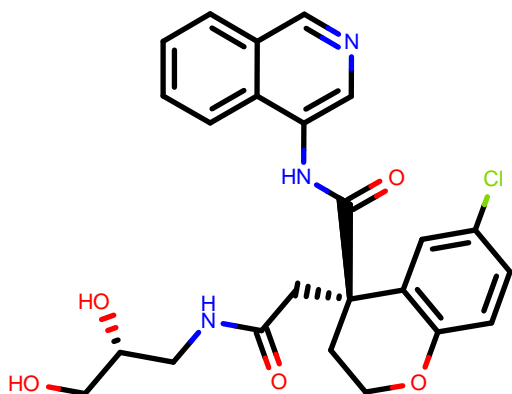
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCS5(=O)=O

RUN: RUN14732

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.23

EN300-50845_1_2



CID: EN300-50845_1_2

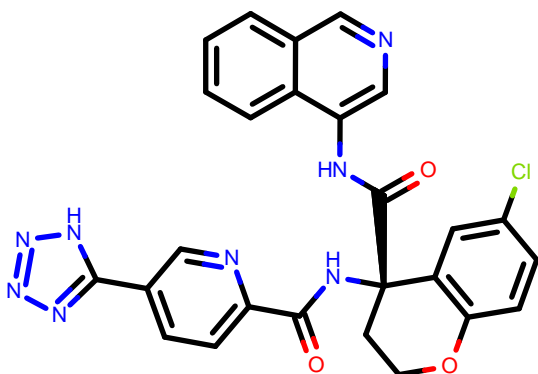
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H](CO)O

RUN: RUN6643

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.34

EN300-306105_1_1



CID: EN300-306105_1_1

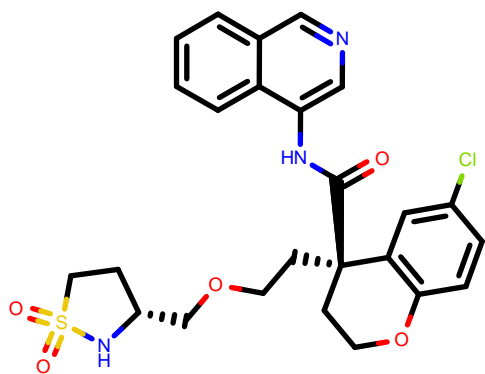
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(nc5)c6[nH]n6

RUN: RUN9895

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.23

EN300-1699871_3_1



CID: EN300-1699871_3_1

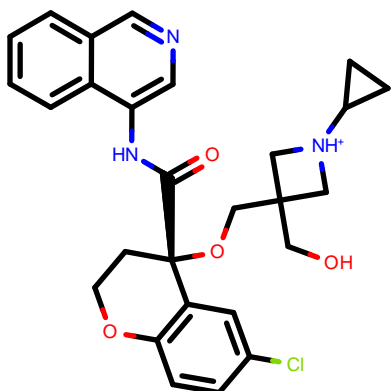
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CCOC[C@H]5CCS(=O)(=O)N5

RUN: RUN2174

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.28

EN300-6735421_1_1



CID: EN300-6735421_1_1

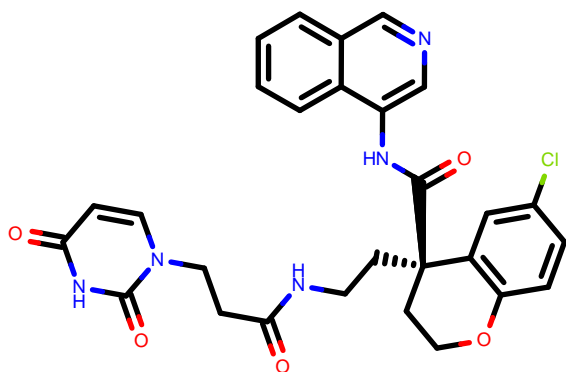
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)OCC5[C[NH+]](C5)C6CC6)CO

RUN: RUN2571

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.29

EN300-106781_3_1



CID: EN300-106781_3_1

SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CCNC(=O)CCn5ccc(=O)[nH]c5=O

RUN: RUN14806

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.31

CID: EN300-266299_1_1

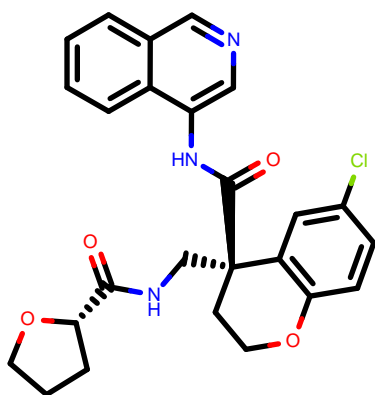
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@](COc4c3cc(cc4)C)CC(=O)N[C@@]5C[C@]([H])(C5)O

RUN: RUN7139

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.21

EN300-104395_2_1



CID: EN300-104395_2_1

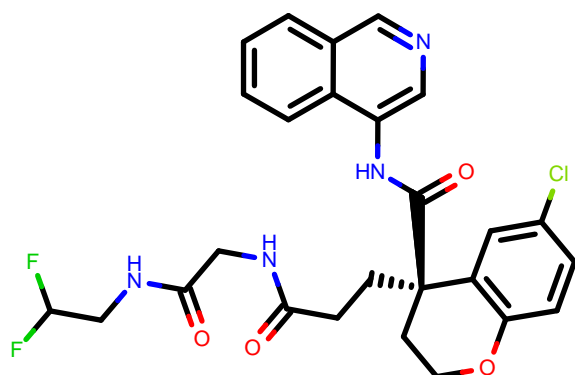
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CCCO5

RUN: RUN5263

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.21

EN300-195464_2_1



CID: EN300-195464_2_1

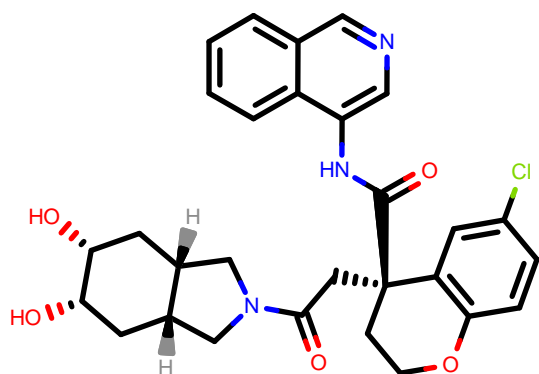
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CNC(=O)NCC(F)F

RUN: RUN10132

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.23

EN300-7355477_1_9



CID: EN300-7355477_1_9

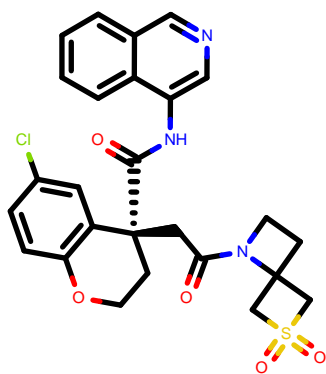
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)N5C[C@@H]6C[C@@H]7[C@@H]3[C@@H]6C5=O

RUN: RUN12752

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.25

EN300-1717443_1_1



CID: EN300-1717443_1_1

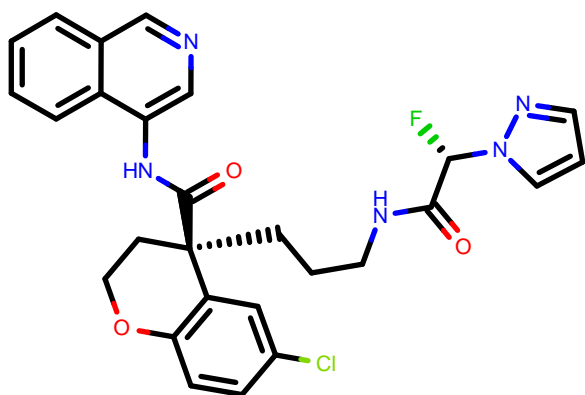
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)C)CC(=O)N5CCCS6CS(=O)(=O)C6

RUN: RUN7483

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.24

EN300-1726277_4_1



CID: EN300-1726277_4_1

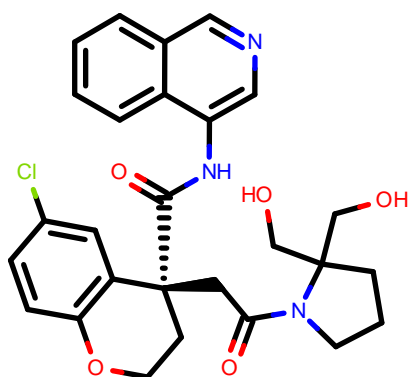
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](n5cccn5)F

RUN: RUN7534

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.24

EN300-1091448_1_1



CID: EN300-1091448_1_1

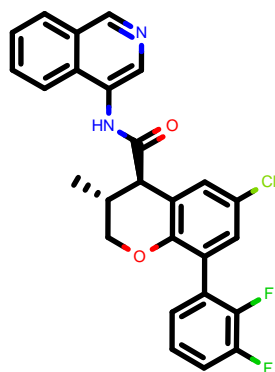
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC5(O)CO

RUN: RUN5365

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.31

DAR-DIA-0d514e7d-14_1



CID: DAR-DIA-0d514e7d-14_1

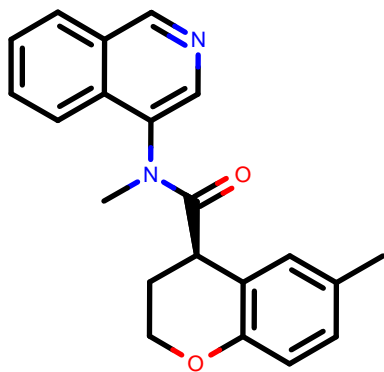
SMILES: C[C@@H]1COc2c(cc(c2)[C@@H]1C(=O)Nc3ncnc4c3ccc4)Cl)c5ccoc(c5)F

RUN: RUN226

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.23

MAK-UNK-3875bbc8-1_2



CID: MAK-UNK-3875bbc8-1_2

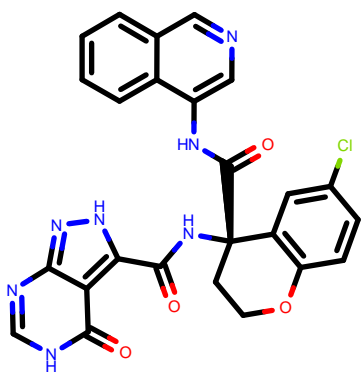
SMILES: Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)C3cncnc4c3ccc4

RUN: RUN20

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.11

EN300-1266218_1_1



CID: EN300-1266218_1_1

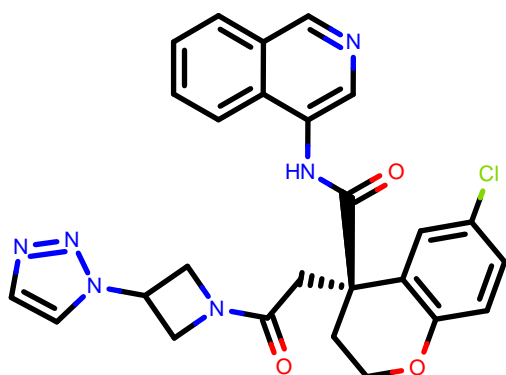
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)C)NC(=O)c5c6c(=O)[nH]cnc6[nH]5

RUN: RUN8540

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.20

EN300-367405_1_1



CID: EN300-367405_1_1

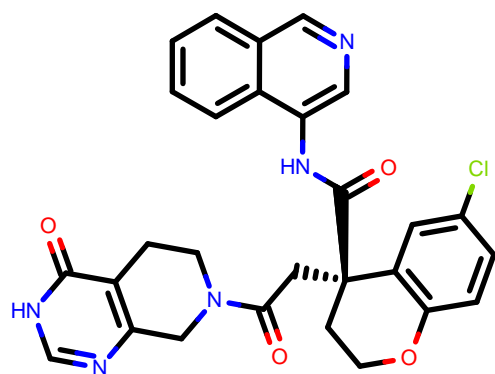
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6cnm6

RUN: RUN9609

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.19

EN300-132141_1_1



CID: EN300-132141_1_1

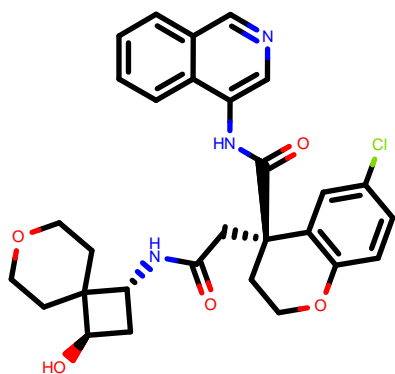
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)N5CCc6c(nc[nH]c6=O)C5

RUN: RUN14260

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.22

EN300-640503_1_1



CID: EN300-640503_1_1

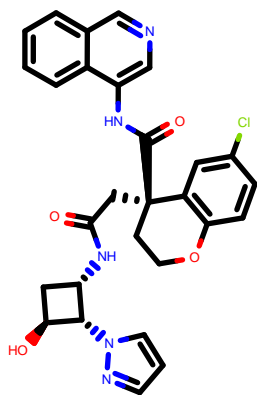
SMILES: c1ccc2c(c1)cncc2NC(=O)C@@3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5[C@@H](C6CCCC6)O

RUN: RUN13840

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.33

EN300-260696_1_6



CID: EN300-260696_1_6

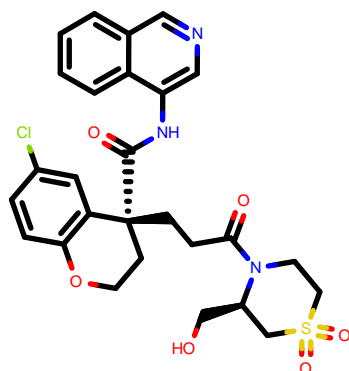
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3c(coc4)C(C)C(=O)N(C@@H)C(C@@H)5c6ccn6O

RUN: RUN585

DDG (kcal/mol): -0.42

dDDG (kcal/mol): 0.25

EN300-157541_2_2



CID: EN300-157541_2_2

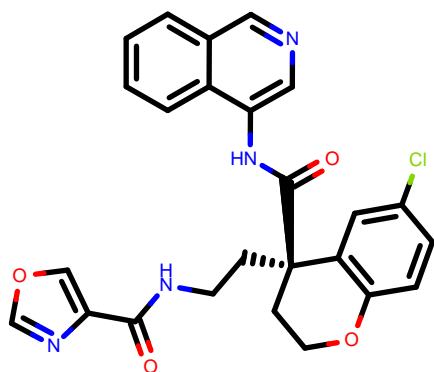
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3c(coc4)C(C)C(=O)N5CCS(=O)(=O)C(C)@H]5CO

RUN: RUN4992

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.38

EN300-68618_3_1



CID: EN300-68618_3_1

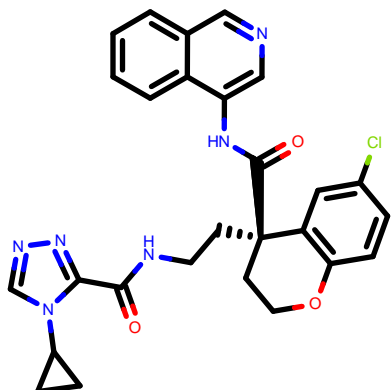
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3c(coc4)C(C)CCNC(=O)c5ccn5

RUN: RUN15235

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.20

EN300-6745581_3_1



CID: EN300-6745581_3_1

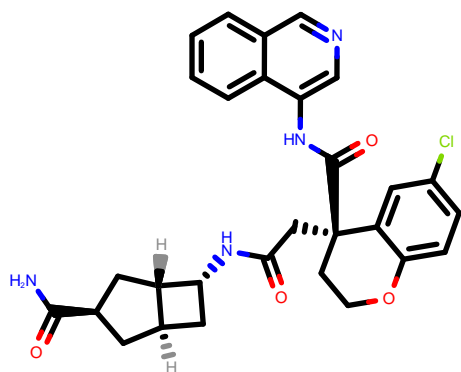
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOC4C3c(coc4)C(C)CCNC(=O)c5nncn5C6CC6

RUN: RUN15008

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.21

EN300-1268016_1_13



CID: EN300-1268016_1_13

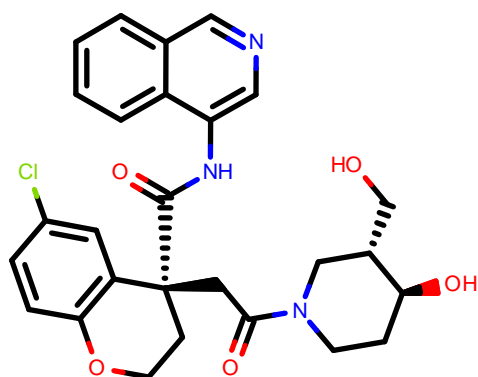
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)CC(=O)N[C@@]3[C@@H](C)C[C@@H](C)C(=O)N

RUN: RUN14948

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.22

EN300-233678_1_1



CID: EN300-233678_1_1

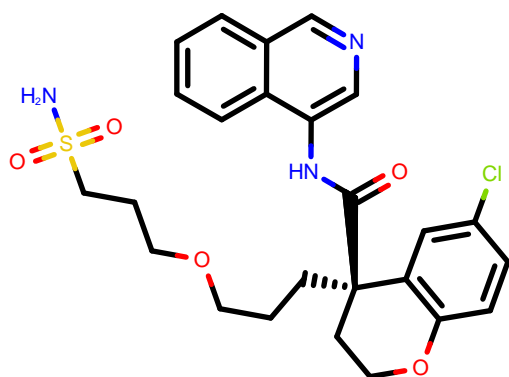
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)C[C@@H]3C(=O)N5CCNCC5O

RUN: RUN9288

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.22

EN300-79588_4_1



CID: EN300-79588_4_1

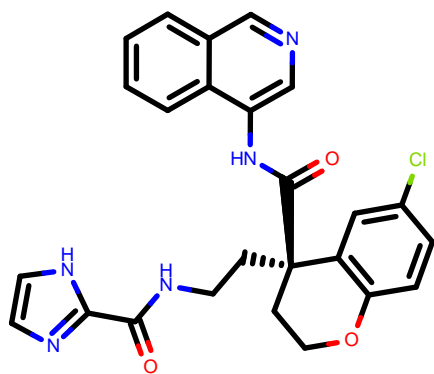
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)C[C@@H]3C(=O)N(S(=O)(=O)O)O

RUN: RUN869

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

EN300-315836_3_1



CID: EN300-315836_3_1

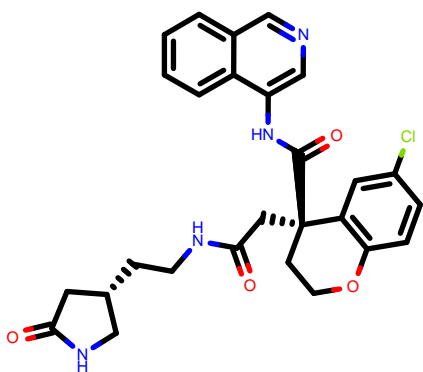
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@O]c4ccc(cc4)C[C@@H]3C(=O)N5C=CN=C5

RUN: RUN15241

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.18

EN300-298582_1_2



CID: EN300-298582_1_2

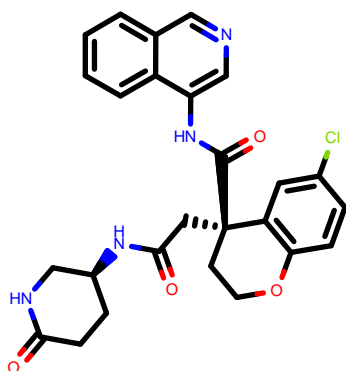
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC[C@H]5CC(=O)NCS

RUN: RUN6280

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EN300-62191_1_2



CID: EN300-62191_1_2

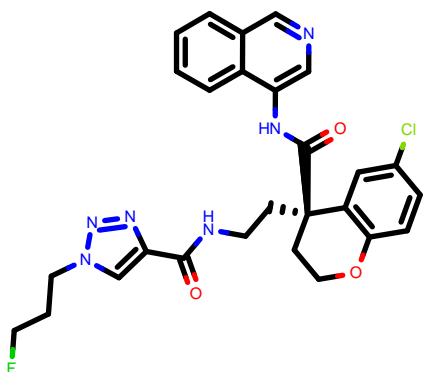
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CC(=O)NCS

RUN: RUN11831

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.21

EN300-1704723_3_1



CID: EN300-1704723_3_1

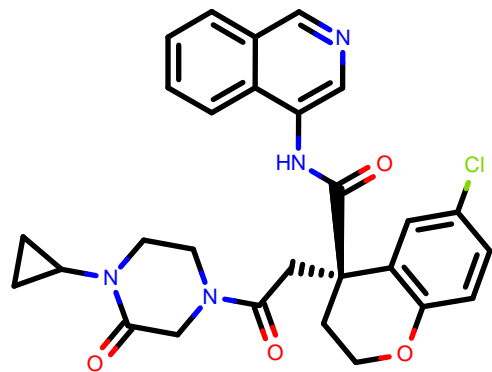
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cn[nH]5)CCCF

RUN: RUN15408

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EN300-202232_1_1



CID: EN300-202232_1_1

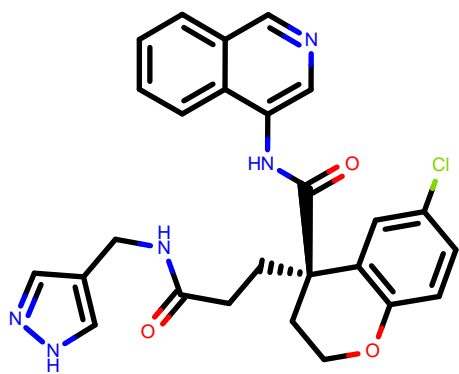
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(C(=O)C5)CC6C6

RUN: RUN11493

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.24

EN300-31562_2_1



CID: EN300-31562_2_1

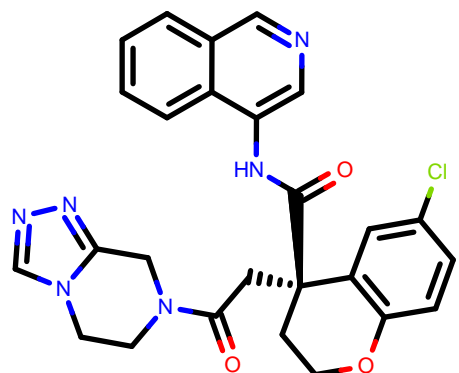
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5c[nH]ne5

RUN: RUN8354

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.25

EN300-71125_1_1



CID: EN300-71125_1_1

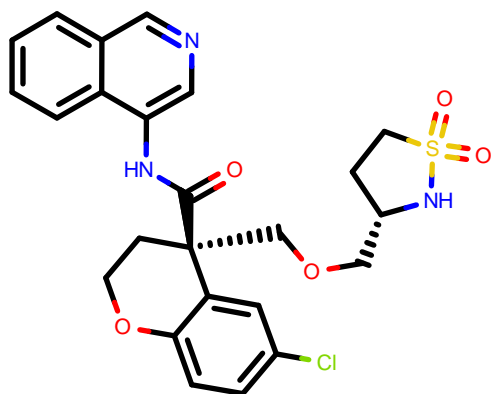
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CNc6nnc6S

RUN: RUN12524

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EN300-1699871_2_2



CID: EN300-1699871_2_2

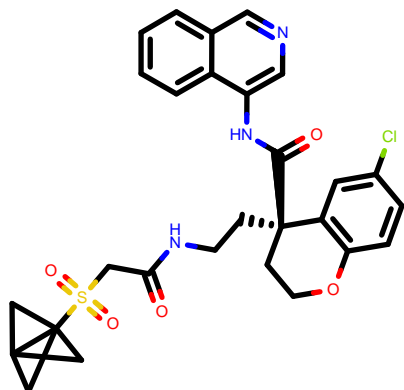
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5SCCS(=O)(=O)N5

RUN: RUN436

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.23

EN300-6763072_3_1



CID: EN300-6763072_3_1

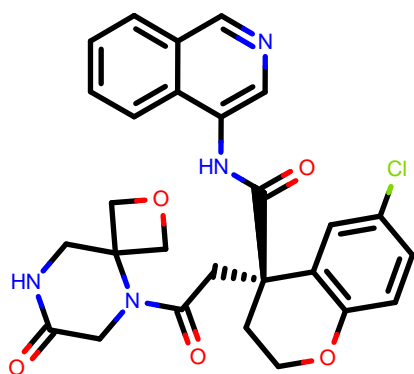
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)C56C(C5)C6

RUN: RUN14840

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.30

EN300-366278_1_1



CID: EN300-366278_1_1

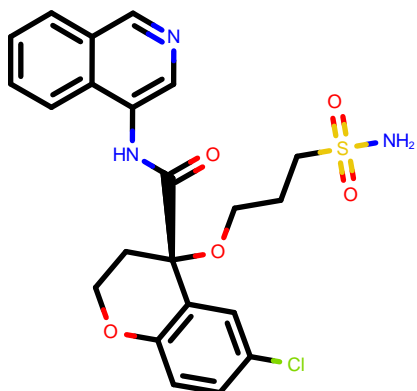
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NCC56COC6

RUN: RUN7703

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.27

EN300-79588_1_1



CID: EN300-79588_1_1

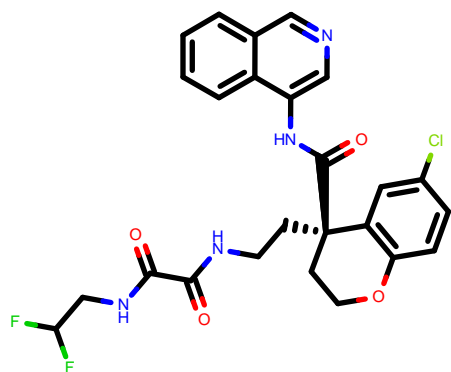
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCS(=O)(=O)N

RUN: RUN927

DDG (kcal/mol): -0.41

dDDG (kcal/mol): 0.28

EN300-128277_3_1



CID: EN300-128277_3_1

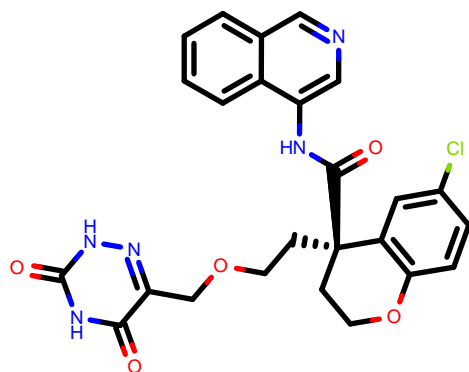
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(F)F

RUN: RUN11393

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.23

EN300-761746_3_1



CID: EN300-761746_3_1

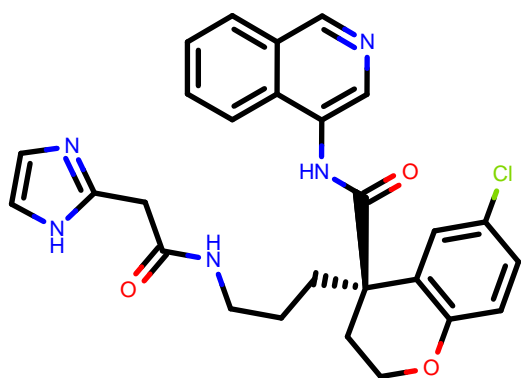
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5c(=O)[nH]c(=O)[nH]n5

RUN: RUN2546

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.25

EN300-220527_4_1



CID: EN300-220527_4_1

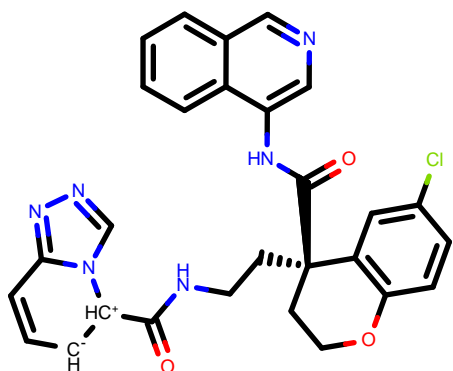
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5[nH]cn5

RUN: RUN7754

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.23

EN300-6488157_3_1



CID: EN300-6488157_3_1

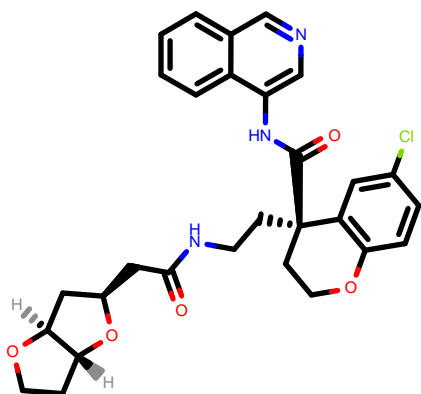
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cccn5

RUN: RUN15132

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.25

EN300-7355519_3_8



CID: EN300-7355519_3_8

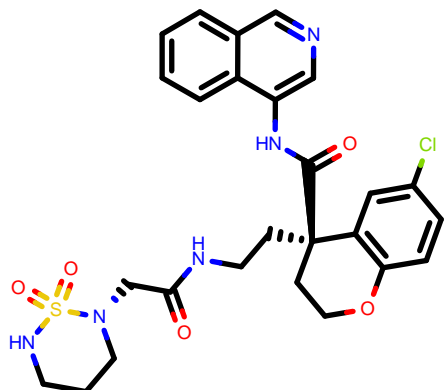
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5[C@H](C)[C@H]6OCCO6

RUN: RUN14586

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

EN300-4726186_3_1



CID: EN300-4726186_3_1

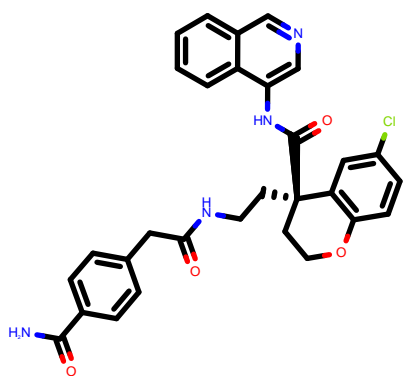
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[N@]5SCCNS5(=O)=O

RUN: RUN8147

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.39

EN300-135123_3_1



CID: EN300-135123_3_1

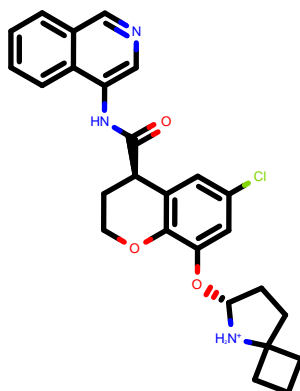
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOCc4ccc(cc4)Cl)CCNC(=O)C5CCOC(C5)=O

RUN: RUN11445

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

DAR-DIA-23e5a6a0-1_1



CID: DAR-DIA-23e5a6a0-1_1

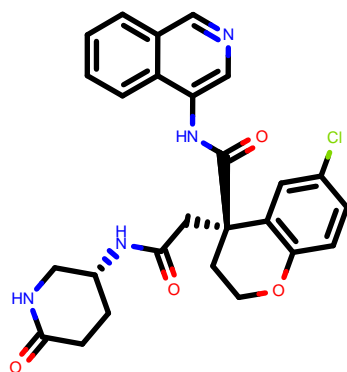
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOCc4ccc(cc4)Cl)C@H5CCCC6([NH2+][5]OCC6)Cl

RUN: RUN183

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.32

EN300-62191_1_1



CID: EN300-62191_1_1

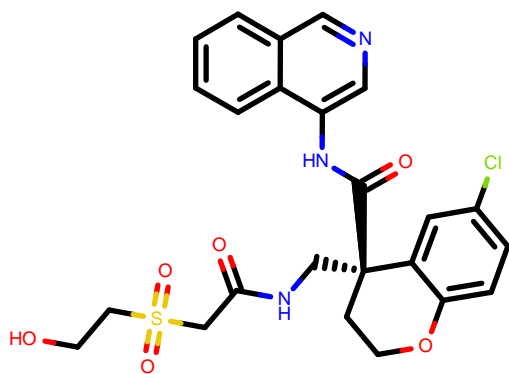
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOCc4ccc(cc4)Cl)CC(=O)N[C@@]5[C@@H](CCOC)N5

RUN: RUN7975

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.22

EN300-4293814_2_1



CID: EN300-4293814_2_1

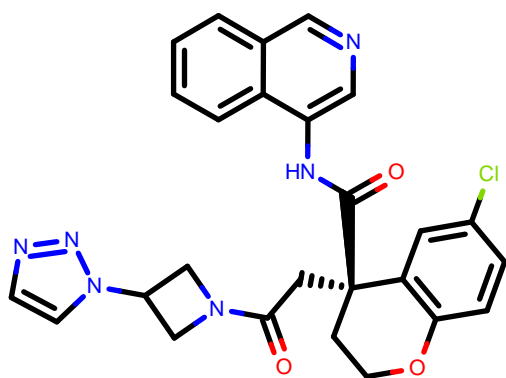
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@H](CCOCc4ccc(cc4)Cl)CNC(=O)CS(=O)(=O)CCO

RUN: RUN446

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.54

EN300-367405_1_1



CID: EN300-367405_1_1

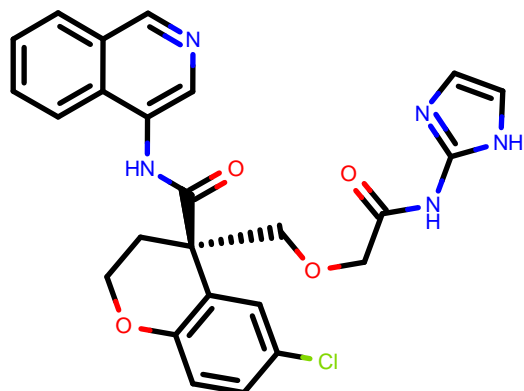
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)n6cnn6

RUN: RUN9606

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.23

EN300-331993_2_1



CID: EN300-331993_2_1

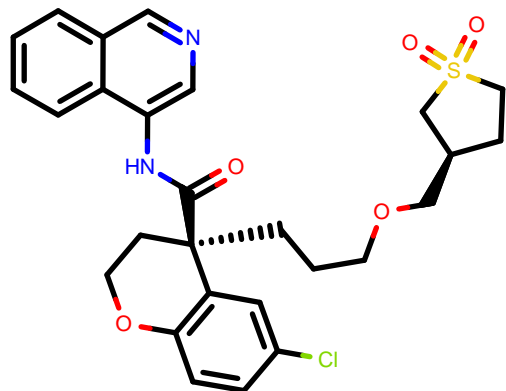
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)COCC(=O)Nc5[nH]cnn5

RUN: RUN2506

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.20

EN300-1448603_4_1



CID: EN300-1448603_4_1

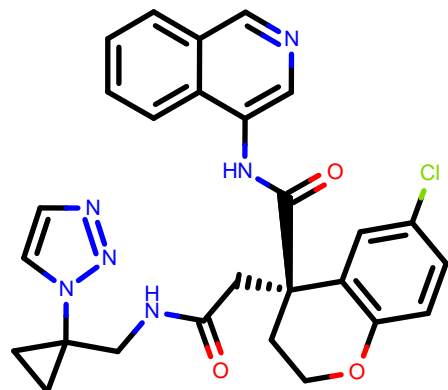
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC(C@@H)5CCS(=O)(=O)C5

RUN: RUN1507

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

EN300-1721883_1_1



CID: EN300-1721883_1_1

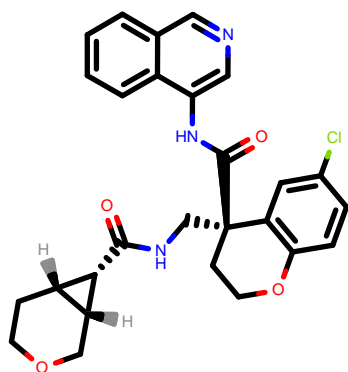
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC5(CC5)n6cnn6

RUN: RUN11078

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.24

EN300-1644723_2_6



CID: EN300-1644723_2_6

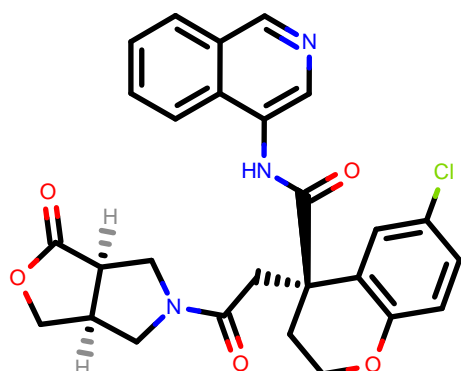
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C[C@@H](O)CNC(=O)[C@@H](O)C[C@@H](O)C

RUN: RUN2563

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.27

EN300-316193_1_1



CID: EN300-316193_1_1

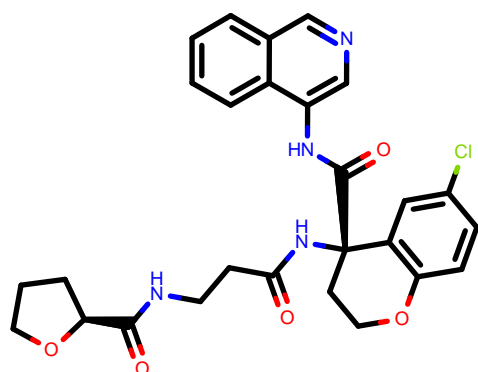
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C[C@@H](O)CNC(=O)[C@@H](O)C

RUN: RUN5969

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.21

EN300-86732_1_1



CID: EN300-86732_1_1

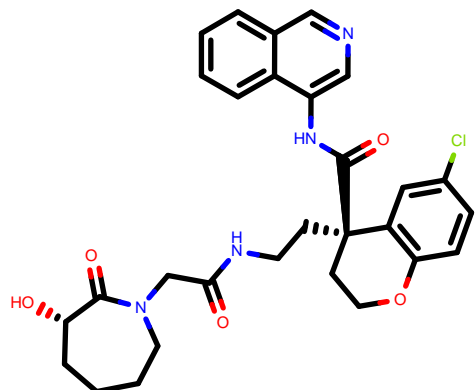
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C[C@@H](O)CNC(=O)CCNC(=O)[C@@H](O)C

RUN: RUN3106

DDG (kcal/mol): -0.40

dDDG (kcal/mol): 0.24

EN300-259849_3_2



CID: EN300-259849_3_2

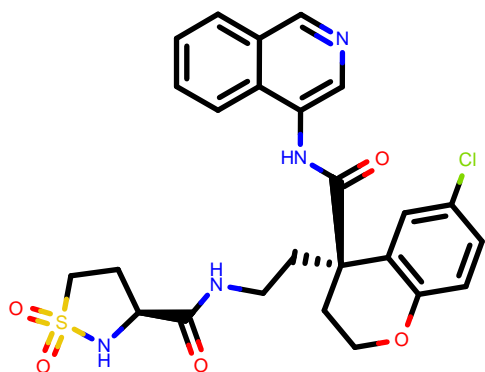
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](Cl)C[C@@H](O)CNC(=O)CCNC(=O)[C@@H](O)C

RUN: RUN13692

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.49

EN300-45049_3_1



CID: EN300-45049_3_1

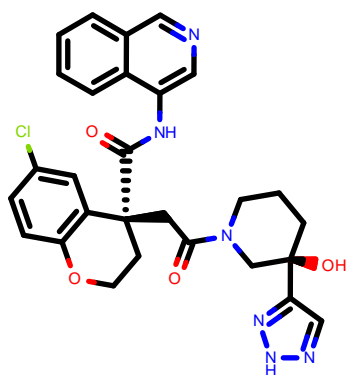
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5SCCS(=O)(=O)N5

RUN: RUN14458

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.26

EN300-222120_1_1



CID: EN300-222120_1_1

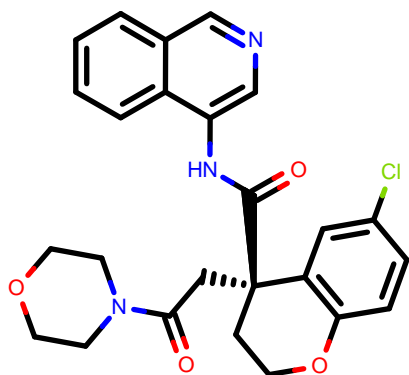
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@]3(C)C5Nc6nc[nH]6O

RUN: RUN3721

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.35

EN300-18064_1_1



CID: EN300-18064_1_1

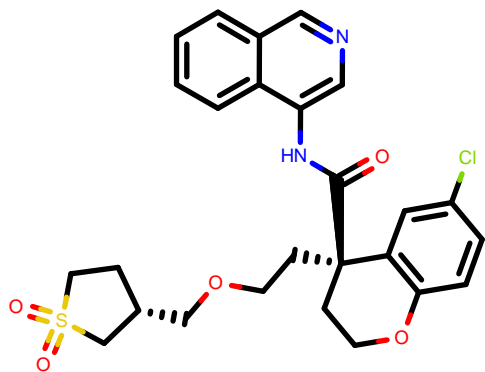
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOCC5

RUN: RUN9735

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.19

EN300-1448603_3_2



CID: EN300-1448603_3_2

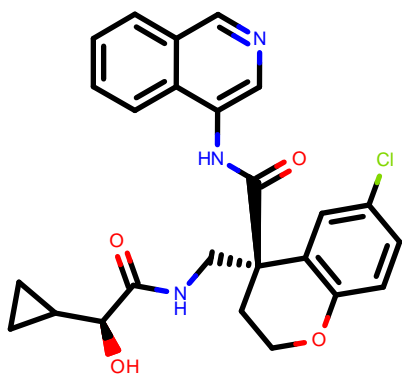
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5SCCS(=O)(=O)C5

RUN: RUN2158

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.28

EN300-72211_2_2



CID: EN300-72211_2_2

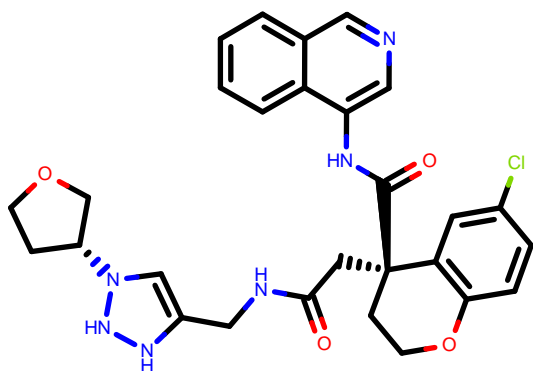
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H](C5CC5)O

RUN: RUN4559

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.25

EN300-1222454_1_1



CID: EN300-1222454_1_1

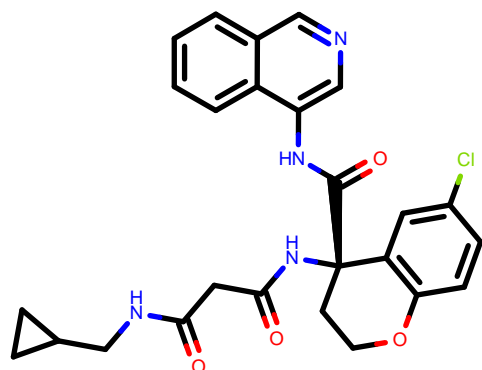
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5Nn5)[C@@]H6COC6

RUN: RUN4513

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-178829_1_1



CID: EN300-178829_1_1

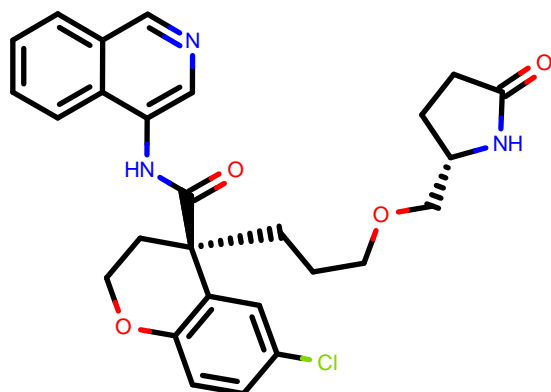
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)NCC5COC5

RUN: RUN7028

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.25

EN300-195756_4_2



CID: EN300-195756_4_2

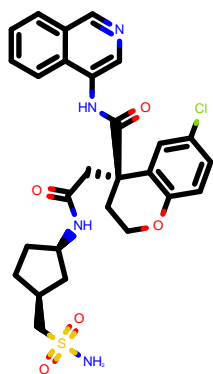
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]H5CCCC(=O)N5

RUN: RUN821

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.24

EN300-1425899_1_1



CID: EN300-1425899_1_1

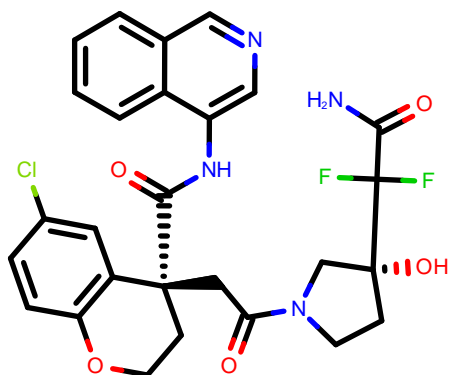
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(C)C(=O)N[C@@H]5CC[C@@H]6C(S(=O)(=O)N)C6=O

RUN: RUN14252

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.34

EN300-1720496_1_1



CID: EN300-1720496_1_1

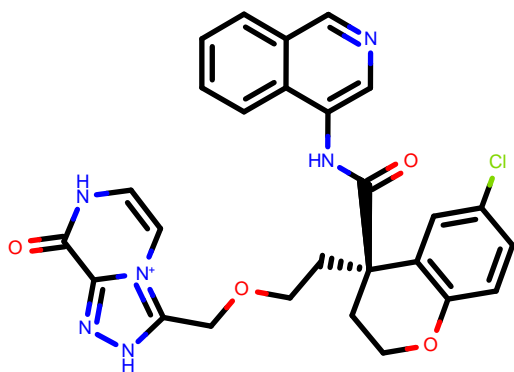
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(C)C(=O)N5CC[C@@H]6C(S(=O)(=O)N)C6=O

RUN: RUN12304

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.26

EN300-378316_3_1



CID: EN300-378316_3_1

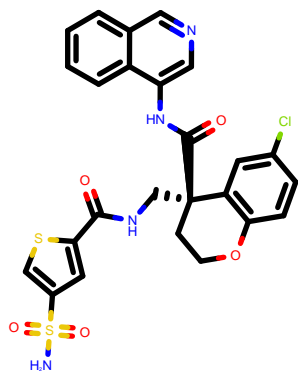
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(C)C(=O)N5CC[C@@H]6C(S(=O)(=O)N)C6=O

RUN: RUN2567

DDG (kcal/mol): -0.39

dDDG (kcal/mol): 0.25

EN300-98099_2_1



CID: EN300-98099_2_1

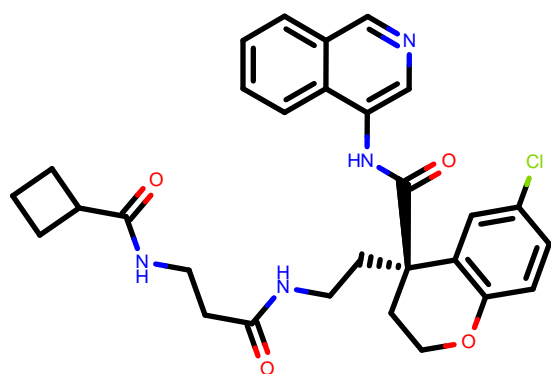
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4cc3cc(c4)C(C)C(=O)N5CC[C@@H]6C(S(=O)(=O)N)C6=O

RUN: RUN9350

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

EN300-62449_3_1



CID: EN300-62449_3_1

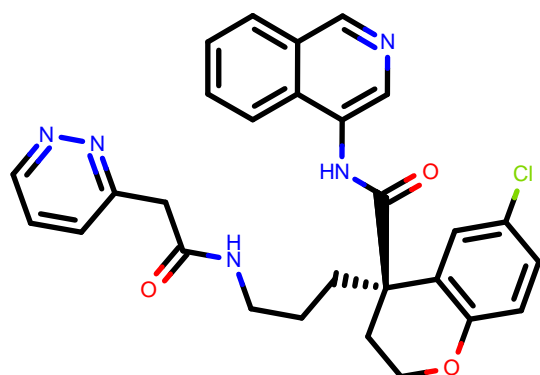
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCNC(=O)C5CCC5

RUN: RUN14630

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.33

EN300-7456948_4_1



CID: EN300-7456948_4_1

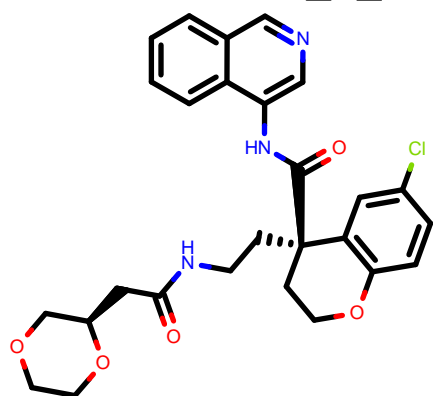
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccnnc5

RUN: RUN12185

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.28

EN300-731622_3_2



CID: EN300-731622_3_2

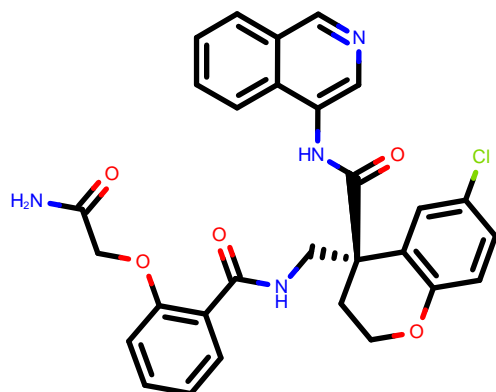
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5OCOC5

RUN: RUN11966

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

EN300-15368_2_1



CID: EN300-15368_2_1

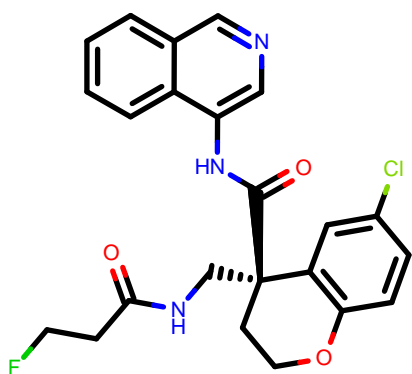
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COc5ccccc5CC(=O)N

RUN: RUN5991

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.33

EN300-97758_2_1



CID: EN300-97758_2_1

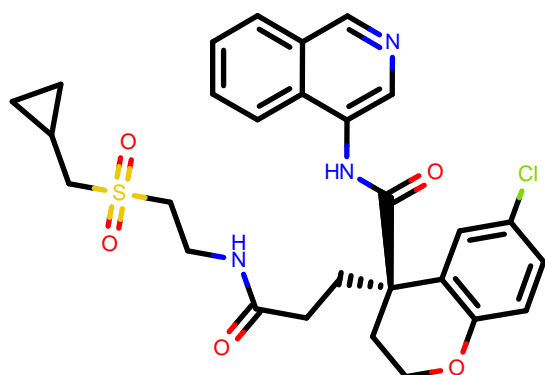
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCF

RUN: RUN1907

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.19

EN300-110245_2_1



CID: EN300-110245_2_1

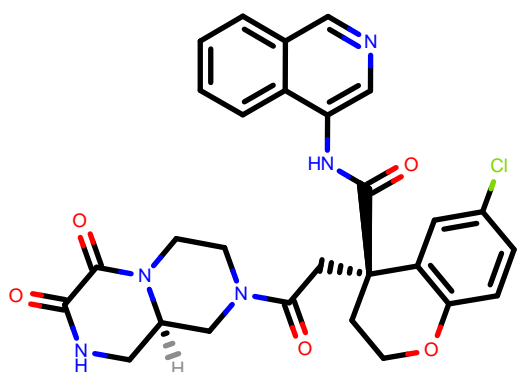
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCS(=O)(=O)CC5CC5

RUN: RUN5820

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.65

EN300-100768_1_2



CID: EN300-100768_1_2

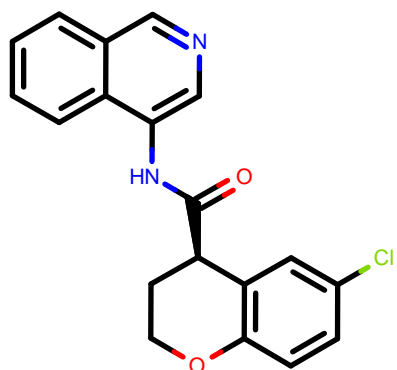
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C(=O)N5CCN6C@@H(C)C5)CNC1=OCC6=O

RUN: RUN10689

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.27

MAT-POS-f7918075-1_1



CID: MAT-POS-f7918075-1_1

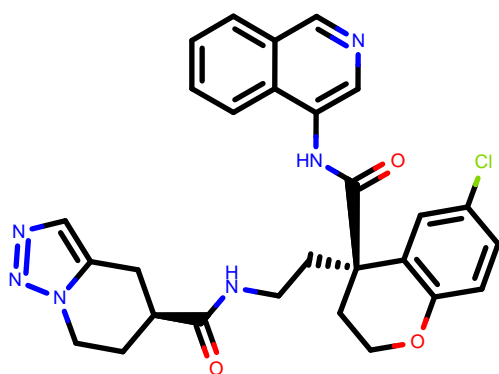
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C

RUN: RUN86

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.06

EN300-7430501_3_1



CID: EN300-7430501_3_1

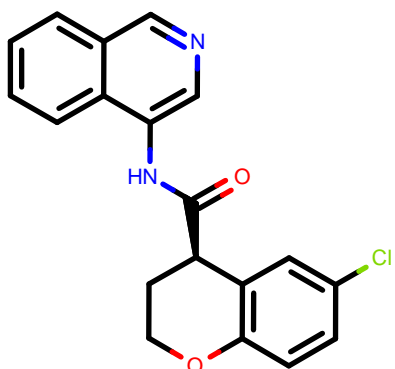
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCn6c(cnn6)C5

RUN: RUN15381

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.29

MAT-POS-f7918075-1_1



CID: MAT-POS-f7918075-1_1

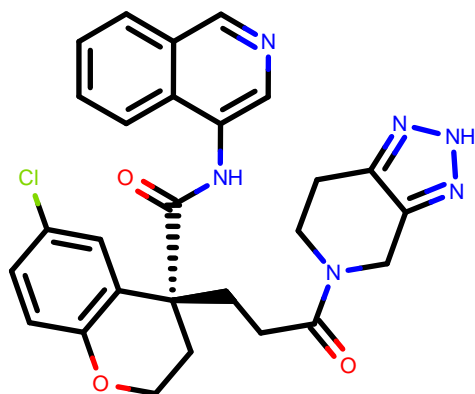
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)

RUN: RUN84

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.06

EN300-90293_2_1



CID: EN300-90293_2_1

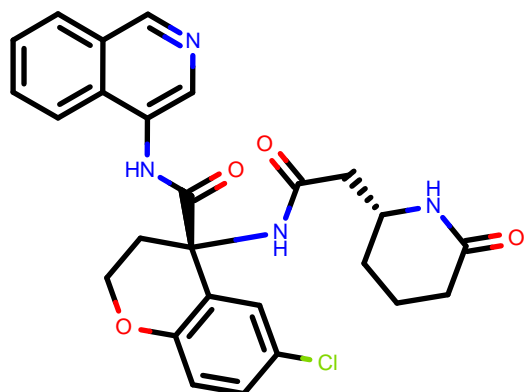
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCc6c(n[nH]n6)C5

RUN: RUN14709

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.24

EN300-210084_1_1



CID: EN300-210084_1_1

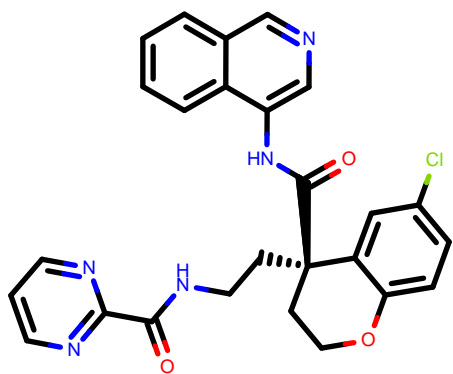
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCC(=O)N5

RUN: RUN7764

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.26

EN300-80230_3_1



CID: EN300-80230_3_1

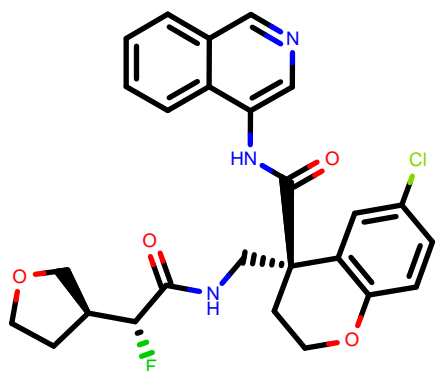
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5nccn5

RUN: RUN15424

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.19

EN300-783124_2_3



CID: EN300-783124_2_3

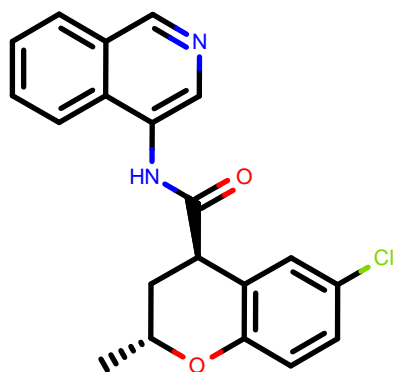
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]H[C@@H]5CCOC5F

RUN: RUN2871

DDG (kcal/mol): -0.38

dDDG (kcal/mol): 0.25

ALP-POS-d3acb8cc-1_1



CID: ALP-POS-d3acb8cc-1_1

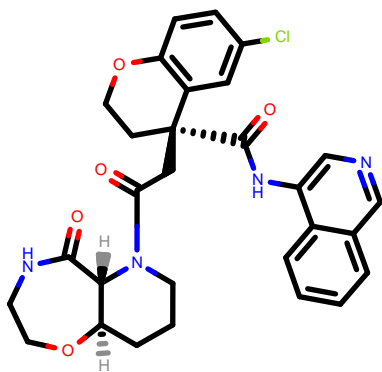
SMILES: C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4

RUN: RUN44

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.07

EN300-364612_1_3



CID: EN300-364612_1_3

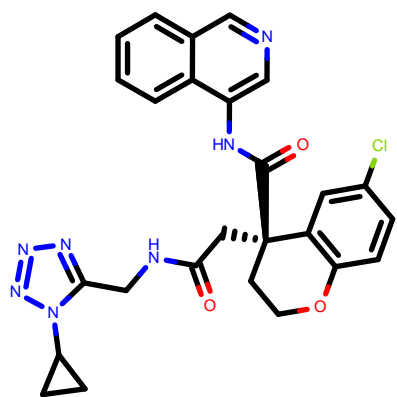
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]6[C@@H]5C1=CNCCO6

RUN: RUN9092

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.24

EN300-93491_1_1



CID: EN300-93491_1_1

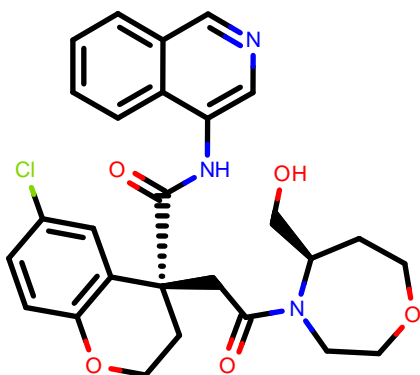
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5nnn5C6CC6

RUN: RUN4313

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.28

EN300-6732376_1_1



CID: EN300-6732376_1_1

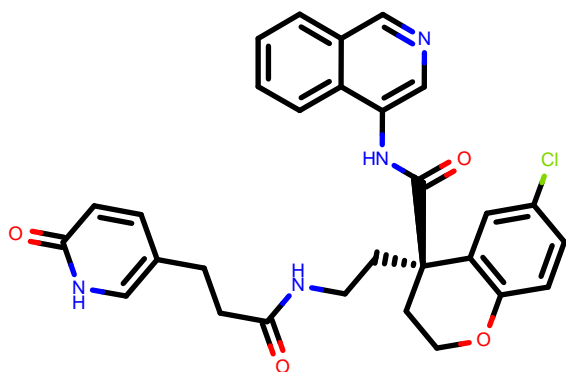
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5COCOC5[C@@]H5CO

RUN: RUN5217

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.28

EN300-187385_3_1



CID: EN300-187385_3_1

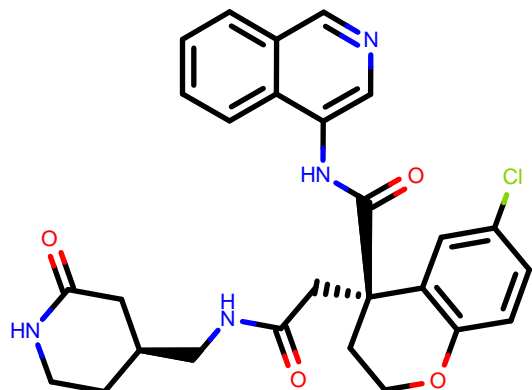
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5ccc(=O)[nH]5

RUN: RUN14414

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.28

EN300-59733_1_1



CID: EN300-59733_1_1

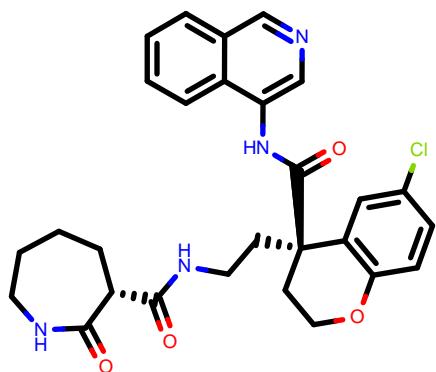
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCNC(=O)C5

RUN: RUN10143

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.24

EN300-6737762_3_2



CID: EN300-6737762_3_2

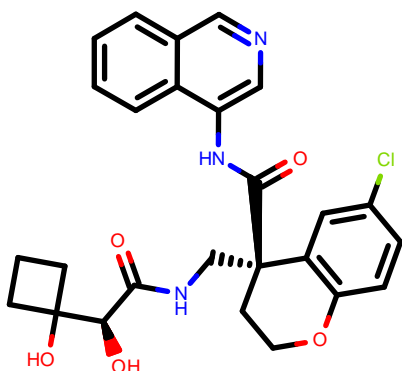
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCCNC5=O

RUN: RUN4389

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.25

EN300-1073320_2_2



CID: EN300-1073320_2_2

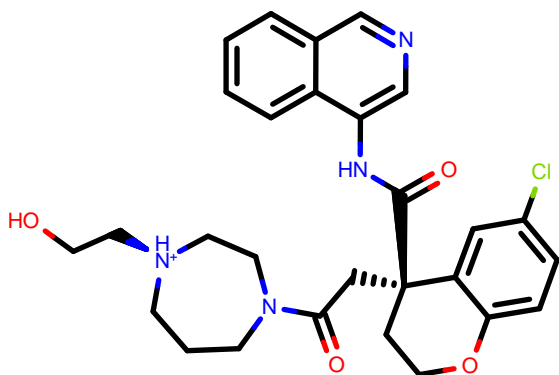
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5(CCC5)O)O

RUN: RUN1460

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.22

EN300-69993_1_2



CID: EN300-69993_1_2

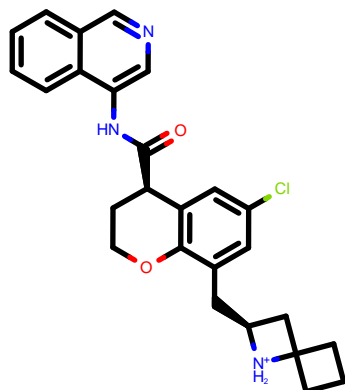
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)CCO

RUN: RUN11625

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.42

DAR-DIA-23e5a6a0-7_1



CID: DAR-DIA-23e5a6a0-7_1

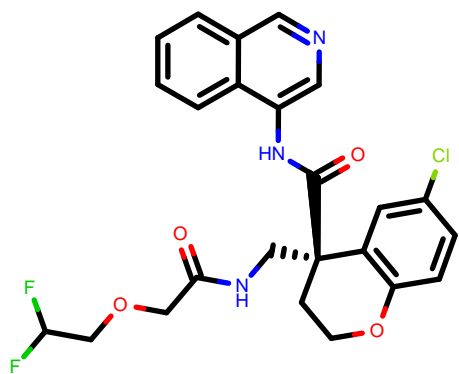
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[NH2+](CC5)CC5Cl

RUN: RUN188

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.29

EN300-315792_2_1



CID: EN300-315792_2_1

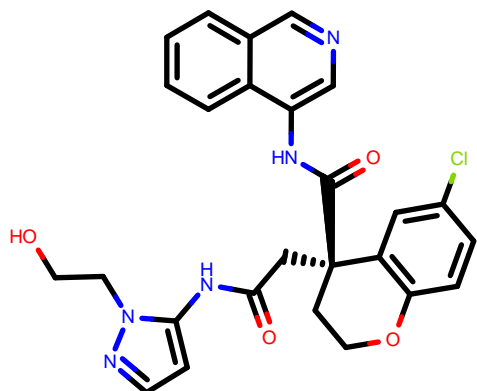
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COCC(F)F

RUN: RUN3551

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.22

EN300-134536_1_1



CID: EN300-134536_1_1

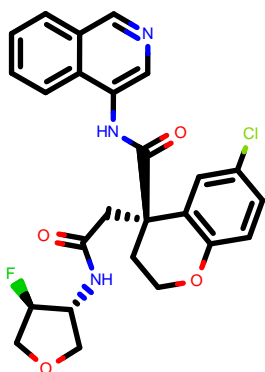
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5cnnc5CO

RUN: RUN5341

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.23

EN300-1657635_1_1



CID: EN300-1657635_1_1

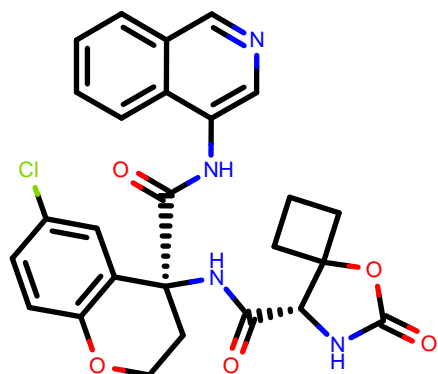
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5COC[C@H]5F

RUN: RUN11815

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.22

EN300-7432415_1_1



CID: EN300-7432415_1_1

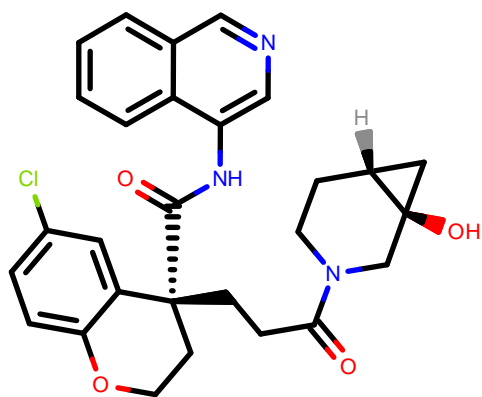
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5C6(CCC6)OC(=O)N5

RUN: RUN7332

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.20

EN300-1267093_2_1



CID: EN300-1267093_2_1

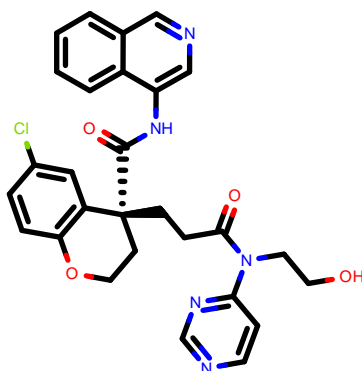
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H]3C=C5O

RUN: RUN9103

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.26

EN300-256174_2_1



CID: EN300-256174_2_1

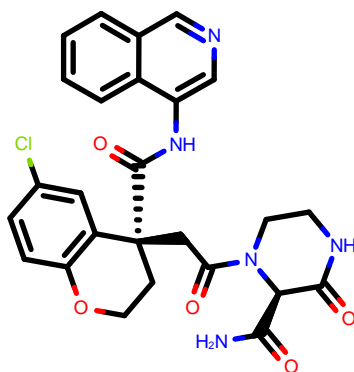
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(CCO)c5ccnnc5

RUN: RUN5252

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.33

EN300-7473032_1_2



CID: EN300-7473032_1_2

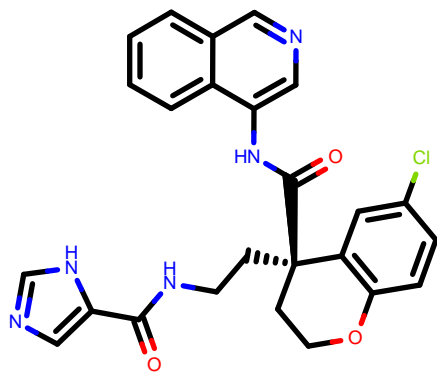
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)[C@H]5C(=O)N

RUN: RUN11857

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.26

EN300-62808_3_1



CID: EN300-62808_3_1

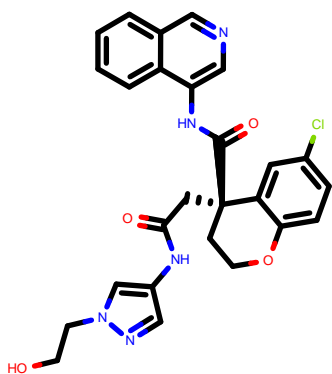
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cnc[nH]5

RUN: RUN15246

DDG (kcal/mol): -0.37

dDDG (kcal/mol): 0.21

EN300-52645_1_1



CID: EN300-52645_1_1

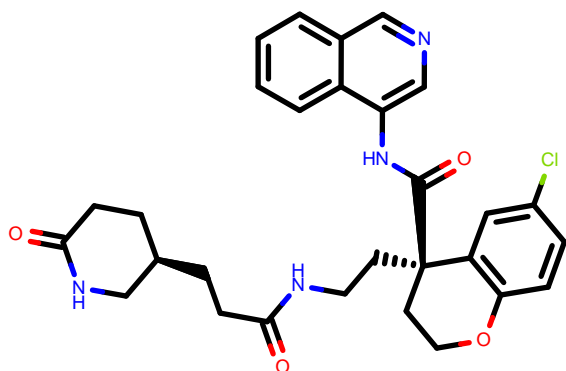
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5enn(c5)CCO

RUN: RUN14234

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.20

EN300-1215738_3_1



CID: EN300-1215738_3_1

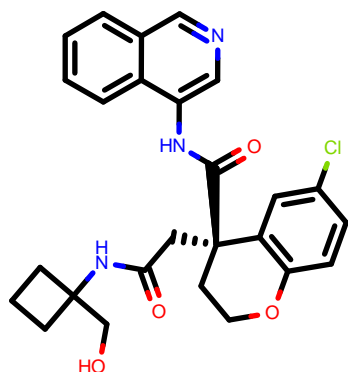
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[C@@]5C5CC(=O)NC5

RUN: RUN9060

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.28

EN300-1723511_1_1



CID: EN300-1723511_1_1

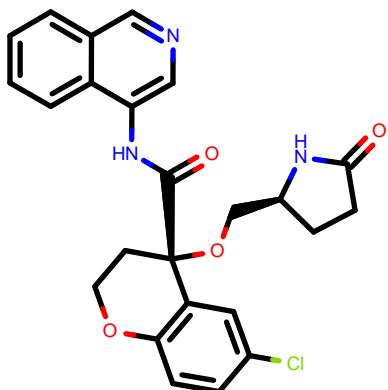
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(CCC5)CO

RUN: RUN13674

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.34

EN300-195756_1_2



CID: EN300-195756_1_2

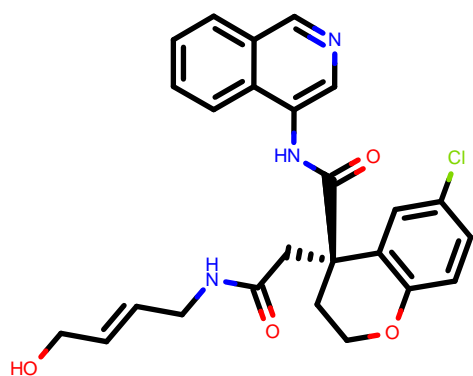
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@]5H5CC(=O)N5

RUN: RUN1956

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.28

EN300-157158_1_2



CID: EN300-157158_1_2

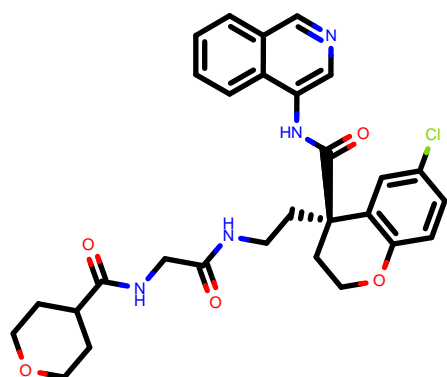
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC/C=C/O

RUN: RUN5185

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.18

EN300-74167_3_1



CID: EN300-74167_3_1

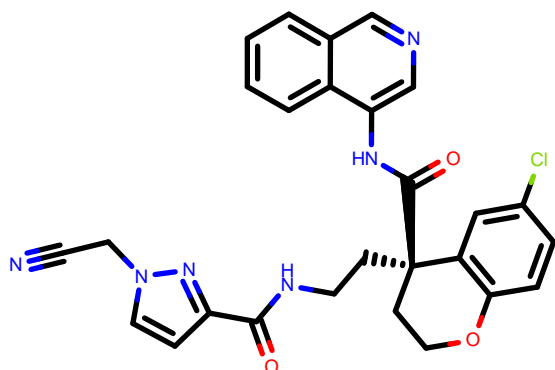
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CCOCC5

RUN: RUN11944

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.27

EN300-1251424_3_1



CID: EN300-1251424_3_1

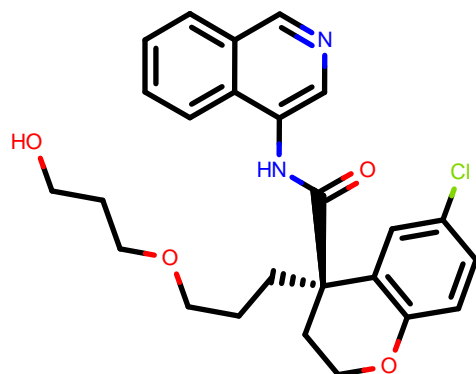
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccn(n5)C#N

RUN: RUN4833

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.20

EN300-221518_4_1



CID: EN300-221518_4_1

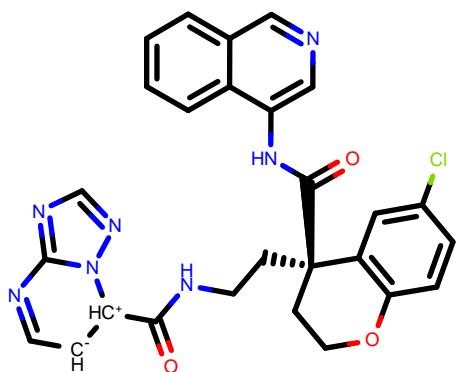
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN709

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.25

EN300-28262_3_1



CID: EN300-28262_3_1

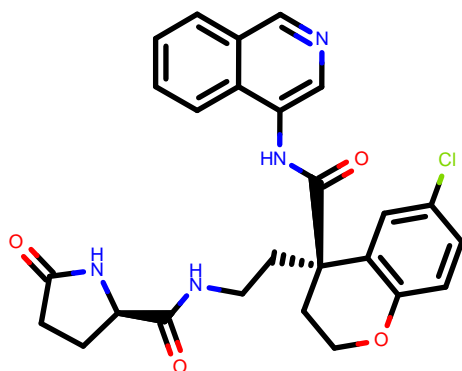
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccnc6r5nc6

RUN: RUN15086

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.26

EN300-54541_3_1



CID: EN300-54541_3_1

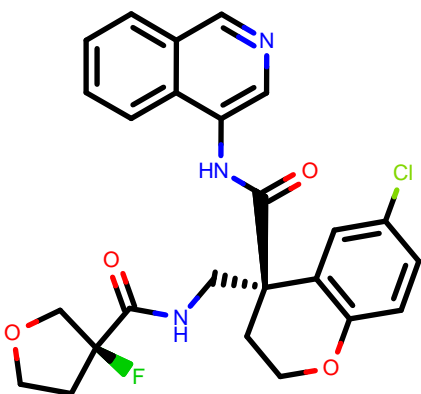
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CC(=O)N5

RUN: RUN865

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.23

EN300-188356_2_1



CID: EN300-188356_2_1

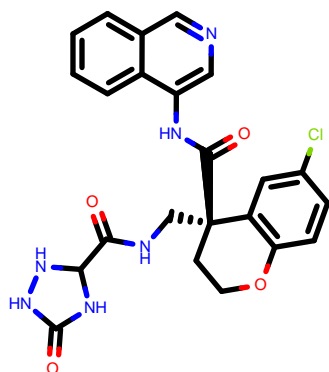
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCOc5)F

RUN: RUN1540

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.21

EN300-35843_2_1



CID: EN300-35843_2_1

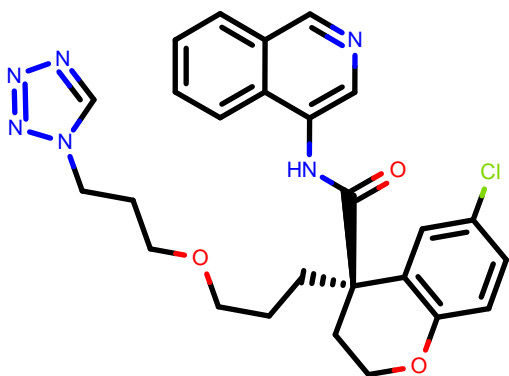
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5[nH]c(=O)[nH]n5

RUN: RUN8545

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.22

EN300-1696962_4_1



CID: EN300-1696962_4_1

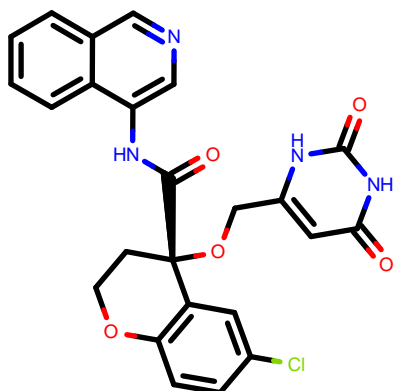
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCn5cnnn5

RUN: RUN829

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.25

EN300-11300_1_1



CID: EN300-11300_1_1

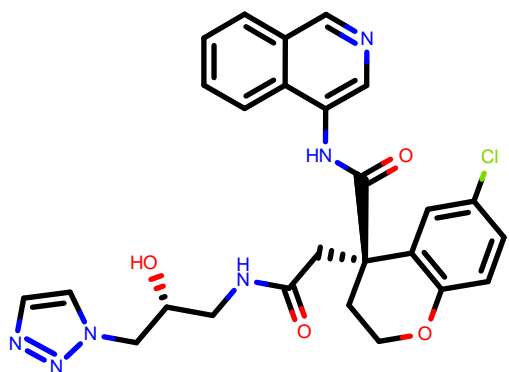
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cc(=O)[nH]c(=O)[nH]5

RUN: RUN2368

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.23

EN300-251752_1_1



CID: EN300-251752_1_1

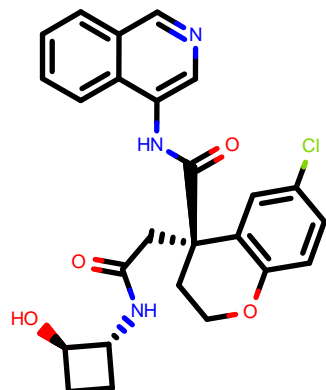
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5Cn5cnn5O

RUN: RUN4225

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.31

EN300-129424_1_1



CID: EN300-129424_1_1

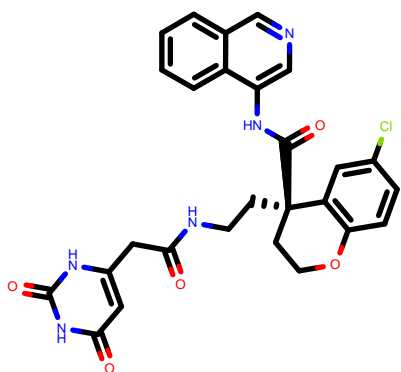
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CC[C@H]5O

RUN: RUN1711

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.21

EN300-11441_3_1



CID: EN300-11441_3_1

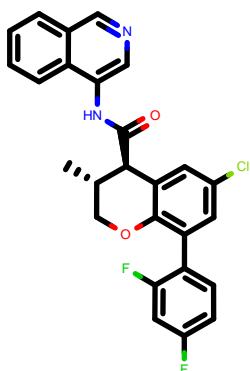
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5ccc(O)[nH]c1=O[nH]5

RUN: RUN15101

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.28

DAR-DIA-0d514e7d-12_1



CID: DAR-DIA-0d514e7d-12_1

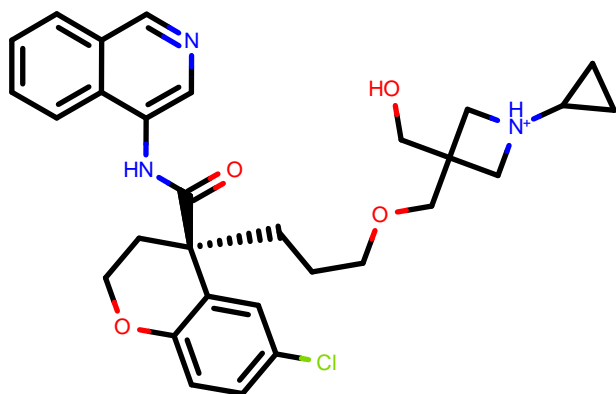
SMILES: C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3ccc4c3ccc4)C)c5ccc(cc5)F

RUN: RUN224

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.20

EN300-6735421_4_1



CID: EN300-6735421_4_1

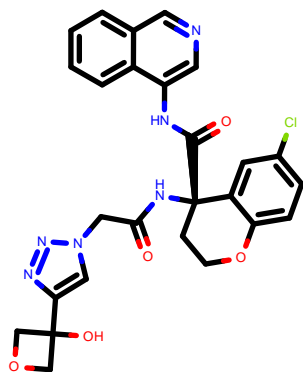
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC5(C)[NH+](C5)C6CC6)CO

RUN: RUN1842

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.26

EN300-7445540_1_1



CID: EN300-7445540_1_1

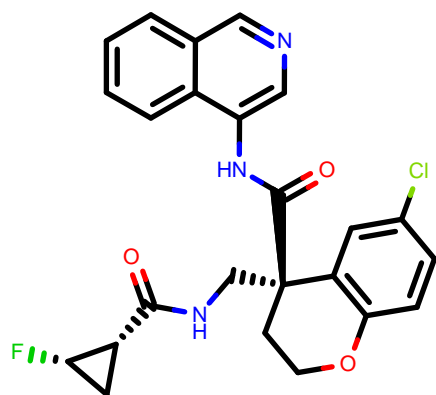
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5cc(nn5)C6(COC6)O

RUN: RUN9237

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.26

EN300-4698402_2_1



CID: EN300-4698402_2_1

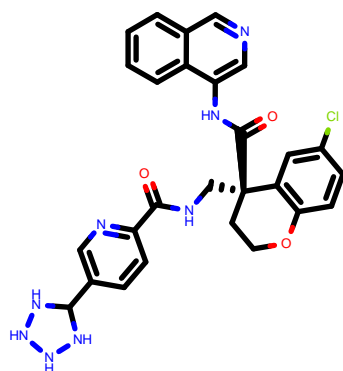
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C[C@@H]5F

RUN: RUN4955

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.20

EN300-306105_2_1



CID: EN300-306105_2_1

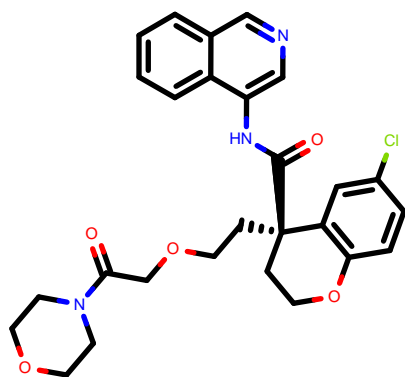
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5ccc(en5)n6[nH]n6

RUN: RUN9530

DDG (kcal/mol): -0.36

dDDG (kcal/mol): 0.28

EN300-1241327_3_1



CID: EN300-1241327_3_1

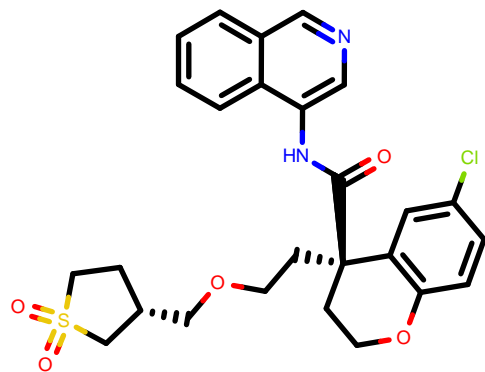
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOCC(=O)N5CCOCC5

RUN: RUN2254

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.25

EN300-1448603_3_2



CID: EN300-1448603_3_2

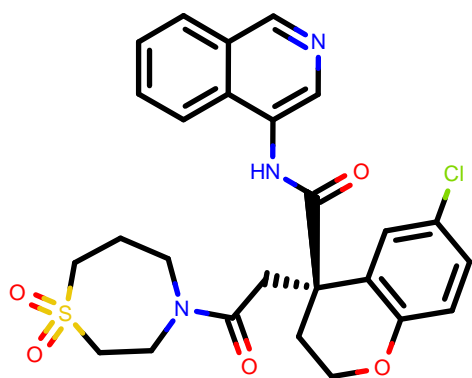
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC(=O)N5SCC(=O)C5

RUN: RUN2166

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.27

EN300-73620_1_1



CID: EN300-73620_1_1

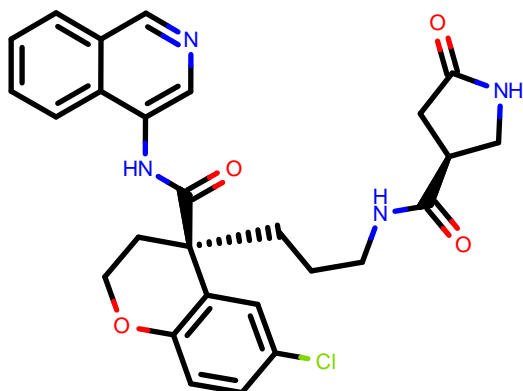
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCS(=O)(=O)CC5

RUN: RUN12542

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.29

EN300-59487_4_2



CID: EN300-59487_4_2

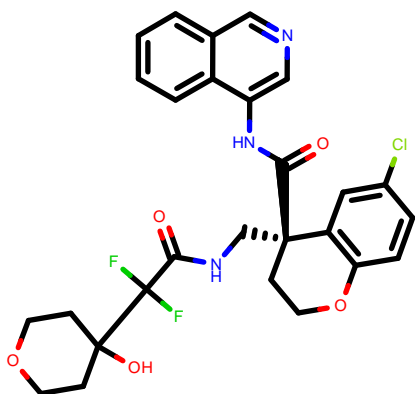
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)N5

RUN: RUN11979

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.22

EN300-706065_2_1



CID: EN300-706065_2_1

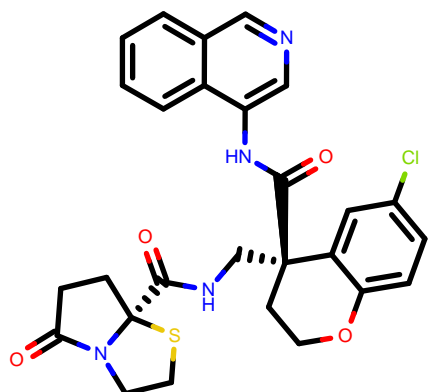
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(C5(COCCO5)O)(F)F

RUN: RUN5063

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.29

EN300-10334_2_1



CID: EN300-10334_2_1

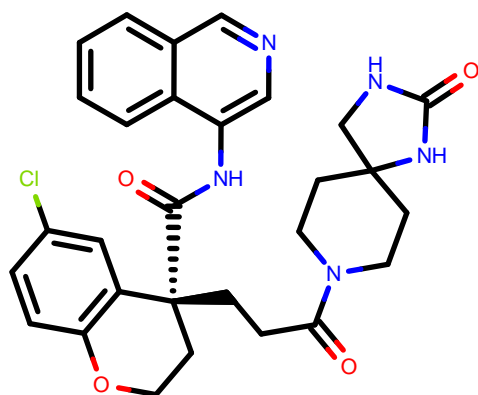
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]56CCCC(=O)N5CCS6

RUN: RUN7693

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.30

EN300-6745712_2_1



CID: EN300-6745712_2_1

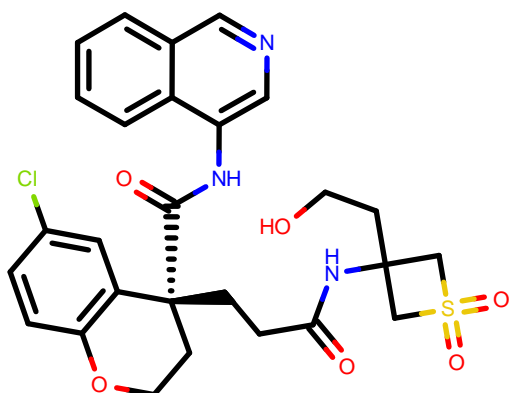
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCOC6(CCS)CNC(=O)N6

RUN: RUN14567

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.25

EN300-6487630_2_1



CID: EN300-6487630_2_1

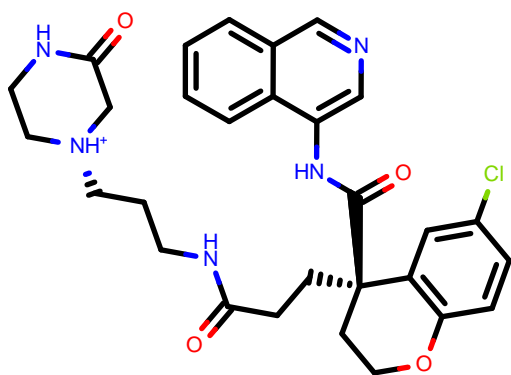
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC5(CS(=O)(=O)C5)CCO

RUN: RUN600

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.37

EN300-81528_2_2



CID: EN300-81528_2_2

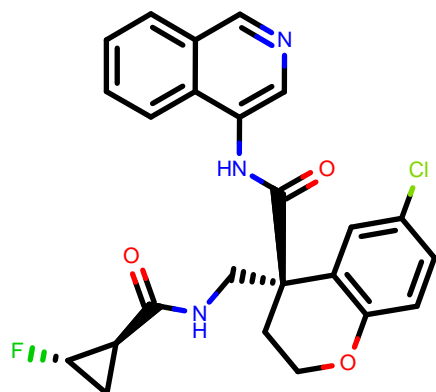
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCN5C(=O)N5

RUN: RUN13125

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.39

EN300-6953121_2_1



CID: EN300-6953121_2_1

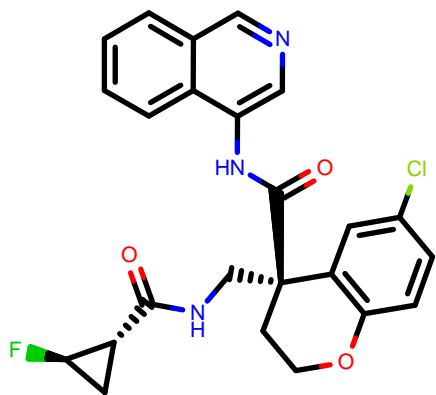
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5C[C@@H]5F

RUN: RUN5291

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.20

EN300-1654606_2_1



CID: EN300-1654606_2_1

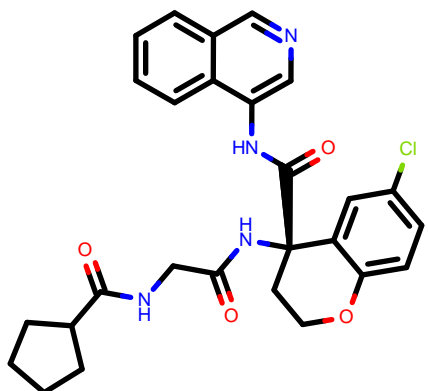
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@H]5F

RUN: RUN5787

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.18

EN300-36845_1_1



CID: EN300-36845_1_1

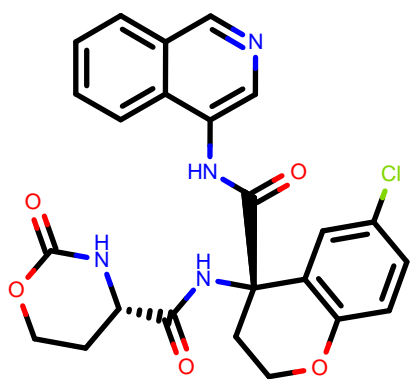
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)C5CCCC5

RUN: RUN9125

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.25

EN300-249804_1_1



CID: EN300-249804_1_1

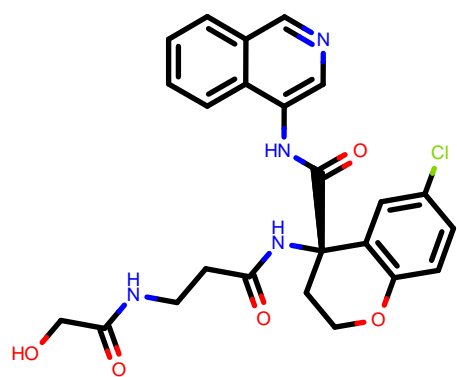
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC(=O)N5

RUN: RUN6269

DDG (kcal/mol): -0.35

dDDG (kcal/mol): 0.21

EN300-383904_1_1



CID: EN300-383904_1_1

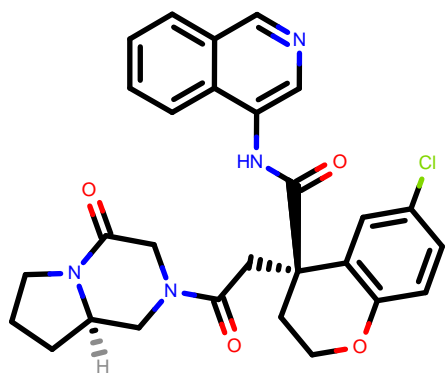
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCNC(=O)CO

RUN: RUN2782

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.27

EN300-1696143_1_1



CID: EN300-1696143_1_1

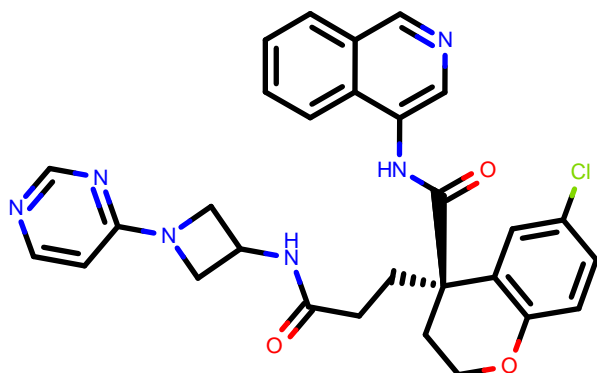
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CCCCN6C(=O)C5

RUN: RUN6591

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.27

EN300-102871_2_1



CID: EN300-102871_2_1

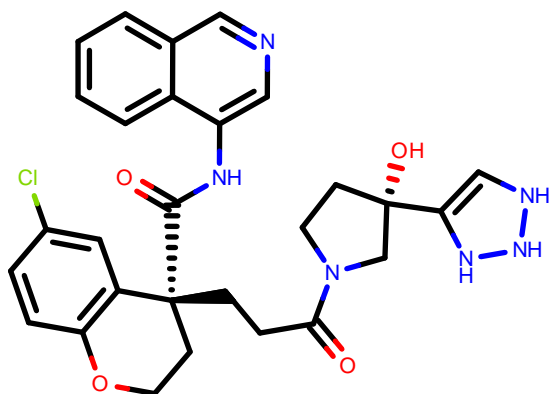
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5CN(C5)c6ccnnc6

RUN: RUN11981

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.21

EN300-221122_2_2



CID: EN300-221122_2_2

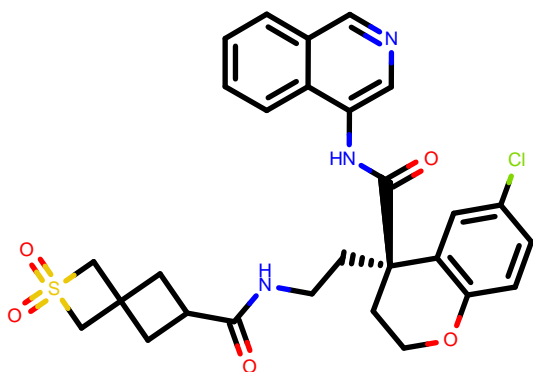
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@]5(C5)(c6cn[nH]n6)O

RUN: RUN13997

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.33

EN300-318305_3_1



CID: EN300-318305_3_1

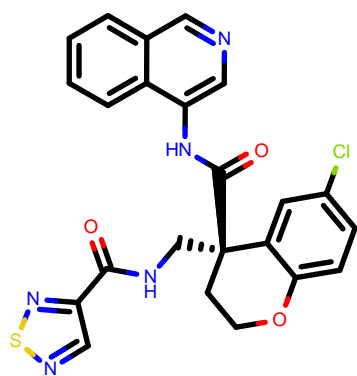
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC6(C5)CS(=O)(=O)C6

RUN: RUN15444

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.27

EN300-42270_2_1



CID: EN300-42270_2_1

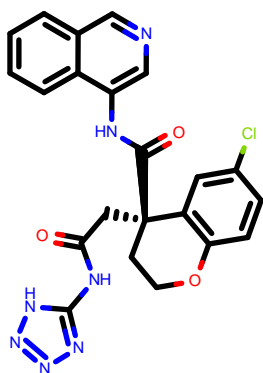
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnsn5

RUN: RUN2604

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.20

EN300-33999_1_1



CID: EN300-33999_1_1

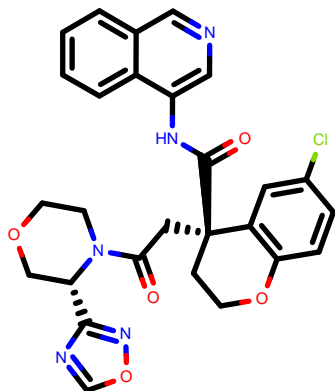
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5n[n-]nn5

RUN: RUN11986

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.19

EN300-122849_1_1



CID: EN300-122849_1_1

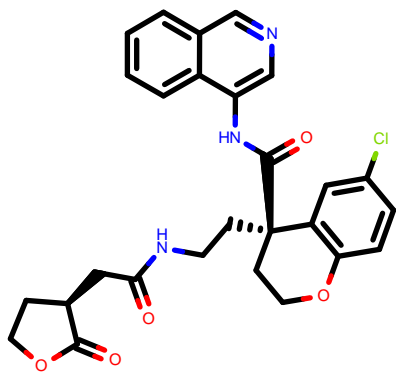
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5c6ncon6

RUN: RUN9753

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.20

EN300-1072972_3_2



CID: EN300-1072972_3_2

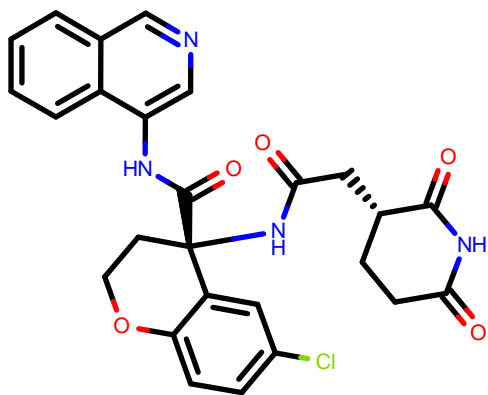
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5=O

RUN: RUN11244

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.28

EN300-3451857_1_1



CID: EN300-3451857_1_1

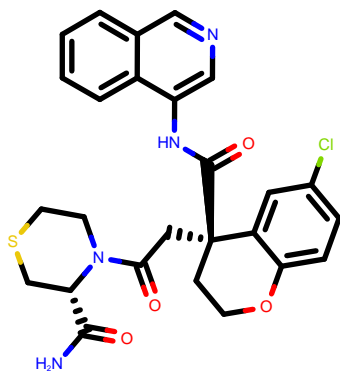
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)NC5=O

RUN: RUN331

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.28

EN300-122866_1_1



CID: EN300-122866_1_1

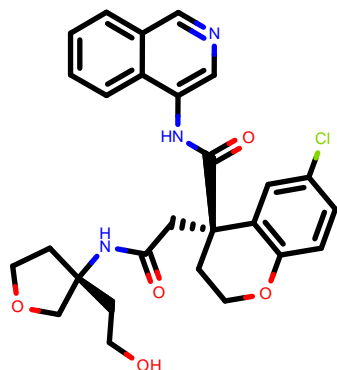
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCSC[C@@H]5C(=O)N

RUN: RUN12246

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.32

EN300-183736_1_1



CID: EN300-183736_1_1

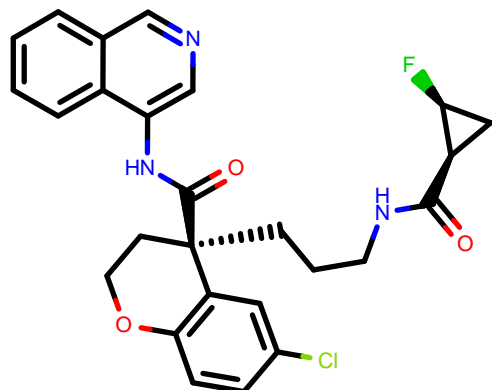
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CCO)C5=O

RUN: RUN13058

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.31

EN300-97300_4_3



CID: EN300-97300_4_3

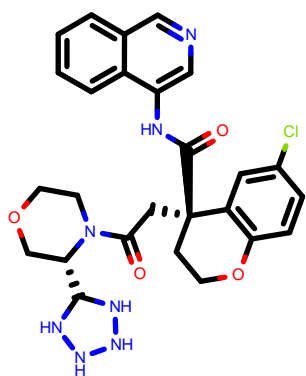
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(C)C[C@@H]5F

RUN: RUN12771

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.21

EN300-239825_1_1



CID: EN300-239825_1_1

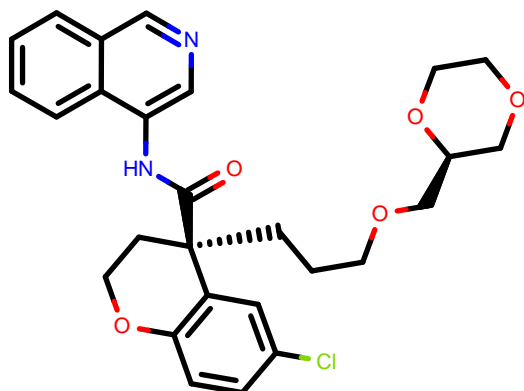
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5c6n[n-]n6

RUN: RUN10777

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.24

EN300-139167_4_2



CID: EN300-139167_4_2

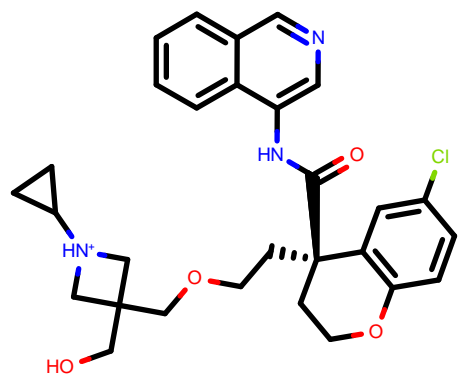
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCOC5

RUN: RUN1139

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.22

EN300-6735421_3_1



CID: EN300-6735421_3_1

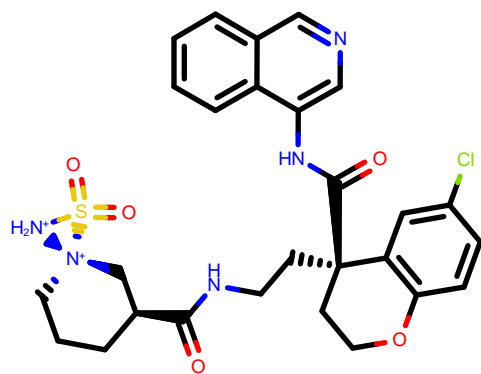
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5(C)[NH+](C5)C6CC6)CO

RUN: RUN250

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.37

EN300-219496_3_2



CID: EN300-219496_3_2

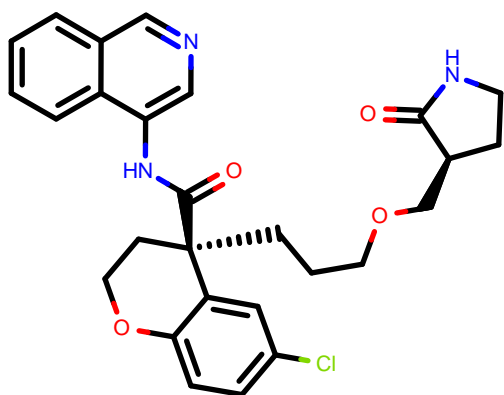
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)N[C@@H]5C(=O)N(S(=O)(=O)N)5

RUN: RUN13634

DDG (kcal/mol): -0.34

dDDG (kcal/mol): 0.71

EN300-246248_4_2



CID: EN300-246248_4_2

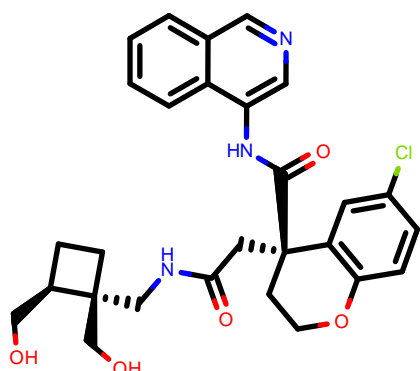
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O

RUN: RUN1411

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.27

EN300-1692359_1_4



CID: EN300-1692359_1_4

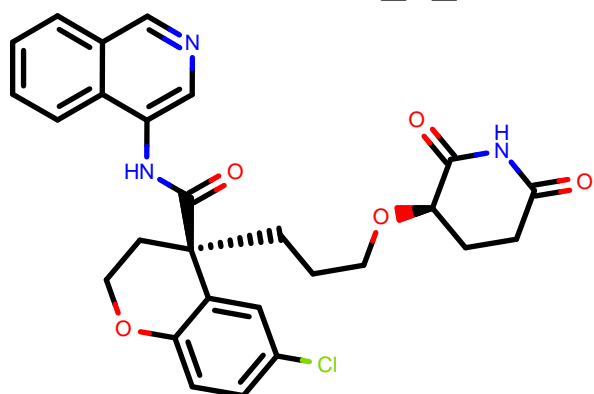
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CC[C@@H]5)CO

RUN: RUN10253

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.26

EN300-120920_4_2



CID: EN300-120920_4_2

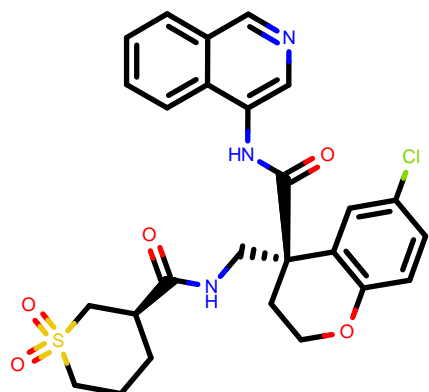
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CC(=O)NC5=O

RUN: RUN949

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.22

EN300-77778_2_2



CID: EN300-77778_2_2

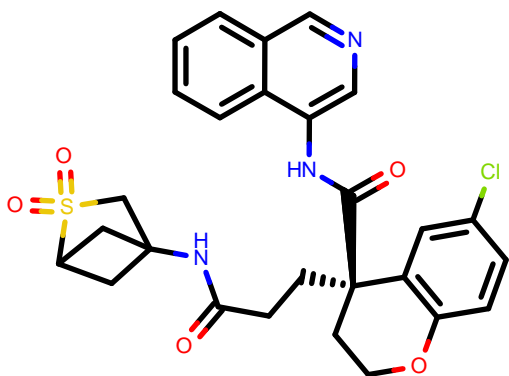
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCCS(=O)(=O)C5

RUN: RUN6003

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.26

EN300-7493768_2_1



CID: EN300-7493768_2_1

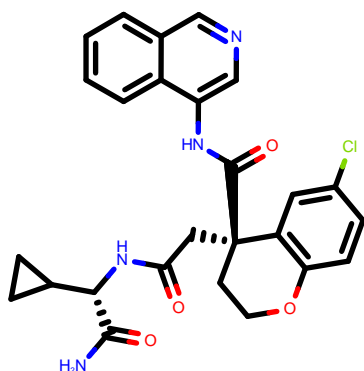
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC56CC(C5)S(=O)(=O)C6

RUN: RUN13733

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.25

EN300-1265434_1_2



CID: EN300-1265434_1_2

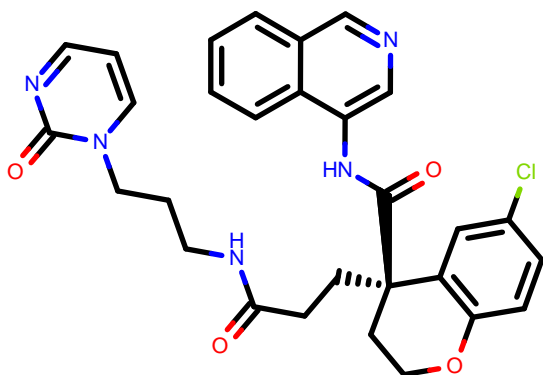
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@]4H(C5CC5)C1=O)N

RUN: RUN12656

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.23

EN300-191114_2_1



CID: EN300-191114_2_1

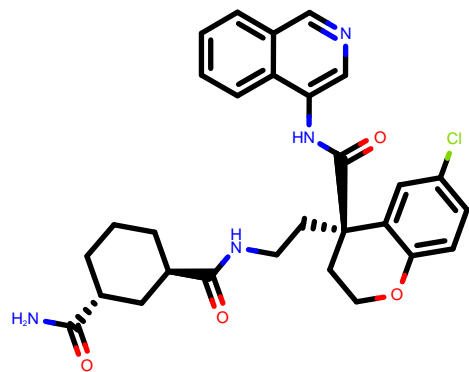
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5=CN=CC=C5=O

RUN: RUN11508

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.23

EN300-90142_3_3



CID: EN300-90142_3_3

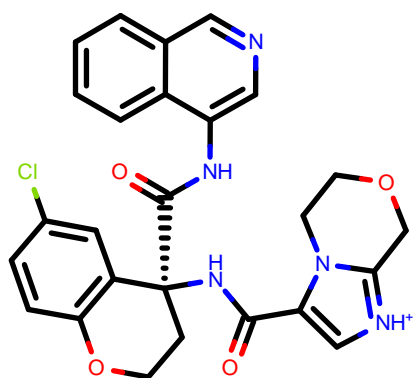
SMILES: c1ccc2c(c1)ncnc2NC1=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN1=O)[C@@]4H5CC[C@@]4H(C5)C1=O)N

RUN: RUN14352

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.25

EN300-307190_1_1



CID: EN300-307190_1_1

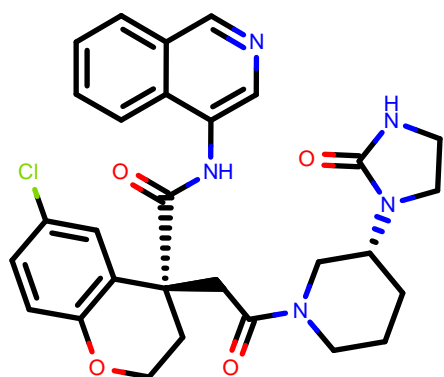
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH+]c6n5CCOC6

RUN: RUN4926

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.29

EN300-55087_1_2



CID: EN300-55087_1_2

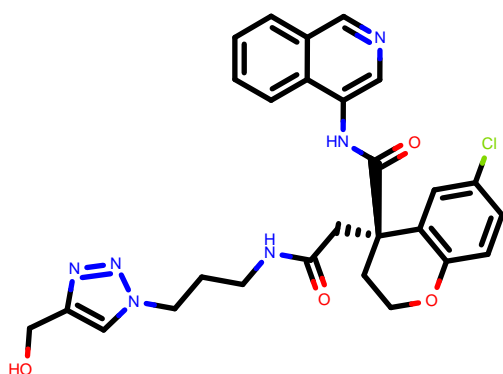
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H]5C6NCCN6=O

RUN: RUN3485

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.28

EN300-215607_1_1



CID: EN300-215607_1_1

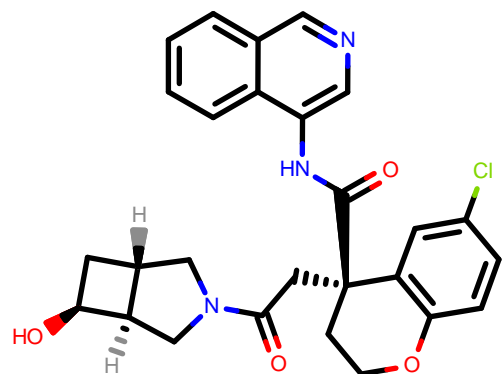
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCc5cc(nn5)CO

RUN: RUN6663

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.28

EN300-305294_1_1



CID: EN300-305294_1_1

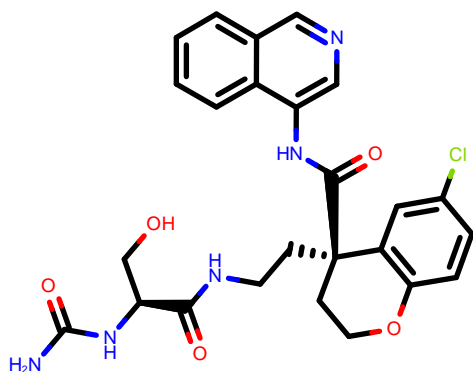
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H]5C[C@H]6C[C@H]6C5=O

RUN: RUN12612

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.21

EN300-10170_3_2



CID: EN300-10170_3_2

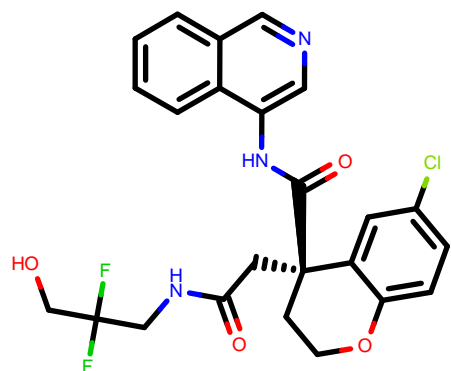
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H](CO)NC(=O)N

RUN: RUN13068

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.45

EN300-139846_1_1



CID: EN300-139846_1_1

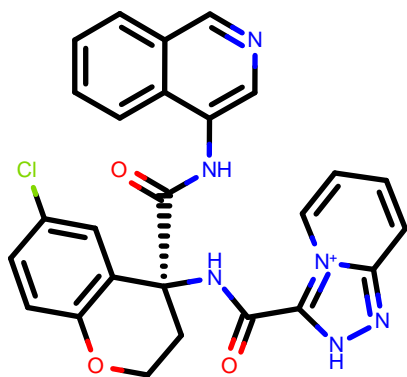
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC(CO)(F)F

RUN: RUN3313

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.27

EN300-6760451_1_1



CID: EN300-6760451_1_1

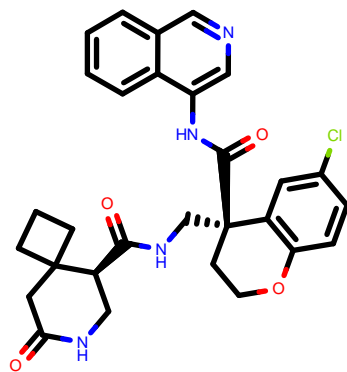
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5nncc6n5ccc6

RUN: RUN3446

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.18

EN300-1704404_2_2



CID: EN300-1704404_2_2

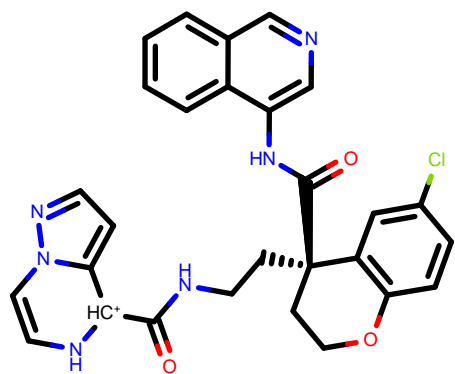
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CNC(=O)CC56CCC6

RUN: RUN3779

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.26

EN300-359842_3_1



CID: EN300-359842_3_1

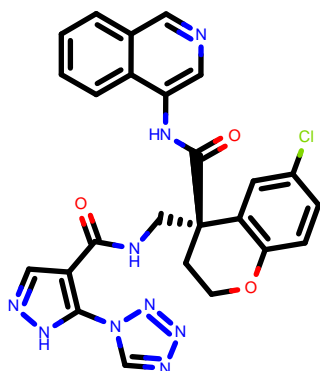
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5c6cn[nH]c56

RUN: RUN15049

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.23

EN300-7549839_2_1



CID: EN300-7549839_2_1

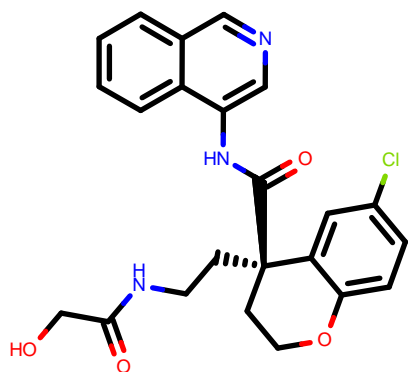
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]c5n6

RUN: RUN8858

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.24

EN300-19242_3_1



CID: EN300-19242_3_1

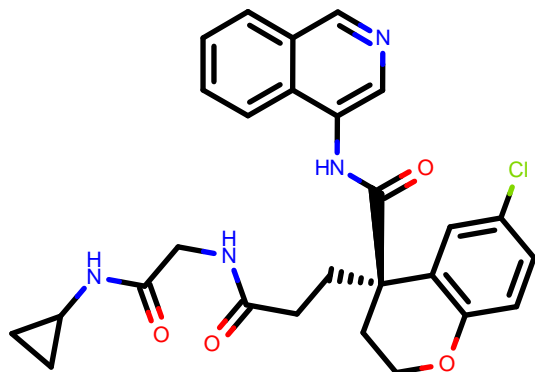
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO

RUN: RUN14578

DDG (kcal/mol): -0.33

dDDG (kcal/mol): 0.16

EN300-35428_2_1



CID: EN300-35428_2_1

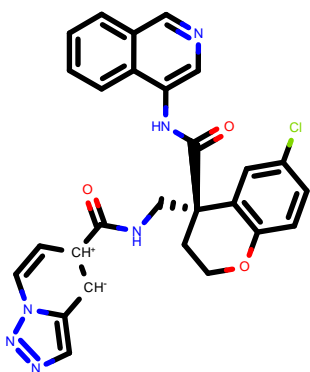
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(=O)NC5CC5

RUN: RUN5220

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.23

EN300-6743433_2_1



CID: EN300-6743433_2_1

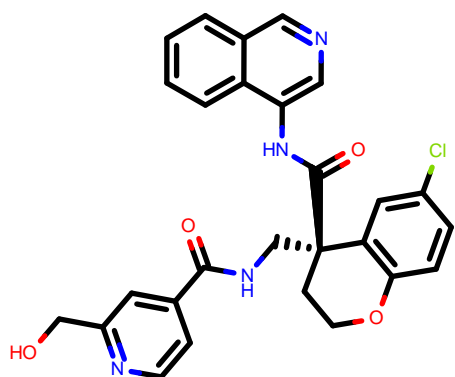
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn6c(c5)cn6

RUN: RUN9266

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.25

EN300-396748_2_1



CID: EN300-396748_2_1

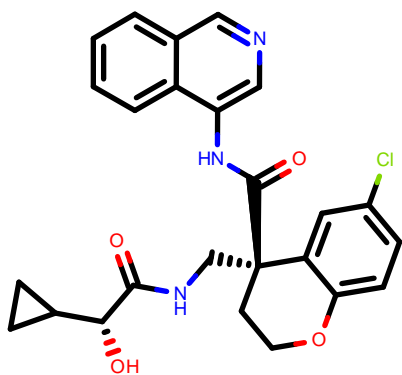
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccn(c5)CO

RUN: RUN8842

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.25

EN300-72211_2_1



CID: EN300-72211_2_1

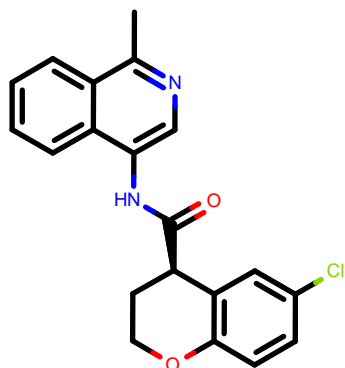
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4(C)C5C5O

RUN: RUN4683

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.26

ADA-UCB-dc2b944c-12_1



CID: ADA-UCB-dc2b944c-12_1

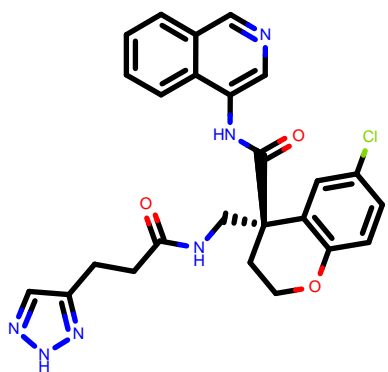
SMILES: Cc1c2ccccc2c(c1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4(C)C5C5O

RUN: RUN46

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.07

EN300-244947_2_1



CID: EN300-244947_2_1

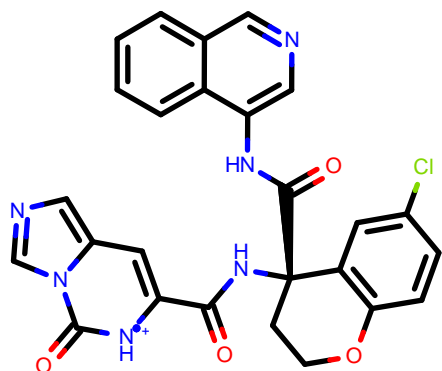
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CCc5cn[nH]5

RUN: RUN2332

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.26

EN300-7443518_1_1



CID: EN300-7443518_1_1

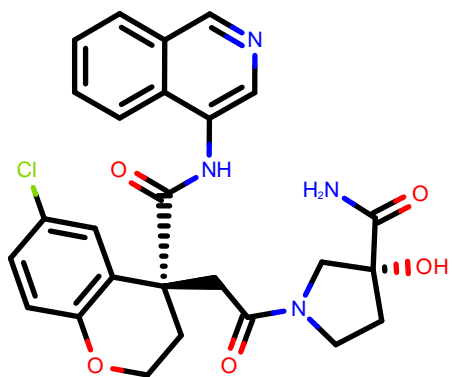
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c6ncn[nH]5

RUN: RUN4062

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.22

EN300-172481_1_1



CID: EN300-172481_1_1

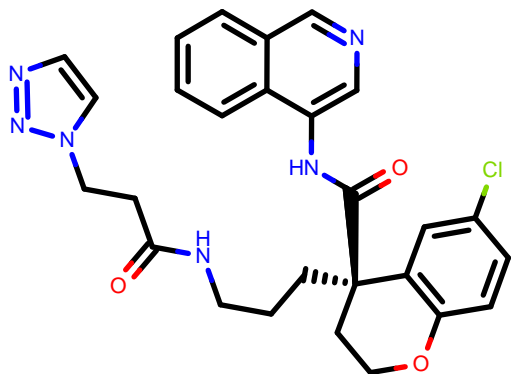
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@]5(C)C(=O)N

RUN: RUN7679

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.35

EN300-28871_4_1



CID: EN300-28871_4_1

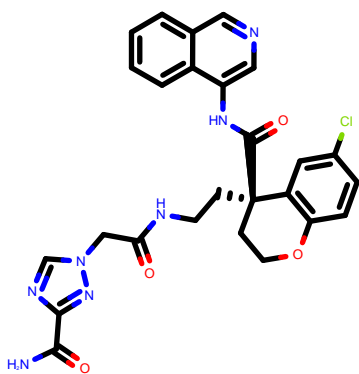
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5cnn5

RUN: RUN10582

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.24

EN300-262604_3_1



CID: EN300-262604_3_1

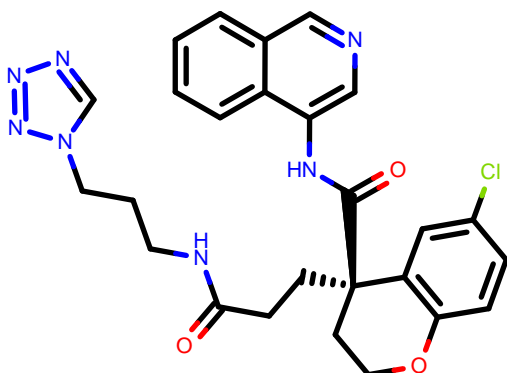
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5ncnc5C(=O)N

RUN: RUN10851

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.25

EN300-1698571_2_1



CID: EN300-1698571_2_1

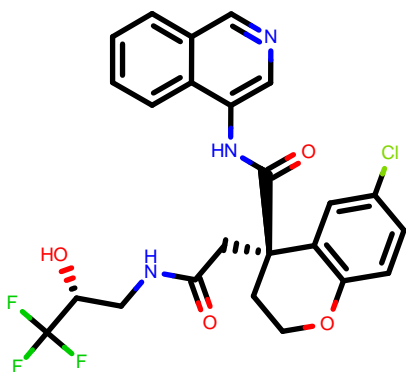
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCCn5nnn5

RUN: RUN9051

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.30

EN300-51459_1_2



CID: EN300-51459_1_2

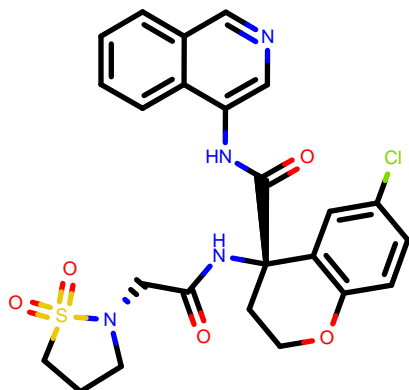
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@H](C(F)(F)F)O

RUN: RUN11811

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.43

EN300-43206_1_1



CID: EN300-43206_1_1

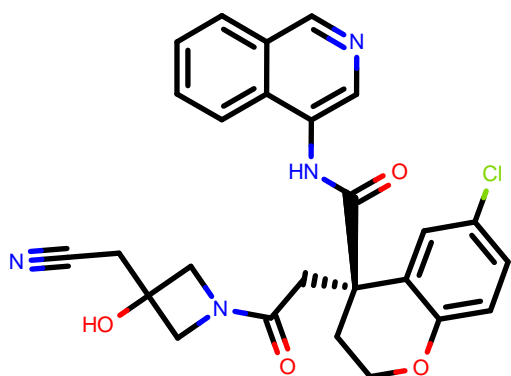
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C[N@]5CCCC5(=O)=O

RUN: RUN3826

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.36

EN300-155823_1_1



CID: EN300-155823_1_1

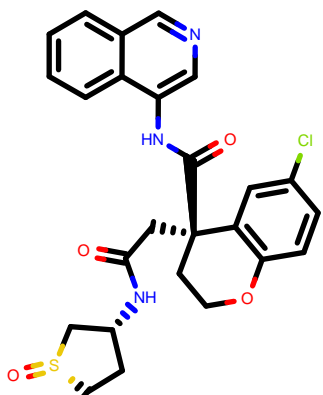
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CC#N)O

RUN: RUN11661

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.23

EN300-93574_1_1



CID: EN300-93574_1_1

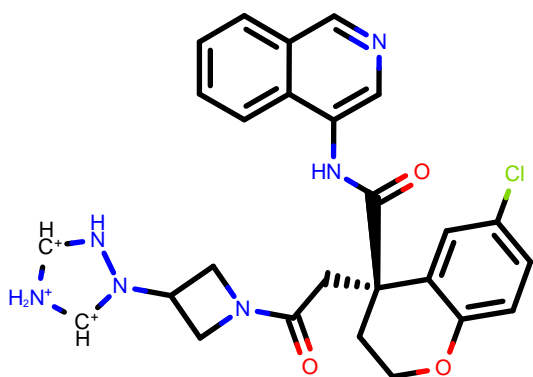
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H5CC(S)H(=O)C5

RUN: RUN6743

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.22

EN300-66518_1_1



CID: EN300-66518_1_1

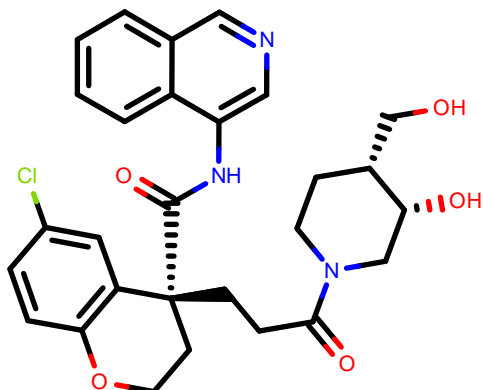
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)n6ncn6

RUN: RUN3833

DDG (kcal/mol): -0.32

dDDG (kcal/mol): 0.18

EN300-95639_2_3



CID: EN300-95639_2_3

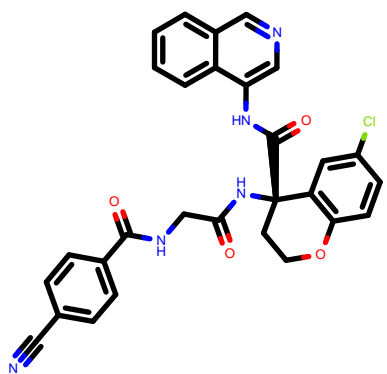
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C)C@H(C)C@H(C5)O)CO

RUN: RUN3380

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.27

EN300-65853_1_1



CID: EN300-65853_1_1

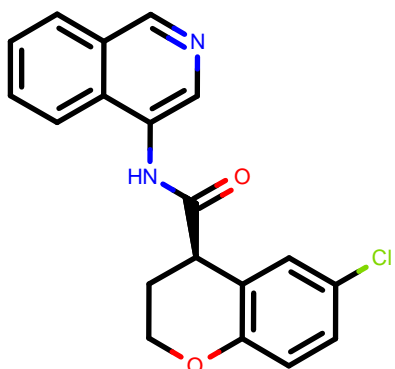
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5ccc(cc5)C#N

RUN: RUN9862

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

MAT-POS-f7918075-1_1



CID: MAT-POS-f7918075-1_1

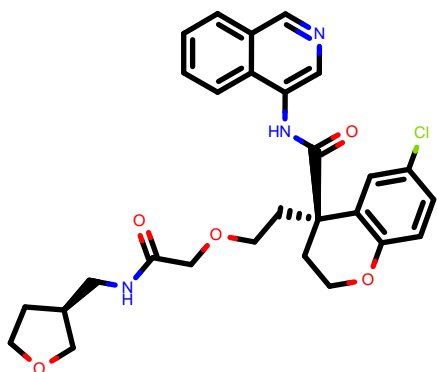
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3C@H3CCOc4c3cc(cc4)Cl

RUN: RUN85

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.06

EN300-46832_3_1



CID: EN300-46832_3_1

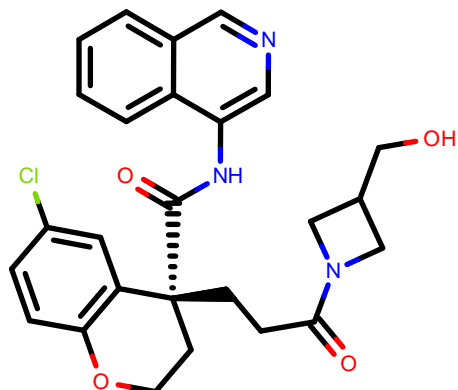
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@@]5CCOC5

RUN: RUN274

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.34

EN300-7370063_2_1



CID: EN300-7370063_2_1

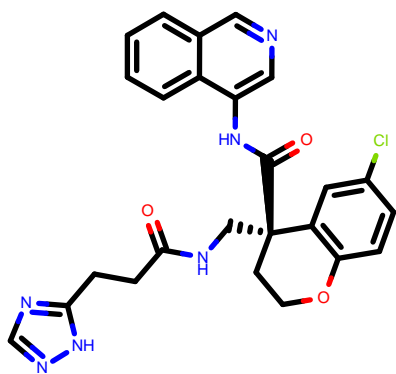
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(C5)C5O

RUN: RUN13447

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

EN300-101197_2_1



CID: EN300-101197_2_1

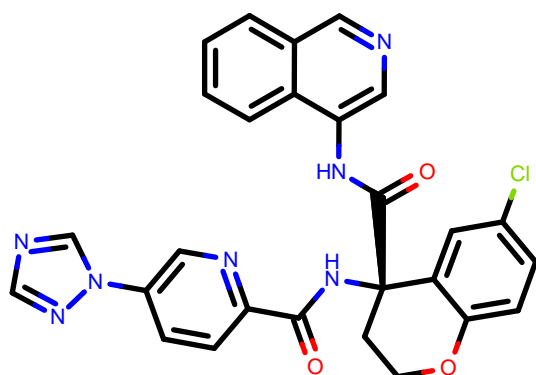
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)CCc5[nH]n5

RUN: RUN1236

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

EN300-195855_1_1



CID: EN300-195855_1_1

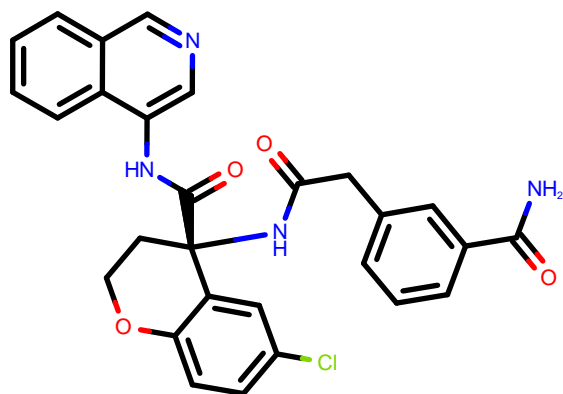
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cccn5n6cn6

RUN: RUN9880

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.19

EN300-1179673_1_1



CID: EN300-1179673_1_1

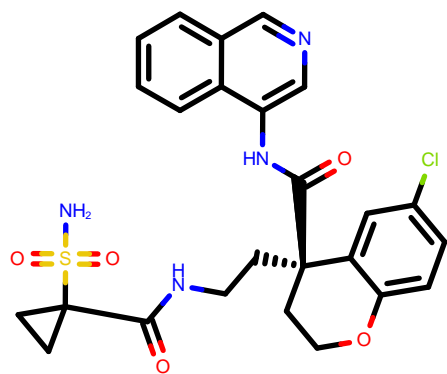
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5ccc(c5)C(=O)N

RUN: RUN9841

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.27

EN300-223741_3_1



CID: EN300-223741_3_1

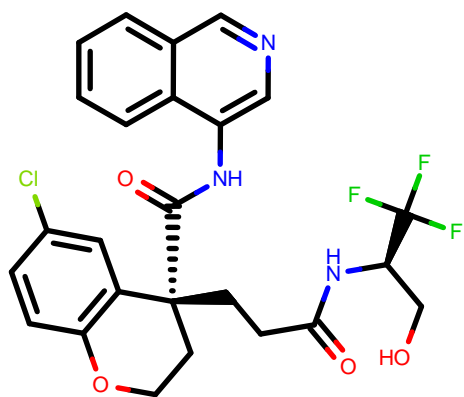
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5(CS(=O)C(=O)N

RUN: RUN13374

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.27

EN300-139403_2_1



CID: EN300-139403_2_1

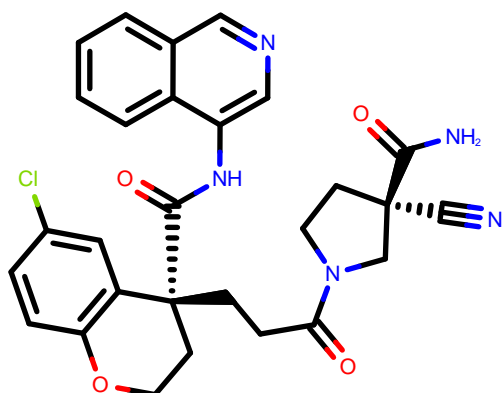
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)C(F)(F)F

RUN: RUN7018

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.33

EN300-1608992_2_1



CID: EN300-1608992_2_1

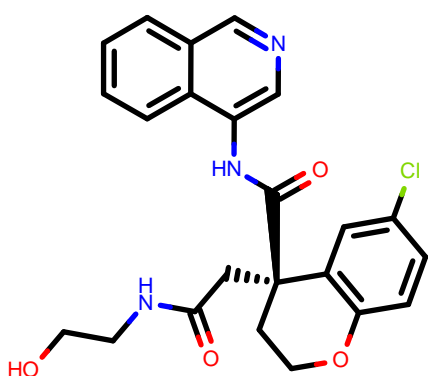
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(=O)NCC#N

RUN: RUN14075

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.27

EN300-19392_1_1



CID: EN300-19392_1_1

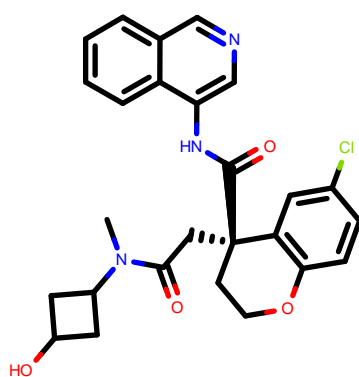
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H](C)C(CO)NCCO

RUN: RUN9825

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.28

EN300-93074_1_1



CID: EN300-93074_1_1

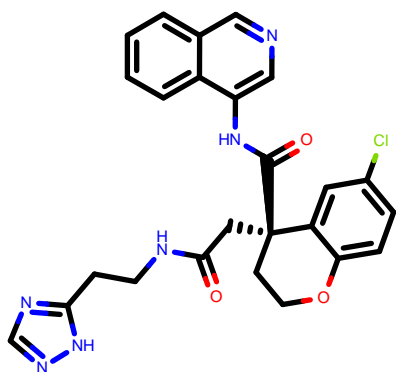
SMILES: CN(C(=O)C[C@@H](c2c(ccc(c2)Cl)OCC1)C(=O)Nc3c4c(nc3)cccc4)[C@@H]5C[C@@H](C5)O

RUN: RUN5873

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.30

EN300-227021_1_1



CID: EN300-227021_1_1

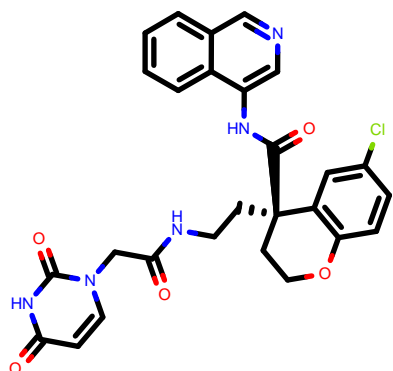
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCc5[nH]n5

RUN: RUN9276

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.24

EN300-13287_3_1



CID: EN300-13287_3_1

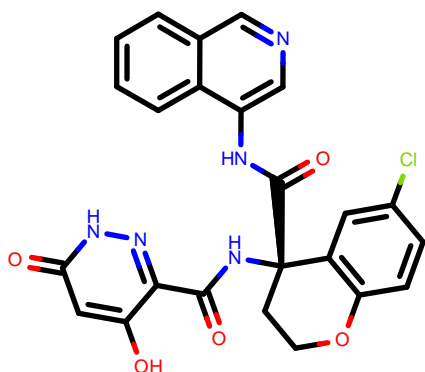
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccc(=O)[nH]5=O

RUN: RUN7619

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.24

EN300-111159_1_1



CID: EN300-111159_1_1

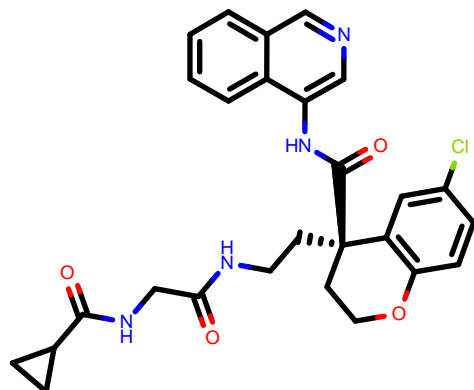
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(cc(=O)[nH]5)[O]

RUN: RUN5714

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.23

EN300-36522_3_1



CID: EN300-36522_3_1

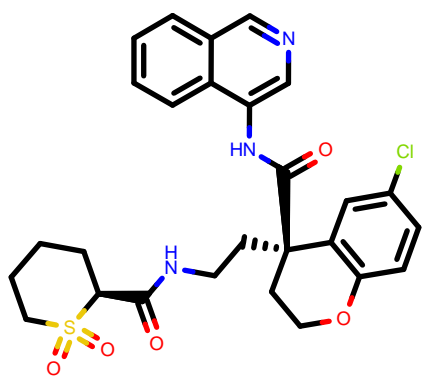
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CC5

RUN: RUN11897

DDG (kcal/mol): -0.31

dDDG (kcal/mol): 0.25

EN300-107435_3_1



CID: EN300-107435_3_1

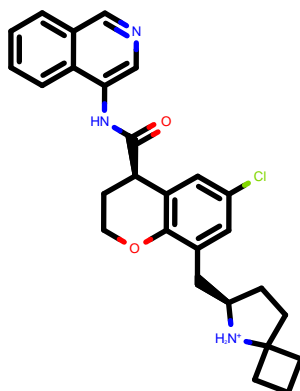
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CCCCSS(=O)=O

RUN: RUN15063

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.24

DAR-DIA-23e5a6a0-6_1



CID: DAR-DIA-23e5a6a0-6_1

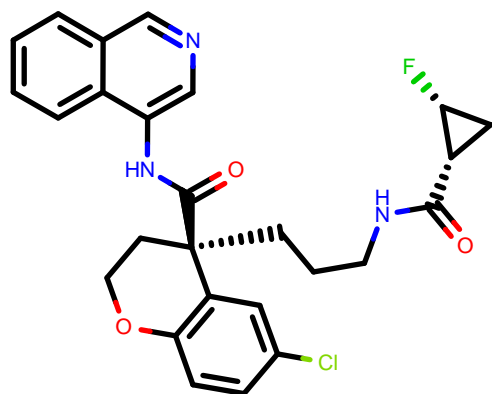
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C[C@H]5CCC6([NH2+][5])COC6Cl

RUN: RUN194

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.30

EN300-97300_4_2



CID: EN300-97300_4_2

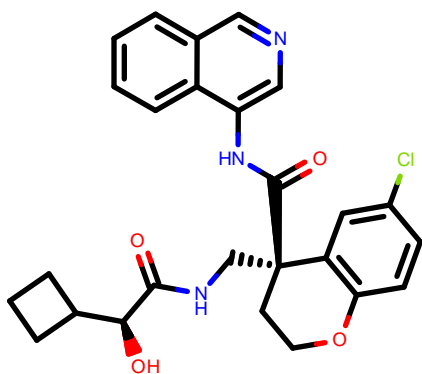
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5C[C@H]5F

RUN: RUN7714

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.18

EN300-249764_2_2



CID: EN300-249764_2_2

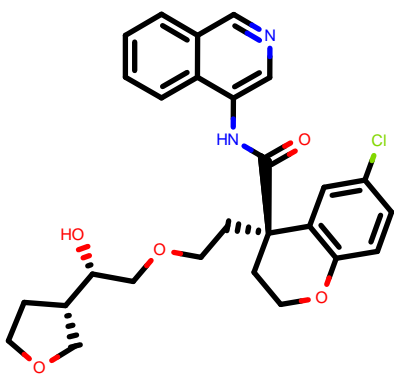
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5C5CC5O

RUN: RUN1172

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

EN300-1911992_3_3



CID: EN300-1911992_3_3

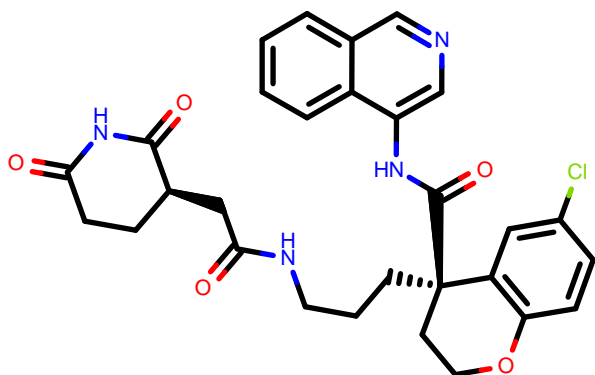
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](C)[H]5CCOC5=O

RUN: RUN1831

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.29

EN300-3451857_4_1



CID: EN300-3451857_4_1

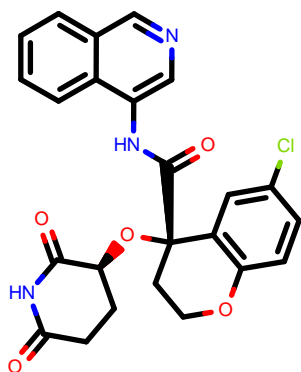
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCC(=O)NC5=O

RUN: RUN11660

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-120920_1_1



CID: EN300-120920_1_1

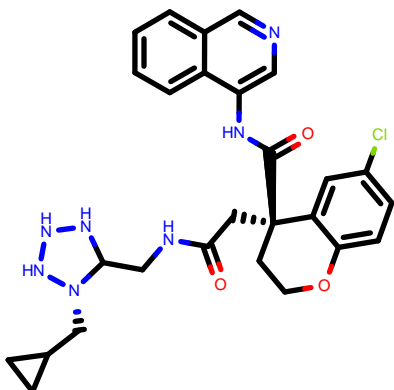
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@H]5CCCC(=O)NC5=O

RUN: RUN1789

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.17

EN300-140751_1_1



CID: EN300-140751_1_1

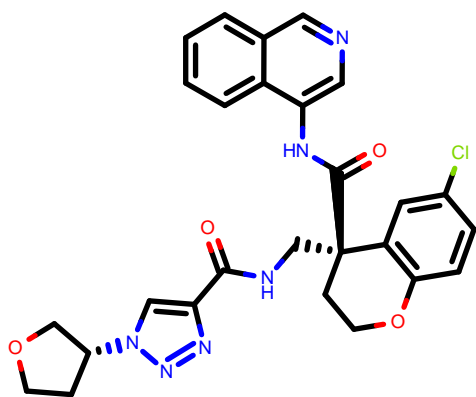
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5nnc5C6CC6

RUN: RUN8575

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

EN300-151461_2_1



CID: EN300-151461_2_1

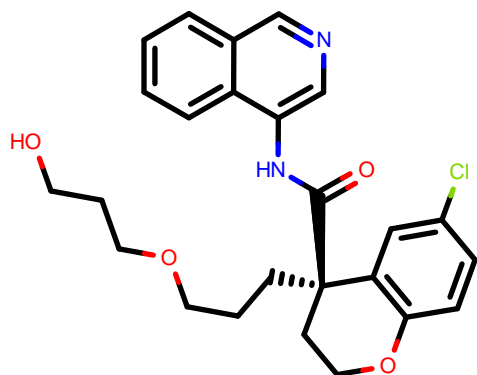
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(n5)C[C@@H]6CCOC6

RUN: RUN3375

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.26

EN300-221518_4_1



CID: EN300-221518_4_1

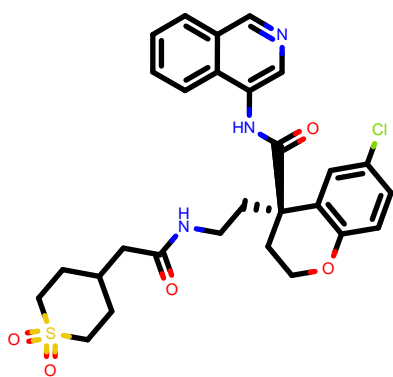
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO

RUN: RUN693

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.20

EN300-250120_3_1



CID: EN300-250120_3_1

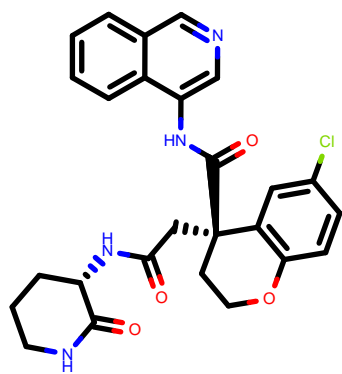
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCS(=O)(=O)CC5

RUN: RUN14712

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-60035_1_1



CID: EN300-60035_1_1

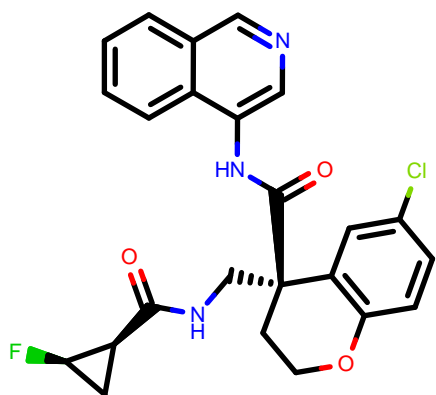
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCNC5=O

RUN: RUN10863

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.23

EN300-97300_2_2



CID: EN300-97300_2_2

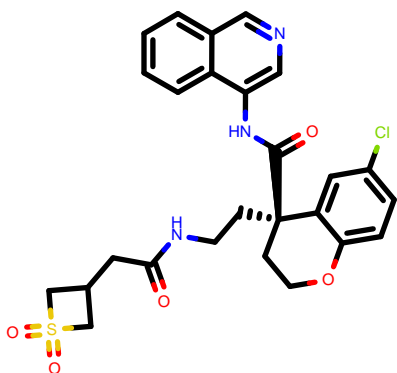
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5C[C@H]5F

RUN: RUN5047

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.20

EN300-256583_3_1



CID: EN300-256583_3_1

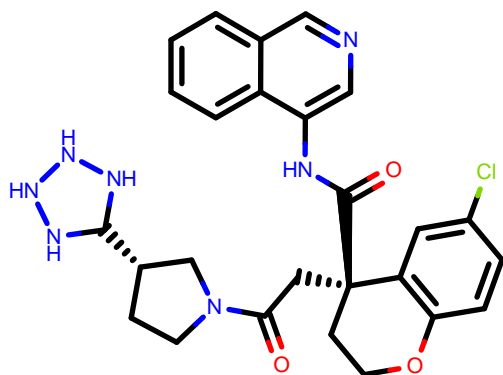
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)CS

RUN: RUN14850

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.32

EN300-366852_1_1



CID: EN300-366852_1_1

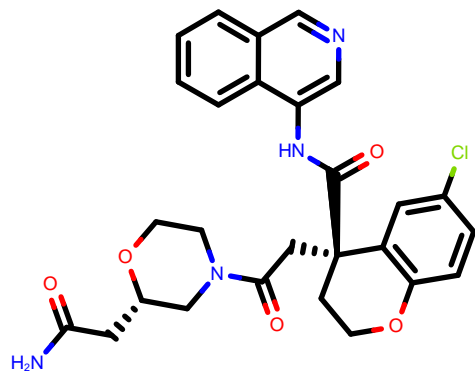
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)c6n[nH]n6

RUN: RUN6236

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.23

EN300-321558_1_2



CID: EN300-321558_1_2

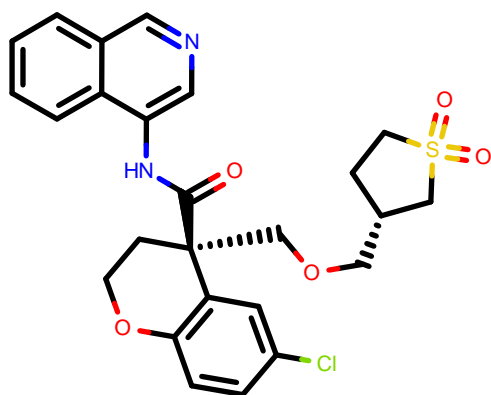
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)CC(=O)N

RUN: RUN3145

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.23

EN300-1448603_2_1



CID: EN300-1448603_2_1

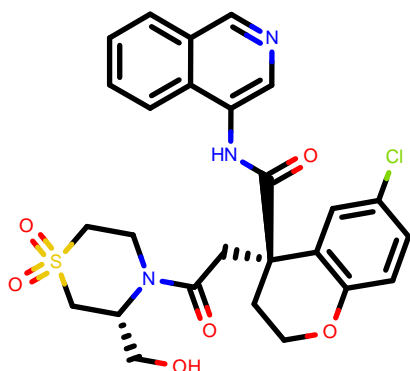
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCS(=O)(=O)C5

RUN: RUN660

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.24

EN300-157541_1_2



CID: EN300-157541_1_2

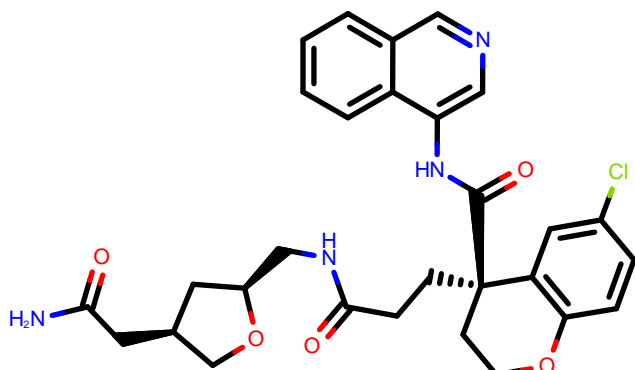
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)C5O

RUN: RUN5909

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.24

EN300-6736649_2_2



CID: EN300-6736649_2_2

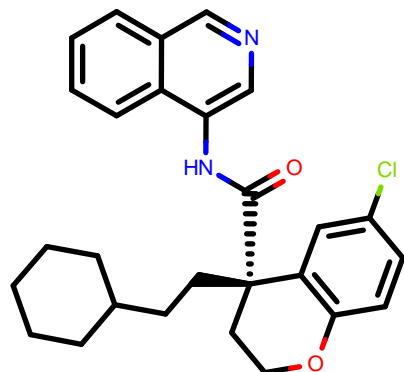
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5C[C@@H](C)CC5=O

RUN: RUN6339

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.25

DAR-DIA-6a508060-9_2



CID: DAR-DIA-6a508060-9_2

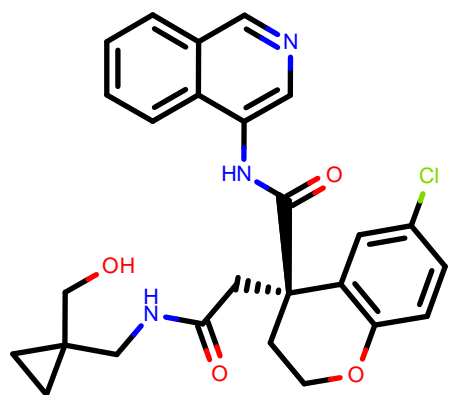
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C)C5CCCC5

RUN: RUN107

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.21

EN300-81512_1_1



CID: EN300-81512_1_1

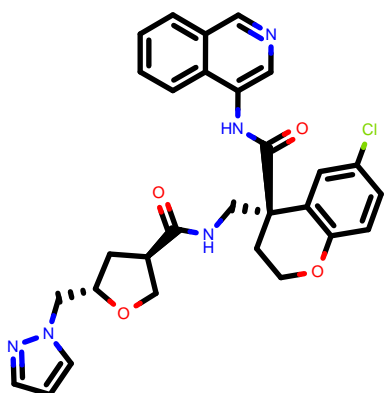
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CC5)CO

RUN: RUN12288

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.20

EN300-6494859_2_1



CID: EN300-6494859_2_1

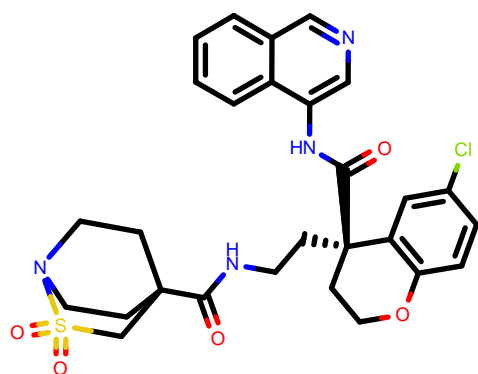
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(C)OC5C6=CN=C6

RUN: RUN7941

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.29

EN300-6731334_3_1



CID: EN300-6731334_3_1

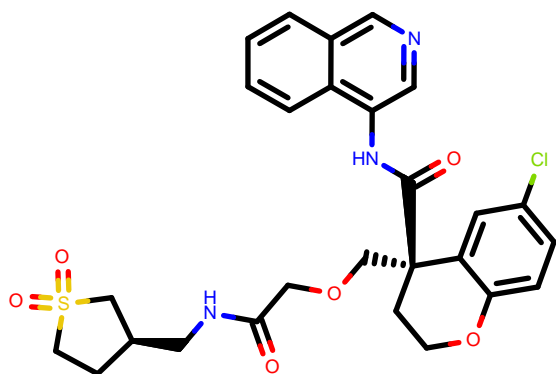
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)C56CCN(CC5)S(=O)(=O)C6

RUN: RUN14906

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.34

EN300-47606_2_2



CID: EN300-47606_2_2

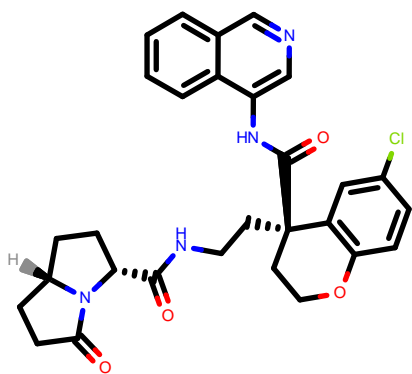
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC(=O)NC[C@@]5(C)SCS(=O)(=O)C5

RUN: RUN2280

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.31

EN300-6479181_3_2



CID: EN300-6479181_3_2

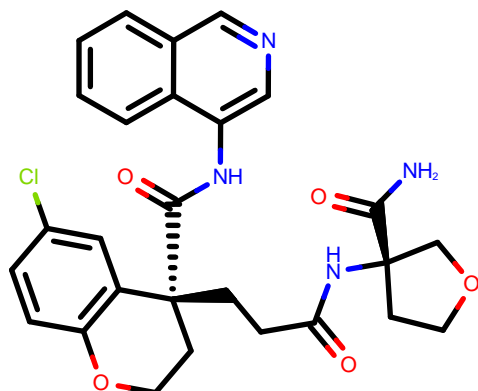
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@@H]5NSC(=O)CC6

RUN: RUN15207

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.24

EN300-124258_2_1



CID: EN300-124258_2_1

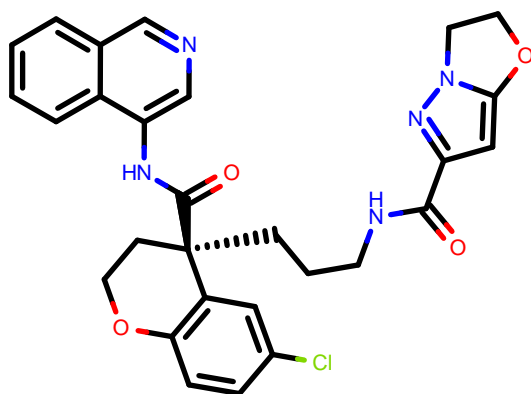
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5(CCOCC5)C(=O)N

RUN: RUN12553

DDG (kcal/mol): -0.30

dDDG (kcal/mol): 0.27

EN300-181688_4_1



CID: EN300-181688_4_1

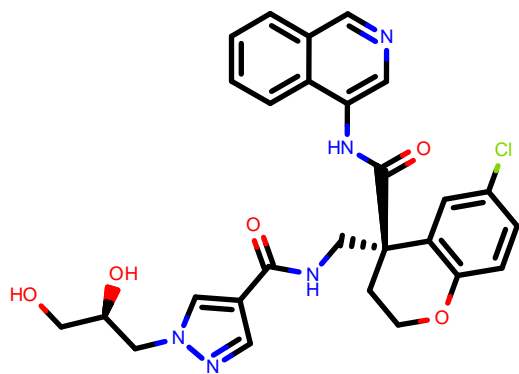
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCCCNC(=O)c5cc6n(n5)CCO6

RUN: RUN14657

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-246178_2_1



CID: EN300-246178_2_1

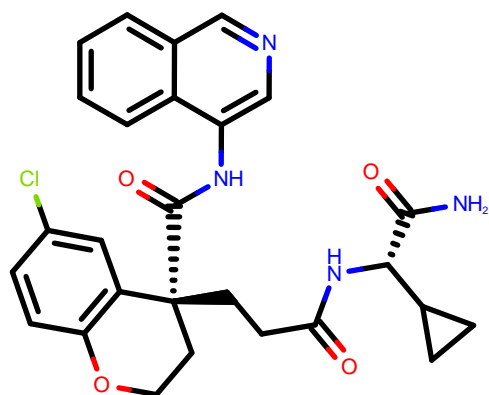
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnn(c5)C[C@@H](Cl)CO

RUN: RUN9286

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.29

EN300-1265434_2_2



CID: EN300-1265434_2_2

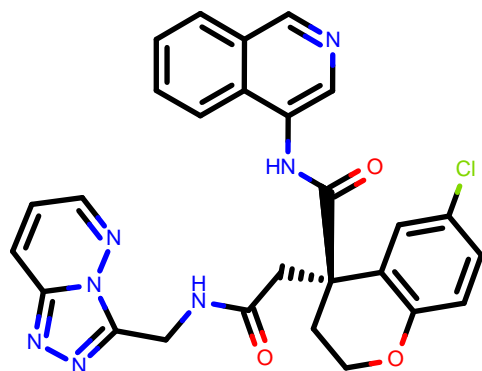
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H](C5CC5)C(=O)N

RUN: RUN4240

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.25

EN300-176135_1_1



CID: EN300-176135_1_1

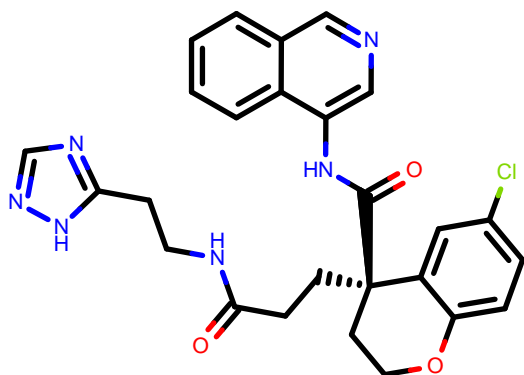
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5nncc6n5nc6

RUN: RUN14918

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.23

EN300-227021_2_1



CID: EN300-227021_2_1

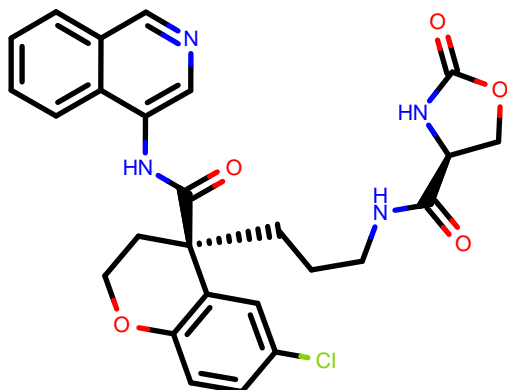
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NCCc5[nH]nc5

RUN: RUN8763

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.26

EN300-126389_4_1



CID: EN300-126389_4_1

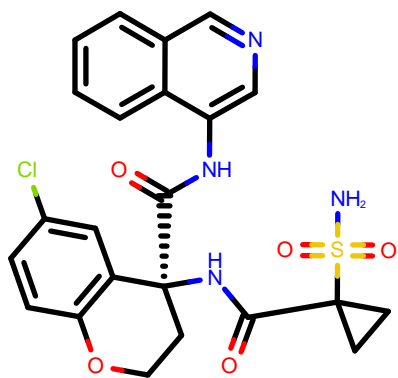
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5COC(=O)N5

RUN: RUN13411

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.23

EN300-223741_1_1



CID: EN300-223741_1_1

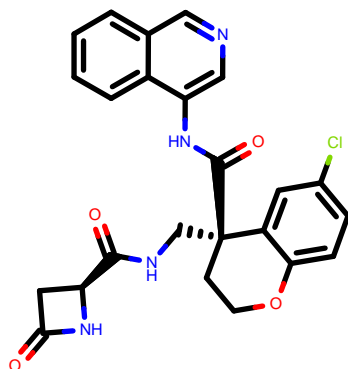
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5(CCS(=O)=O)N

RUN: RUN6265

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.29

EN300-103219_2_1



CID: EN300-103219_2_1

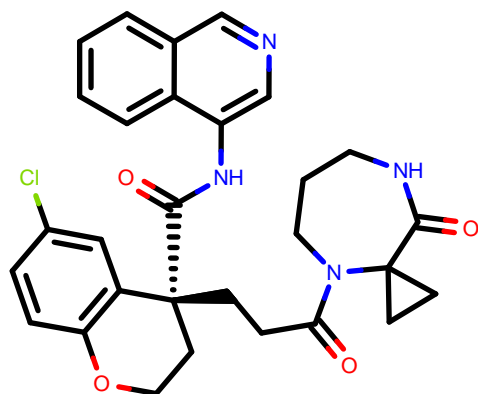
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CC(=O)N5

RUN: RUN6509

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.23

EN300-716218_2_1



CID: EN300-716218_2_1

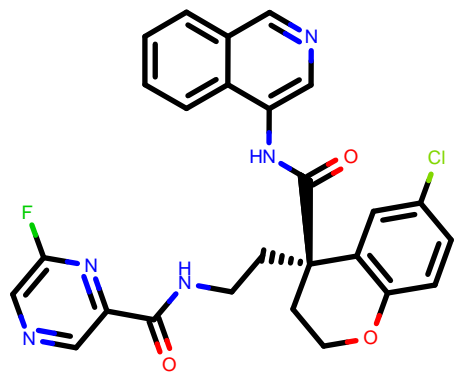
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCNC(=O)C56CC6

RUN: RUN6144

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.24

EN300-373552_3_1



CID: EN300-373552_3_1

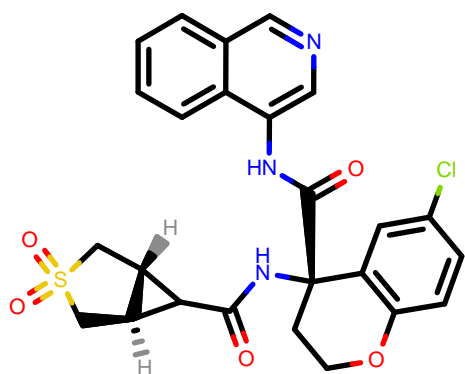
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5cncnc5F

RUN: RUN9248

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.21

EN300-6779469_1_1



CID: EN300-6779469_1_1

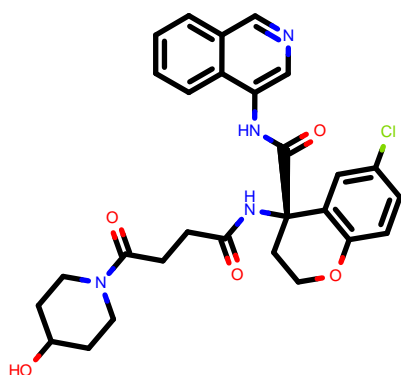
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(C@@H)C@@H5CS(=O)(=O)C6

RUN: RUN9349

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.22

EN300-51889_1_1



CID: EN300-51889_1_1

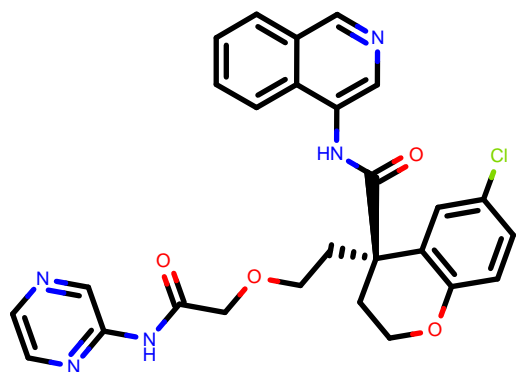
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCC(=O)N5CCCC(CS)O

RUN: RUN4314

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.31

EN300-105267_3_1



CID: EN300-105267_3_1

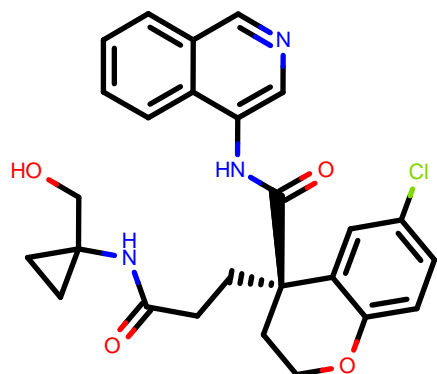
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5nccn5

RUN: RUN2553

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.32

EN300-117059_2_1



CID: EN300-117059_2_1

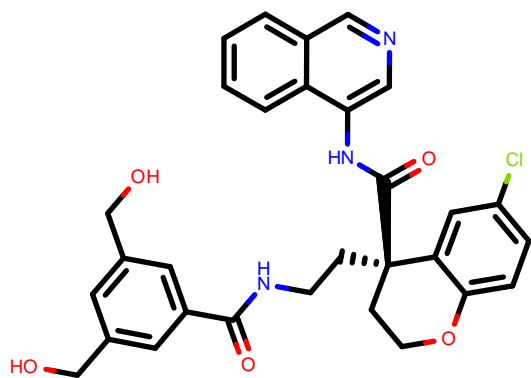
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CS)CO

RUN: RUN4656

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.26

EN300-211158_3_1



CID: EN300-211158_3_1

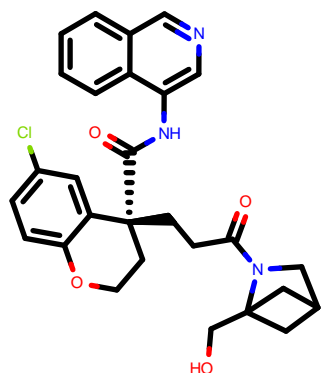
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccc(cc5)CO

RUN: RUN14985

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.29

EN300-298031_2_1



CID: EN300-298031_2_1

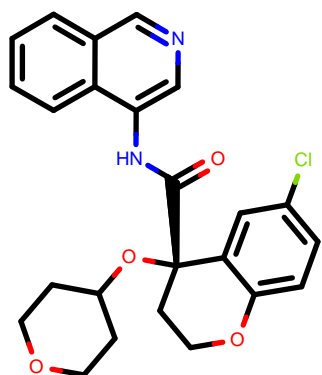
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6CC5(C6)CO

RUN: RUN14259

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.29

EDJ-MED-28ec730d-3_1



CID: EDJ-MED-28ec730d-3_1

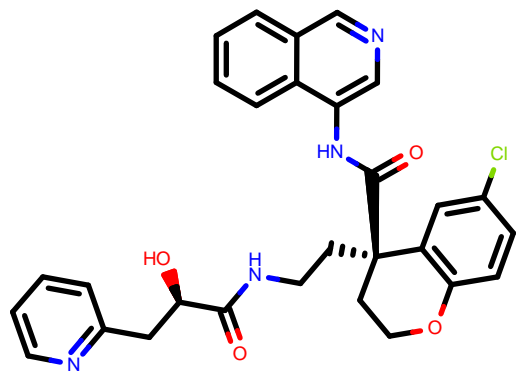
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5CCOCC5

RUN: RUN228

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.16

EN300-6762327_3_1



CID: EN300-6762327_3_1

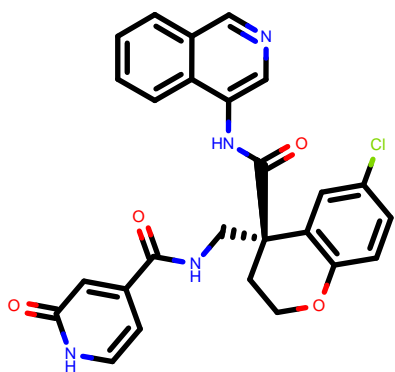
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]4H(C5c5ccoc5)O

RUN: RUN14678

DDG (kcal/mol): -0.29

dDDG (kcal/mol): 0.32

EN300-97661_2_1



CID: EN300-97661_2_1

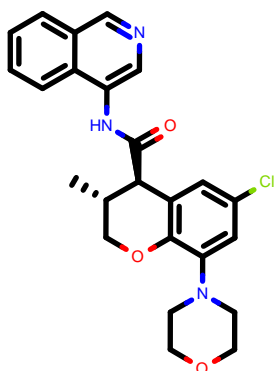
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc[nH]c5=O

RUN: RUN8734

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.21

DAR-DIA-0d514e7d-20_1



CID: DAR-DIA-0d514e7d-20_1

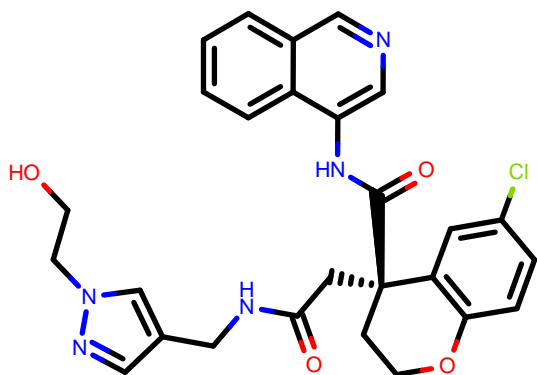
SMILES: C[C@H]1COc2c(cc2N3CCOCC3)Cl][C@@H]1C(=O)Nc4cnc5c4cccc5

RUN: RUN180

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.21

EN300-1692858_1_1



CID: EN300-1692858_1_1

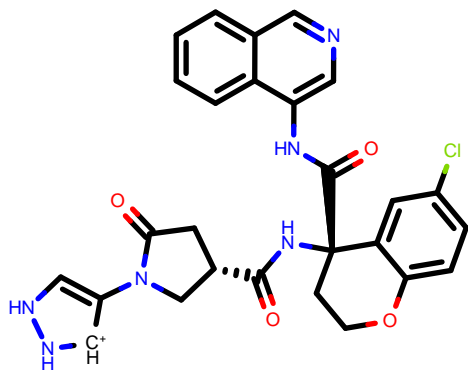
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5cnc1c5)CCO

RUN: RUN3257

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.26

EN300-99064_1_2



CID: EN300-99064_1_2

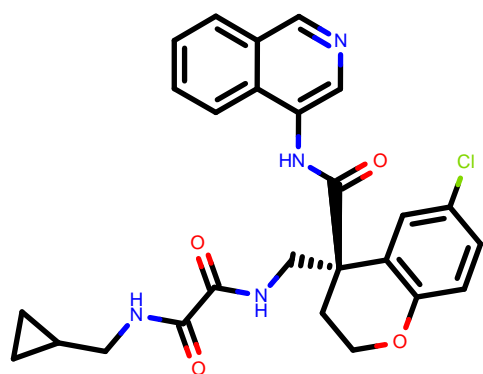
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC(=O)NC5)c6c[nH]c6

RUN: RUN9817

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.20

EN300-173216_2_1



CID: EN300-173216_2_1

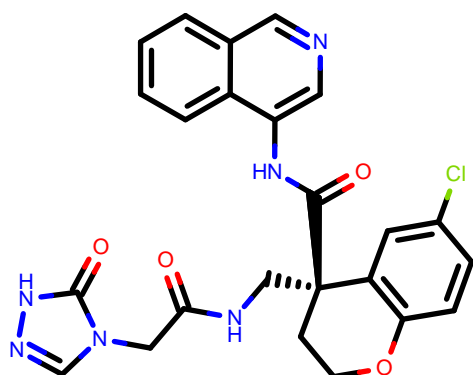
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(=O)NCC5CC5

RUN: RUN6254

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.25

EN300-120820_2_1



CID: EN300-120820_2_1

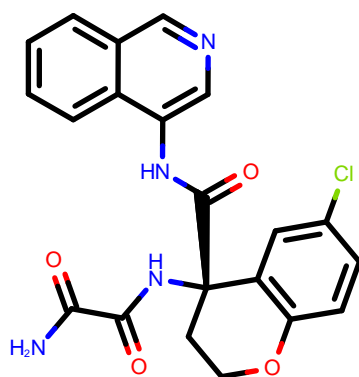
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5n[nH]c5=O

RUN: RUN486

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.21

EN300-113507_1_1



CID: EN300-113507_1_1

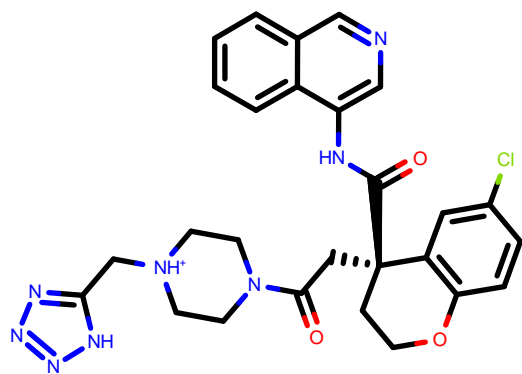
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)N

RUN: RUN4162

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.16

EN300-1268020_1_1



CID: EN300-1268020_1_1

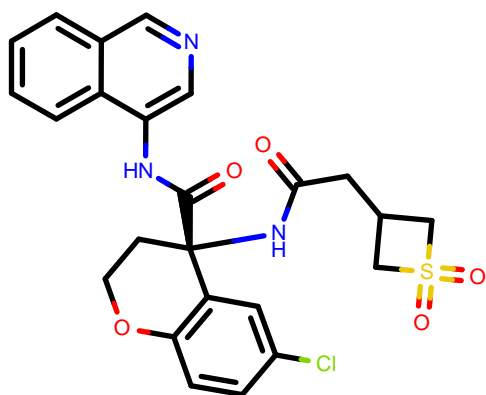
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)C6n[n-]nn6

RUN: RUN11623

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.31

EN300-256583_1_1



CID: EN300-256583_1_1

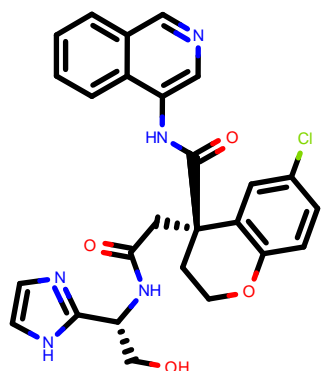
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)CC5CS(=O)=O)C5

RUN: RUN3622

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.29

EN300-657410_1_1



CID: EN300-657410_1_1

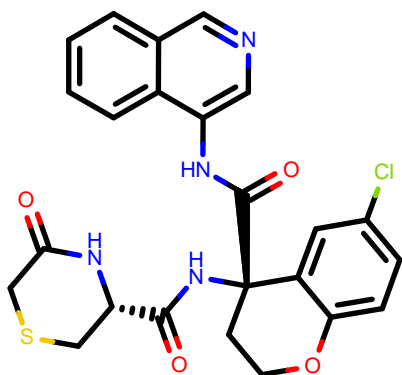
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC@H(CO)c5[nH]cn5

RUN: RUN8984

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.39

EN300-657320_1_1



CID: EN300-657320_1_1

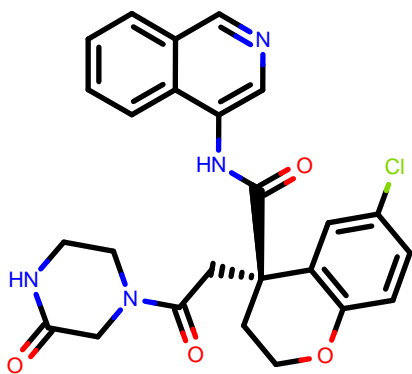
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@]4H5CSCC(=O)N5

RUN: RUN6532

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.24

EN300-08705_1_1



CID: EN300-08705_1_1

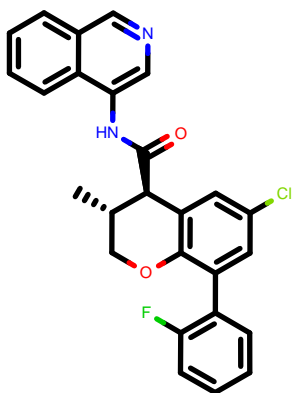
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCNC(=O)C5

RUN: RUN10157

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.22

DAR-DIA-0d514e7d-16_1



CID: DAR-DIA-0d514e7d-16_1

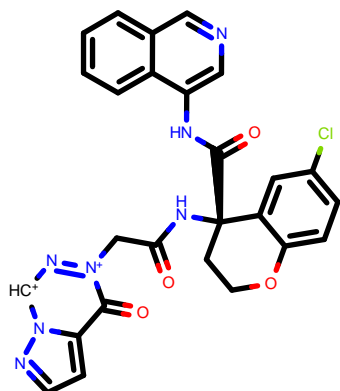
SMILES: C[C@H]1COc2c(cc2[C@@H]1C(=O)Nc3ncnc4c3cccc4Cl)c5ccccc5F

RUN: RUN222

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.20

EN300-75464_1_1



CID: EN300-75464_1_1

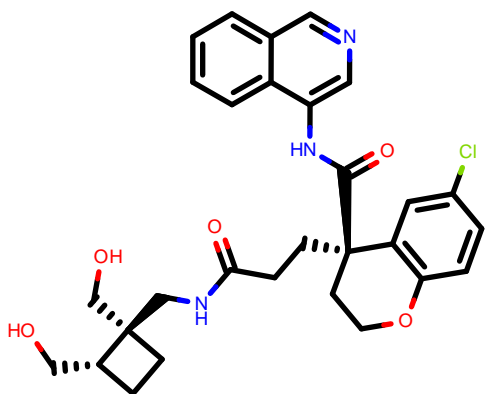
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc5

RUN: RUN9814

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.31

EN300-1692359_2_4



CID: EN300-1692359_2_4

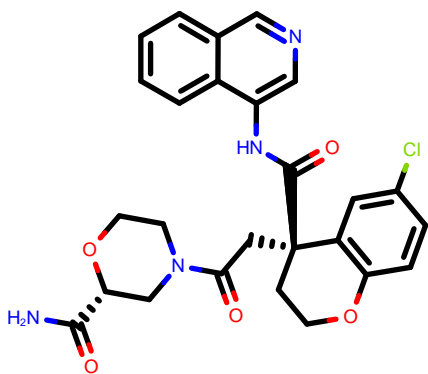
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(C)C[C@H]5O

RUN: RUN5980

DDG (kcal/mol): -0.28

dDDG (kcal/mol): 0.27

EN300-60862_1_1



CID: EN300-60862_1_1

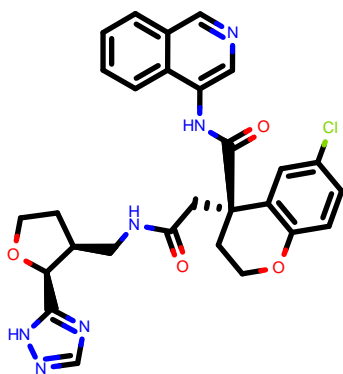
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC5

RUN: RUN10221

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.23

EN300-1272707_1_1



CID: EN300-1272707_1_1

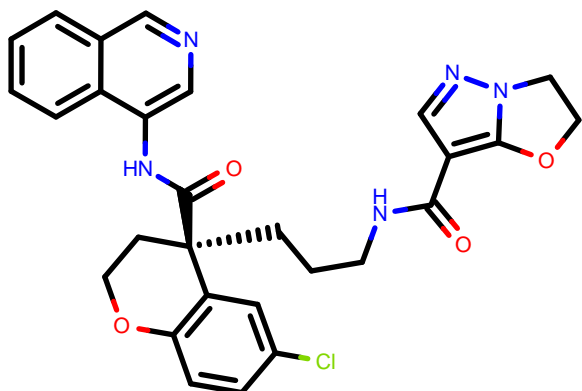
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)O[C@@H]5COC(=O)C@H5c6c[nH]n6

RUN: RUN7603

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.31

EN300-303519_4_1



CID: EN300-303519_4_1

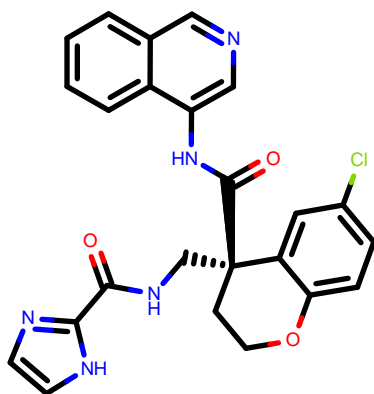
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)O[C@@H]5COC(=O)C@H5c6c[nH]n6

RUN: RUN13463

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.25

EN300-315836_2_1



CID: EN300-315836_2_1

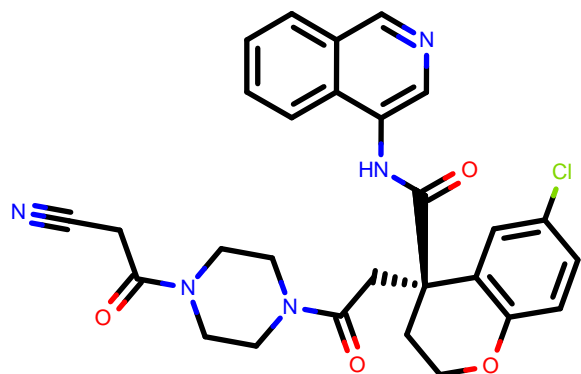
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)O[C@@H]5COC(=O)C@H5c6c[nH]n6

RUN: RUN2813

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.20

EN300-109060_1_1



CID: EN300-109060_1_1

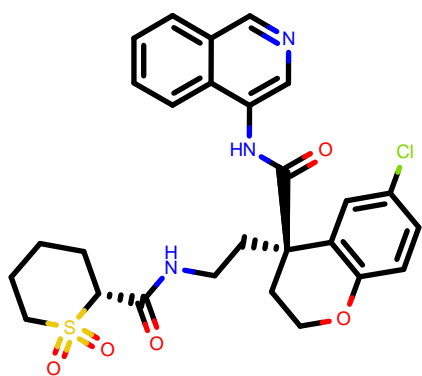
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3ccc4)O[C@@H]5COC(=O)C@H5c6c[nH]n6

RUN: RUN12760

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.28

EN300-107435_3_2



CID: EN300-107435_3_2

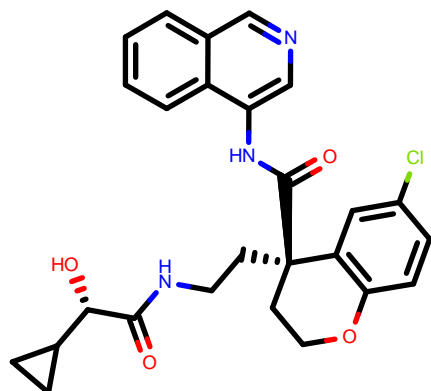
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCCS5(=O)=O

RUN: RUN14516

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.26

EN300-72211_3_2



CID: EN300-72211_3_2

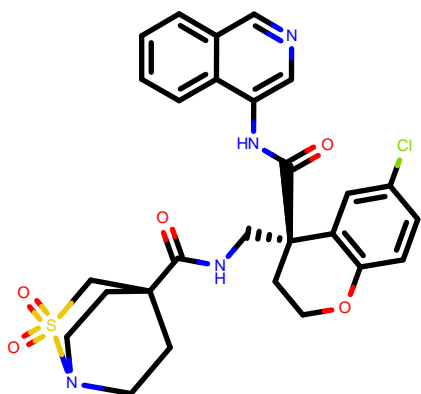
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CC5)O

RUN: RUN2356

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.22

EN300-6731334_2_1



CID: EN300-6731334_2_1

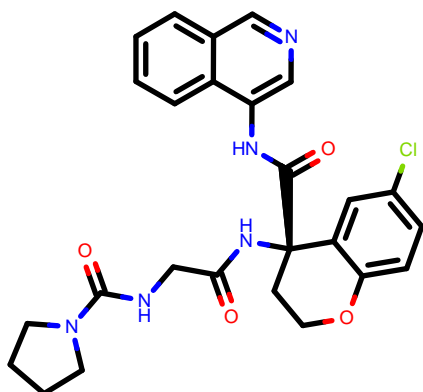
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CCN(CC5)S(=O)(=O)C6

RUN: RUN9198

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.28

EN300-383906_1_1



CID: EN300-383906_1_1

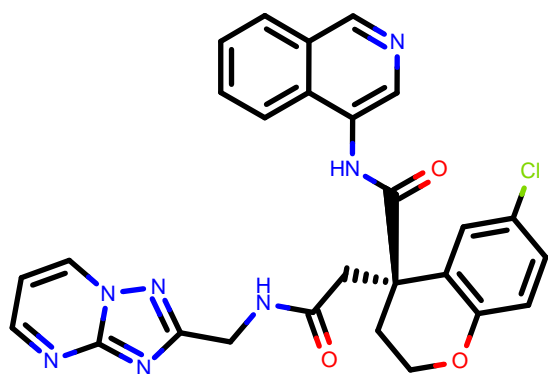
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N5CCCC5

RUN: RUN9730

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.27

EN300-250416_1_1



CID: EN300-250416_1_1

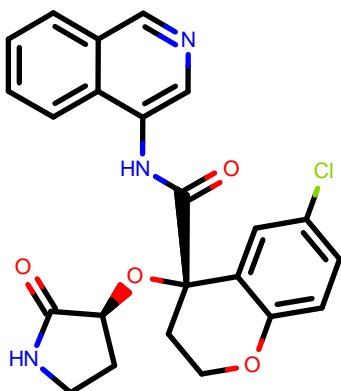
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5nc6nccn6n5

RUN: RUN12030

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.24

EN300-6736413_1_1



CID: EN300-6736413_1_1

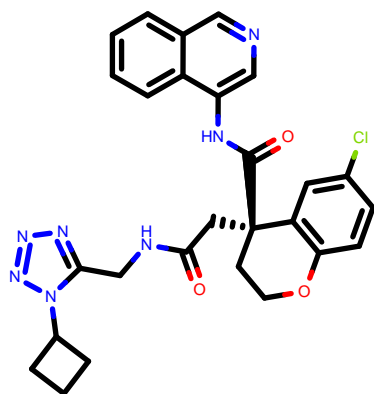
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@H]5CCNC5=O

RUN: RUN1717

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.16

EN300-7426624_1_1



CID: EN300-7426624_1_1

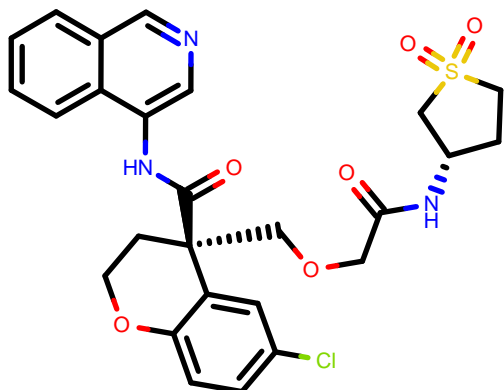
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5nnnn5C6CC6

RUN: RUN13730

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.25

EN300-05512_2_2



CID: EN300-05512_2_2

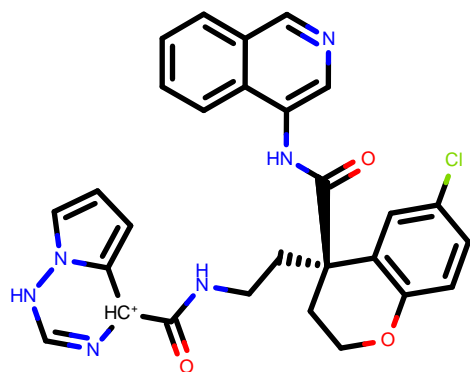
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N[C@H]5SCCS(=O)(=O)C5

RUN: RUN2088

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.36

EN300-7426781_3_1



CID: EN300-7426781_3_1

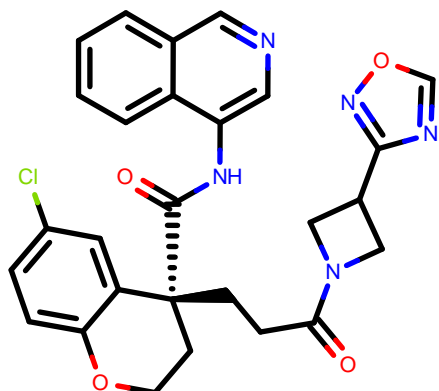
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)CCNC(=O)c5c6cccn6nc5

RUN: RUN14598

DDG (kcal/mol): -0.27

dDDG (kcal/mol): 0.23

EN300-1700143_2_1



CID: EN300-1700143_2_1

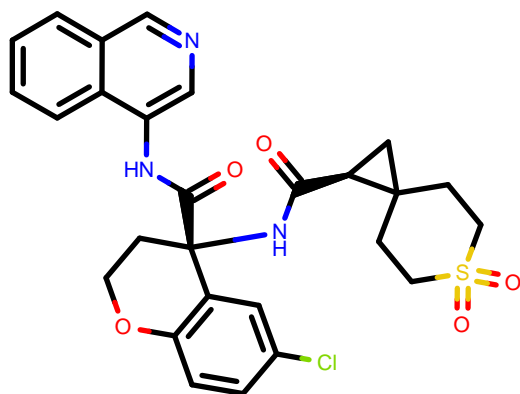
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)CCC(=O)N5CC(C5)c6ncn6

RUN: RUN14797

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.23

EN300-141809_1_2



CID: EN300-141809_1_2

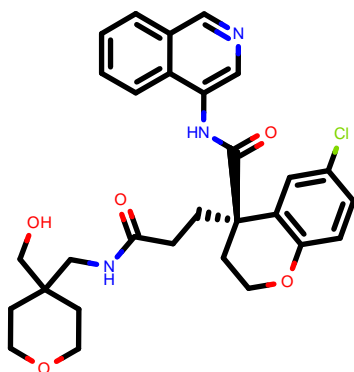
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)N(C=O)[C@@]5(C)S(=O)(=O)C5

RUN: RUN9778

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.24

EN300-115011_2_1



CID: EN300-115011_2_1

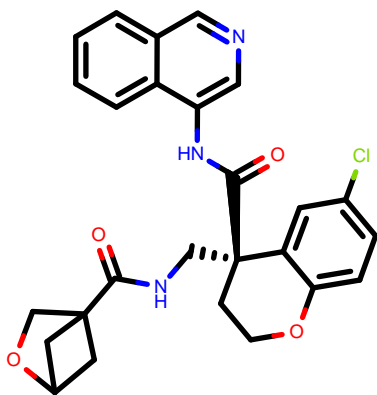
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)C)CCC(=O)NCC5(CCOCC5)CO

RUN: RUN2972

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.22

EN300-1604607_2_1



CID: EN300-1604607_2_1

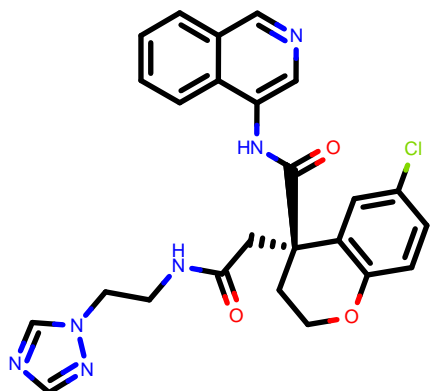
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C56CC(C5)OC6

RUN: RUN8197

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.21

EN300-69553_1_1



CID: EN300-69553_1_1

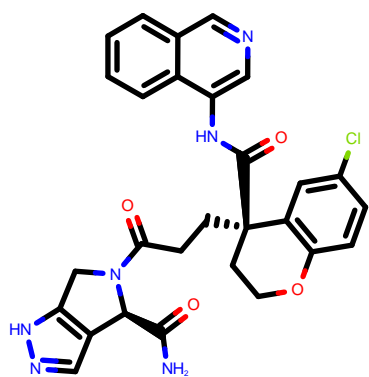
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCn5cn5

RUN: RUN9597

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.21

EN300-1704047_2_1



CID: EN300-1704047_2_1

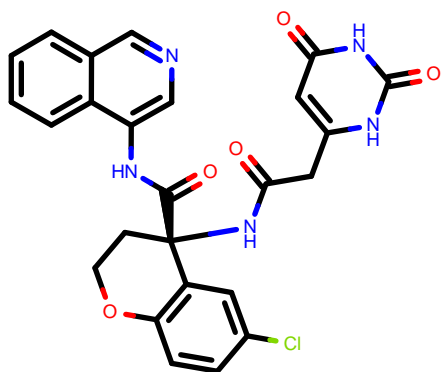
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5C6c6c(c7[nH]c8c7[nH]c8)C@H9[C@@]9N

RUN: RUN6140

DDG (kcal/mol): -0.26

dDDG (kcal/mol): 0.46

EN300-11441_1_1



CID: EN300-11441_1_1

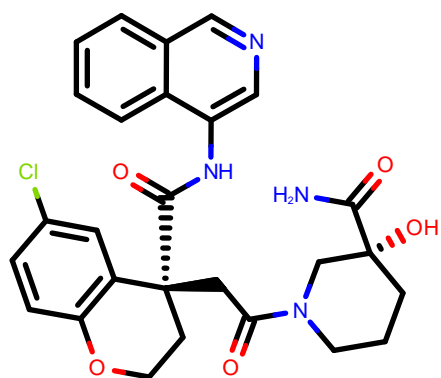
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)C5cc(=O)[nH]c(=O)[nH]5

RUN: RUN9441

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.23

EN300-210553_1_1



CID: EN300-210553_1_1

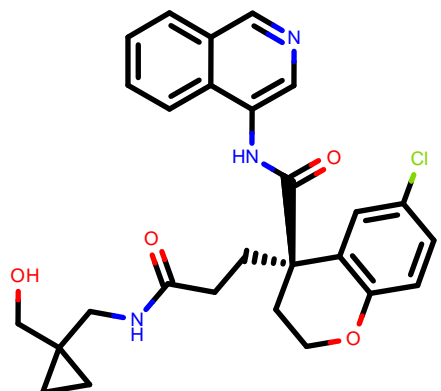
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@]3(C5)C(=O)N5O

RUN: RUN12242

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.24

EN300-81512_2_1



CID: EN300-81512_2_1

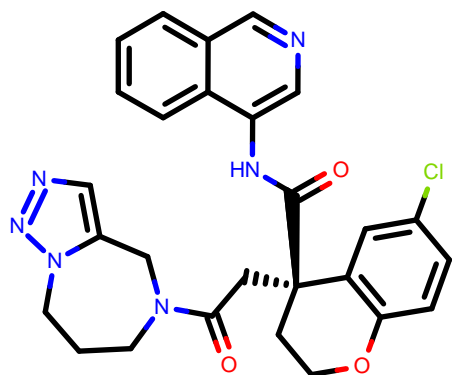
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(C)C5O

RUN: RUN2411

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.22

EN300-175400_1_1



CID: EN300-175400_1_1

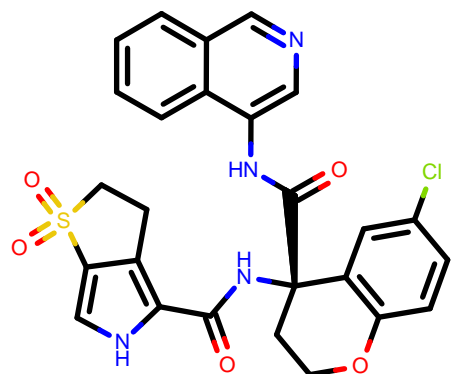
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN6c(cnn6)C5

RUN: RUN7943

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.24

EN300-205047_1_1



CID: EN300-205047_1_1

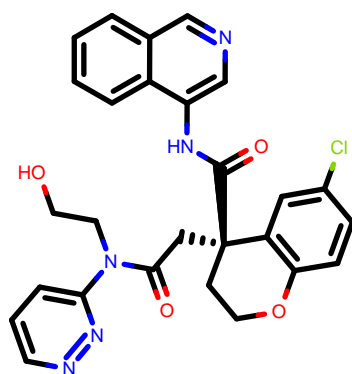
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c(c[nH]5)S(=O)(=O)CC6

RUN: RUN6221

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.22

EN300-99899_1_1



CID: EN300-99899_1_1

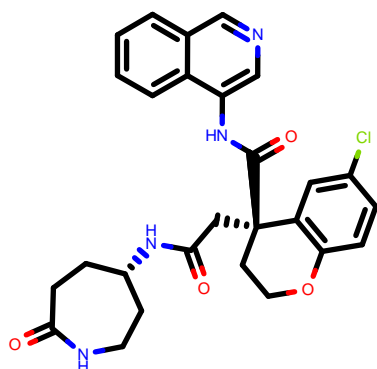
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5ccocn5

RUN: RUN4009

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.31

EN300-256759_1_2



CID: EN300-256759_1_2

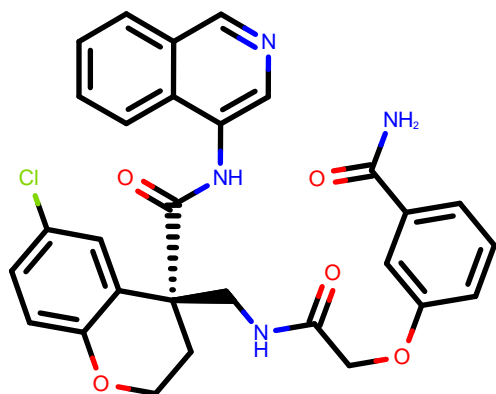
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(C@H)5CCCC(=O)NC5

RUN: RUN9152

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.23

EN300-51736_2_1



CID: EN300-51736_2_1

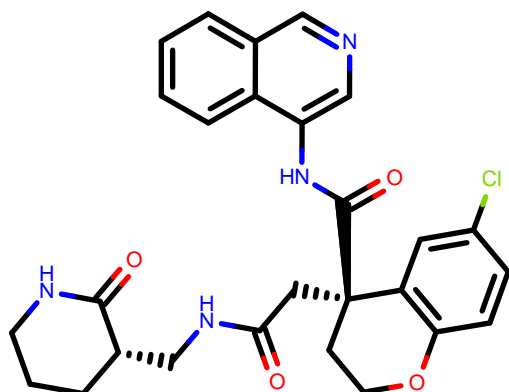
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COc5ccccc5Cl(=O)N

RUN: RUN5623

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.27

EN300-59757_1_2



CID: EN300-59757_1_2

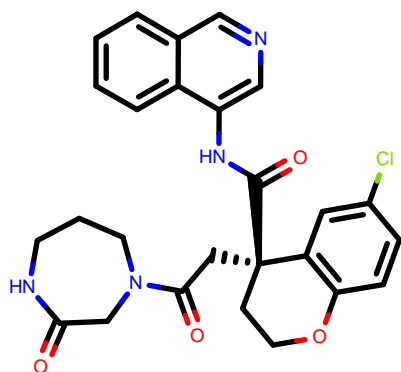
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]4H5CCNCC5=O

RUN: RUN11072

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.37

EN300-366468_1_1



CID: EN300-366468_1_1

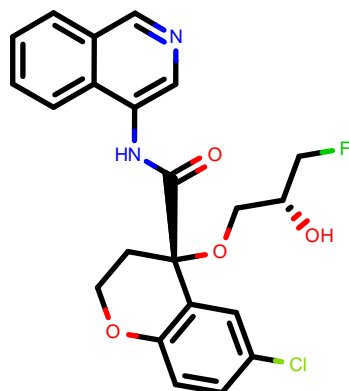
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCCN5C(=O)C5

RUN: RUN7687

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.26

EN300-1968342_1_2



CID: EN300-1968342_1_2

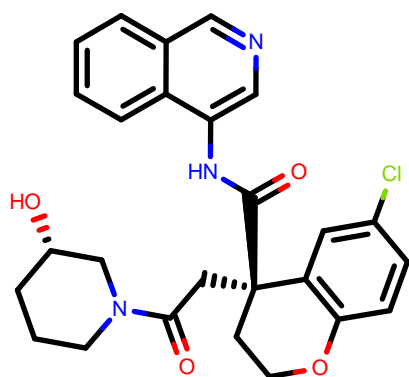
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CF)O

RUN: RUN2591

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.25

EN300-188582_1_1



CID: EN300-188582_1_1

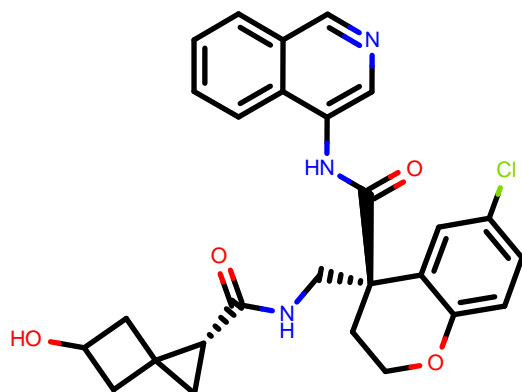
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H](C5)O

RUN: RUN9444

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.19

EN300-1717166_2_1



CID: EN300-1717166_2_1

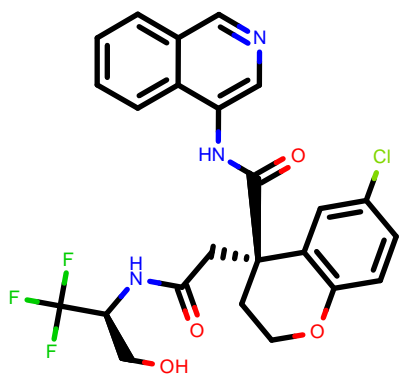
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(C)CC5C(C)O

RUN: RUN5007

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.23

EN300-142130_1_1



CID: EN300-142130_1_1

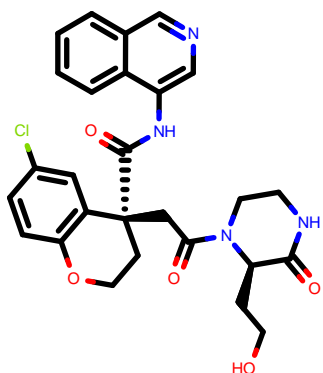
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)C(F)(F)F

RUN: RUN8067

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.36

EN300-1587691_1_2



CID: EN300-1587691_1_2

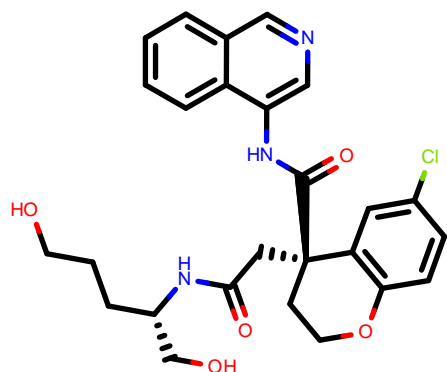
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)[C@H]5CO

RUN: RUN10041

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.30

EN300-7499295_1_1



CID: EN300-7499295_1_1

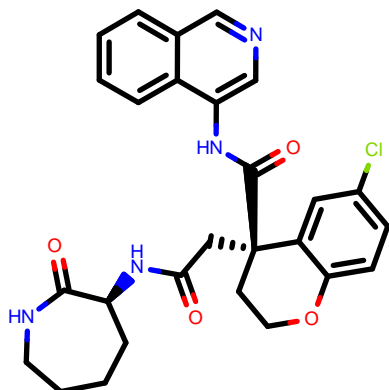
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CCCCO)CO

RUN: RUN3333

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.31

EN300-129384_1_1



CID: EN300-129384_1_1

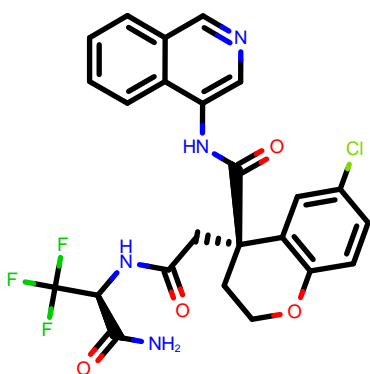
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN13960

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.21

EN300-6763470_1_1



CID: EN300-6763470_1_1

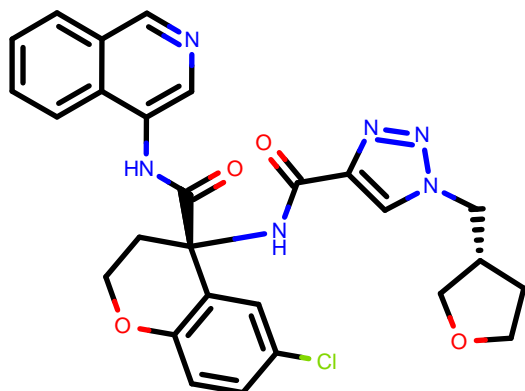
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](C(=O)N)C(F)(F)F

RUN: RUN4329

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.24

EN300-317272_1_1



CID: EN300-317272_1_1

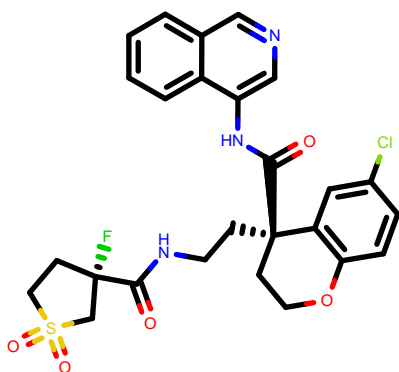
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@H]6CCOC6

RUN: RUN579

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.23

EN300-311920_3_1



CID: EN300-311920_3_1

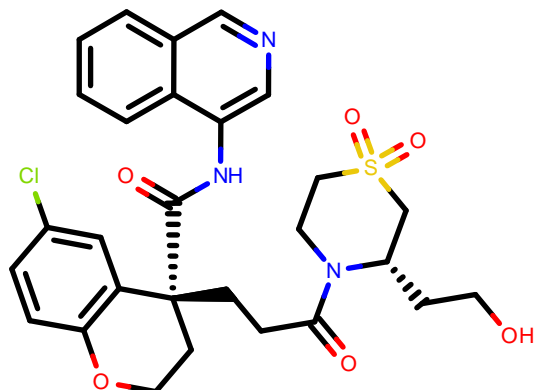
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCS(=O)=O)C5F

RUN: RUN15051

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.29

EN300-393056_2_1



CID: EN300-393056_2_1

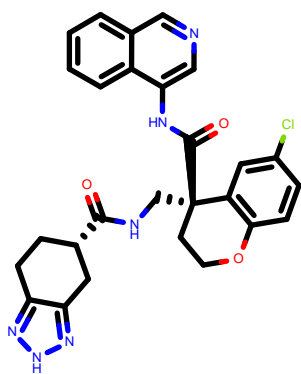
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)C5[C@@H]6CCO

RUN: RUN5336

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.34

EN300-185729_2_1



CID: EN300-185729_2_1

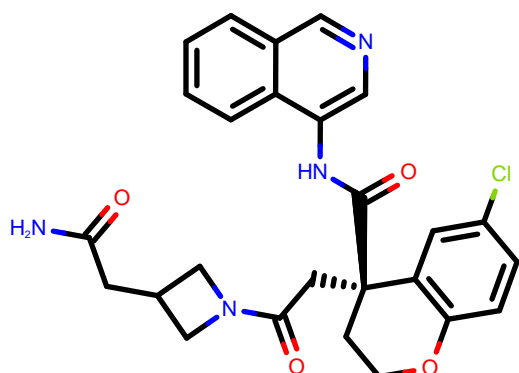
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCc6c(n[nH]6)C5

RUN: RUN7341

DDG (kcal/mol): -0.25

dDDG (kcal/mol): 0.26

EN300-194172_1_1



CID: EN300-194172_1_1

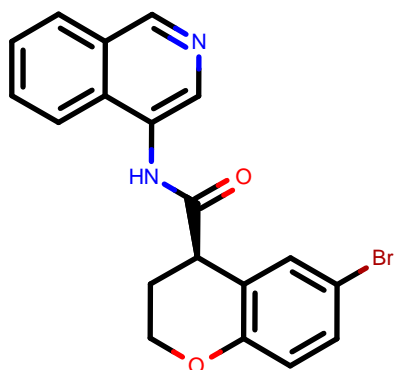
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)CC(=O)N

RUN: RUN6475

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.21

MAT-POS-11b63608-1_1



CID: MAT-POS-11b63608-1_1

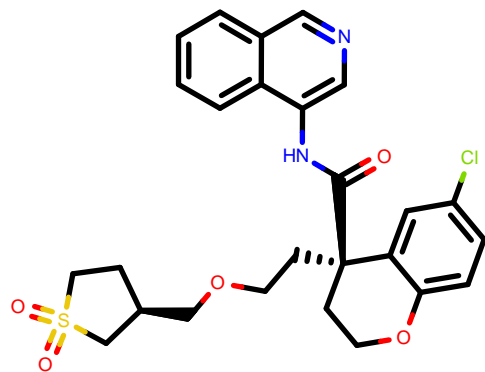
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Br

RUN: RUN93

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.08

EN300-1448603_3_1



CID: EN300-1448603_3_1

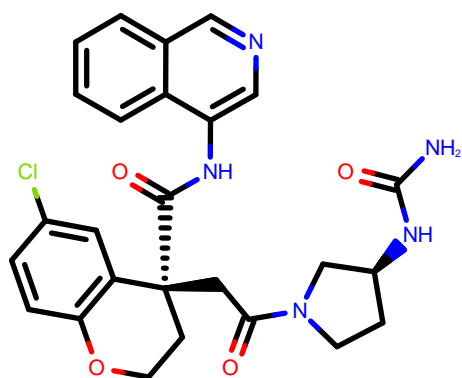
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5CCS(=O)(=O)C5

RUN: RUN2206

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.27

EN300-118869_1_1



CID: EN300-118869_1_1

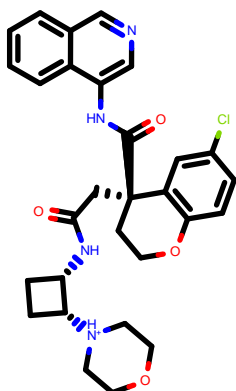
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@]@H(C5)NC(=O)N

RUN: RUN5405

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.21

EN300-1425963_1_2



CID: EN300-1425963_1_2

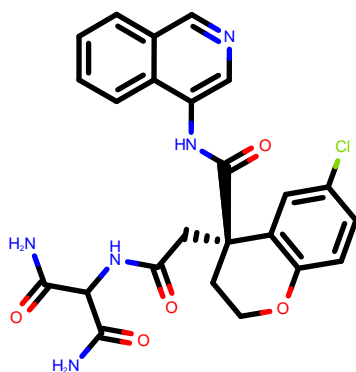
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N(C@H)5CC[C@@]@H5[NH+]#CCCCO6

RUN: RUN15167

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.30

EN300-26953_1_1



CID: EN300-26953_1_1

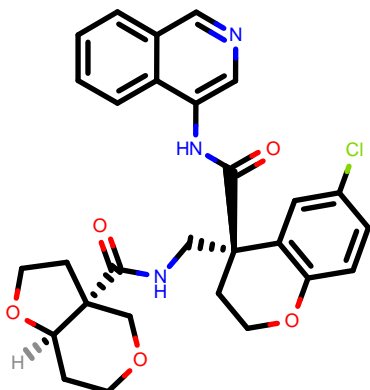
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC(C(=O)N)C(=O)N

RUN: RUN14028

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.25

EN300-341337_2_2



CID: EN300-341337_2_2

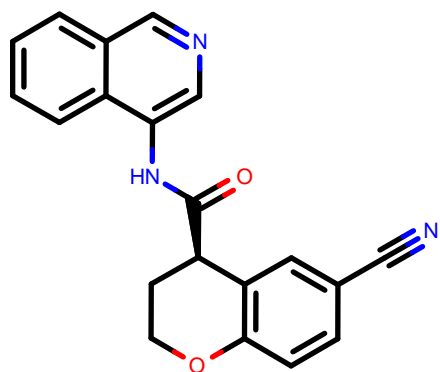
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C@H56CCO[C@@]@H56CCCC6

RUN: RUN8129

DDG (kcal/mol): -0.24

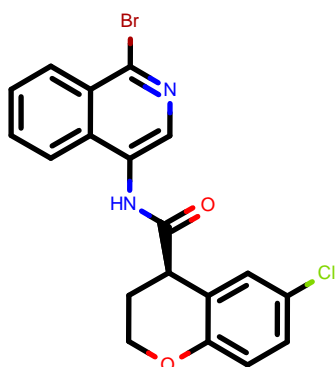
dDDG (kcal/mol): 0.31

DAR-DIA-6a508060-3_1



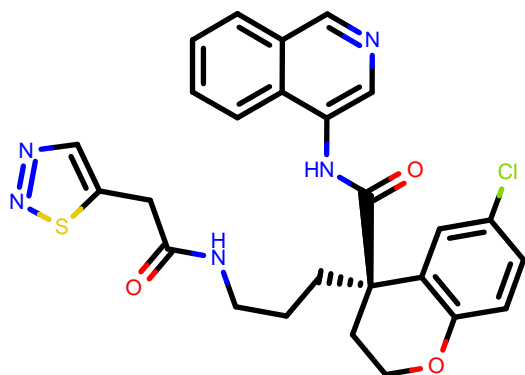
CID:	DAR-DIA-6a508060-3_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOCc4c3cc(cc4)C#N</chem>
RUN:	RUN88
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.08

ADA-UCB-dc2b944c-11_1



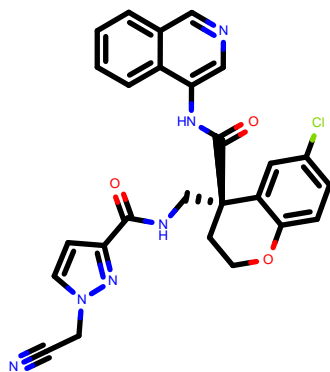
CID:	ADA-UCB-dc2b944c-11_1
SMILES:	<chem>c1ccc2c(c1)c(nc2Br)NC(=O)[C@@H]3CCOCc4c3cc(cc4)Cl</chem>
RUN:	RUN138
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.08

EN300-260152_4_1



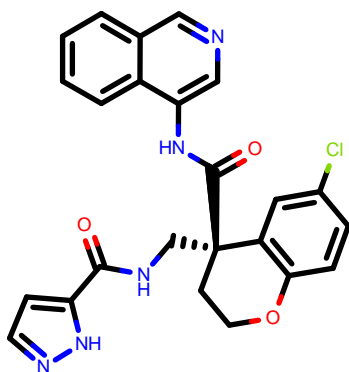
CID:	EN300-260152_4_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnns5</chem>
RUN:	RUN10846
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.23

EN300-1251424_2_1



CID:	EN300-1251424_2_1
SMILES:	<chem>c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccn(n5)C#N</chem>
RUN:	RUN3187
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.24

EN300-37077_2_1



CID: EN300-37077_2_1

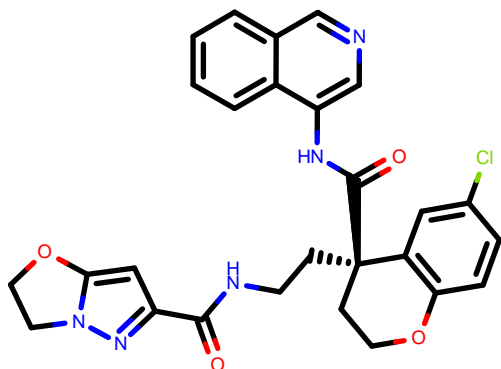
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn[nH]5

RUN: RUN422

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.19

EN300-181688_3_1



CID: EN300-181688_3_1

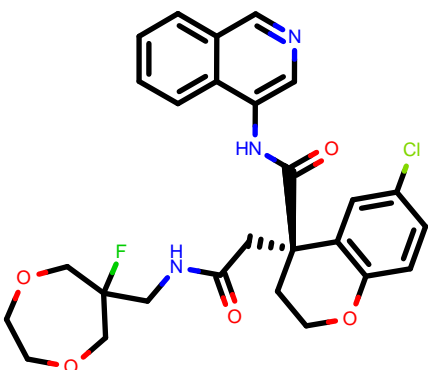
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5c6n(n5)CCO6

RUN: RUN15538

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.23

EN300-7500507_1_1



CID: EN300-7500507_1_1

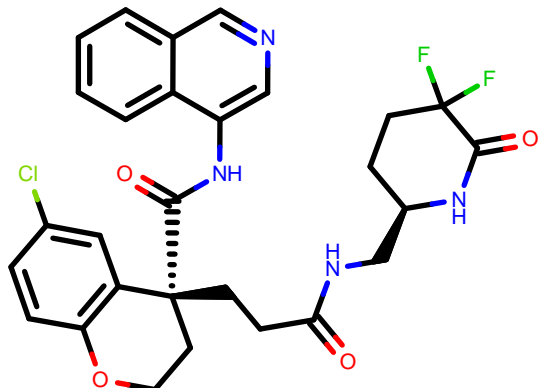
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC5(COCCOC5)F

RUN: RUN8003

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.30

EN300-1087098_2_1



CID: EN300-1087098_2_1

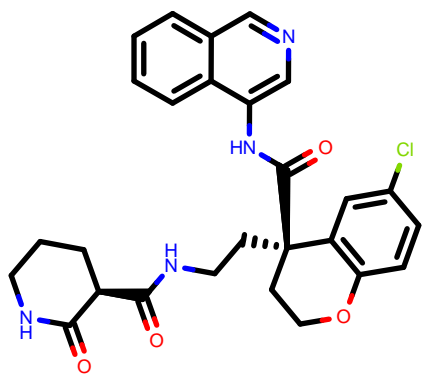
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N[C@@H]5CC(C(=O)N5)F/F

RUN: RUN7046

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.27

EN300-82616_3_1



CID: EN300-82616_3_1

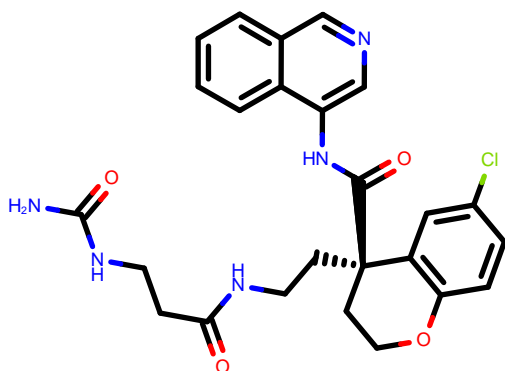
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5H5CCNC(=O)

RUN: RUN457

DDG (kcal/mol): -0.24

dDDG (kcal/mol): 0.26

EN300-10729_3_1



CID: EN300-10729_3_1

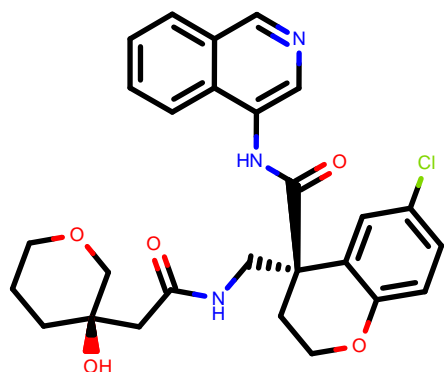
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCNC(=O)N

RUN: RUN13592

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-1071940_2_1



CID: EN300-1071940_2_1

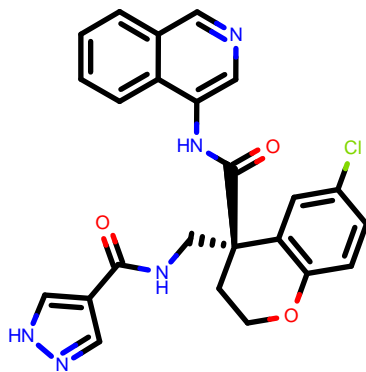
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(C)CCOC5O

RUN: RUN2570

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.28

EN300-41863_2_1



CID: EN300-41863_2_1

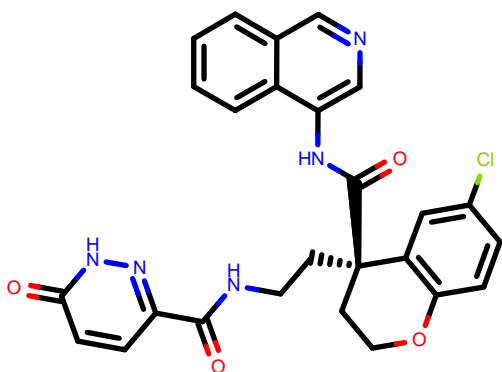
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c[nH]c5

RUN: RUN7841

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.22

EN300-04614_3_1



CID: EN300-04614_3_1

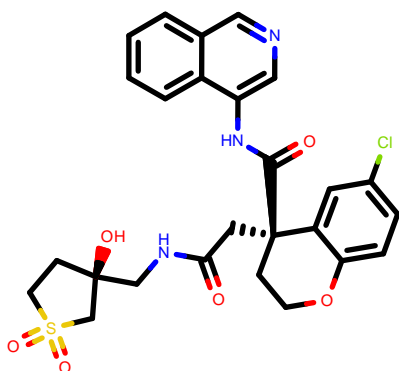
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)O)CCNC(=O)c5ccc(=O)[nH]n5

RUN: RUN15509

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.21

EN300-233786_1_2



CID: EN300-233786_1_2

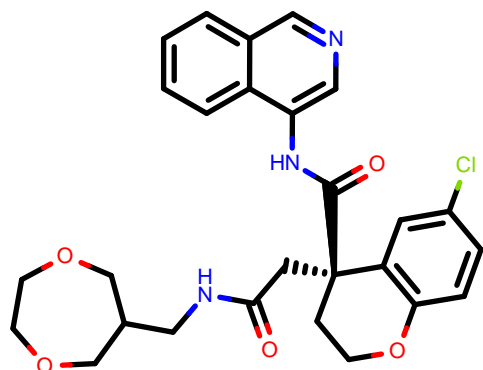
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CCS(=O)(=O)C5)O

RUN: RUN6827

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.32

EN300-7542483_1_1



CID: EN300-7542483_1_1

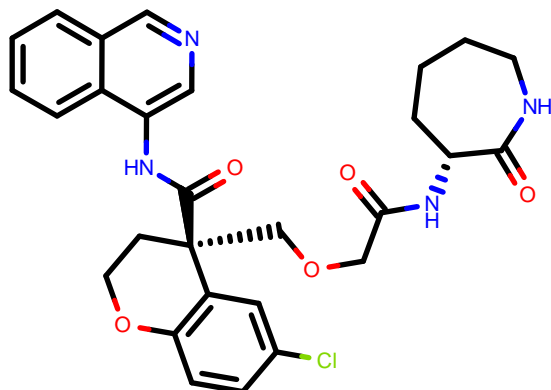
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5COCCO5

RUN: RUN8131

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.24

EN300-37195_2_2



CID: EN300-37195_2_2

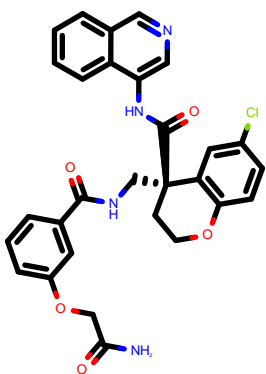
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N[C@@]5(C)CCNCC5=O

RUN: RUN1602

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.24

EN300-30687_2_1



CID: EN300-30687_2_1

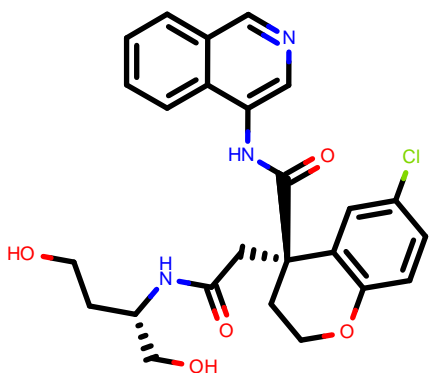
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccccc5)OCC(=O)N

RUN: RUN9398

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.32

EN300-195790_1_1



CID: EN300-195790_1_1

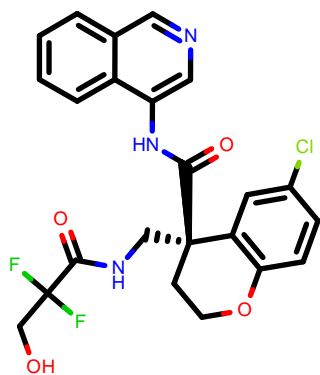
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]H(CCO)CO

RUN: RUN3841

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.26

EN300-123489_2_1



CID: EN300-123489_2_1

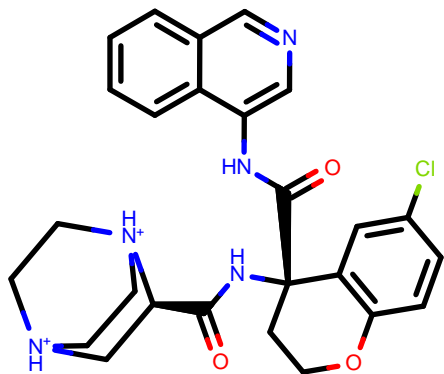
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(CO)(F)F

RUN: RUN5463

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.25

EN300-1605566_1_2



CID: EN300-1605566_1_2

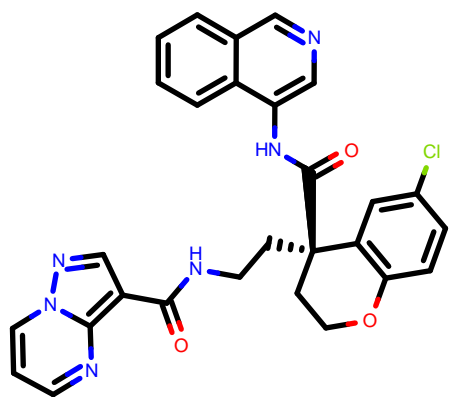
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CN6CC[NH+]5CC6

RUN: RUN8885

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.26

EN300-29520_3_1



CID: EN300-29520_3_1

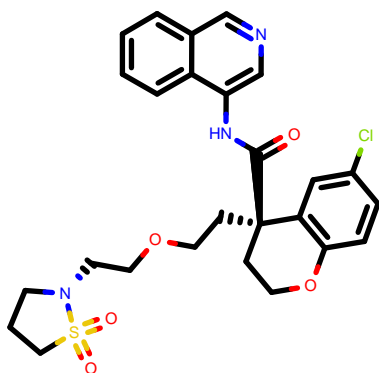
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnnc5

RUN: RUN9244

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.23

EN300-114134_3_1



CID: EN300-114134_3_1

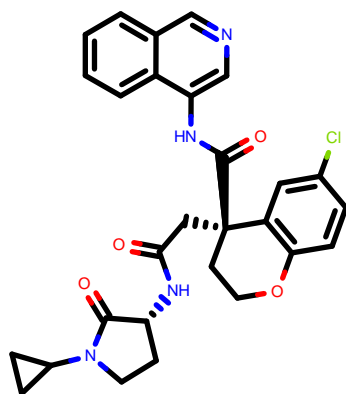
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N[C@@]5(CCS(=O)(=O)O)O

RUN: RUN2413

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.30

EN300-77438_1_2



CID: EN300-77438_1_2

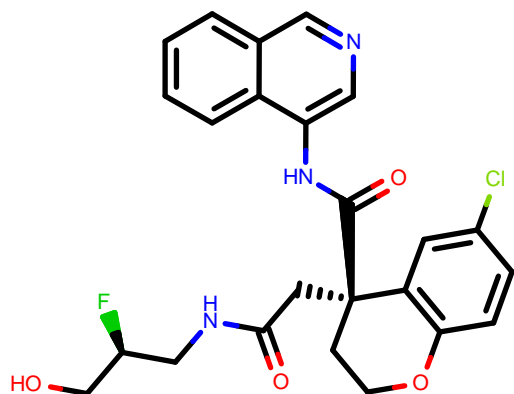
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(C)CCN(C5=O)C6CC6

RUN: RUN12416

DDG (kcal/mol): -0.23

dDDG (kcal/mol): 0.24

EN300-7353971_1_1



CID: EN300-7353971_1_1

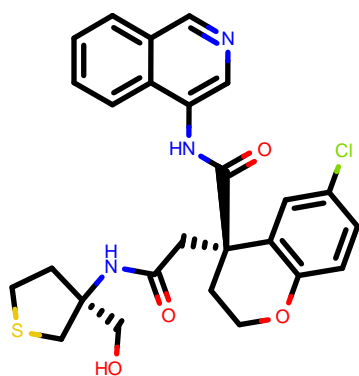
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(C)C(F)CO

RUN: RUN10397

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.28

EN300-1260794_1_2



CID: EN300-1260794_1_2

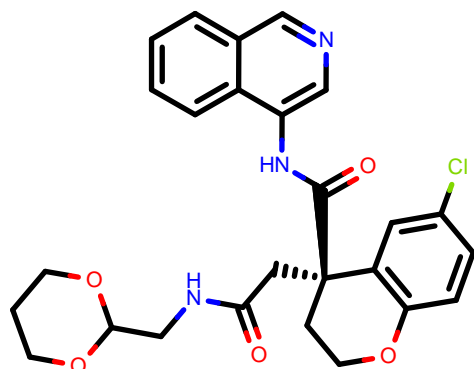
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5(CCSC5)CO

RUN: RUN12826

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.38

EN300-170720_1_1



CID: EN300-170720_1_1

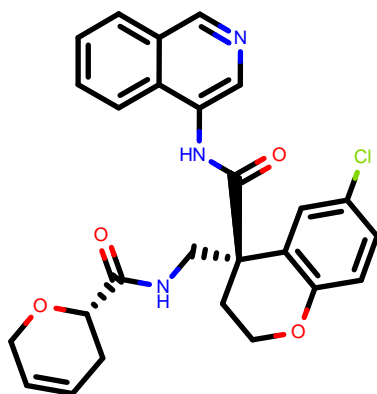
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC5OCCO5

RUN: RUN11116

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.25

EN300-378044_2_1



CID: EN300-378044_2_1

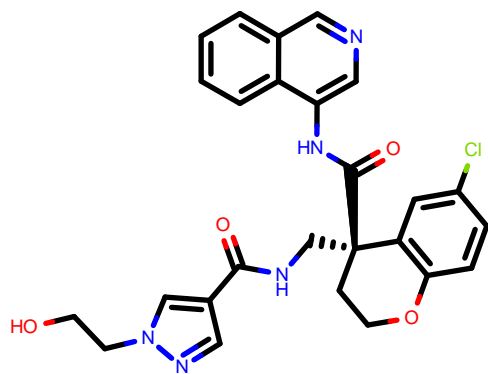
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@H]5CC=COC5

RUN: RUN5135

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.21

EN300-761209_2_1



CID: EN300-761209_2_1

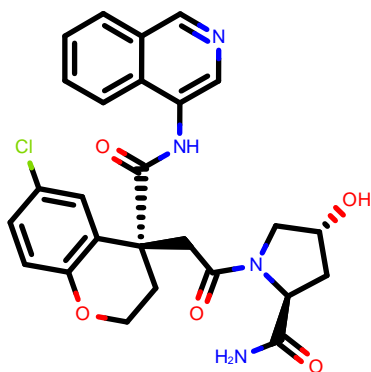
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5nn(c5)CCO

RUN: RUN3211

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.23

EN300-07752_1_2



CID: EN300-07752_1_2

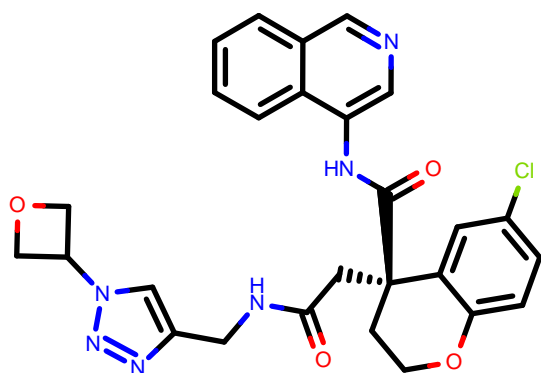
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3ccc(cc4)Cl)CC(=O)N5C[C@@H]5C[C@@H]5Cl(=O)N5O

RUN: RUN7063

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.25

EN300-1709745_1_1



CID: EN300-1709745_1_1

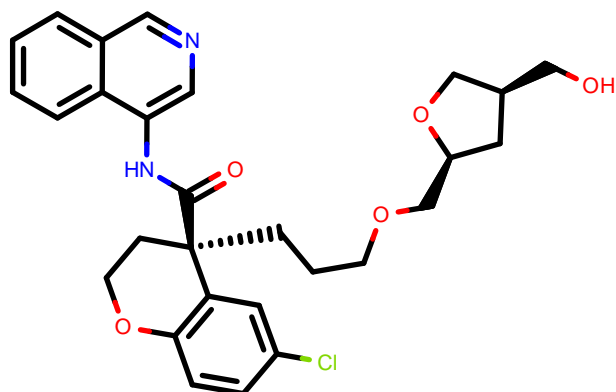
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3ccc(cc4)Cl)CC(=O)Nc5cn(nn5)C6COC6

RUN: RUN4605

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

EN300-6494158_4_2



CID: EN300-6494158_4_2

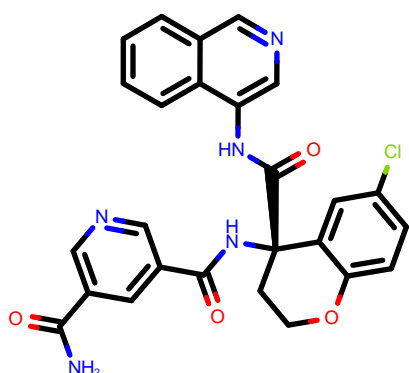
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3ccc(cc4)Cl)CCCOC[C@@H]5C[C@@H]5C[C@@H]5CO

RUN: RUN1834

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-44993_1_1



CID: EN300-44993_1_1

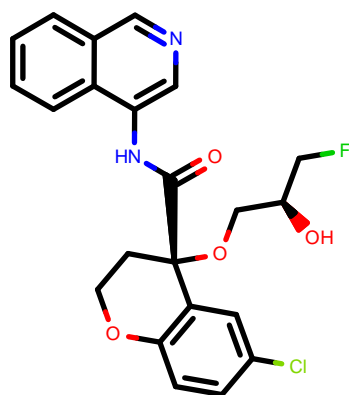
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@H]3(CCOc4c3ccc(cc4)Cl)NC(=O)c5ccn(cnc5)C(=O)N

RUN: RUN2962

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.23

EN300-1968342_1_1



CID: EN300-1968342_1_1

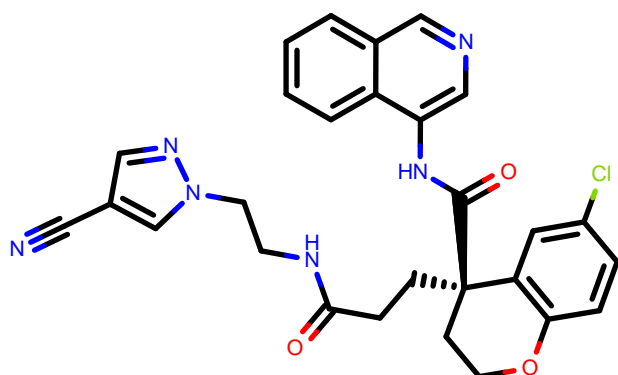
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](CF)O

RUN: RUN1637

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.29

EN300-80001_2_1



CID: EN300-80001_2_1

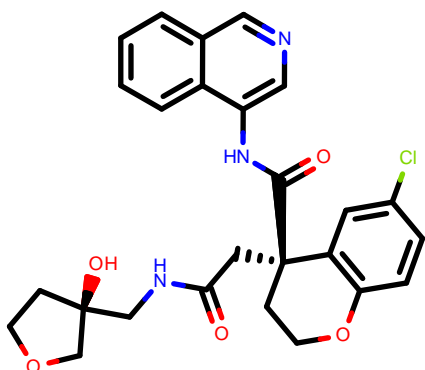
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCn5cc(cn5)C#N

RUN: RUN12091

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.22

EN300-200699_1_2



CID: EN300-200699_1_2

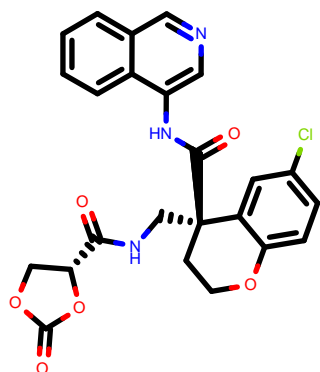
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCOCS)O

RUN: RUN2093

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.25

EN300-5253939_2_2



CID: EN300-5253939_2_2

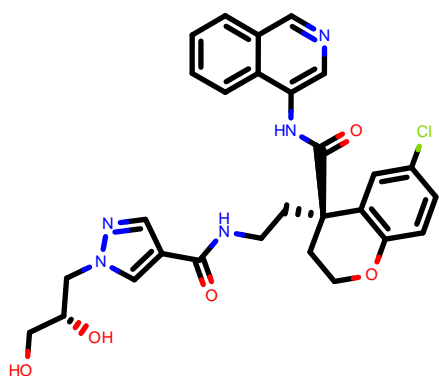
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COC(=O)O5

RUN: RUN2521

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.19

EN300-246178_3_1



CID: EN300-246178_3_1

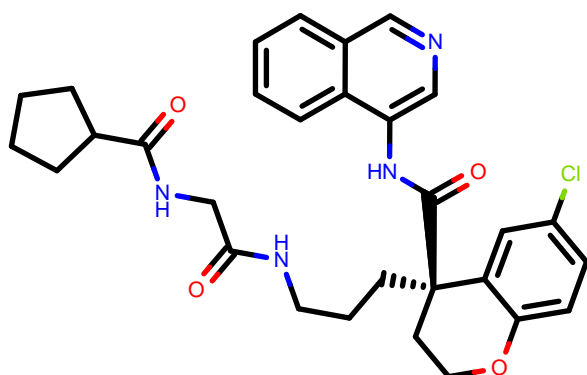
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cnn(c5)C[C@@H](CO)O

RUN: RUN15406

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.35

EN300-36845_4_1



CID: EN300-36845_4_1

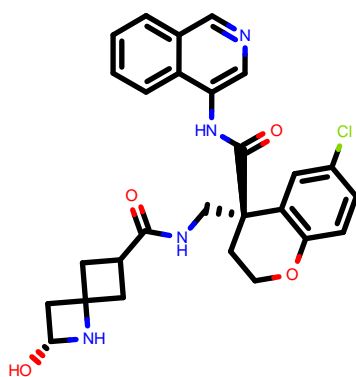
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CCCC5

RUN: RUN11332

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.27

EN300-1700760_2_1



CID: EN300-1700760_2_1

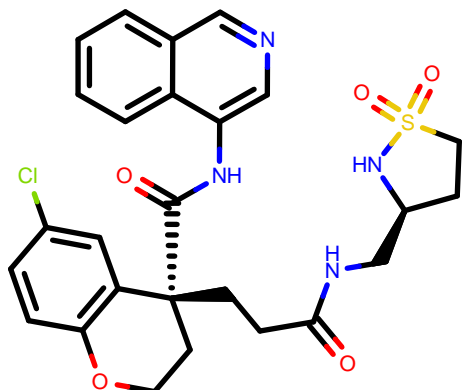
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC6(C5)CC(=O)N6

RUN: RUN7381

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

EN300-1266316_2_2



CID: EN300-1266316_2_2

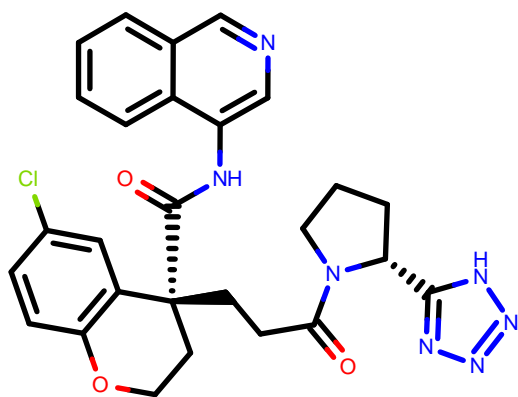
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCS(=O)(=O)N5

RUN: RUN4228

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.30

EN300-43282_2_2



CID: EN300-43282_2_2

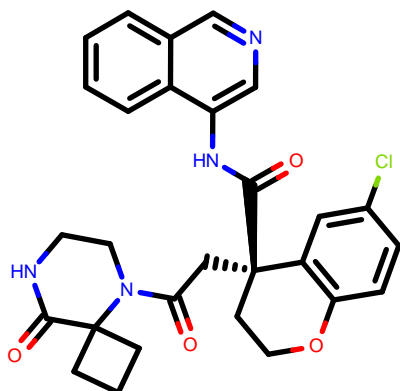
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)CCC(=O)N5CCCC[C@@H]5c6[nH]n6

RUN: RUN3580

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

EN300-1242134_1_1



CID: EN300-1242134_1_1

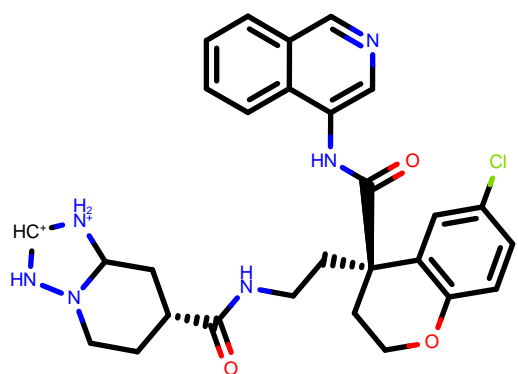
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)CC(=O)N5CCNC(=O)C56CCC6

RUN: RUN11635

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.32

EN300-1448674_3_2



CID: EN300-1448674_3_2

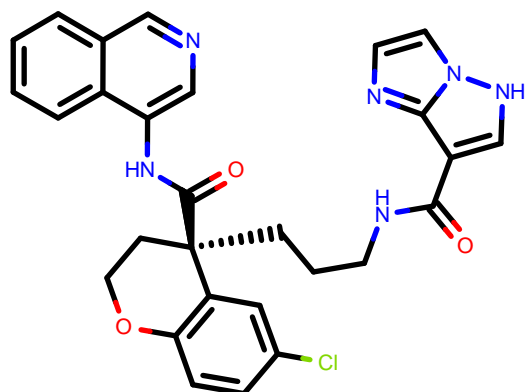
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)CCNC(=O)[C@@H]5C6Cn6c(n6)C5

RUN: RUN15356

DDG (kcal/mol): -0.22

dDDG (kcal/mol): 0.26

EN300-135238_4_1



CID: EN300-135238_4_1

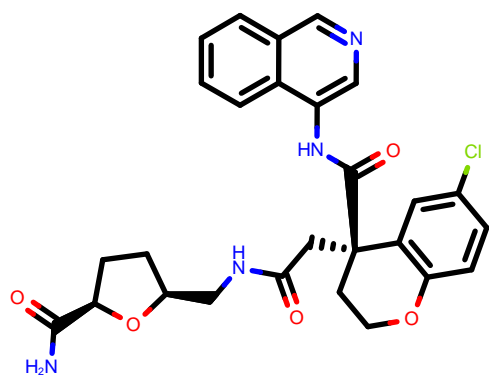
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)COCc4c3cc(cc4)C)CCCNC(=O)c5c[nH]n6c5nc6

RUN: RUN13583

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-107700_1_2



CID: EN300-107700_1_2

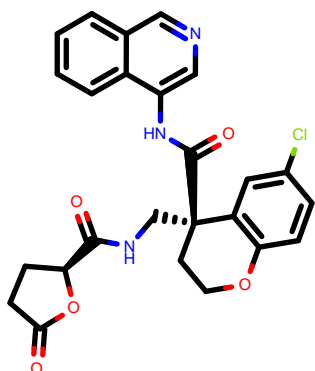
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H]5CC[C@@H](O5)C(=O)N

RUN: RUN7079

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.22

EN300-359750_2_1



CID: EN300-359750_2_1

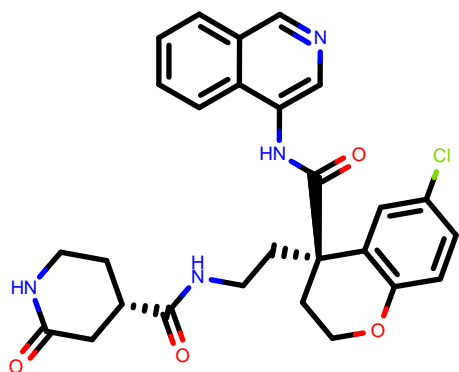
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CC(=O)O5

RUN: RUN6429

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.22

EN300-107493_3_1



CID: EN300-107493_3_1

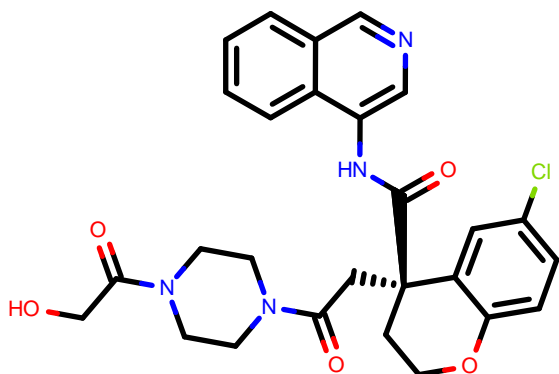
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCNC(=O)C5

RUN: RUN4793

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.22

EN300-58821_1_1



CID: EN300-58821_1_1

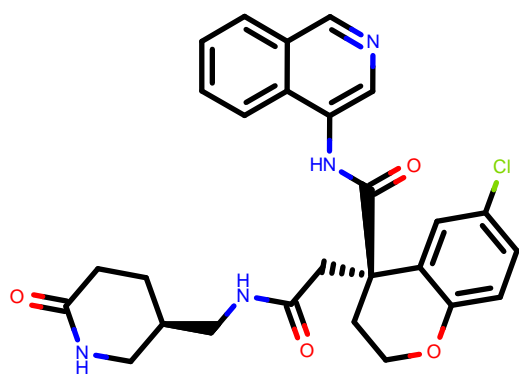
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN(CC5)C(=O)CO

RUN: RUN9320

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-6746326_1_1



CID: EN300-6746326_1_1

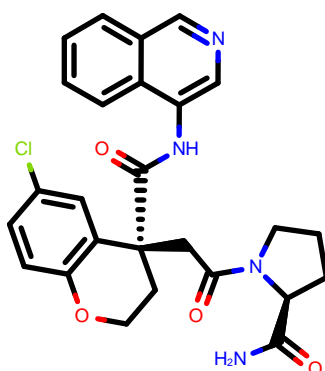
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCCC(=O)NCS

RUN: RUN5721

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.25

EN300-07127_1_1



CID: EN300-07127_1_1

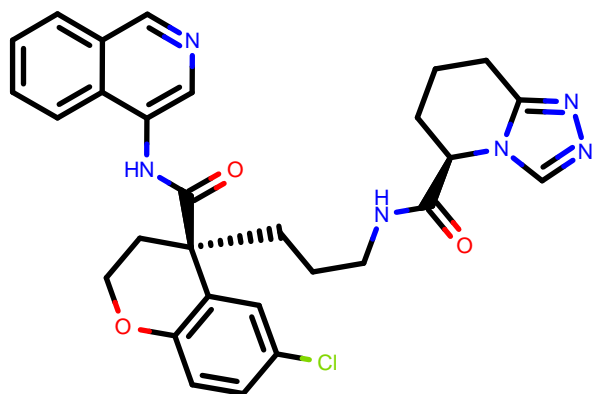
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5C(=O)N

RUN: RUN10153

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.26

EN300-6478631_4_2



CID: EN300-6478631_4_2

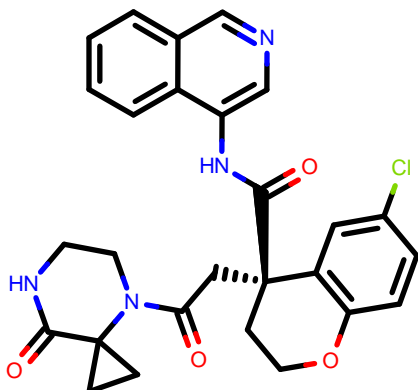
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC6N6

RUN: RUN8783

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.23

EN300-1067786_1_1



CID: EN300-1067786_1_1

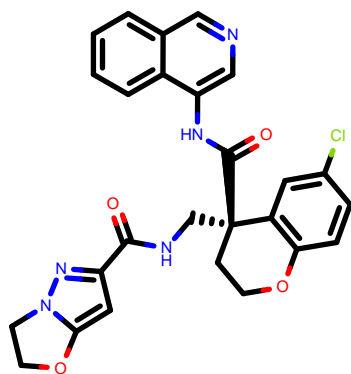
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)[C@H]5C6C6

RUN: RUN13534

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.27

EN300-181688_2_1



CID: EN300-181688_2_1

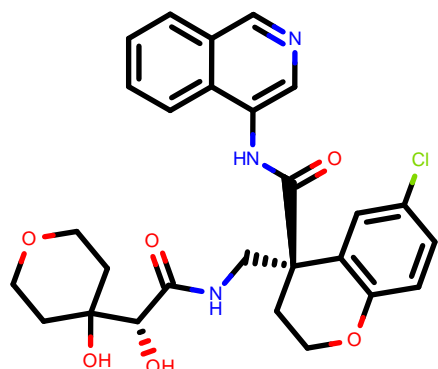
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5ccn(n5)CCO6

RUN: RUN3359

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.20

EN300-749499_2_1



CID: EN300-749499_2_1

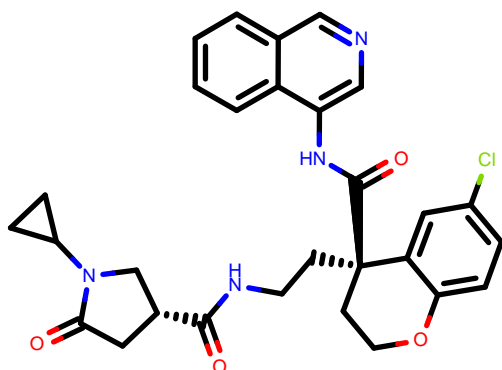
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]H(C5(CCOCC5)O)O

RUN: RUN5203

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.33

EN300-12440_3_1



CID: EN300-12440_3_1

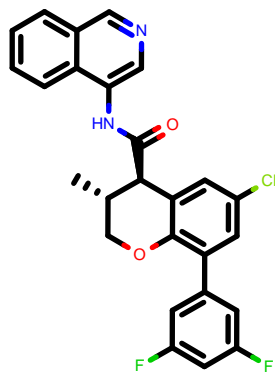
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]H5C(CO)N(C5)C6C6

RUN: RUN15212

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.30

DAR-DIA-0d514e7d-17_1



CID: DAR-DIA-0d514e7d-17_1

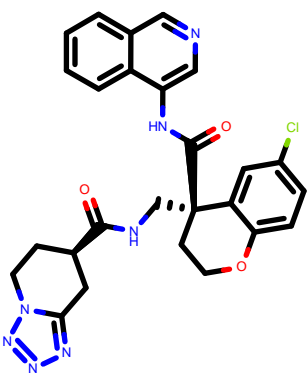
SMILES: C[C@@H]1COc2c(ccc2[C@@]H1C(=O)Nc3nc4c3cccc4)C)c5cc(cc5)F)F

RUN: RUN225

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.21

EN300-1653482_2_2



CID: EN300-1653482_2_2

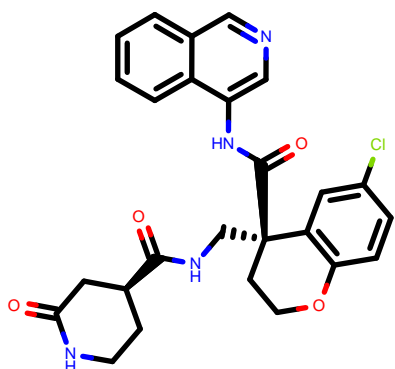
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5Cn6c(nnn6)C5

RUN: RUN6601

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.25

EN300-107493_2_1



CID: EN300-107493_2_1

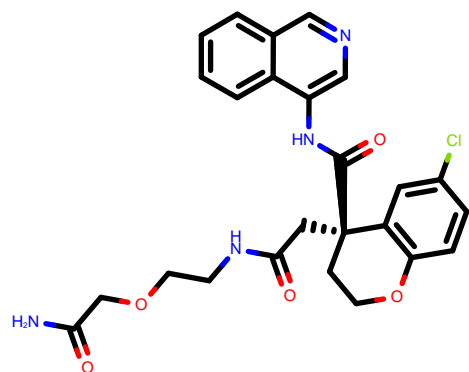
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCNCC(=O)C5

RUN: RUN6067

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.22

EN300-108305_1_1



CID: EN300-108305_1_1

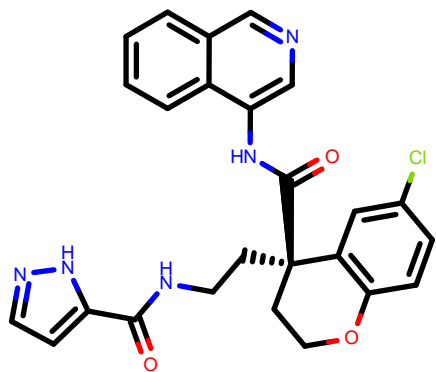
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCOCC(=O)N

RUN: RUN5889

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.32

EN300-37077_3_1



CID: EN300-37077_3_1

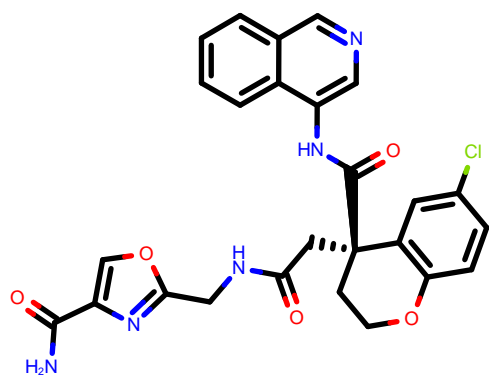
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccn[nH]5

RUN: RUN15286

DDG (kcal/mol): -0.21

dDDG (kcal/mol): 0.19

EN300-266460_1_1



CID: EN300-266460_1_1

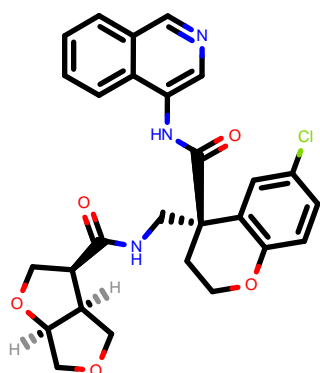
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCCOc4c3cc(cc4)Cl)CC(=O)NCc5nc(cc5)C(=O)N

RUN: RUN4177

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.21

EN300-6482296_2_1



CID: EN300-6482296_2_1

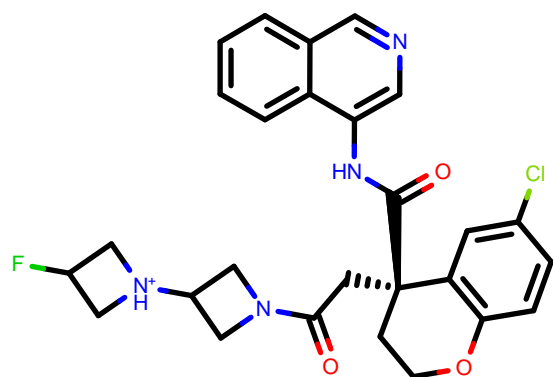
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CO)C@H(C)C@H5COO6

RUN: RUN7085

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-6731820_1_1



CID: EN300-6731820_1_1

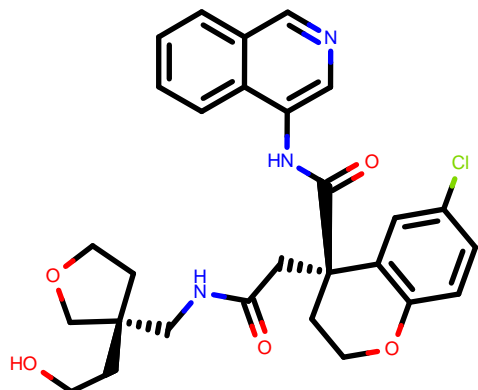
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[NH+]6CC(C6)F

RUN: RUN13088

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-105829_1_1



CID: EN300-105829_1_1

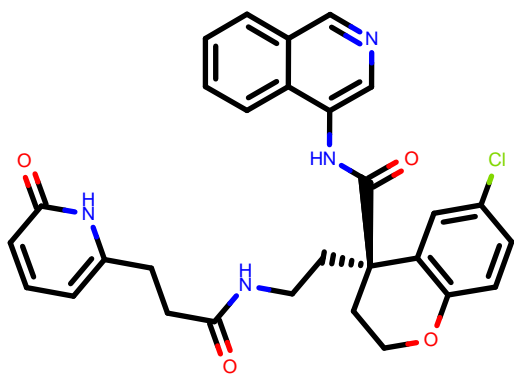
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(C)COC5)CCO

RUN: RUN10465

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.21

EN300-6491697_3_1



CID: EN300-6491697_3_1

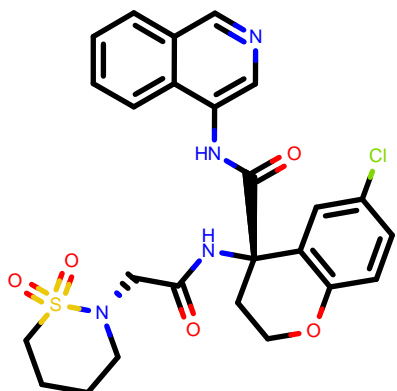
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)CCc5ccoc(=O)[nH]5

RUN: RUN4881

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.30

EN300-378836_1_2



CID: EN300-378836_1_2

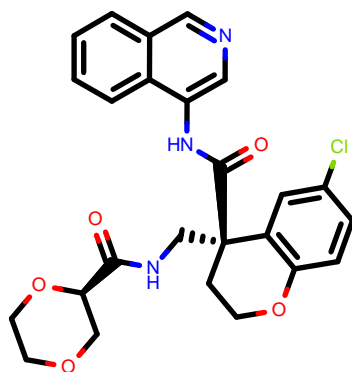
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)N[C@@]5CCCCS(=O)=O

RUN: RUN5158

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.29

EN300-36158_2_2



CID: EN300-36158_2_2

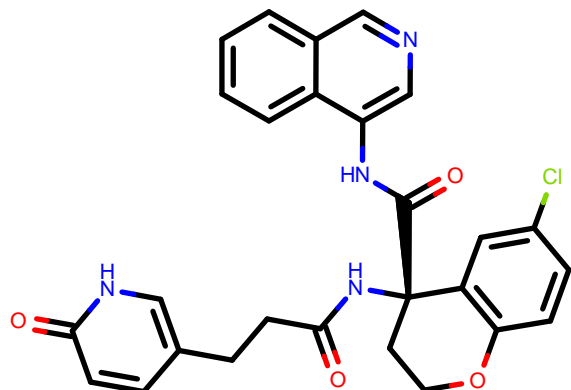
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@@H]5COCOC5

RUN: RUN2416

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.20

EN300-187385_1_1



CID: EN300-187385_1_1

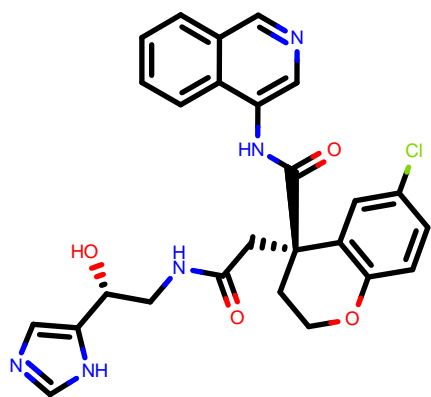
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)CCc5ccoc(=O)[nH]5

RUN: RUN6193

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.23

EN300-384557_1_1



CID: EN300-384557_1_1

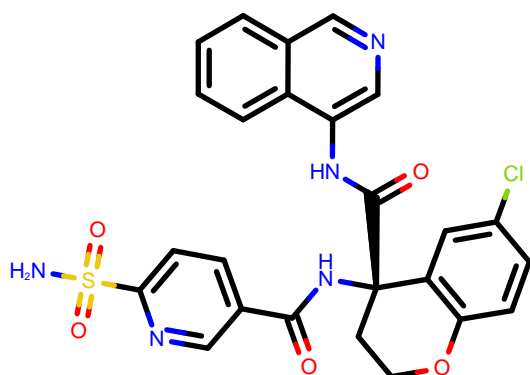
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@H](c5cn[nH]5)O

RUN: RUN3709

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.28

EN300-120480_1_1



CID: EN300-120480_1_1

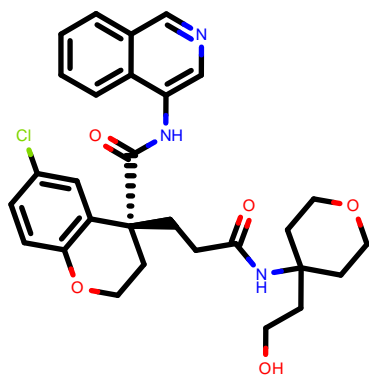
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc[nH]5S(=O)(=O)N

RUN: RUN7092

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.34

EN300-300825_2_1



CID: EN300-300825_2_1

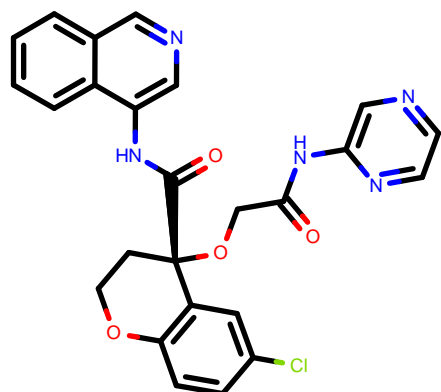
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCOCC5OCCO

RUN: RUN680

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.29

EN300-105267_1_1



CID: EN300-105267_1_1

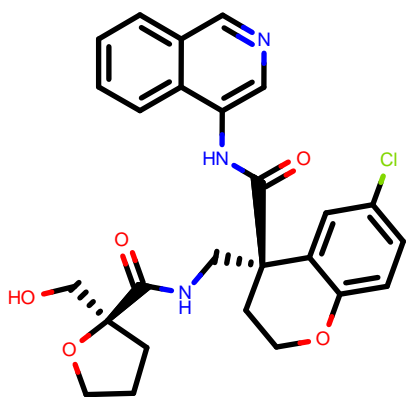
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5ccncc5

RUN: RUN1813

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.29

EN300-1425677_2_1



CID: EN300-1425677_2_1

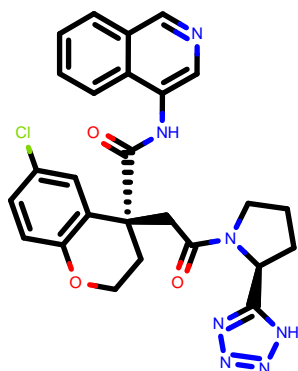
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C@H5(CCCO5)CO

RUN: RUN2250

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.31

EN300-2908043_1_1



CID: EN300-2908043_1_1

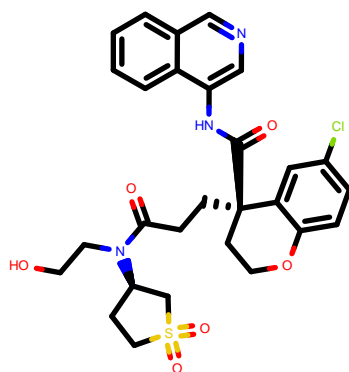
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5c6n[nH]n6

RUN: RUN9949

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.25

EN300-10673_2_1



CID: EN300-10673_2_1

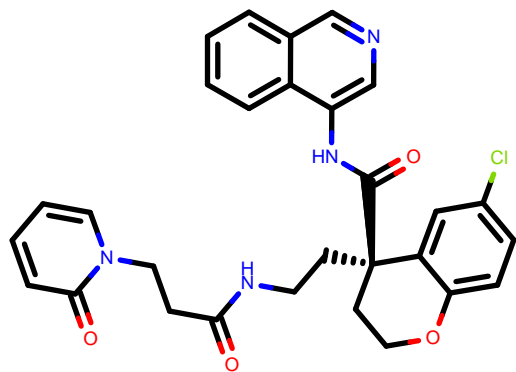
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCS(=O)(=O)C)C5

RUN: RUN10160

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.52

EN300-36622_3_1



CID: EN300-36622_3_1

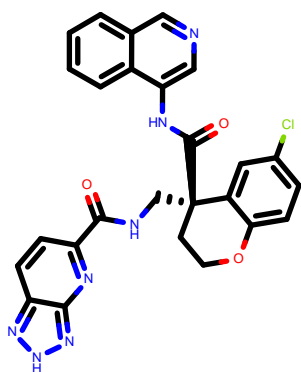
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cccc5=O

RUN: RUN14330

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.32

EN300-133058_2_1



CID: EN300-133058_2_1

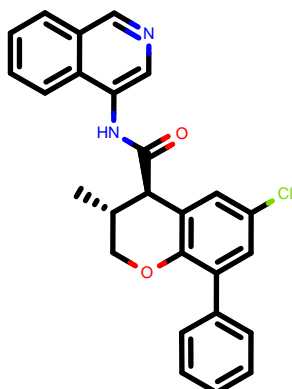
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6c(n5)n[nH]6

RUN: RUN3275

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.23

DAR-DIA-0d514e7d-9_1



CID: DAR-DIA-0d514e7d-9_1

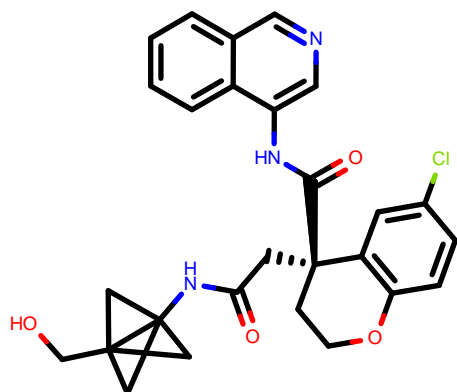
SMILES: C[C@H]1COc2c(cc2[C@@H]1C(=O)Nc3cnc4c3cccc4)Cl)c5ccccc5

RUN: RUN220

DDG (kcal/mol): -0.20

dDDG (kcal/mol): 0.18

EN300-6478040_1_1



CID: EN300-6478040_1_1

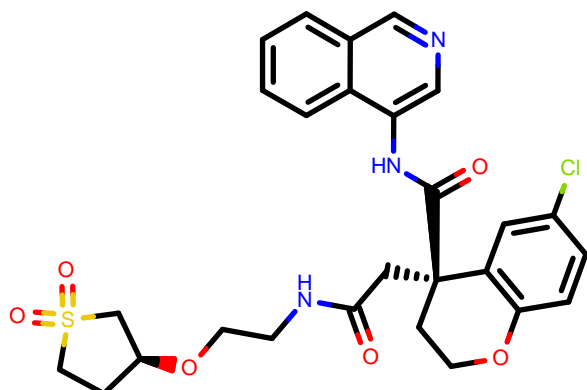
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC56CC(C5)(C6)CO

RUN: RUN12910

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.19

EN300-6474933_1_2



CID: EN300-6474933_1_2

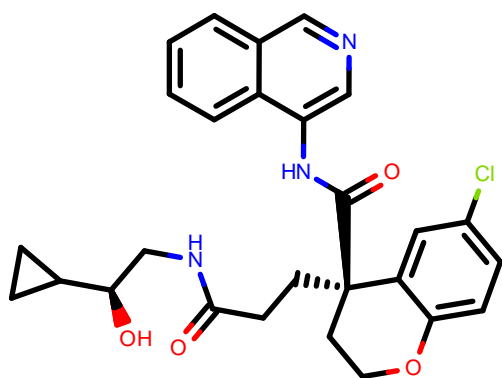
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCO[C@@H]5CCS(C5)(=O)C5

RUN: RUN11779

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.30

EN300-67533_2_1



CID: EN300-67533_2_1

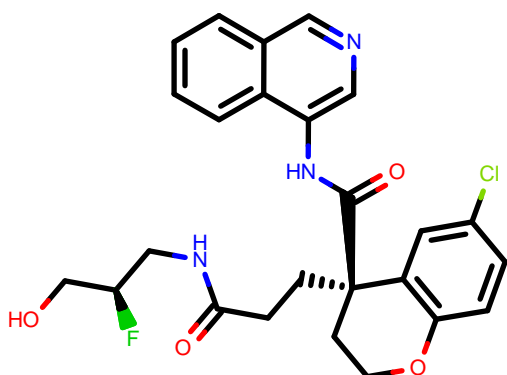
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H](C5CC5)O

RUN: RUN4836

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-7353973_2_2



CID: EN300-7353973_2_2

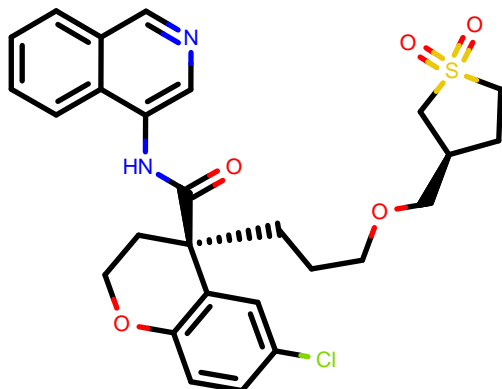
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H](CO)F

RUN: RUN2298

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.26

EN300-1448603_4_1



CID: EN300-1448603_4_1

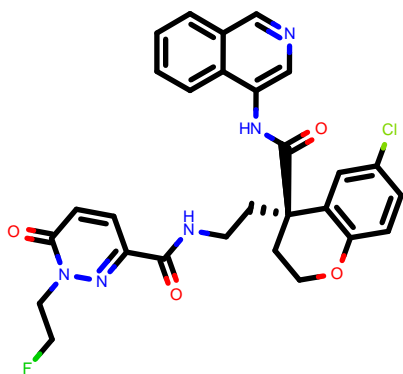
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@]5H5CCS(=O)(=O)C5

RUN: RUN1515

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.29

EN300-263456_3_1



CID: EN300-263456_3_1

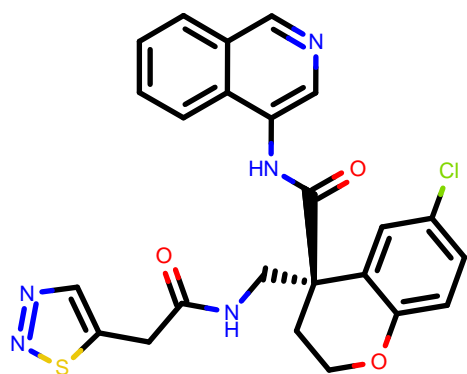
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccc(=O)n(n5)CCF

RUN: RUN14482

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.25

EN300-260152_2_1



CID: EN300-260152_2_1

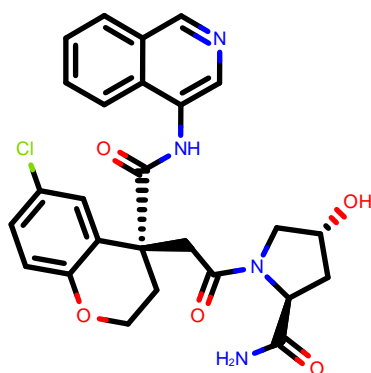
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5cnns5

RUN: RUN5671

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.21

EN300-07752_1_2



CID: EN300-07752_1_2

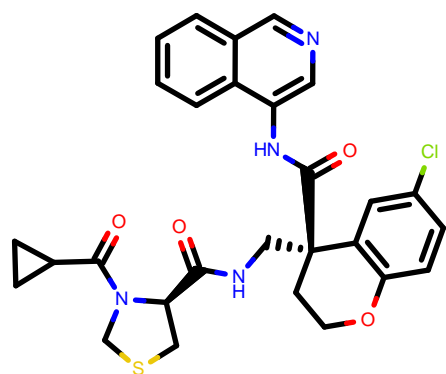
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(C1=O)N5C[C@@H](C1)H5C1=O)N1

RUN: RUN7059

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

EN300-18928_2_2



CID: EN300-18928_2_2

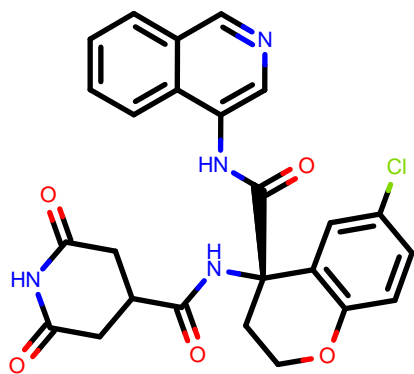
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CSCN5C(=O)C6CC6

RUN: RUN3695

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.26

EN300-62192_1_1



CID: EN300-62192_1_1

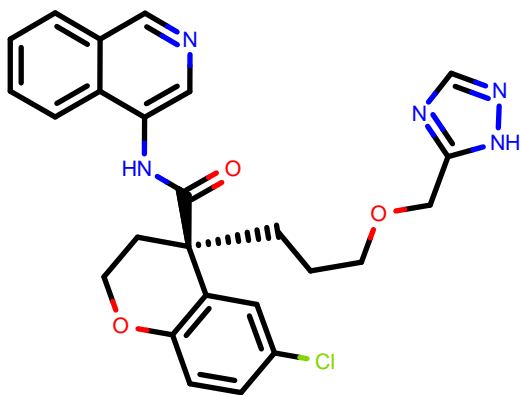
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CC(=O)NC(=O)C5

RUN: RUN9313

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.24

EN300-306316_4_1



CID: EN300-306316_4_1

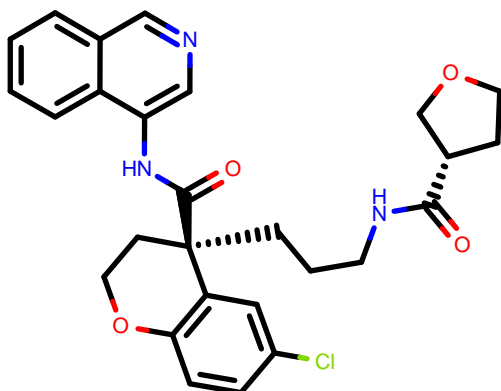
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOc5[nH]jncn5

RUN: RUN1227

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.19

EN300-53423_4_2



CID: EN300-53423_4_2

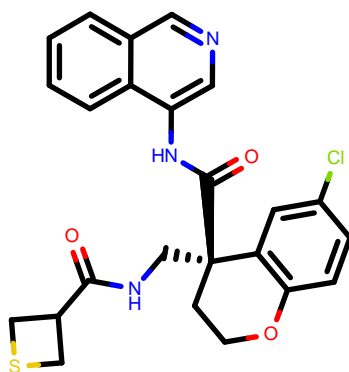
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5

RUN: RUN11824

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.20

EN300-95094_2_1



CID: EN300-95094_2_1

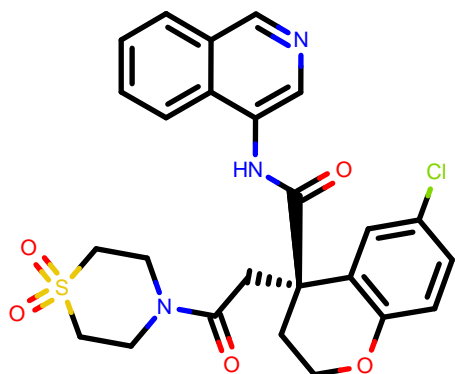
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CSC5

RUN: RUN1268

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.20

EN300-67050_1_1



CID: EN300-67050_1_1

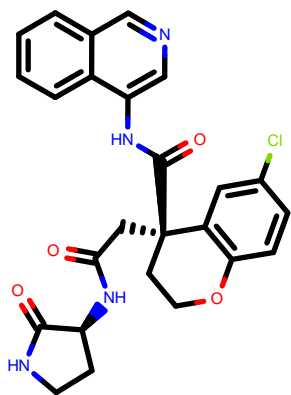
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)CC5

RUN: RUN5305

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.25

EN300-298184_1_1



CID: EN300-298184_1_1

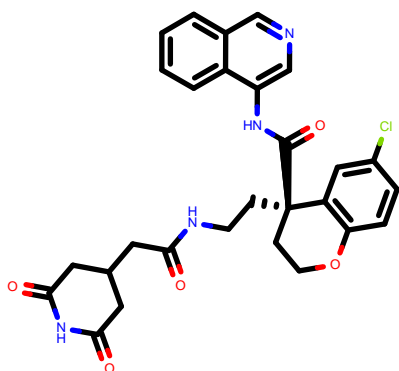
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@H]5CCNC5=O

RUN: RUN3777

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.20

EN300-225165_3_1



CID: EN300-225165_3_1

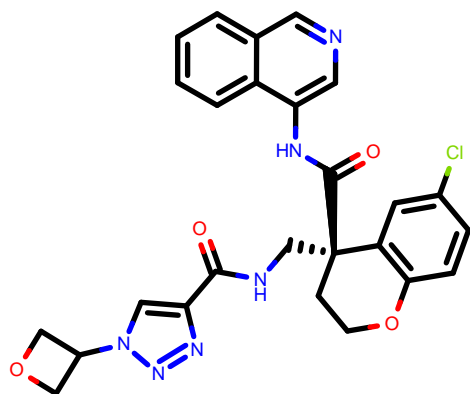
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC5CC(=O)NC(=O)C5

RUN: RUN15201

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

EN300-1696043_2_1



CID: EN300-1696043_2_1

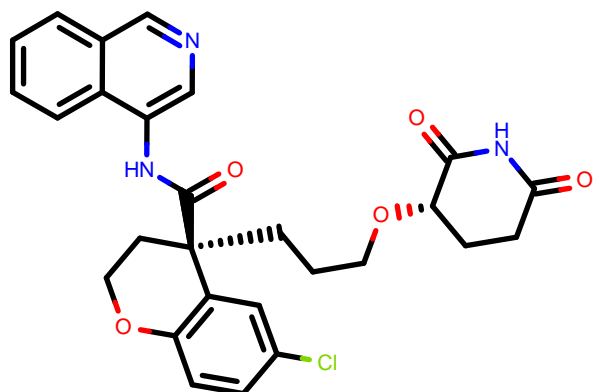
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn(nn5)C6COC6

RUN: RUN3343

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.26

EN300-120920_4_1



CID: EN300-120920_4_1

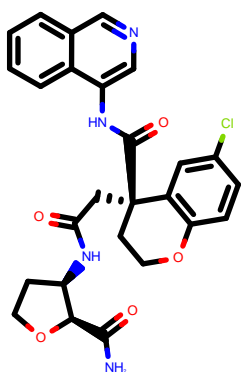
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCCO[C@@H]5CCCC(=O)NC5=O

RUN: RUN2193

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.21

EN300-7435545_1_1



CID: EN300-7435545_1_1

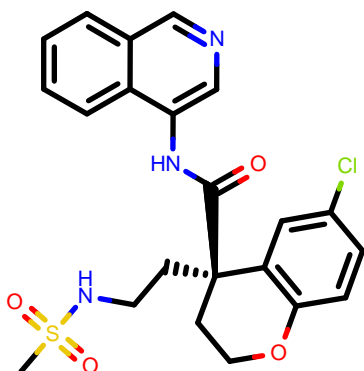
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4ccc(cc4)Cl)CC(=O)NC@@H5CCO[C@@H]5Cl-OH

RUN: RUN12446

DDG (kcal/mol): -0.19

dDDG (kcal/mol): 0.27

DAR-DIA-6a508060-13_1



CID: DAR-DIA-6a508060-13_1

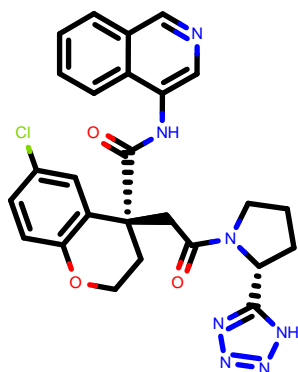
SMILES: CS(=O)(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3ncc4c3ccc4

RUN: RUN153

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-195173_1_1



CID: EN300-195173_1_1

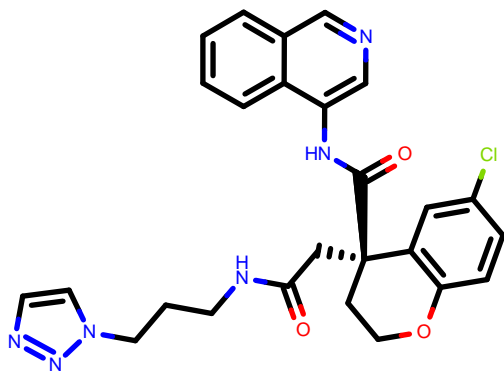
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5c6n[n-]n6

RUN: RUN4973

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.21

EN300-1698650_1_1



CID: EN300-1698650_1_1

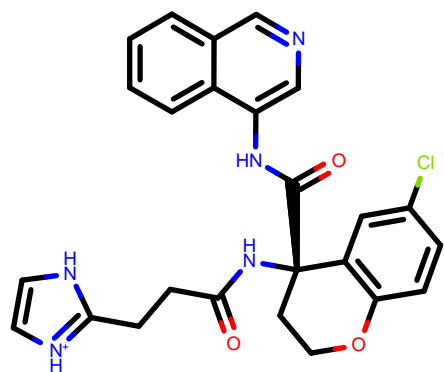
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCc5cnn5

RUN: RUN12098

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.21

EN300-188650_1_1



CID: EN300-188650_1_1

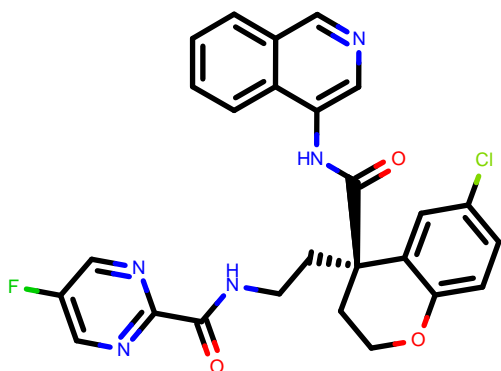
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5[nH]cd[nH+]5

RUN: RUN7112

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-149296_3_1



CID: EN300-149296_3_1

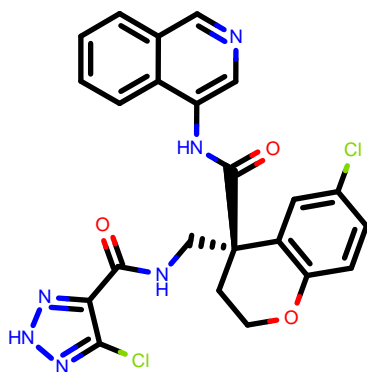
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ncnc(n5)F

RUN: RUN15517

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.20

EN300-149013_2_1



CID: EN300-149013_2_1

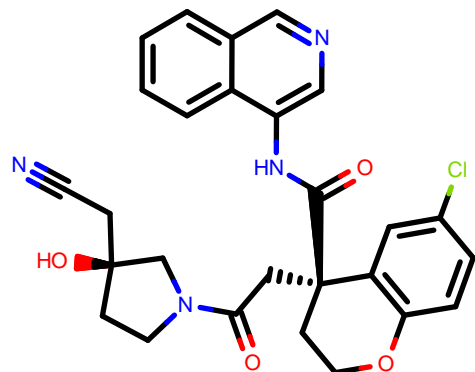
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c[nH]n5Cl

RUN: RUN8189

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-257405_1_1



CID: EN300-257405_1_1

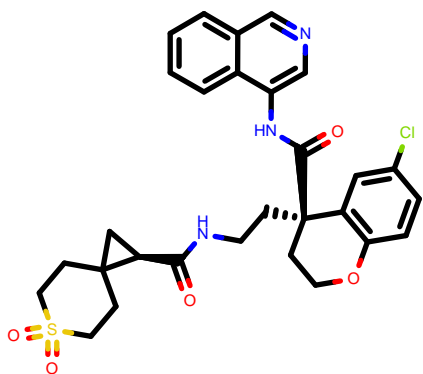
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]3(C5)CC#N

RUN: RUN3221

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.23

EN300-141809_3_1



CID: EN300-141809_3_1

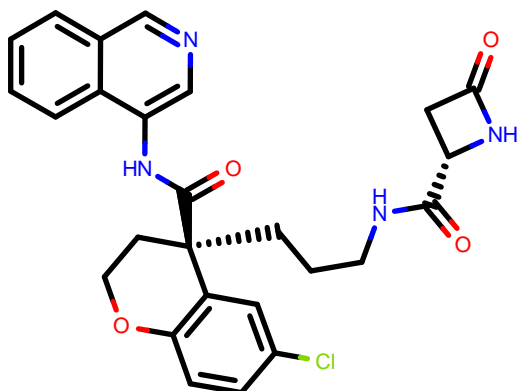
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C56C5(-O)-O5C6

RUN: RUN15326

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.35

EN300-103219_4_1



CID: EN300-103219_4_1

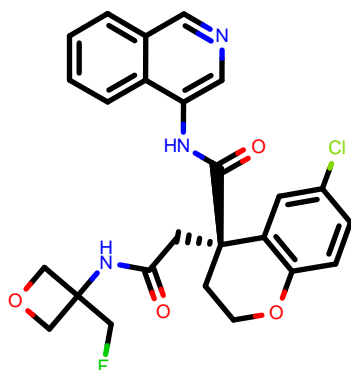
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)N5

RUN: RUN13497

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.22

EN300-6970573_1_1



CID: EN300-6970573_1_1

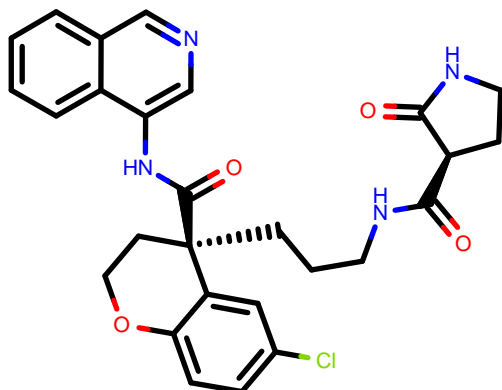
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(COC5)CF

RUN: RUN13024

DDG (kcal/mol): -0.18

dDDG (kcal/mol): 0.31

EN300-94945_4_1



CID: EN300-94945_4_1

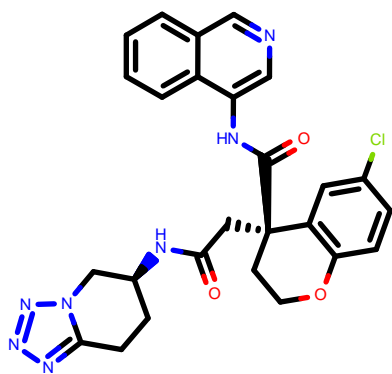
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCNC5=O

RUN: RUN11969

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-7444106_1_2



CID: EN300-7444106_1_2

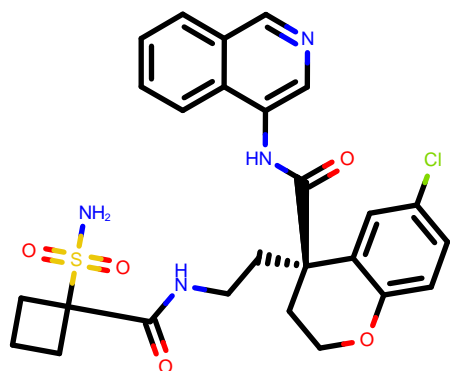
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCc6nnnn6C5

RUN: RUN11337

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-1440321_3_1



CID: EN300-1440321_3_1

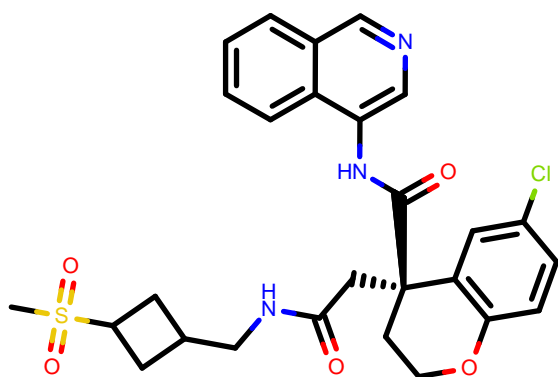
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)S(=O)(=O)N

RUN: RUN4897

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.28

EN300-7562761_1_1



CID: EN300-7562761_1_1

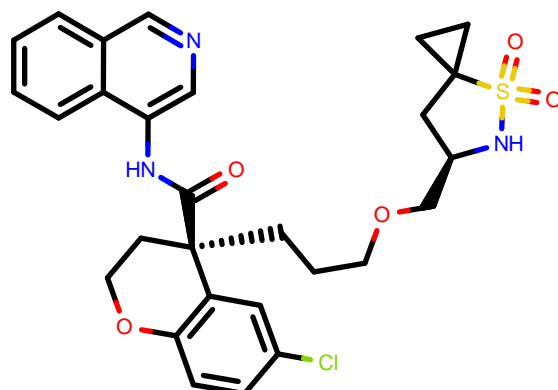
SMILES: CS(=O)(=O)[C@@H]1C[C@@H](C1)CNC(=O)[C@@]2(C3c4ccc(c3)Cl)OCC2(C)=O)Nc4c5cnc4ccccc5

RUN: RUN6991

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.22

EN300-6504697_4_1



CID: EN300-6504697_4_1

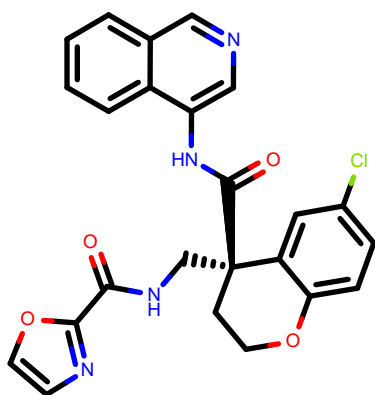
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CC6CC6S(=O)(=O)N5

RUN: RUN1435

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.29

EN300-318344_2_1



CID: EN300-318344_2_1

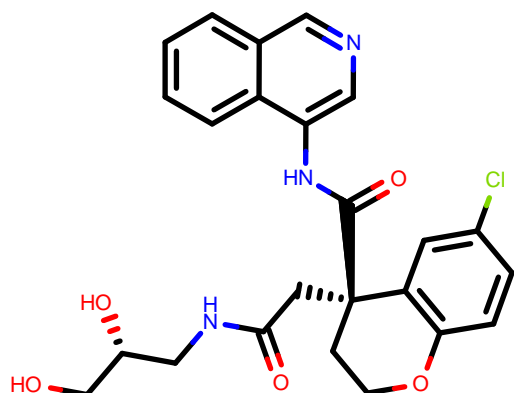
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5ncco5

RUN: RUN2798

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-50845_1_2



CID: EN300-50845_1_2

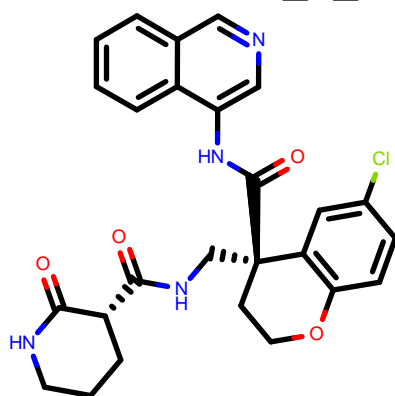
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@H](CO)O

RUN: RUN6647

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.33

EN300-82616_2_1



CID: EN300-82616_2_1

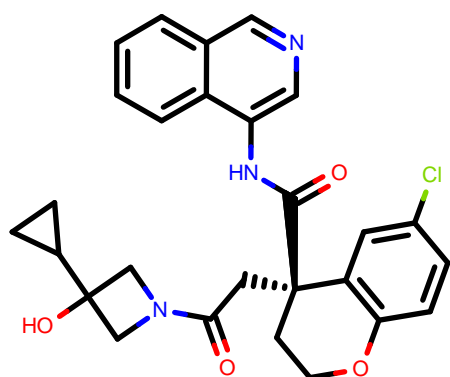
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]4H[C@@H]5CCNCC5=O

RUN: RUN7697

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.27

EN300-126127_1_1



CID: EN300-126127_1_1

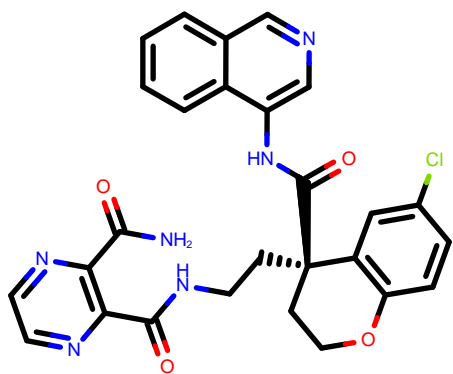
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)C6CC6O

RUN: RUN7867

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.23

EN300-21200_3_1



CID: EN300-21200_3_1

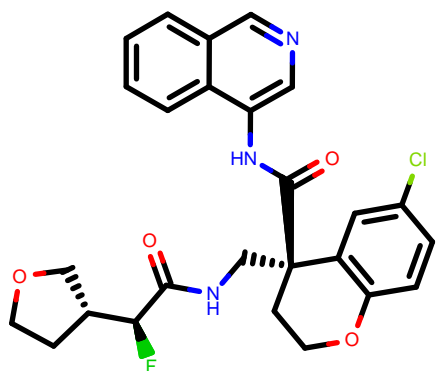
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c(ncn5)C(=O)N

RUN: RUN5085

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.28

EN300-783124_2_2



CID: EN300-783124_2_2

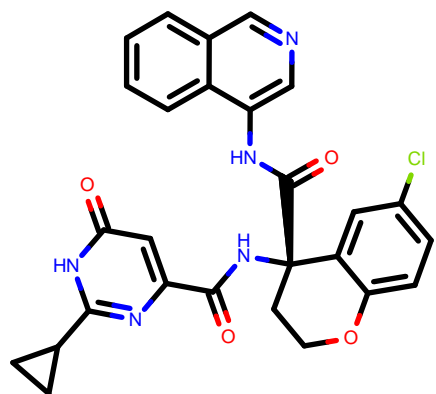
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]([C@@H]5CCOC5)F

RUN: RUN6063

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.26

EN300-204239_1_1



CID: EN300-204239_1_1

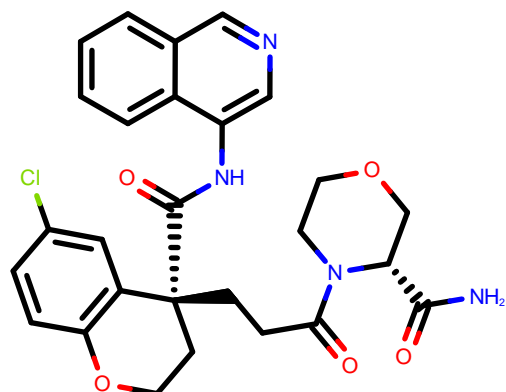
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]c6c5C6C6

RUN: RUN3510

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.23

EN300-124383_2_2



CID: EN300-124383_2_2

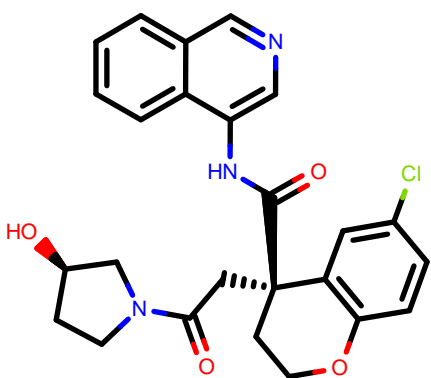
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@@H]5C(=O)N

RUN: RUN4144

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.28

EN300-69313_1_1



CID: EN300-69313_1_1

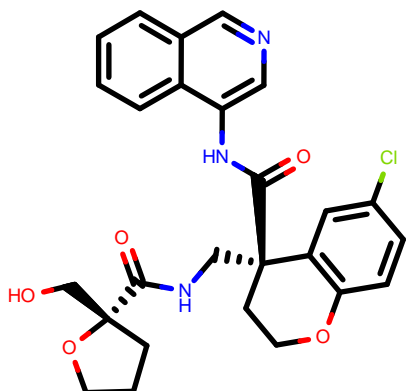
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@H](C5)O

RUN: RUN1679

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-1425677_2_2



CID: EN300-1425677_2_2

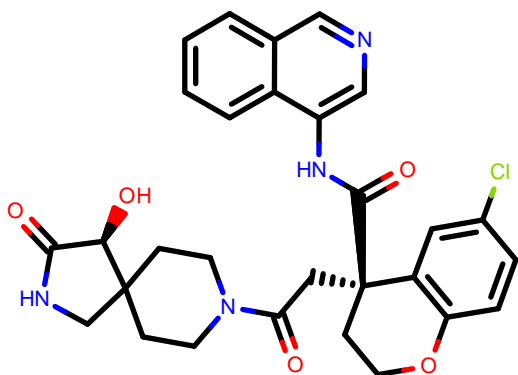
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5(CCCO5)CO

RUN: RUN5119

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.26

EN300-6478434_1_1



CID: EN300-6478434_1_1

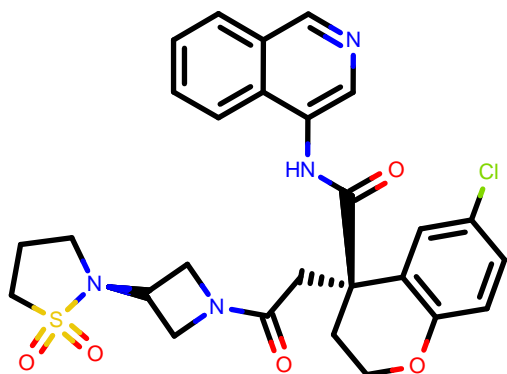
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(C1=O)N5CC(C5)N[C@@]6(C)C1

RUN: RUN10265

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.31

EN300-1272295_1_2



CID: EN300-1272295_1_2

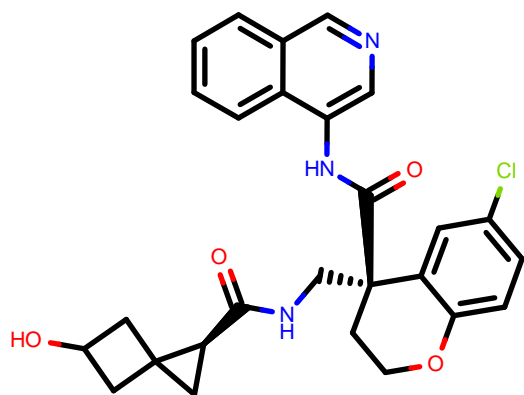
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(C1=O)N5CC(C5)N[C@@]6(C)C1

RUN: RUN4429

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.26

EN300-1717166_2_2



CID: EN300-1717166_2_2

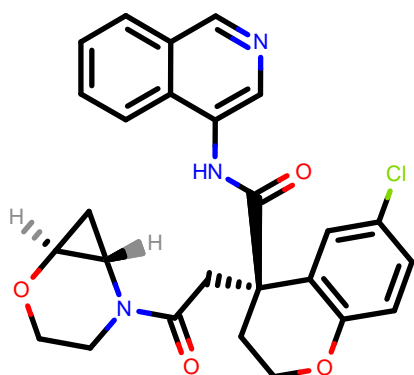
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC56CC(C6)O

RUN: RUN6445

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.20

EN300-91609_1_4



CID: EN300-91609_1_4

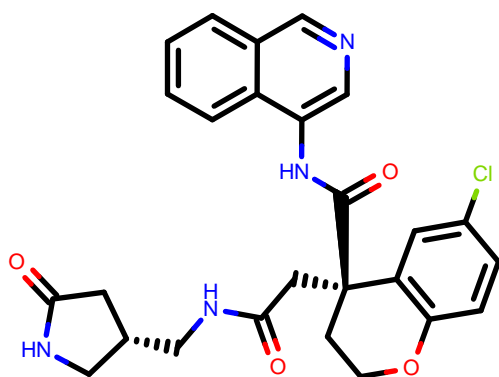
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H]6[C@@H]5C6

RUN: RUN10133

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.18

EN300-238405_1_2



CID: EN300-238405_1_2

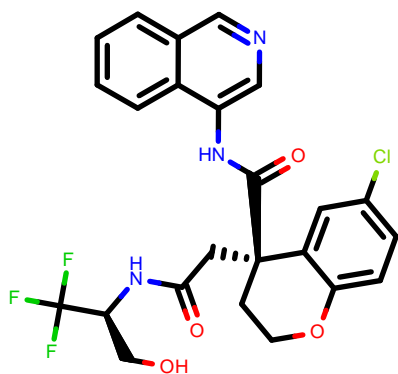
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@H]5CC(=O)N5C5

RUN: RUN1535

DDG (kcal/mol): -0.17

dDDG (kcal/mol): 0.22

EN300-142130_1_1



CID: EN300-142130_1_1

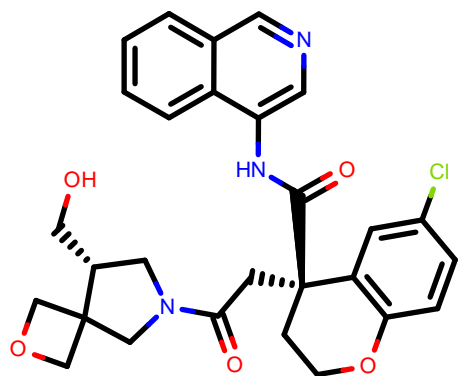
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CO)C(F)F

RUN: RUN8063

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.34

EN300-395654_1_2



CID: EN300-395654_1_2

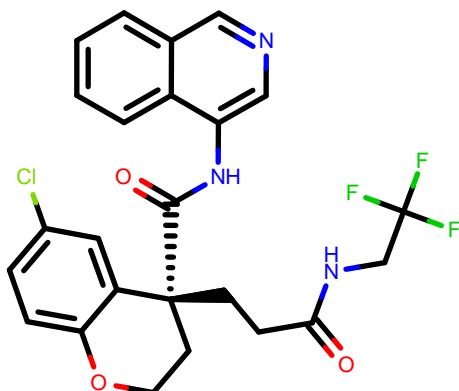
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C6(C5)COC6)CO

RUN: RUN12522

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.19

JAG-UCB-706446eb-1_1



CID: JAG-UCB-706446eb-1_1

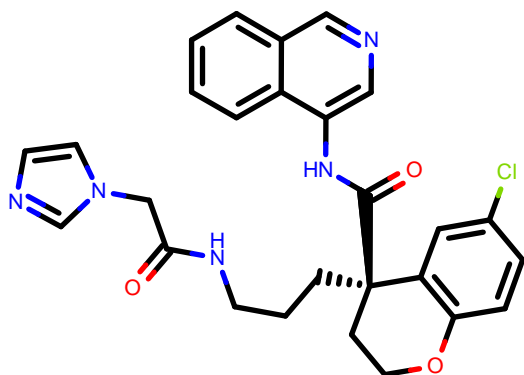
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N(C(F)(F)F)F

RUN: RUN235

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.20

EN300-38979_4_1



CID: EN300-38979_4_1

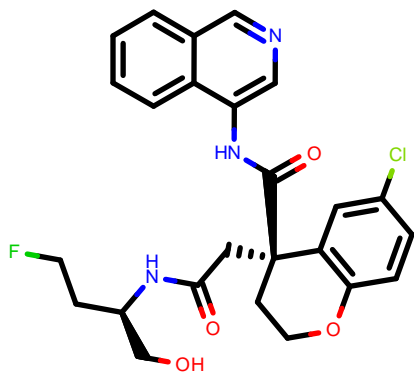
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCN(C=O)Cn5cnc5

RUN: RUN7898

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.22

EN300-175608_1_2



CID: EN300-175608_1_2

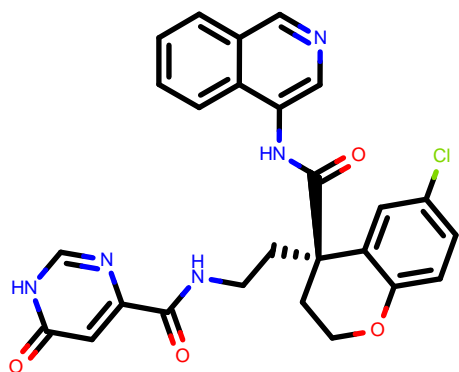
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CC(F)CO)CO

RUN: RUN6248

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-817811_3_1



CID: EN300-817811_3_1

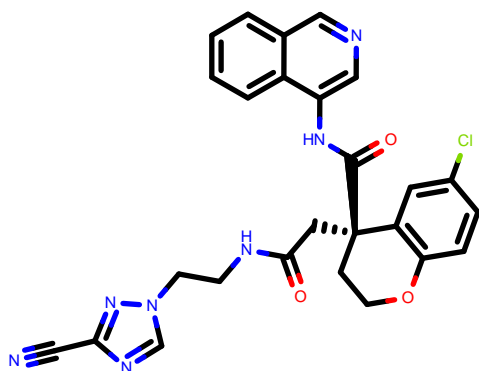
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc(=O)[nH]cn5

RUN: RUN14454

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.28

EN300-210104_1_1



CID: EN300-210104_1_1

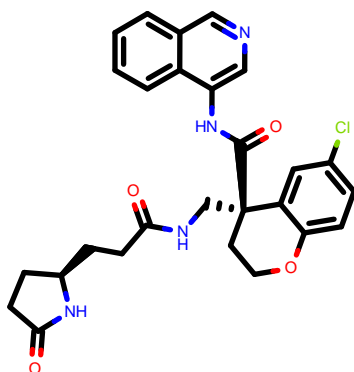
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncn(c5)C#N

RUN: RUN10908

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.27

EN300-104592_2_2



CID: EN300-104592_2_2

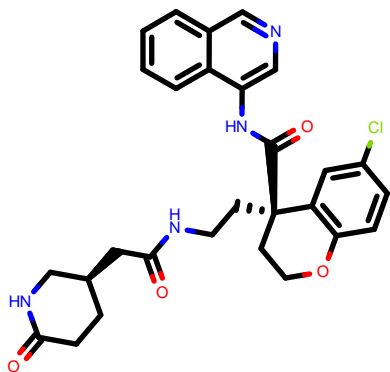
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CC[C@@]5H5CCC(=O)N5

RUN: RUN5455

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.24

EN300-246992_3_2



CID: EN300-246992_3_2

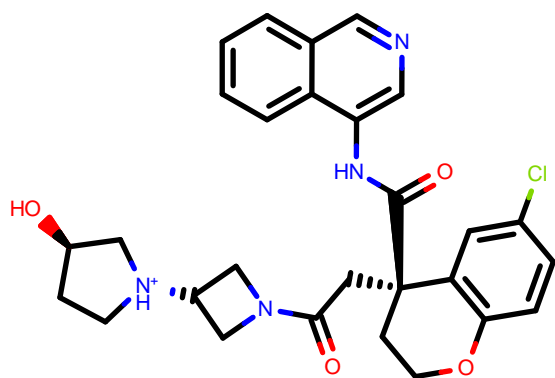
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5H5CCC(=O)N5

RUN: RUN11289

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.30

EN300-260405_1_3



CID: EN300-260405_1_3

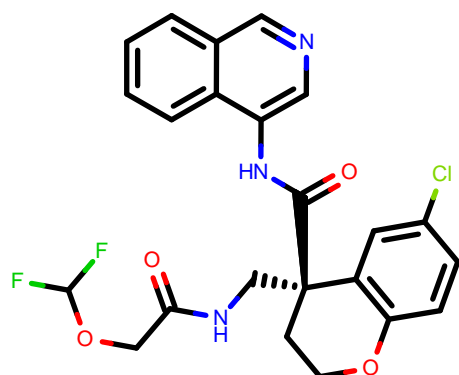
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)[N+](H)CC[C@@H](C)O

RUN: RUN13930

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.27

EN300-179091_2_1



CID: EN300-179091_2_1

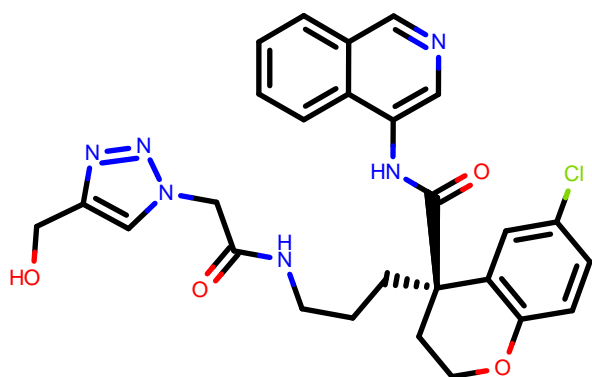
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)COC(F)F

RUN: RUN4595

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.21

EN300-108236_4_1



CID: EN300-108236_4_1

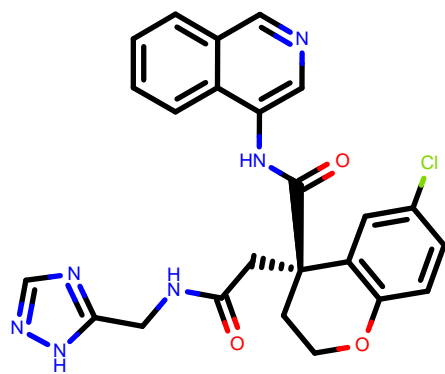
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)Cn5cc(nn5)CO

RUN: RUN9359

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

EN300-43972_1_1



CID: EN300-43972_1_1

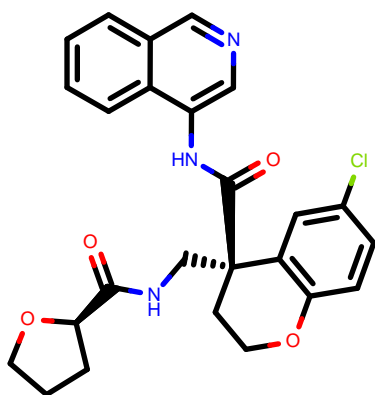
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5[nH]n5

RUN: RUN1391

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.21

EN300-21009_2_2



CID: EN300-21009_2_2

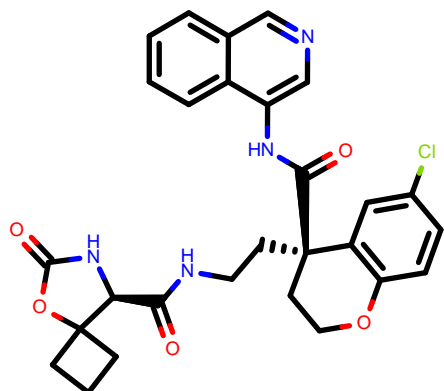
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCOC5

RUN: RUN3591

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.19

EN300-7432415_3_2



CID: EN300-7432415_3_2

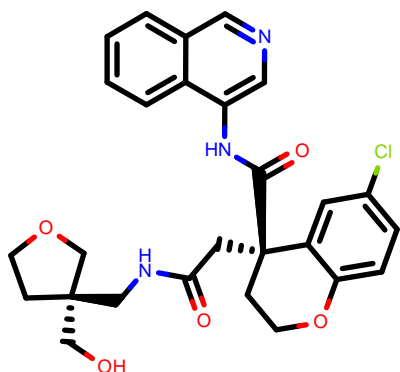
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5C6(CCC6)OC1=O)N5

RUN: RUN4957

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.23

EN300-682529_1_2



CID: EN300-682529_1_2

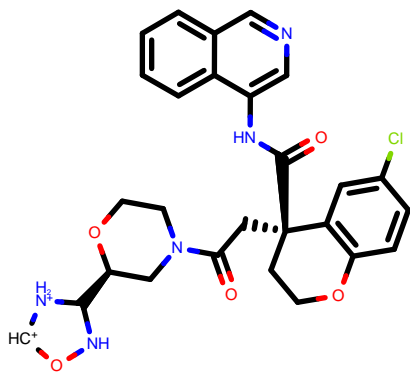
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@]5(CCOc5)CO

RUN: RUN10383

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.27

EN300-131690_1_2



CID: EN300-131690_1_2

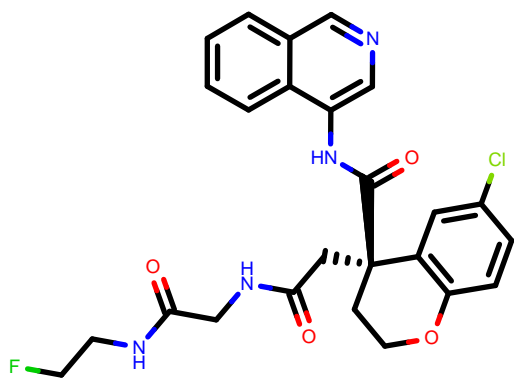
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCO[C@@]H(C5)c6nc[nH+]6

RUN: RUN8760

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.25

EN300-196612_1_1



CID: EN300-196612_1_1

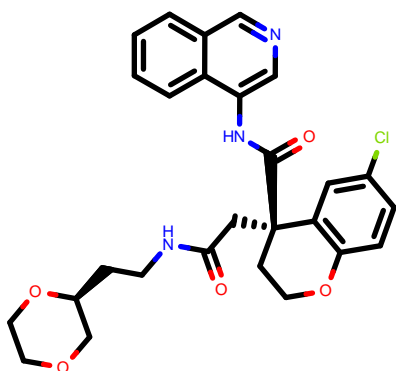
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC(=O)NCCF

RUN: RUN10207

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

EN300-1600887_1_1



CID: EN300-1600887_1_1

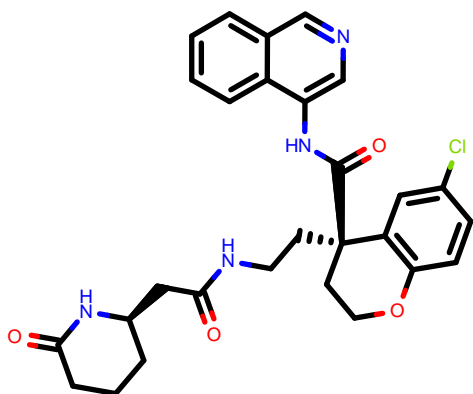
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC[C@H]5OCCO5

RUN: RUN9846

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.26

EN300-210084_3_1



CID: EN300-210084_3_1

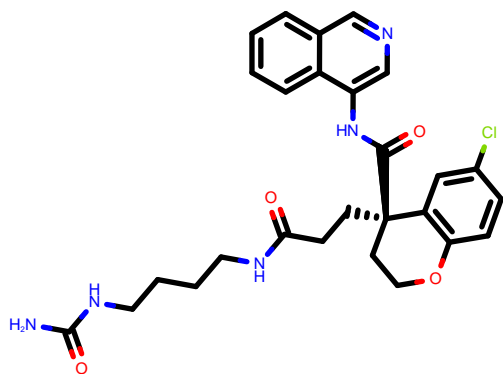
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCC(=O)N5

RUN: RUN14220

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.35

EN300-79606_2_1



CID: EN300-79606_2_1

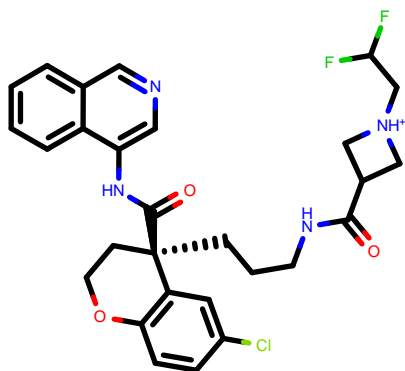
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCNC(=O)N

RUN: RUN14185

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.24

EN300-182579_4_1



CID: EN300-182579_4_1

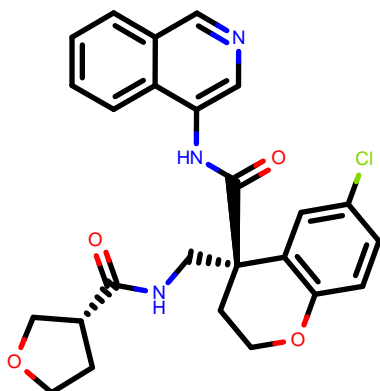
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5CN(C5)CC(F)F

RUN: RUN11682

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.32

EN300-53423_2_1



CID: EN300-53423_2_1

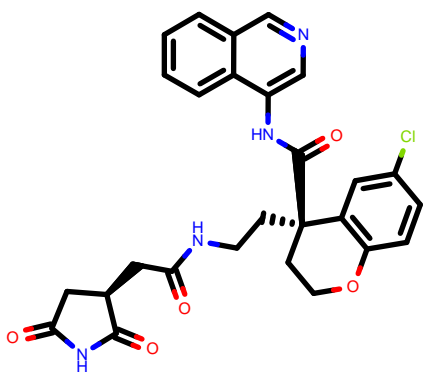
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@@]5C@H5CCOC5

RUN: RUN5667

DDG (kcal/mol): -0.16

dDDG (kcal/mol): 0.21

EN300-227055_3_2



CID: EN300-227055_3_2

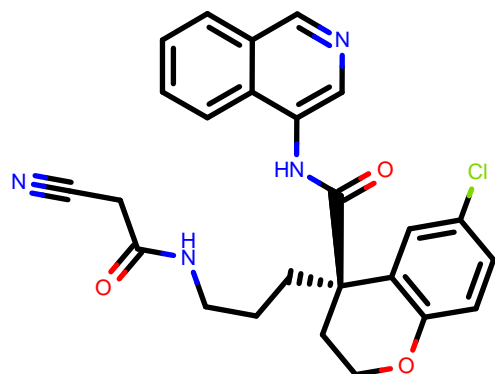
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C[C@@]5C@H5C(=O)NC5=O

RUN: RUN14166

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.28

EN300-19926_4_1



CID: EN300-19926_4_1

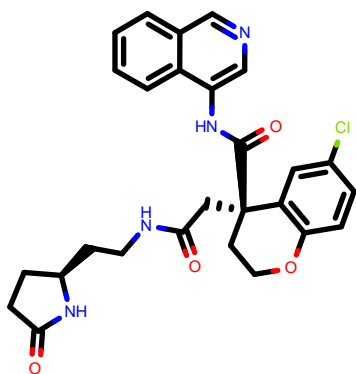
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CC#N

RUN: RUN10676

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.19

EN300-205779_1_2



CID: EN300-205779_1_2

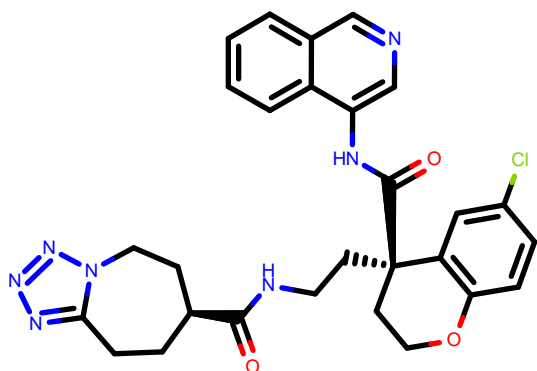
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC[C@@]5H5CCC(=O)N5

RUN: RUN3509

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.31

EN300-253571_3_2



CID: EN300-253571_3_2

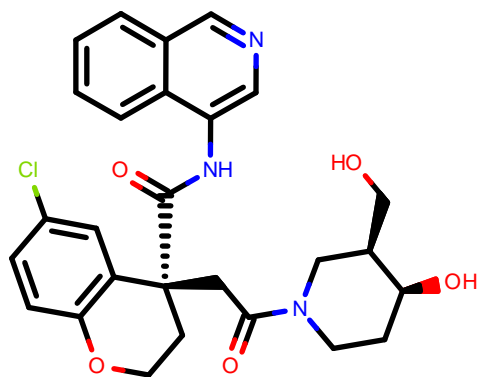
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5H5CCc6nnc6C5

RUN: RUN15171

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.30

EN300-233678_1_3



CID: EN300-233678_1_3

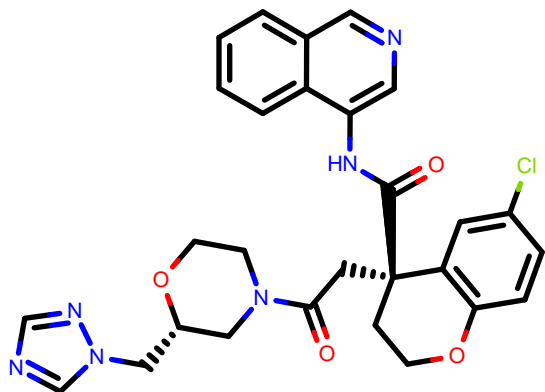
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@]5H[C@@]5(O)C5(O)

RUN: RUN1303

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.25

EN300-80241_1_2



CID: EN300-80241_1_2

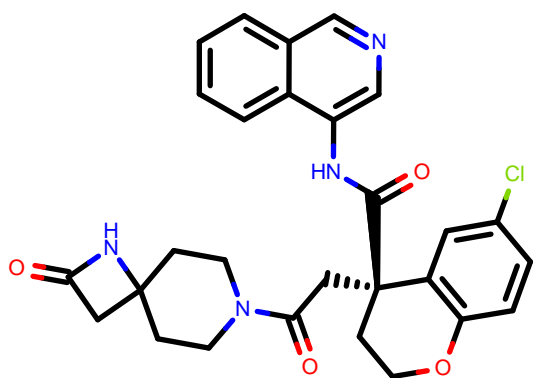
SMILES: c1ccc2c(c1)nc(=O)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@]5H[C@@]5Cn6cn6

RUN: RUN5509

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-52210_1_1



CID: EN300-52210_1_1

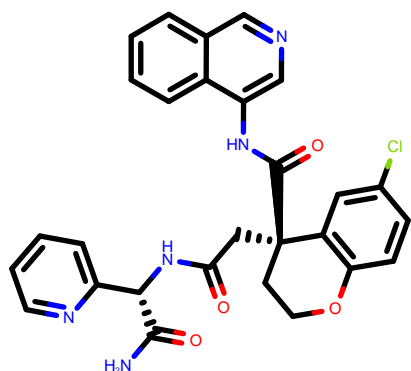
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC6(CC5)CC(=O)N6

RUN: RUN10509

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.25

EN300-225920_1_1



CID: EN300-225920_1_1

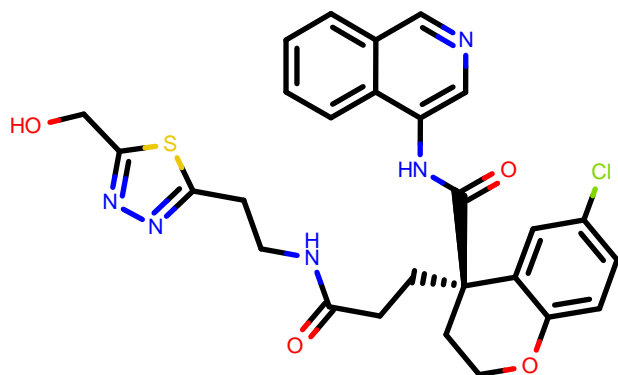
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5CNC6=CC=CC=C6

RUN: RUN13696

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-7549247_2_1



CID: EN300-7549247_2_1

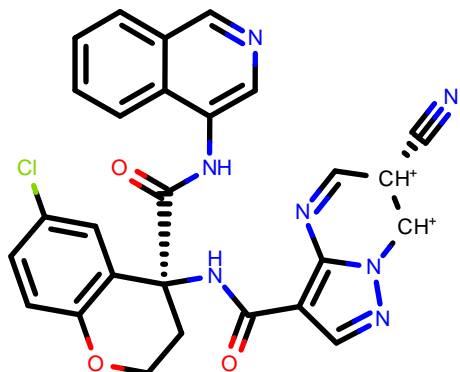
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCc5nnc(s5)CO

RUN: RUN13673

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-255990_1_1



CID: EN300-255990_1_1

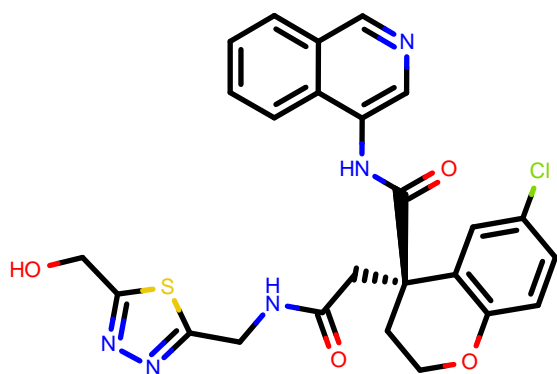
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5ncc(s6)C#N

RUN: RUN9197

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.22

EN300-7550655_1_1



CID: EN300-7550655_1_1

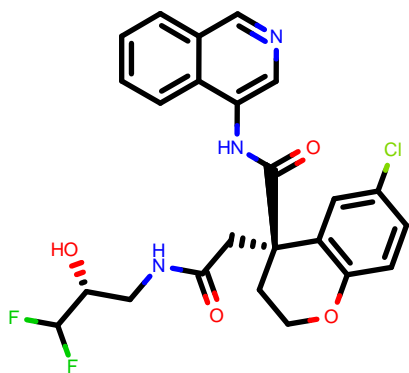
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCc5nn(s5)CO

RUN: RUN10956

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.22

EN300-175160_1_2



CID: EN300-175160_1_2

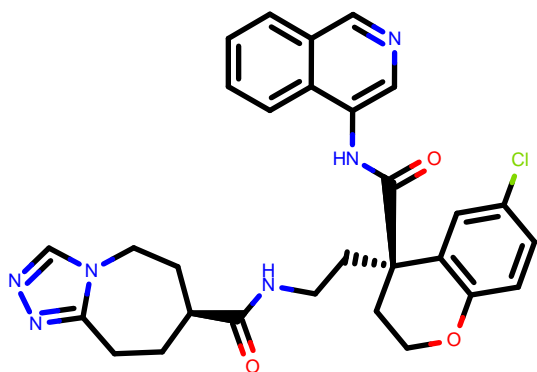
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@H](C(F)F)O

RUN: RUN11603

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.42

EN300-366687_3_2



CID: EN300-366687_3_2

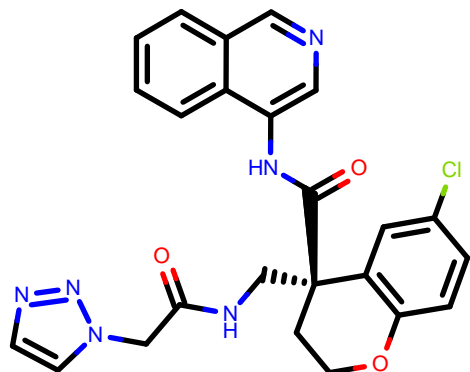
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)[C@H]5CCc6nnnc6C5

RUN: RUN15210

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-100467_2_1



CID: EN300-100467_2_1

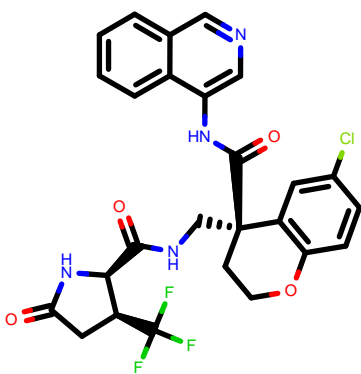
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)Cn5cenn5

RUN: RUN3683

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.19

EN300-169955_2_2



CID: EN300-169955_2_2

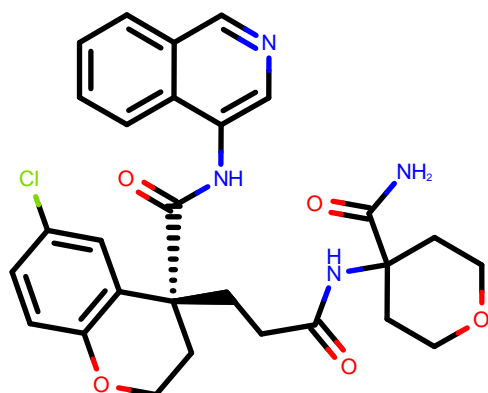
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5C[C@@H](C1=O)N5)C(F)F

RUN: RUN9158

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.26

EN300-301703_2_1



CID: EN300-301703_2_1

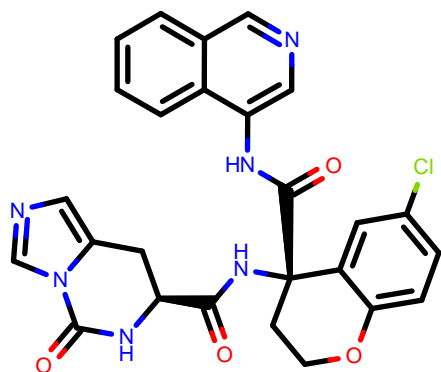
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC5(CCOCC5)C(=O)N

RUN: RUN13333

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.30

EN300-1428805_1_1



CID: EN300-1428805_1_1

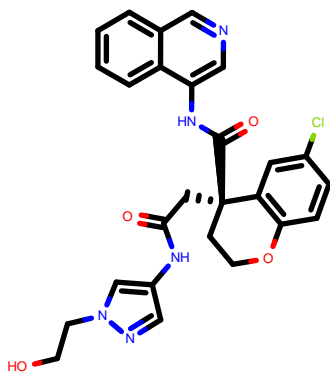
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5C6c6ncn6C(=O)N5

RUN: RUN8969

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.22

EN300-52645_1_1



CID: EN300-52645_1_1

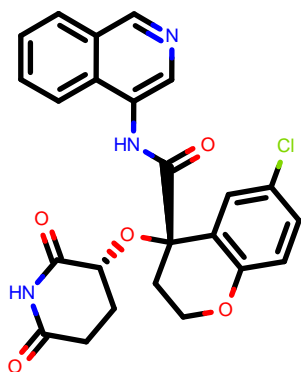
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5enn(c5)CCO

RUN: RUN14236

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.24

EN300-120920_1_2



CID: EN300-120920_1_2

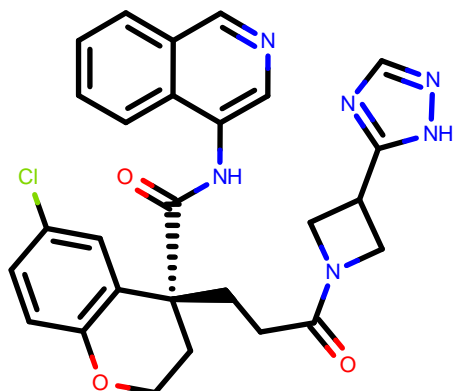
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)O[C@@H]5CCCC(=O)NC5=O

RUN: RUN2290

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.22

EN300-1707980_2_1



CID: EN300-1707980_2_1

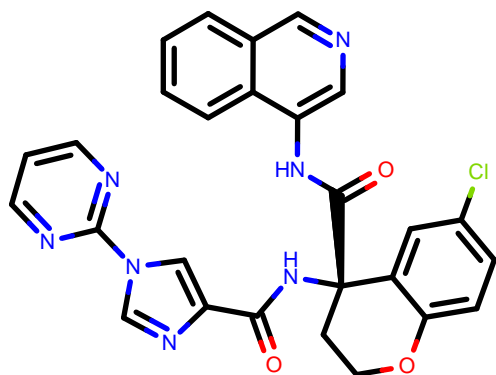
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC(C5)c6[nH]nnc6

RUN: RUN14831

DDG (kcal/mol): -0.15

dDDG (kcal/mol): 0.21

EN300-261056_1_1



CID: EN300-261056_1_1

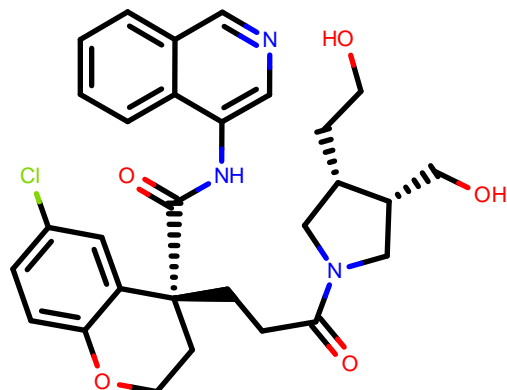
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5cn(cn5)c6nccn6

RUN: RUN859

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.17

EN300-1425608_2_3



CID: EN300-1425608_2_3

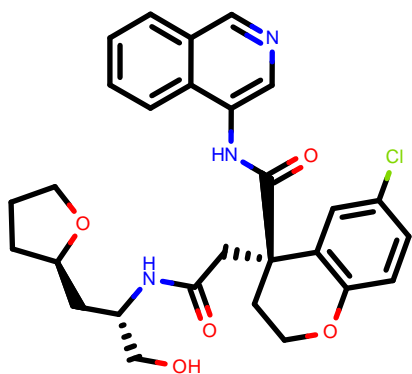
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5C[C@@H](C5)C(O)C(O)C5

RUN: RUN1638

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.36

EN300-386232_1_1



CID: EN300-386232_1_1

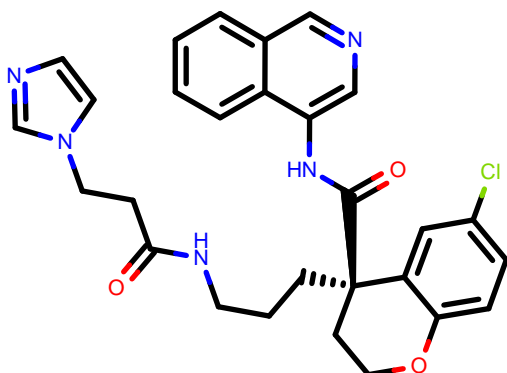
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)N[C@@H](C)C@H5CCOC5CO

RUN: RUN5777

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.26

EN300-75342_4_1



CID: EN300-75342_4_1

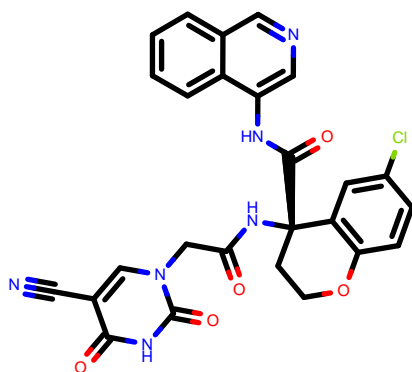
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)CCn5cnc5

RUN: RUN12161

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.31

EN300-235010_1_1



CID: EN300-235010_1_1

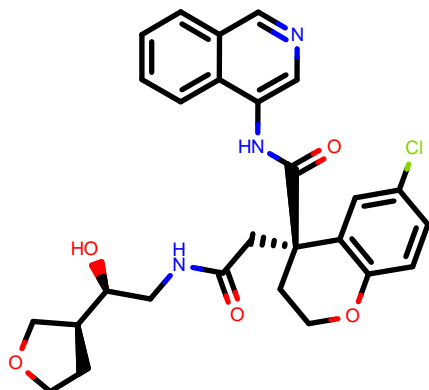
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)Cn5cc(c(=O)[nH]c5=O)C#N

RUN: RUN9859

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.26

EN300-80855_1_4



CID: EN300-80855_1_4

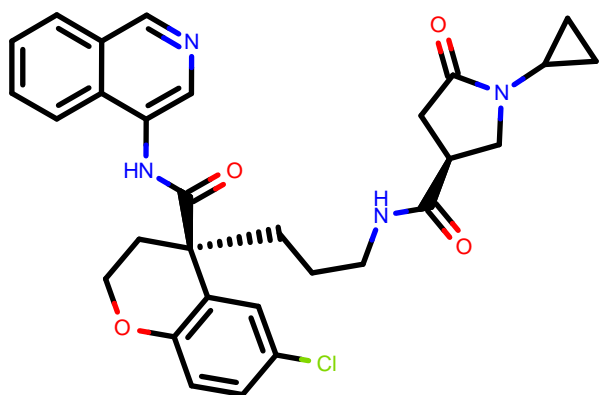
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)C(=O)NC[C@@H](C)C@H5CCOC5O

RUN: RUN12834

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.35

EN300-12440_4_2



CID: EN300-12440_4_2

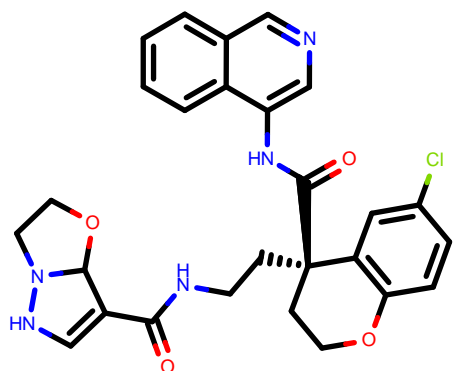
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C@H]5CC(=O)N(C)C6CC6

RUN: RUN12849

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.27

EN300-303519_3_1



CID: EN300-303519_3_1

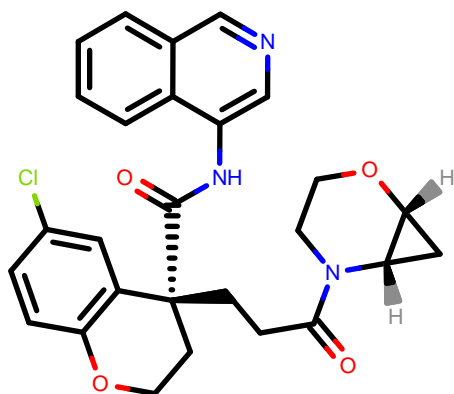
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)C5Cnnc6c5OCC6

RUN: RUN13964

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.22

EN300-91609_2_3



CID: EN300-91609_2_3

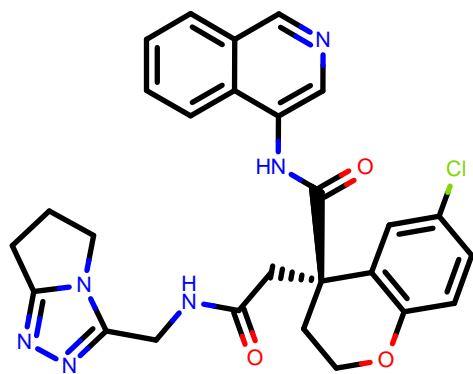
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCO[C@H]6[C@@H]5C6

RUN: RUN11310

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.23

EN300-26031_1_1



CID: EN300-26031_1_1

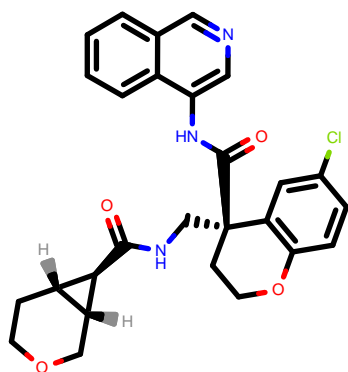
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC5nnc6n5CC6

RUN: RUN11861

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.24

EN300-1644723_2_5



CID: EN300-1644723_2_5

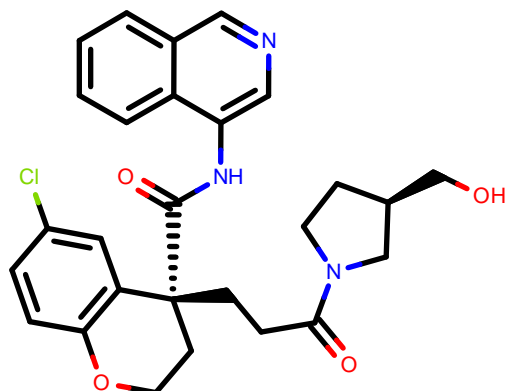
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@@]H[C@@]H[C@@]H[C@@]H5COCc6

RUN: RUN3795

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.21

EN300-144970_2_1



CID: EN300-144970_2_1

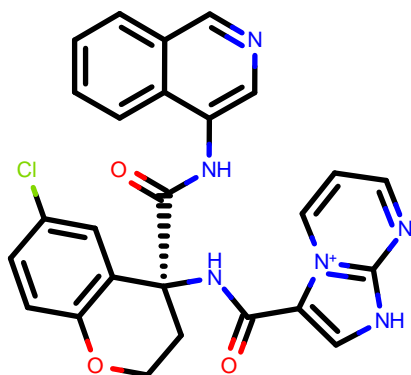
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC[C@H](C5)CO

RUN: RUN13739

DDG (kcal/mol): -0.14

dDDG (kcal/mol): 0.29

EN300-98690_1_1



CID: EN300-98690_1_1

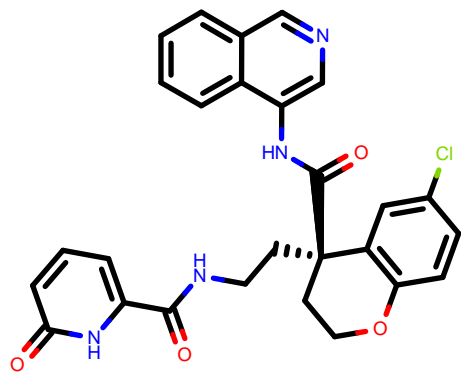
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)NC(=O)c5c[nH+]c6n5cccn6

RUN: RUN5046

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.20

EN300-34636_3_1



CID: EN300-34636_3_1

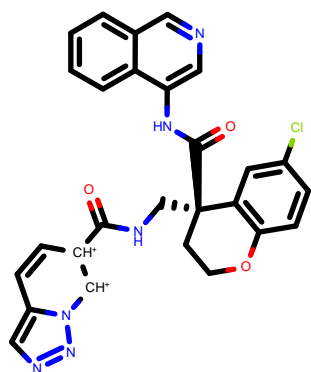
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccc(=O)[nH]5

RUN: RUN15508

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.24

EN300-6491316_2_1



CID: EN300-6491316_2_1

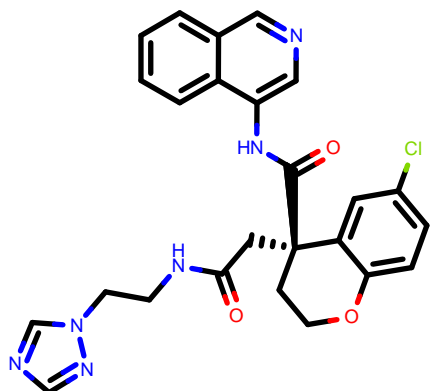
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6cnnn6c5

RUN: RUN9294

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.26

EN300-69553_1_1



CID: EN300-69553_1_1

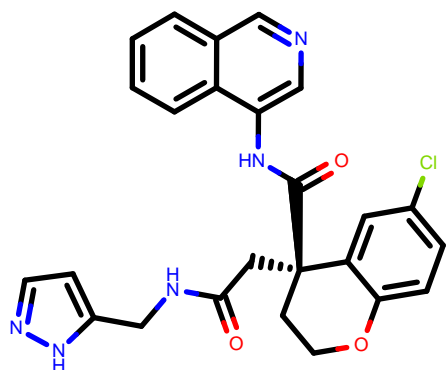
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5cnnn5

RUN: RUN9600

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.25

EN300-39785_1_1



CID: EN300-39785_1_1

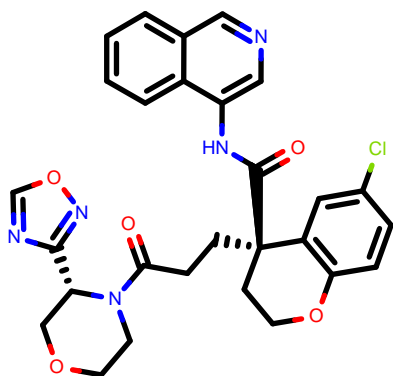
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5cnn[nH]5

RUN: RUN3113

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.20

EN300-122849_2_2



CID: EN300-122849_2_2

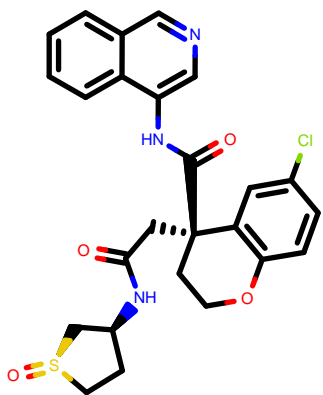
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@@]3H5c6nccn6

RUN: RUN5304

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.30

EN300-93574_1_4



CID: EN300-93574_1_4

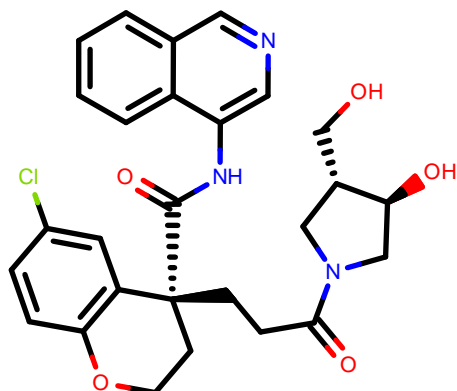
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@H]5CC[S@@]3(=O)C5

RUN: RUN11853

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.22

EN300-248521_2_1



CID: EN300-248521_2_1

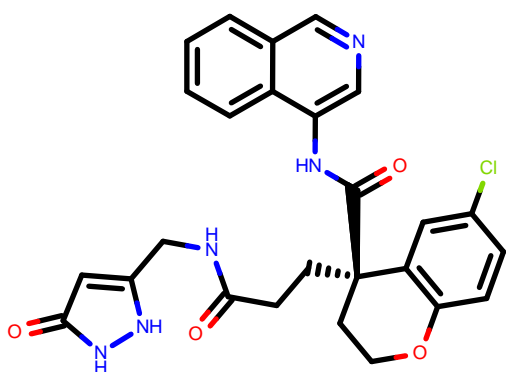
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5C[C@H](O)[C@H](O)C5

RUN: RUN6570

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.33

EN300-260760_2_1



CID: EN300-260760_2_1

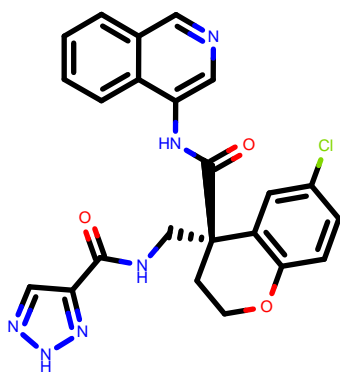
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)Nc5cc(=O)[nH]n5

RUN: RUN5108

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.23

EN300-31998_2_1



CID: EN300-31998_2_1

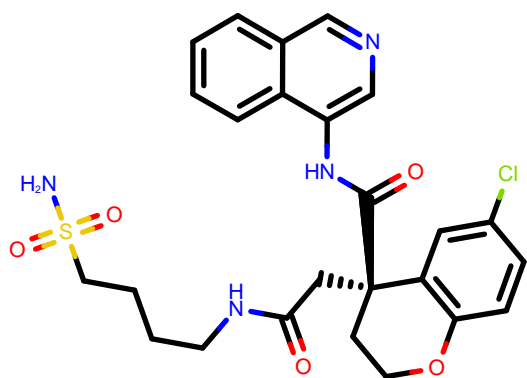
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cn[nH]5

RUN: RUN2549

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.19

EN300-223198_1_1



CID: EN300-223198_1_1

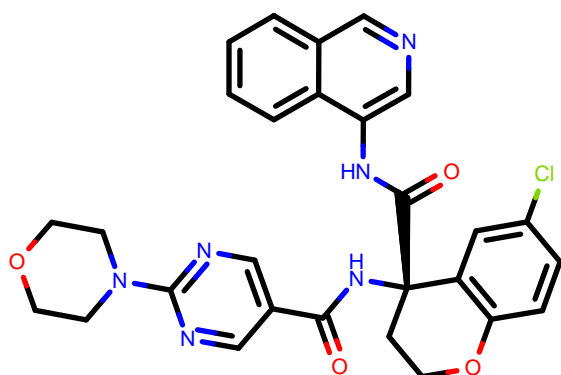
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCCS(=O)(=O)N

RUN: RUN6947

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.38

EN300-5340532_1_1



CID: EN300-5340532_1_1

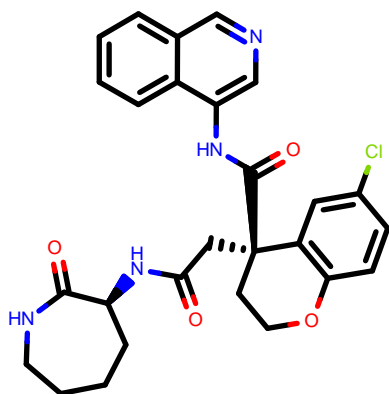
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc(nc5)N6CCOCC6

RUN: RUN9925

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.26

EN300-129384_1_1



CID: EN300-129384_1_1

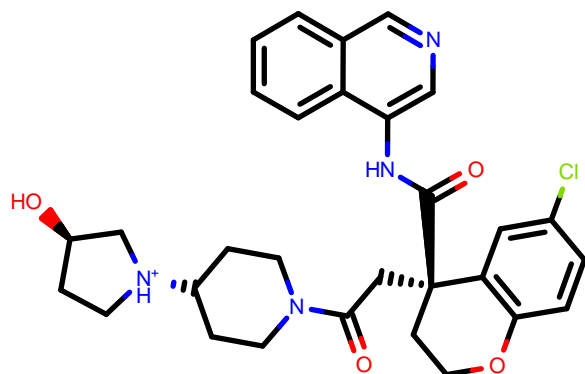
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCCNC5=O

RUN: RUN13962

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.24

EN300-241988_1_3



CID: EN300-241988_1_3

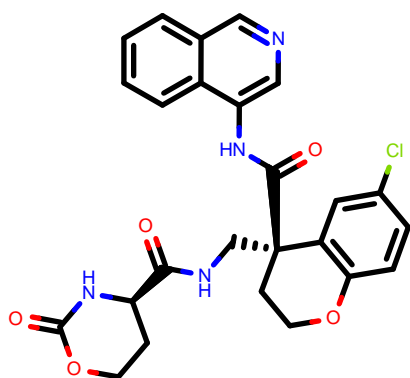
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N6CCCC(C5)N[B@@H]6CC[C@@H]5O

RUN: RUN4273

DDG (kcal/mol): -0.13

dDDG (kcal/mol): 0.33

EN300-249804_2_2



CID: EN300-249804_2_2

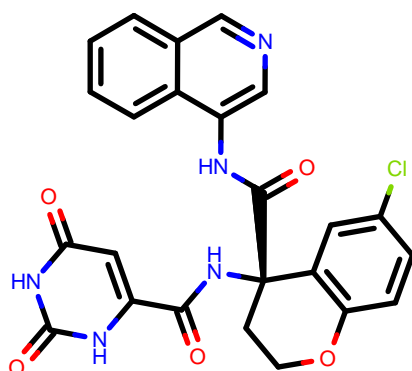
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)[C@H]5CCOC(=O)N5

RUN: RUN6489

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.23

EN300-30039_1_1



CID: EN300-30039_1_1

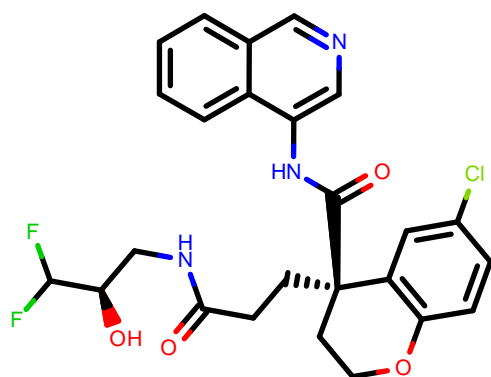
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cc(=O)[nH]c(=O)[nH]5

RUN: RUN5498

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.21

EN300-175160_2_2



CID: EN300-175160_2_2

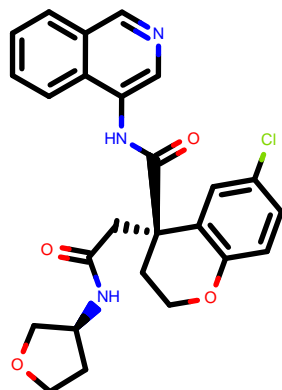
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)NC[C@H](C(F)F)O

RUN: RUN11023

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.47

EN300-171752_1_2



CID: EN300-171752_1_2

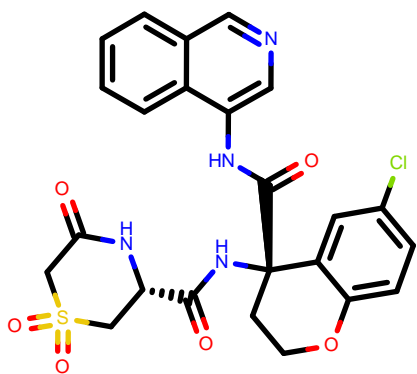
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@H]5CCOC5

RUN: RUN11469

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.22

EN300-702756_1_1



CID: EN300-702756_1_1

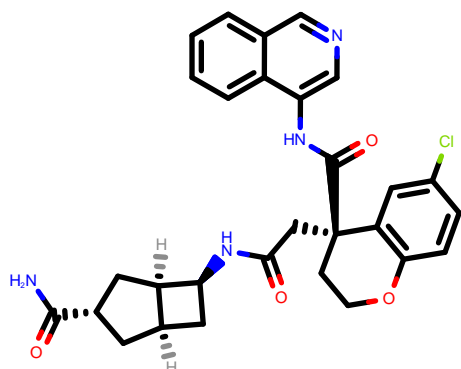
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)C1NC(=O)C@@H3C(S(=O)(=O)N)OC1=O

RUN: RUN7272

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.25

EN300-1268016_1_2



CID: EN300-1268016_1_2

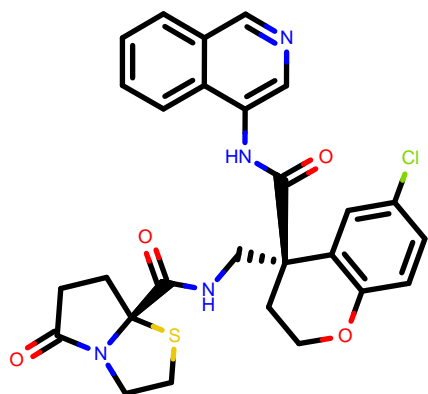
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)C1NC(=O)C@@H3C(N)C1=O

RUN: RUN3293

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-10334_2_2



CID: EN300-10334_2_2

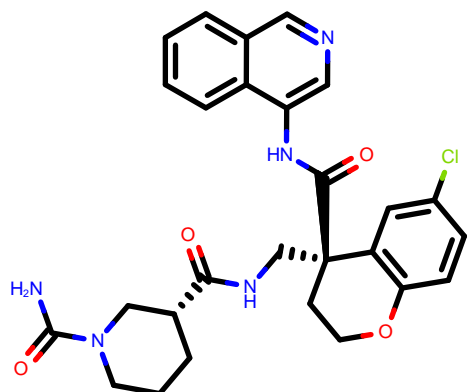
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)C1NC(=O)C@H3C(=O)N5CCCS6

RUN: RUN6147

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.29

EN300-14767_2_1



CID: EN300-14767_2_1

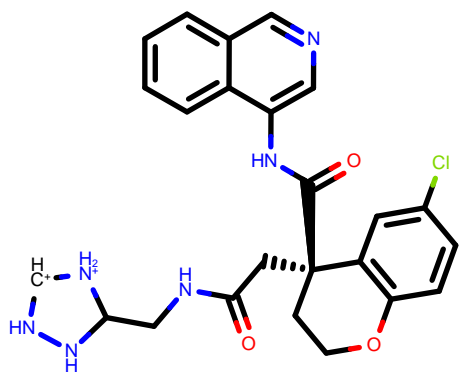
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(C)CCOc4ccc(cc4)C1CNC(=O)C@H3C(=O)N

RUN: RUN4003

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-43972_1_1



CID: EN300-43972_1_1

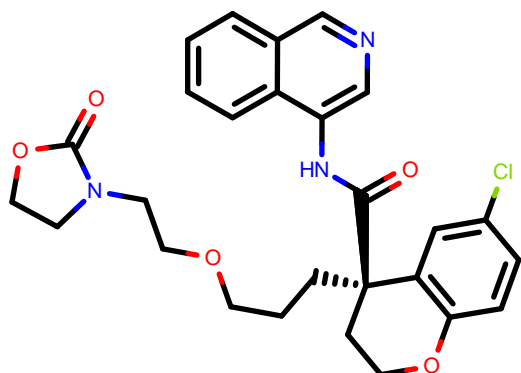
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5[nH]ncn5

RUN: RUN1399

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.22

EN300-370967_4_1



CID: EN300-370967_4_1

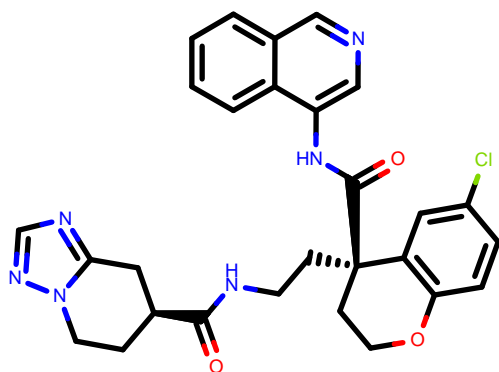
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5NCCOC5=O

RUN: RUN1195

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-1448674_3_1



CID: EN300-1448674_3_1

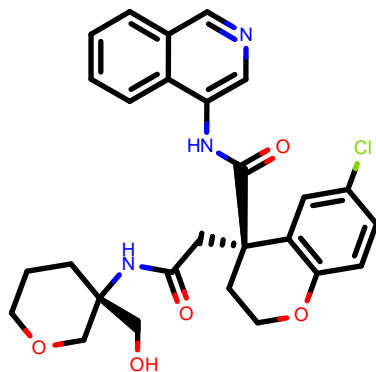
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CNc6c[nH]n6)C5

RUN: RUN15366

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.26

EN300-2969289_1_1



CID: EN300-2969289_1_1

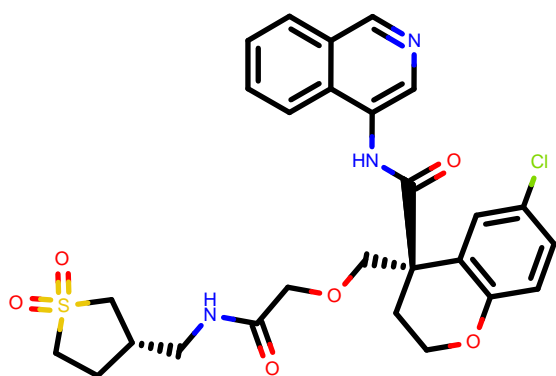
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]5(CCCOC5)CO

RUN: RUN11960

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.34

EN300-47606_2_1



CID: EN300-47606_2_1

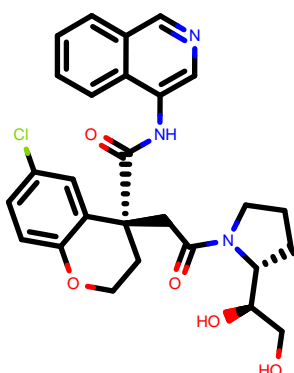
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C1C(C)C(=O)NC1C@H)[C@@H](O)C(=O)S

RUN: RUN2264

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-7459540_1_1



CID: EN300-7459540_1_1

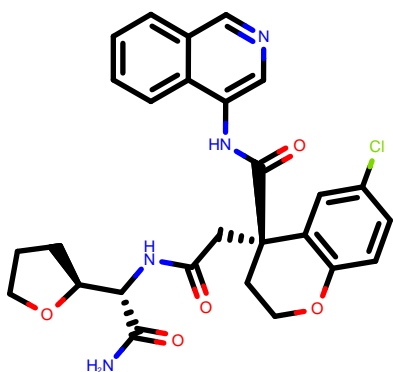
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C1C(C)C(=O)NC1C@H)[C@@H](O)C(=O)O

RUN: RUN3073

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.33

EN300-191187_1_4



CID: EN300-191187_1_4

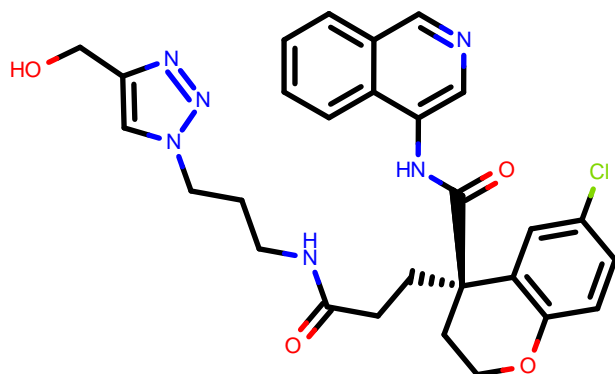
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C1C(C)C(=O)NC1C@H)[C@@H](O)C(=O)N

RUN: RUN7383

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.23

EN300-215607_2_1



CID: EN300-215607_2_1

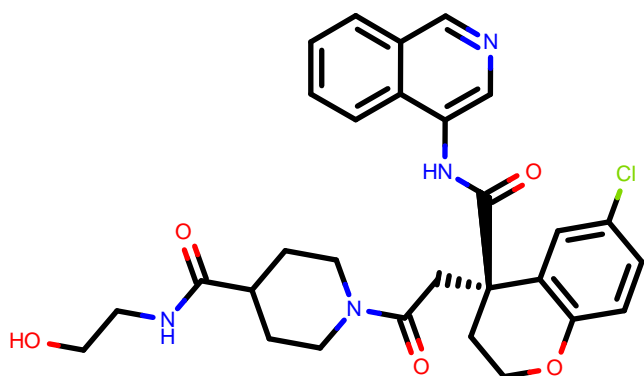
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H](C)C(=O)C1C(C)C(=O)NC1C@H)[C@@H](O)C(=O)N

RUN: RUN10138

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.25

EN300-344753_1_1



CID: EN300-344753_1_1

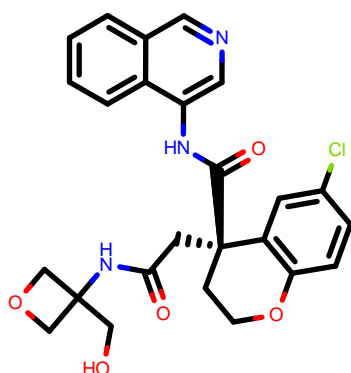
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSCCC(Cc5c(O)NCCO

RUN: RUN10753

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.36

EN300-307198_1_1



CID: EN300-307198_1_1

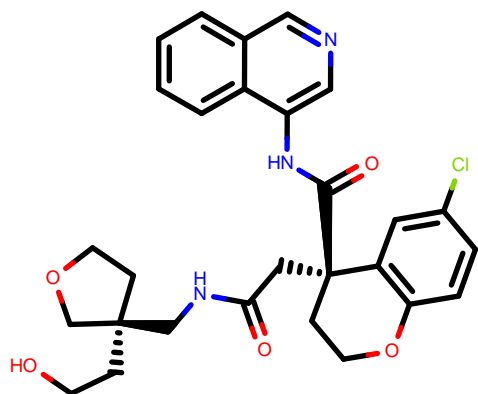
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5(COC5)CO

RUN: RUN13356

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.37

EN300-105829_1_2



CID: EN300-105829_1_2

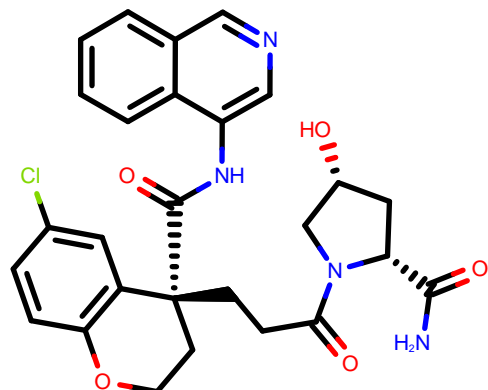
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(COC5)CCO

RUN: RUN10321

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.28

EN300-07752_2_4



CID: EN300-07752_2_4

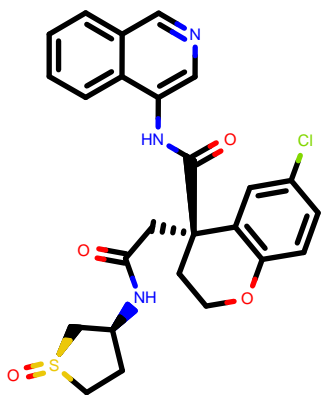
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSC[C@@]5(C)C[C@@]5(C)CO

RUN: RUN1965

DDG (kcal/mol): -0.12

dDDG (kcal/mol): 0.26

EN300-93574_1_4



CID: EN300-93574_1_4

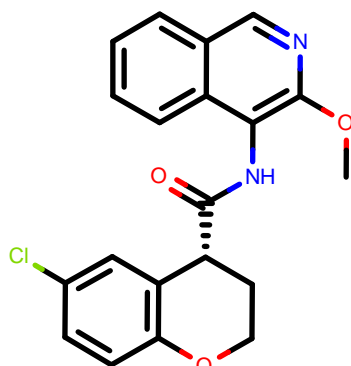
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC@H]5CC[S@@]3(=O)C5

RUN: RUN11851

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.26

JOH-UNI-f51e3bbc-4_1



CID: JOH-UNI-f51e3bbc-4_1

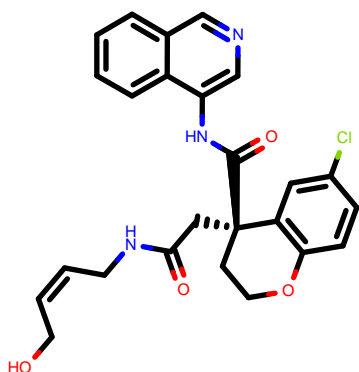
SMILES: COc1c(c2ccccc2cn1)NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C

RUN: RUN143

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.13

EN300-157158_1_1



CID: EN300-157158_1_1

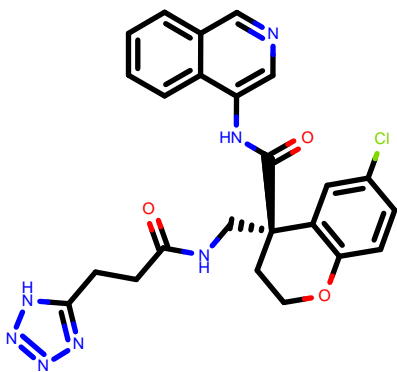
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC/C=C/C(O)C

RUN: RUN5497

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.18

EN300-251851_2_1



CID: EN300-251851_2_1

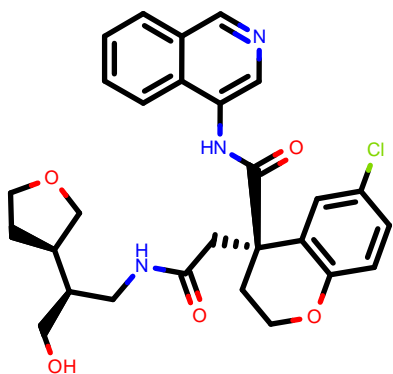
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCc5n[nH]n5

RUN: RUN1979

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.27

EN300-188316_1_3



CID: EN300-188316_1_3

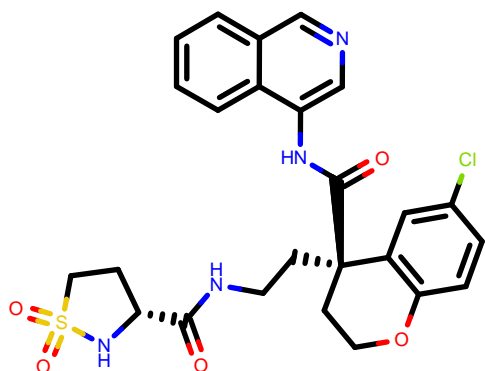
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(c4)C)CC(=O)N[C@@H](CO)C@H5CCOC5

RUN: RUN12544

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.27

EN300-45049_3_2



CID: EN300-45049_3_2

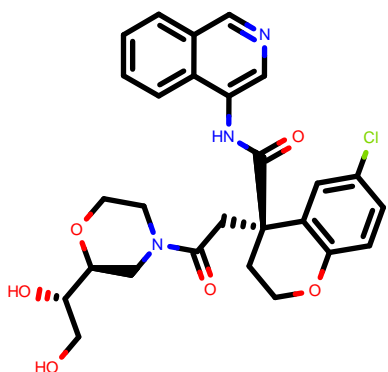
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(c4)C)CCNC(=O)[C@@H]5CCS(=O)(=O)N5

RUN: RUN15147

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.23

EN300-373446_1_1



CID: EN300-373446_1_1

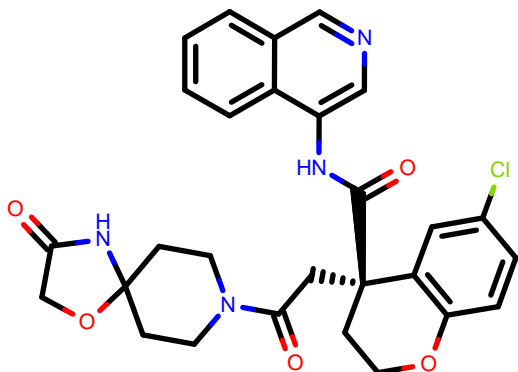
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(c4)C)CC(=O)N5CCOC[C@@H](CS)C@H6CO6

RUN: RUN10241

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.42

EN300-6472952_1_1



CID: EN300-6472952_1_1

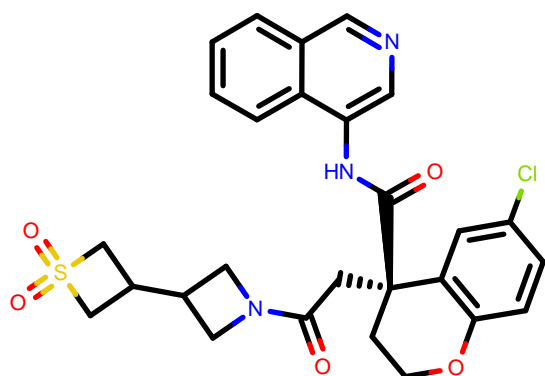
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@H]3(CCOc4c3cc(c4)C)CC(=O)N5CCOC(CS)N(C=O)CO6

RUN: RUN12230

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.26

EN300-246501_1_1



CID: EN300-246501_1_1

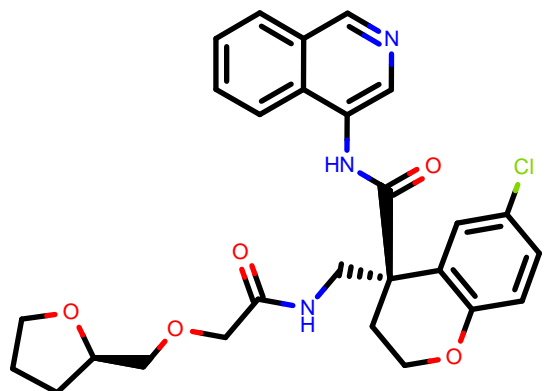
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C6CS(=O)(=O)C6

RUN: RUN12984

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.24

EN300-60033_2_1



CID: EN300-60033_2_1

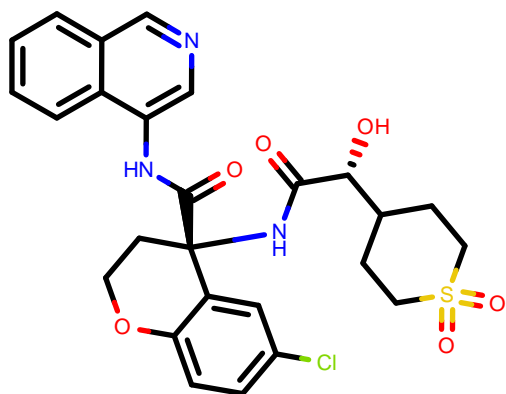
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COC[C@H]5CCOC5

RUN: RUN7037

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.25

EN300-210907_1_1



CID: EN300-210907_1_1

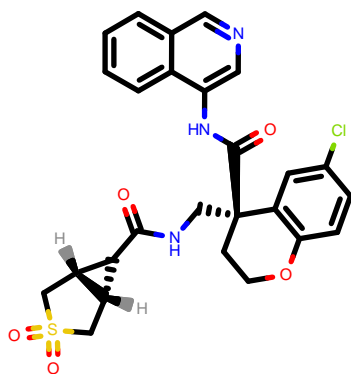
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4(C)CSCS(=O)(=O)C4

RUN: RUN9241

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.35

EN300-6779469_2_2



CID: EN300-6779469_2_2

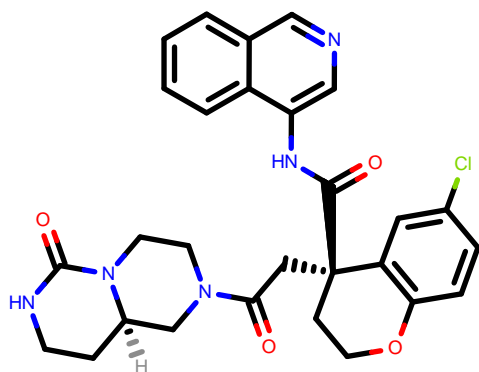
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(C@H)C(C@H)5CS(=O)(=O)C5

RUN: RUN6973

DDG (kcal/mol): -0.11

dDDG (kcal/mol): 0.27

EN300-6474647_1_2



CID: EN300-6474647_1_2

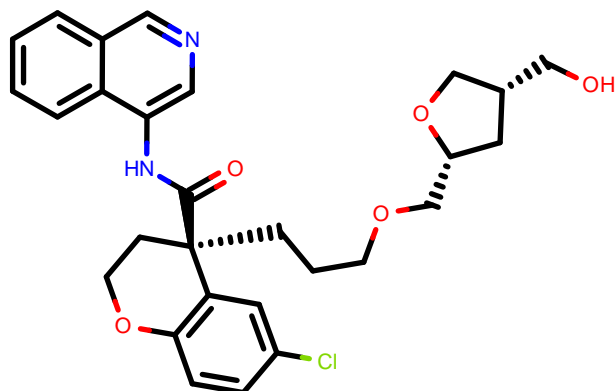
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCN(C@@H)C5CCNC6=O

RUN: RUN4237

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.23

EN300-6494158_4_3



CID: EN300-6494158_4_3

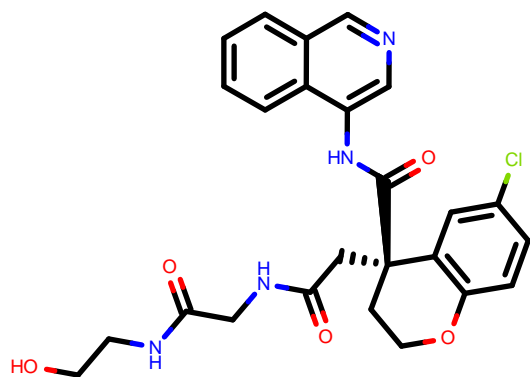
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCOC[C@@H]5C[C@@H](CO)5CO

RUN: RUN1914

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.27

EN300-82181_1_1



CID: EN300-82181_1_1

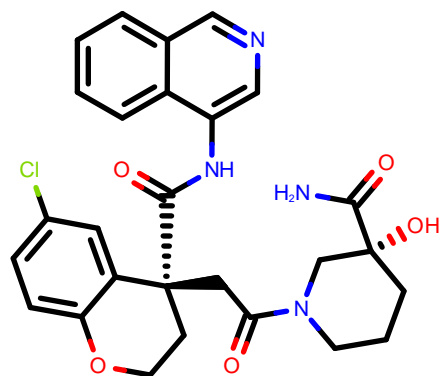
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCC(=O)NCCO

RUN: RUN5569

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.27

EN300-210553_1_1



CID: EN300-210553_1_1

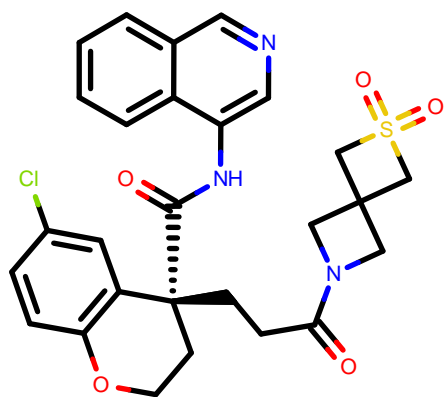
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CCC(C@@H)C5(C(=O)N)O

RUN: RUN12240

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.25

EN300-255498_2_1



CID: EN300-255498_2_1

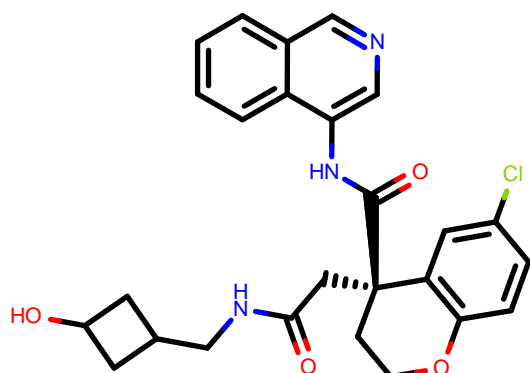
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6(C5)CS(=O)(=O)C6

RUN: RUN14781

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.27

EN300-94856_1_1



CID: EN300-94856_1_1

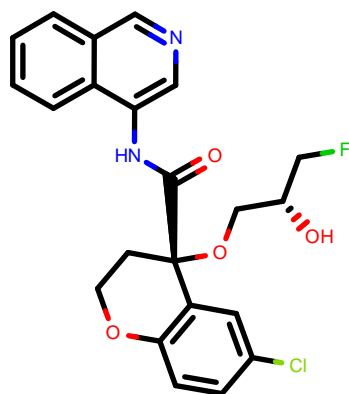
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5CC(C5)O

RUN: RUN6033

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.21

EN300-1968342_1_2



CID: EN300-1968342_1_2

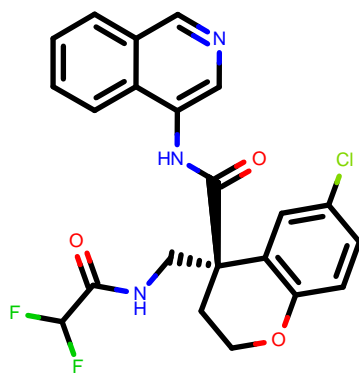
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CF)O

RUN: RUN2584

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.24

EN300-19507_2_1



CID: EN300-19507_2_1

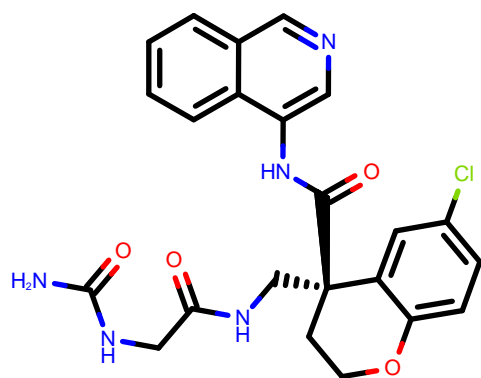
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(F)F

RUN: RUN4635

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.18

EN300-10397_2_1



CID: EN300-10397_2_1

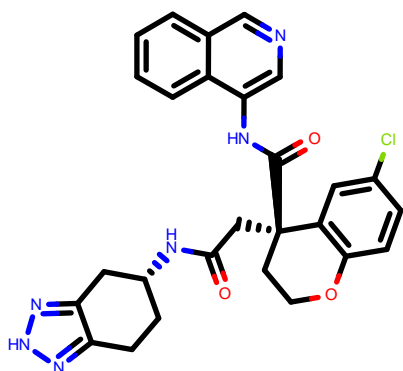
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CNC(=O)N

RUN: RUN606

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.20

EN300-6491682_1_2



CID: EN300-6491682_1_2

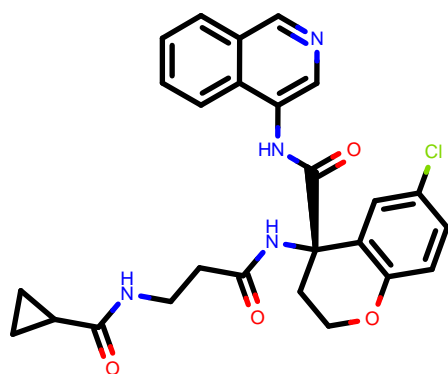
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCc6c(n[nH]6)C5

RUN: RUN4537

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.24

EN300-31147_1_1



CID: EN300-31147_1_1

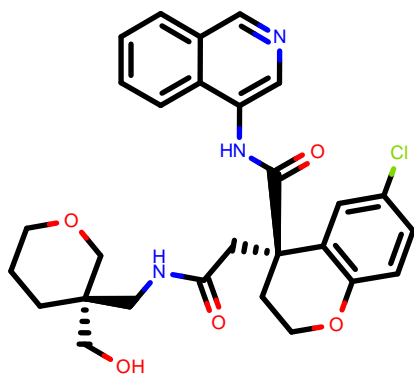
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5CC5

RUN: RUN6273

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.26

EN300-7500408_1_2



CID: EN300-7500408_1_2

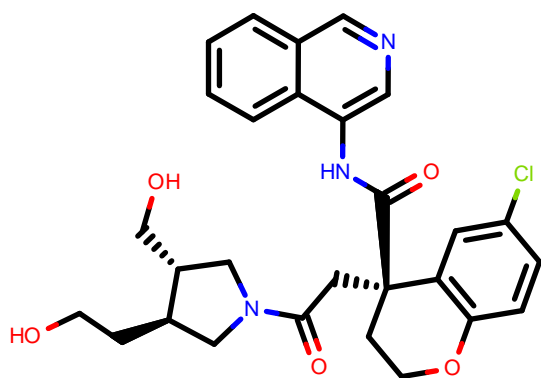
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCCOC5)CO

RUN: RUN12392

DDG (kcal/mol): -0.10

dDDG (kcal/mol): 0.28

EN300-1425608_1_4



CID: EN300-1425608_1_4

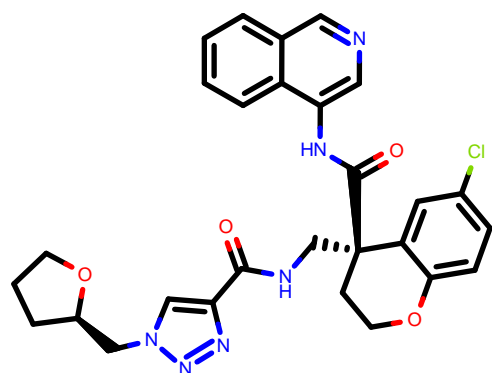
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5C[C@@H](C#N)C5OCCO

RUN: RUN537

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.23

EN300-368758_2_1



CID: EN300-368758_2_1

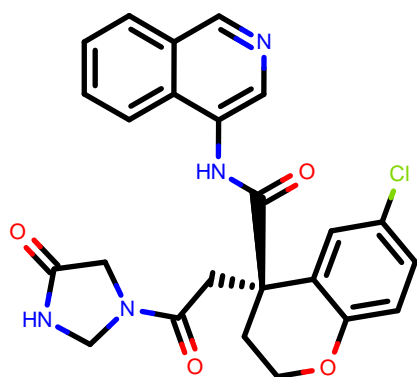
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(n5)C[C@@H]6CCCC6

RUN: RUN9262

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.28

EN300-154156_1_1



CID: EN300-154156_1_1

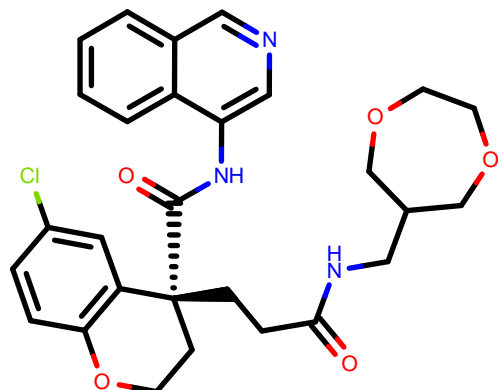
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)N5CC(=O)N5

RUN: RUN10225

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.19

EN300-7542483_2_1



CID: EN300-7542483_2_1

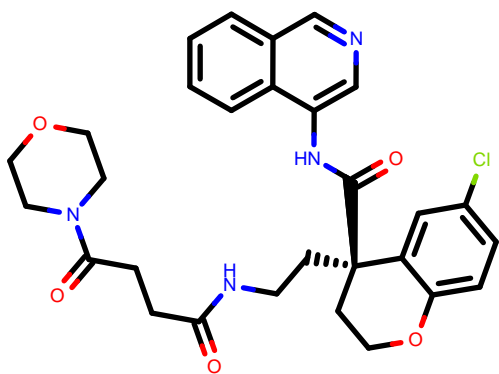
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)NCC5OCCOC5

RUN: RUN4812

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.34

EN300-05277_3_1



CID: EN300-05277_3_1

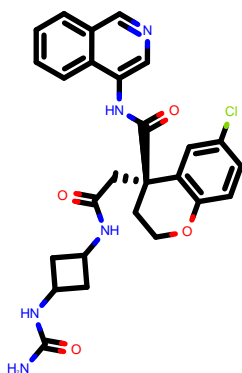
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCC(=O)N5CCOC55

RUN: RUN7871

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.28

EN300-1702911_1_1



CID: EN300-1702911_1_1

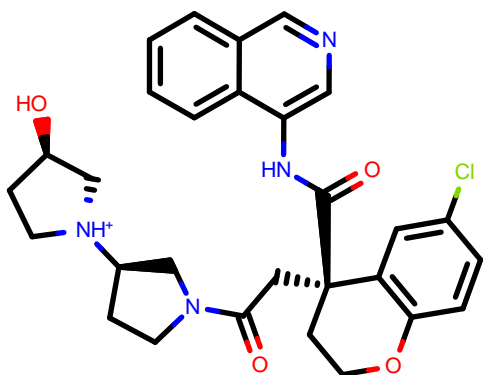
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)NC(=O)N

RUN: RUN3797

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.26

EN300-213215_1_6



CID: EN300-213215_1_6

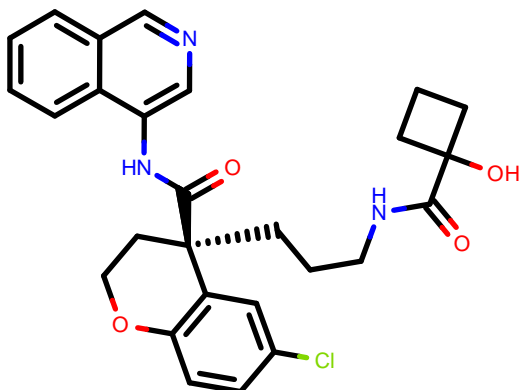
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(O)N5CC(C@H)C5(N)N8[H]8CC[C@@H]C8O

RUN: RUN13738

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.31

EN300-52009_4_1



CID: EN300-52009_4_1

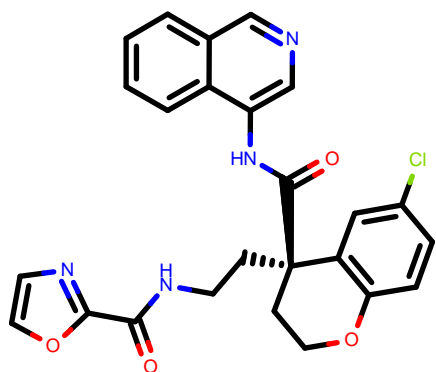
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCN(C(=O)C5(CCC5)O

RUN: RUN12749

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.23

EN300-318344_3_1



CID: EN300-318344_3_1

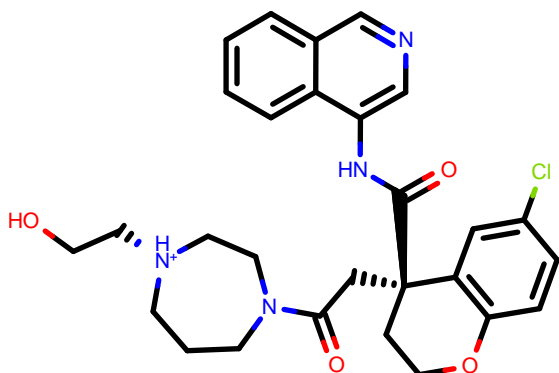
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ncco5

RUN: RUN15279

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.20

EN300-69993_1_1



CID: EN300-69993_1_1

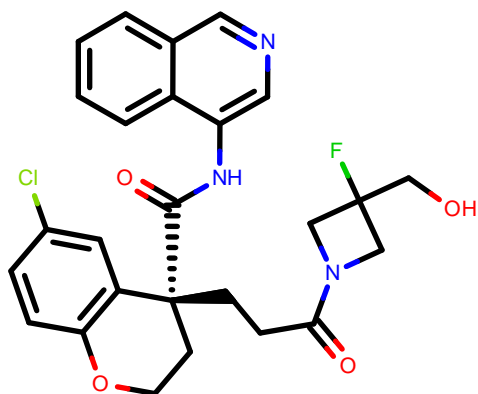
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[N@@H+]([C5])CO

RUN: RUN11819

DDG (kcal/mol): -0.09

dDDG (kcal/mol): 0.39

EN300-204507_2_1



CID: EN300-204507_2_1

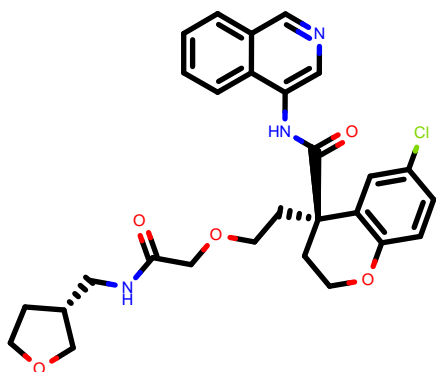
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)(CO)F

RUN: RUN13479

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.27

EN300-46832_3_2



CID: EN300-46832_3_2

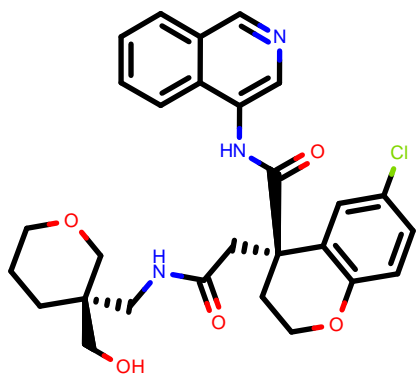
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@@H]5CCOC5

RUN: RUN474

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.27

EN300-7500408_1_1



CID: EN300-7500408_1_1

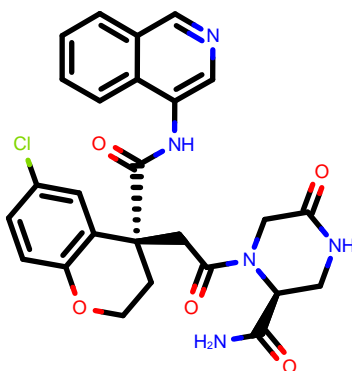
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCCOC5)CO

RUN: RUN7199

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.30

EN300-2009745_1_1



CID: EN300-2009745_1_1

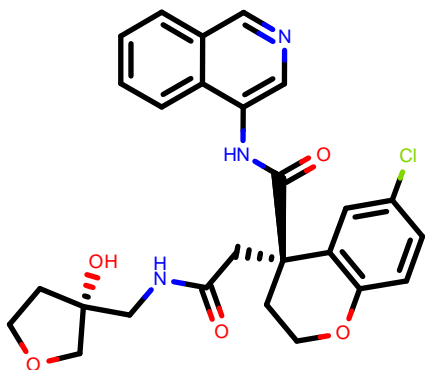
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NC[C@H]5C(=O)N

RUN: RUN3589

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.26

EN300-200699_1_1



CID: EN300-200699_1_1

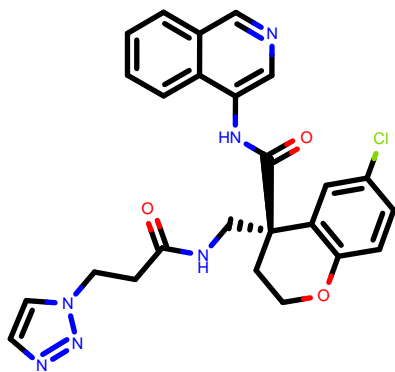
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCCOC5)O

RUN: RUN4289

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.27

EN300-28871_2_1



CID: EN300-28871_2_1

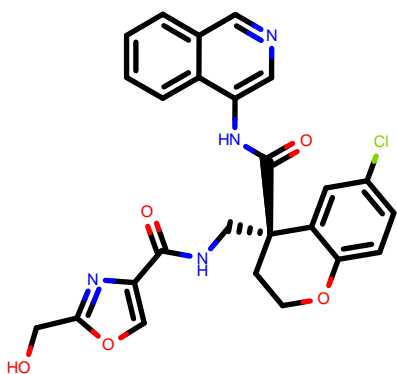
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cncn5

RUN: RUN1724

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.23

EN300-7549555_2_1



CID: EN300-7549555_2_1

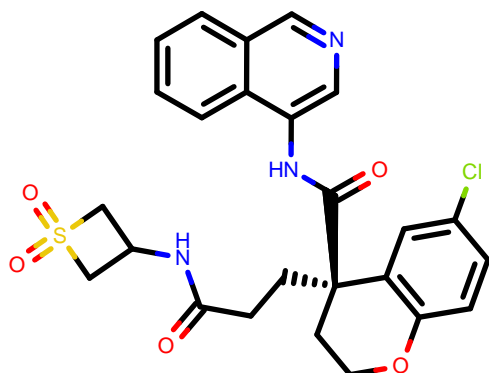
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5COCC5

RUN: RUN3019

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.26

EN300-123291_2_1



CID: EN300-123291_2_1

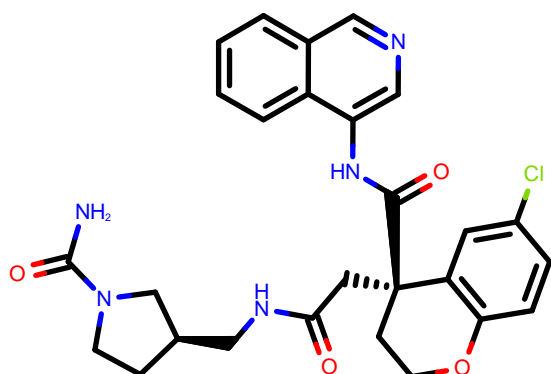
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5CS(=O)C5

RUN: RUN3012

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.31

EN300-210933_1_2



CID: EN300-210933_1_2

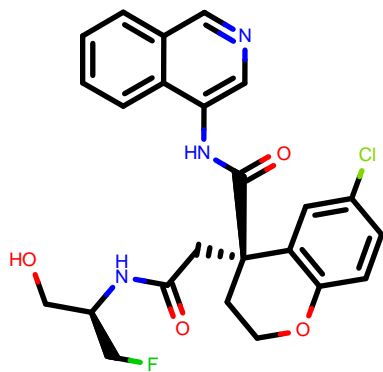
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCN(C5)C(=O)N

RUN: RUN12660

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.25

EN300-6498726_1_1



CID: EN300-6498726_1_1

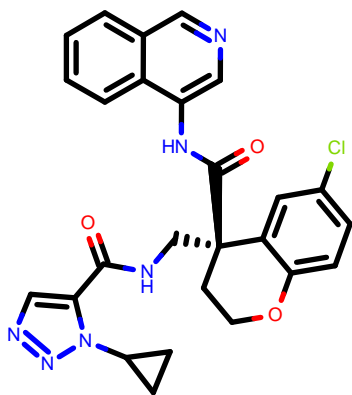
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](C)CF

RUN: RUN11938

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.30

EN300-1718675_2_1



CID: EN300-1718675_2_1

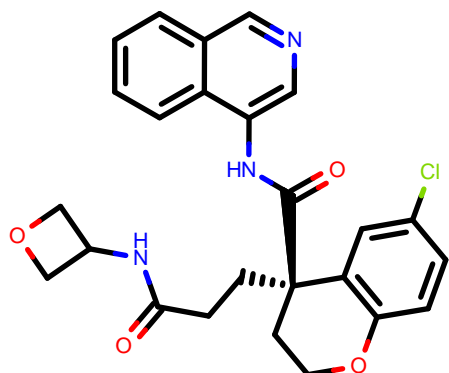
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnmn5C6CC6

RUN: RUN6294

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.27

EN300-49064_2_1



CID: EN300-49064_2_1

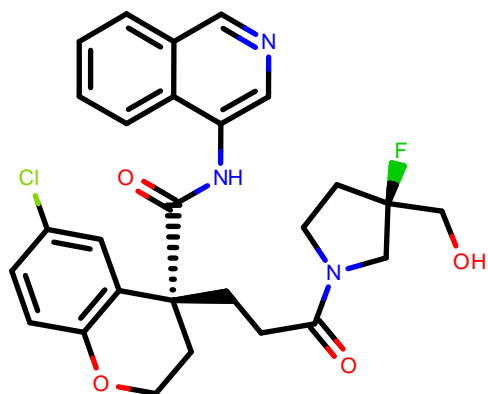
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5COC5

RUN: RUN9303

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.23

EN300-203118_2_1



CID: EN300-203118_2_1

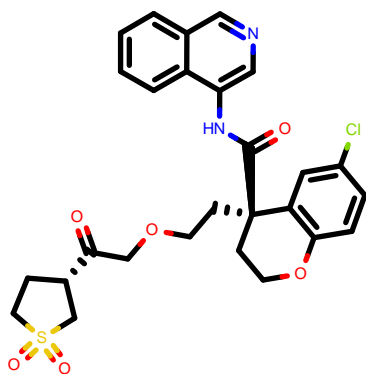
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@]3(C5)COF

RUN: RUN10878

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.35

EN300-226314_3_2



CID: EN300-226314_3_2

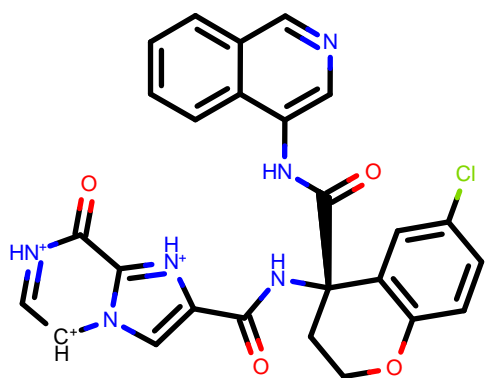
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@@H]5SCS(=O)(=O)C5

RUN: RUN298

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.34

EN300-746646_1_1



CID: EN300-746646_1_1

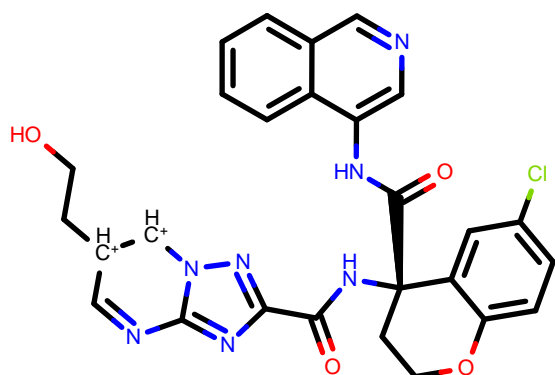
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)c5cn6cc[nH]c(=O)c6[nH+]5

RUN: RUN4542

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.22

EN300-92635_1_1



CID: EN300-92635_1_1

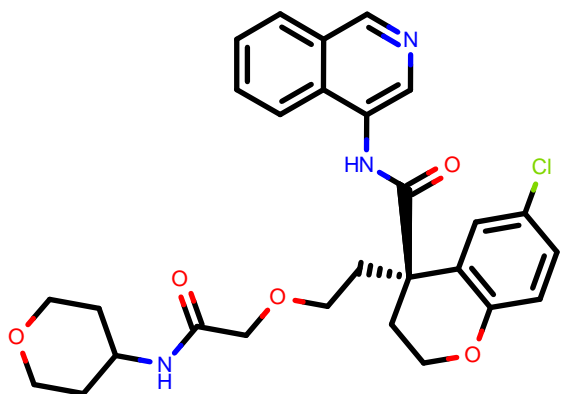
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6ncc[nH+]c5O

RUN: RUN9922

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.24

EN300-67573_3_1



CID: EN300-67573_3_1

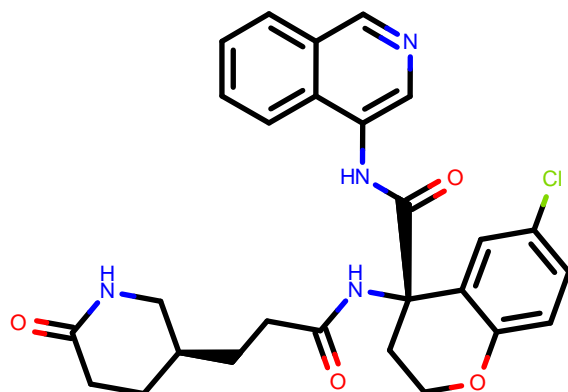
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)COC(=O)N5CCCC5

RUN: RUN330

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.31

EN300-1215738_1_2



CID: EN300-1215738_1_2

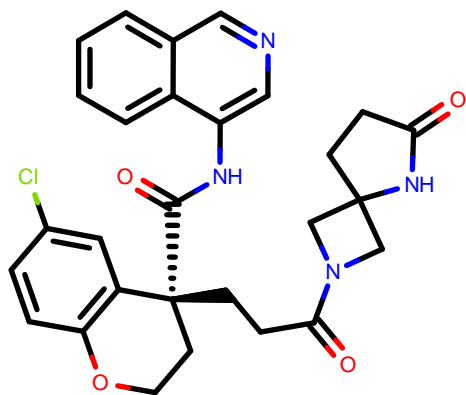
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3[C@@]4(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@@H]5CCCC(=O)N5

RUN: RUN9493

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.25

EN300-2010267_2_1



CID: EN300-2010267_2_1

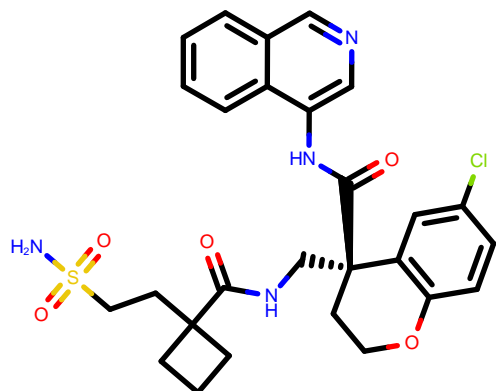
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CC6(C5)CCC(=O)N6

RUN: RUN14823

DDG (kcal/mol): -0.08

dDDG (kcal/mol): 0.31

EN300-7438227_2_1



CID: EN300-7438227_2_1

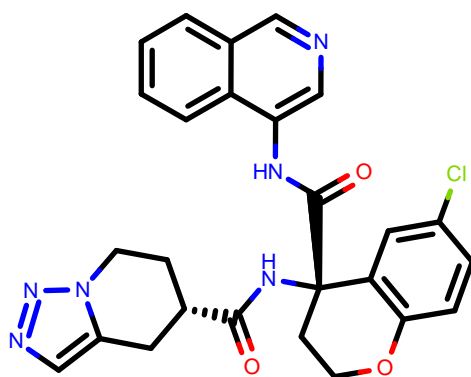
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C5(CCC5)CCS(=O)(=O)N

RUN: RUN6286

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.47

EN300-7430501_1_1



CID: EN300-7430501_1_1

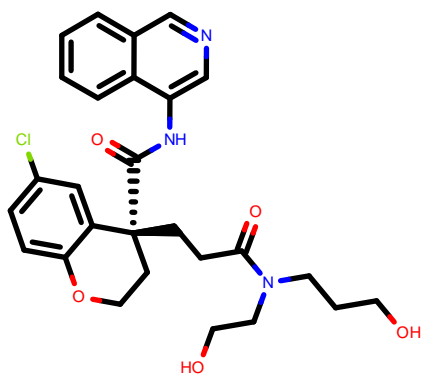
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@H]5CCn6c(cnn6)C5

RUN: RUN7528

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.24

EN300-74200_2_1



CID: EN300-74200_2_1

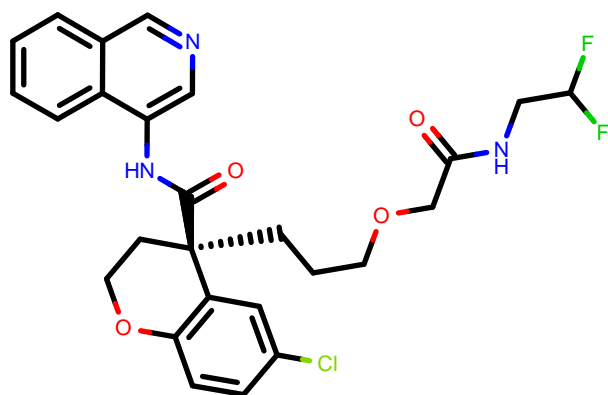
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N(CCCO)CCO

RUN: RUN2196

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.27

EN300-120586_4_1



CID: EN300-120586_4_1

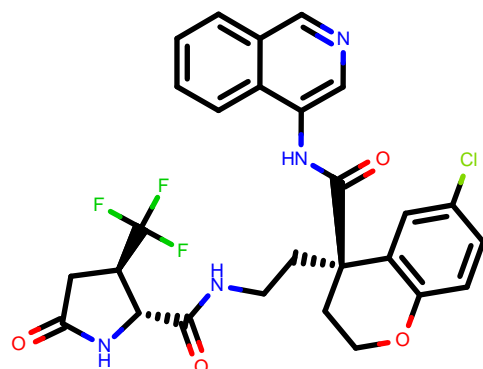
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC(=O)NCC(F)F

RUN: RUN1403

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.24

EN300-169955_3_4



CID: EN300-169955_3_4

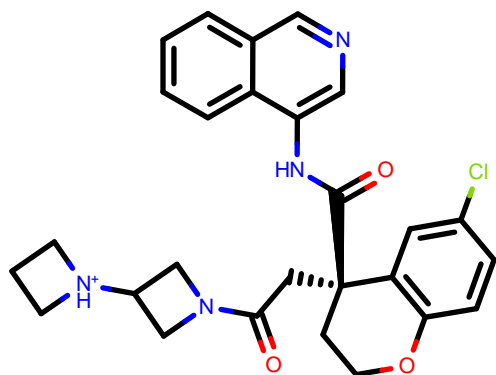
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H5C@H(C)CC(=O)N5C(F)F

RUN: RUN14720

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.30

EN300-262136_1_1



CID: EN300-262136_1_1

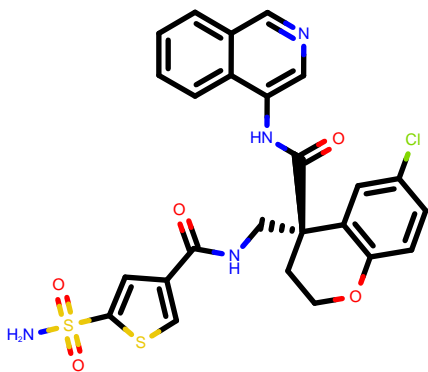
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[NH+]6CCCC6

RUN: RUN10715

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.22

EN300-23792_2_1



CID: EN300-23792_2_1

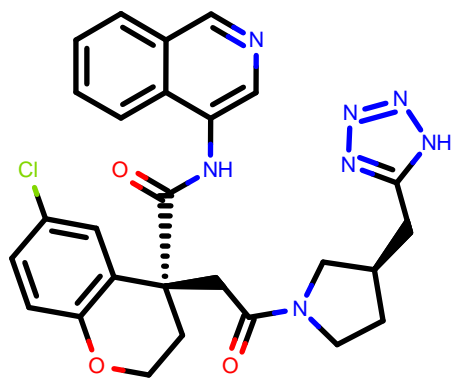
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(s5)S(=O)(=O)N

RUN: RUN5431

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.25

EN300-818709_1_1



CID: EN300-818709_1_1

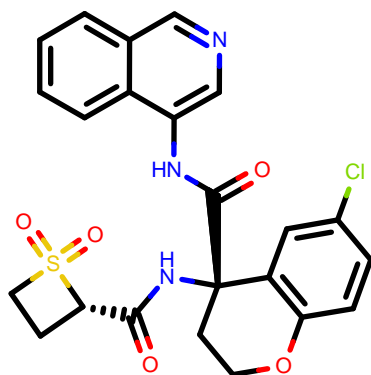
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC[C@@H](C5)Cc6[nH]n6

RUN: RUN1279

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.30

EN300-1387104_1_1



CID: EN300-1387104_1_1

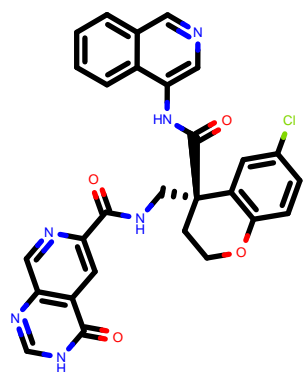
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)NC(=O)[C@@H]5CCS5(=O)=O

RUN: RUN3398

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.22

EN300-151756_2_1



CID: EN300-151756_2_1

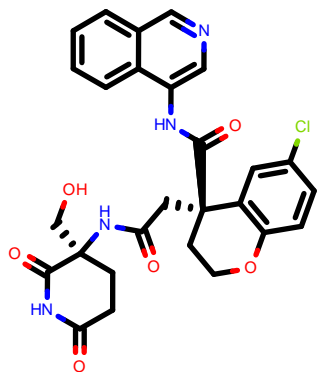
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cc6c(n5)nd[nH]6=O

RUN: RUN2154

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.25

EN300-7537340_1_2



CID: EN300-7537340_1_2

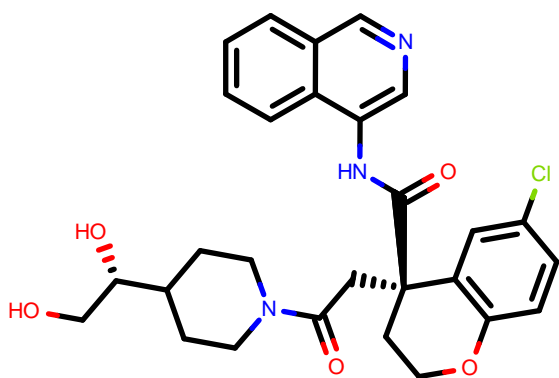
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N[C@@]5(CCC(=O)NC5=O)CO

RUN: RUN14490

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.28

EN300-1699332_1_2



CID: EN300-1699332_1_2

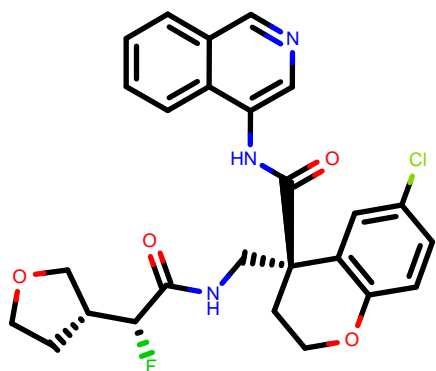
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)[C@H](CO)O

RUN: RUN3277

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.28

EN300-783124_2_1



CID: EN300-783124_2_1

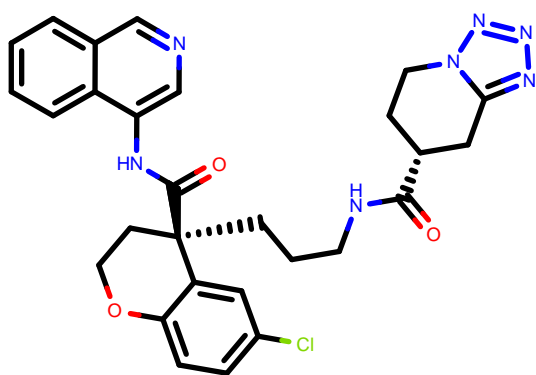
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]4H[C@@]5CCOC5F

RUN: RUN1500

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.25

EN300-1653482_4_2



CID: EN300-1653482_4_2

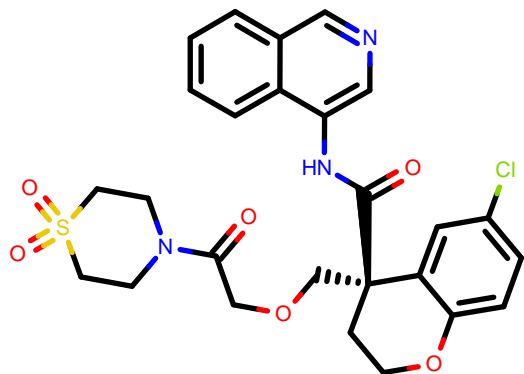
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]4H5CCn6c(nn6)C5

RUN: RUN13435

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.24

EN300-1265948_2_1



CID: EN300-1265948_2_1

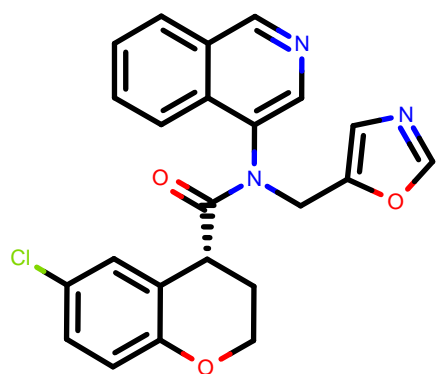
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCS(=O)(=O)CC5

RUN: RUN1066

DDG (kcal/mol): -0.07

dDDG (kcal/mol): 0.25

ALP-UNI-44c99a80-3_1



CID: ALP-UNI-44c99a80-3_1

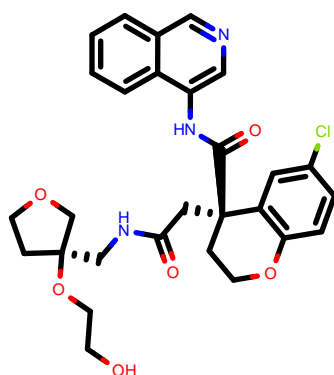
SMILES: c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@H]4CCOCc5c4cc(cc5)Cl

RUN: RUN171

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.20

EN300-298869_1_1



CID: EN300-298869_1_1

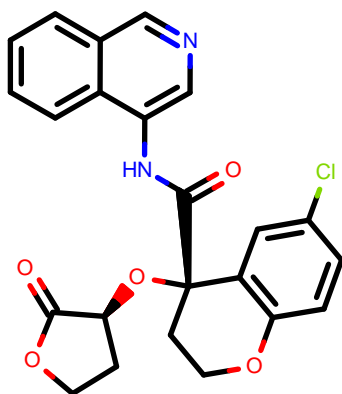
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCOc5)OCCO

RUN: RUN3345

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.27

EN300-20496_1_1



CID: EN300-20496_1_1

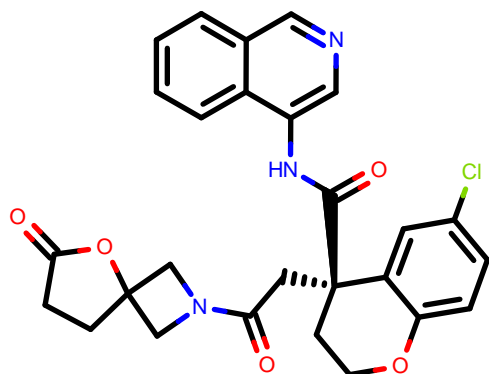
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@H]5CCOC5=O

RUN: RUN1445

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.16

EN300-7534935_1_1



CID: EN300-7534935_1_1

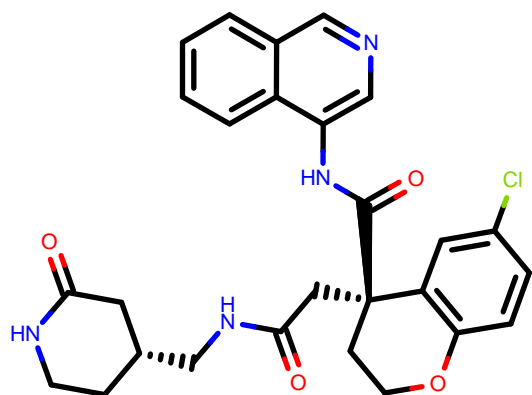
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CCC(=O)O6

RUN: RUN5677

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.23

EN300-59733_1_2



CID: EN300-59733_1_2

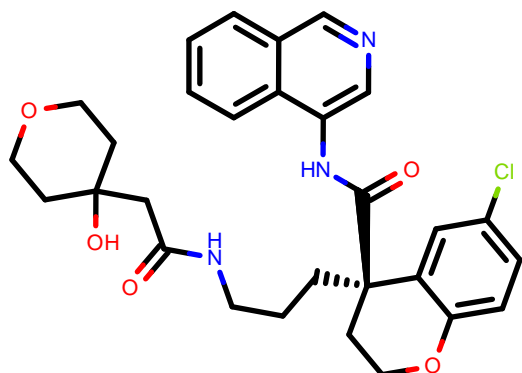
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCNC(=O)C5

RUN: RUN11513

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.24

EN300-151423_4_1



CID: EN300-151423_4_1

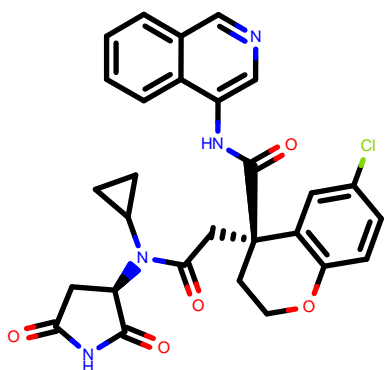
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CCOCC5)O

RUN: RUN12679

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.30

EN300-61086_1_2



CID: EN300-61086_1_2

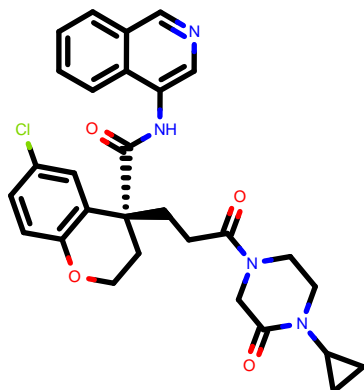
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC1(=O)NC5=O)C6CC6

RUN: RUN12940

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.33

EN300-202232_2_1



CID: EN300-202232_2_1

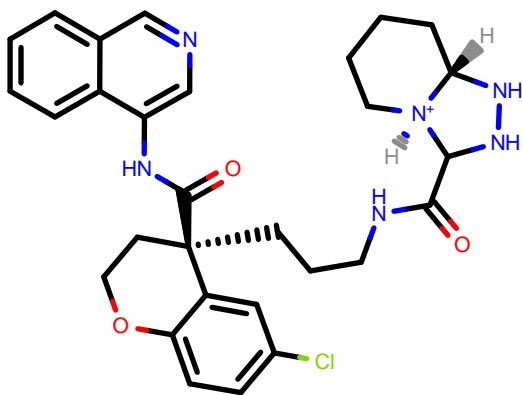
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(C(=O)C5)C6CC6

RUN: RUN14199

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.26

EN300-6746631_4_1



CID: EN300-6746631_4_1

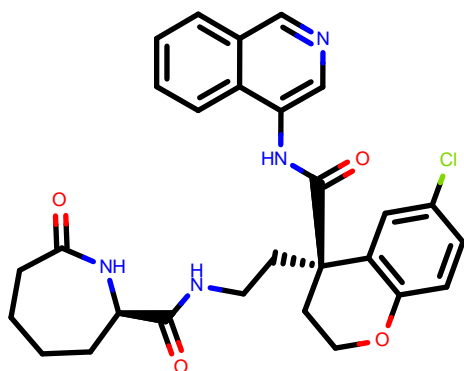
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5nnc6n5CCCC6

RUN: RUN10526

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.30

EN300-80083_3_2



CID: EN300-80083_3_2

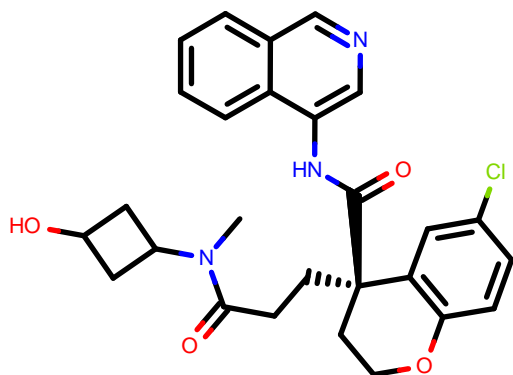
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)N5

RUN: RUN14764

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.25

EN300-93074_2_1



CID: EN300-93074_2_1

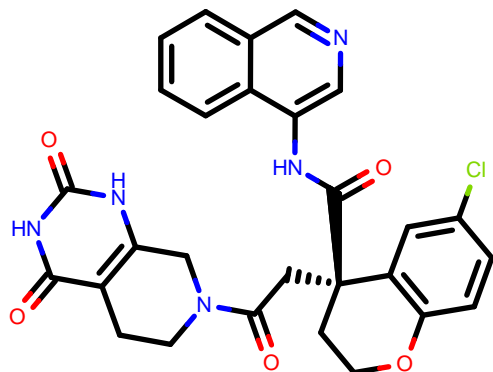
SMILES: CN(C=O)CC[C@@]1(c2ccc(c2)C)OCC1C(=O)Nc3c4cnc3cccc4[C@H]5C[C@@H]5C5O

RUN: RUN6794

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.28

EN300-7427115_1_1



CID: EN300-7427115_1_1

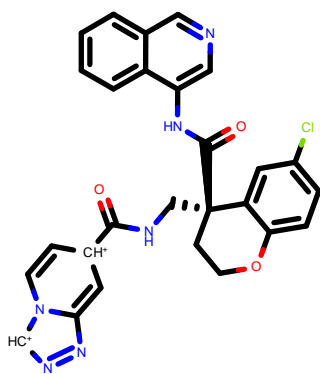
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Coc6c[H]c(-O)[H]d6-O/C5

RUN: RUN8736

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.25

EN300-7537194_2_1



CID: EN300-7537194_2_1

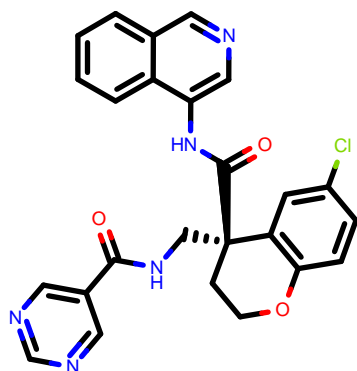
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnc6enn6c5

RUN: RUN9258

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.23

EN300-64297_2_1



CID: EN300-64297_2_1

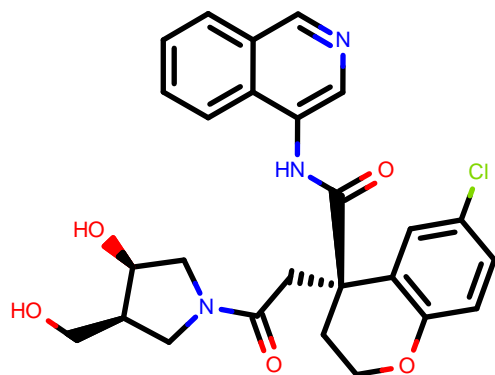
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncnc5

RUN: RUN8694

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.23

EN300-248521_1_2



CID: EN300-248521_1_2

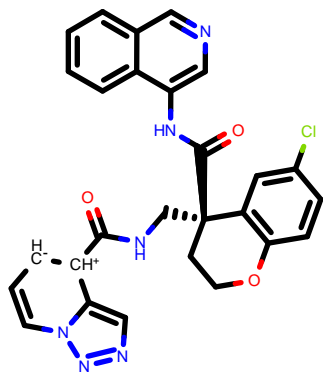
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]([C@H](C5)O)CO

RUN: RUN3133

DDG (kcal/mol): -0.06

dDDG (kcal/mol): 0.28

EN300-1074262_2_1



CID: EN300-1074262_2_1

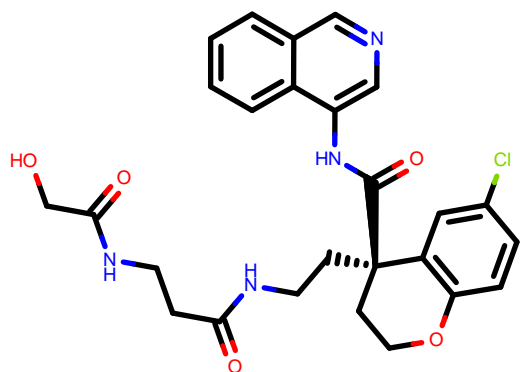
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncn6c5enn6

RUN: RUN6071

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.27

EN300-383904_3_1



CID: EN300-383904_3_1

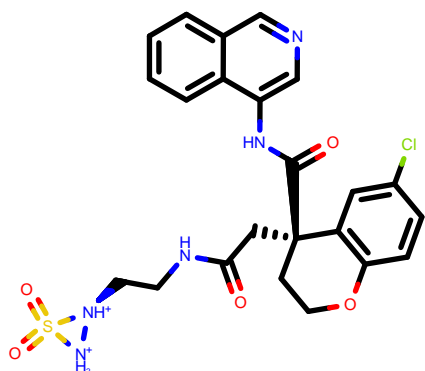
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CCNC(=O)CCO

RUN: RUN2022

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.29

EN300-6740040_1_1



CID: EN300-6740040_1_1

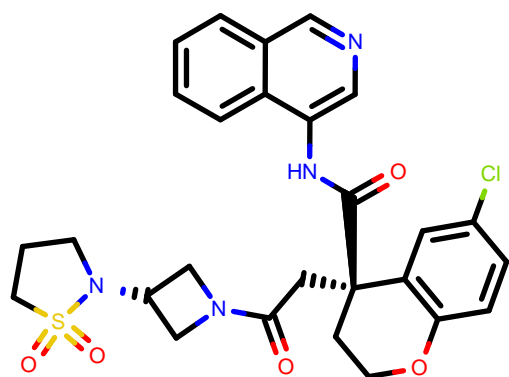
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CC(=O)NCS(=O)(=O)N

RUN: RUN10273

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.56

EN300-1272295_1_1



CID: EN300-1272295_1_1

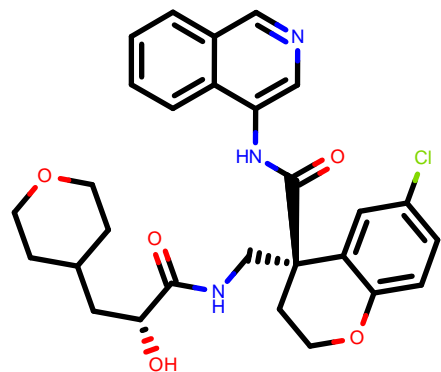
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CC(=O)NSC(C5)N(C5)S(=O)(=O)O

RUN: RUN11082

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.29

EN300-1452069_2_1



CID: EN300-1452069_2_1

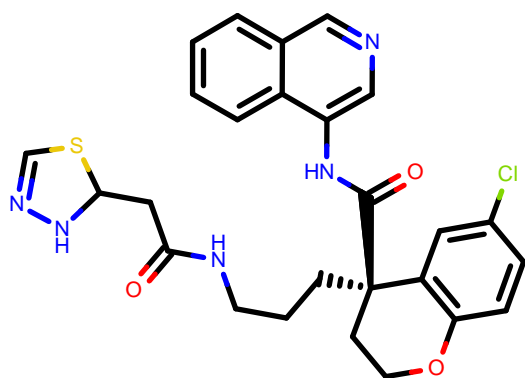
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3[C@@](CCO4c3cc(cc4)Cl)CNC(=O)[C@@]5[C@@H](CC5COCOC5)O

RUN: RUN4367

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.41

EN300-6488240_4_1



CID: EN300-6488240_4_1

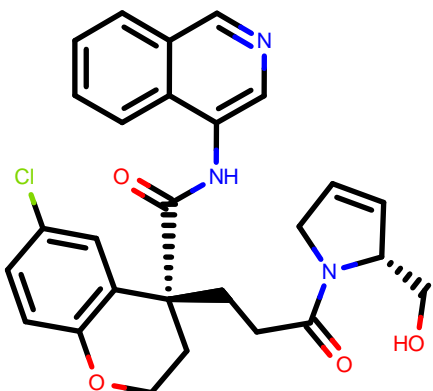
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5nncs5

RUN: RUN10844

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.22

EN300-378343_2_1



CID: EN300-378343_2_1

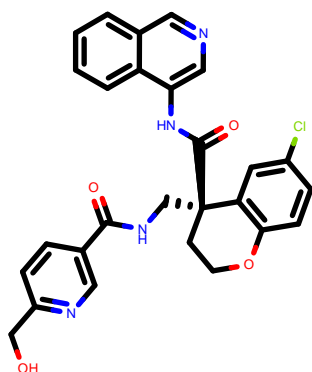
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC=C[C@@]H5CO

RUN: RUN10584

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.25

EN300-146051_2_1



CID: EN300-146051_2_1

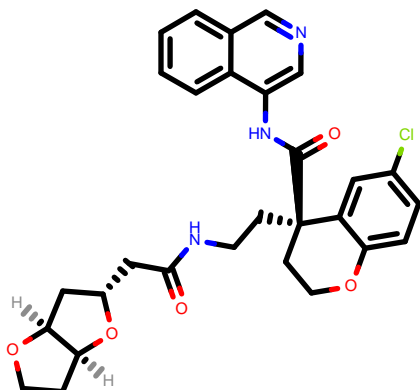
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(nc5)CO

RUN: RUN3191

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-7355519_3_3



CID: EN300-7355519_3_3

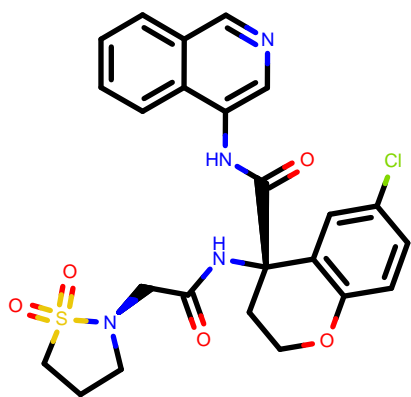
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5C[C@@H]6[C@H](O)COC6

RUN: RUN11102

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.34

EN300-43206_1_2



CID: EN300-43206_1_2

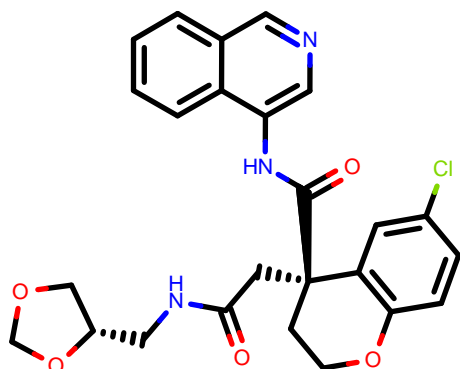
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)NC(=O)C[N@@]5CCCS5(=O)=O

RUN: RUN3738

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.34

EN300-253187_1_1



CID: EN300-253187_1_1

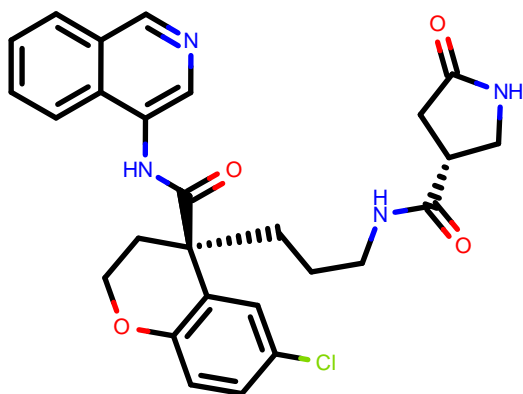
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CC(=O)NC[C@@H]5COCOC5

RUN: RUN10223

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.25

EN300-59487_4_1



CID: EN300-59487_4_1

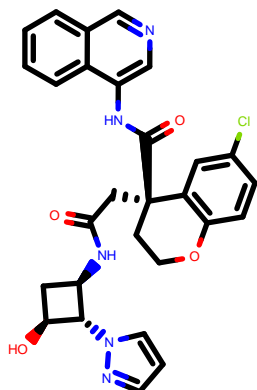
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)CCNC(=O)[C@@H]5CC(=O)NC5

RUN: RUN11991

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.21

EN300-260696_1_5



CID: EN300-260696_1_5

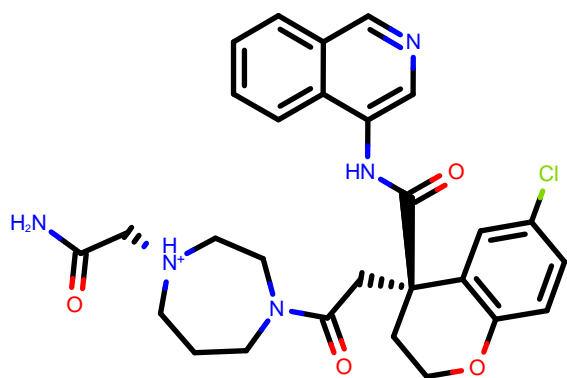
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(C)CCOc4c3cc(cc4)C)C(C1=CN=CN1)C(=O)O

RUN: RUN14524

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.25

EN300-42007_1_1



CID: EN300-42007_1_1

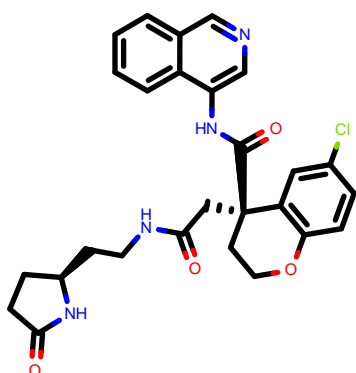
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N6CCCN6@H)CC5CC(=O)N

RUN: RUN9931

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.31

EN300-205779_1_2



CID: EN300-205779_1_2

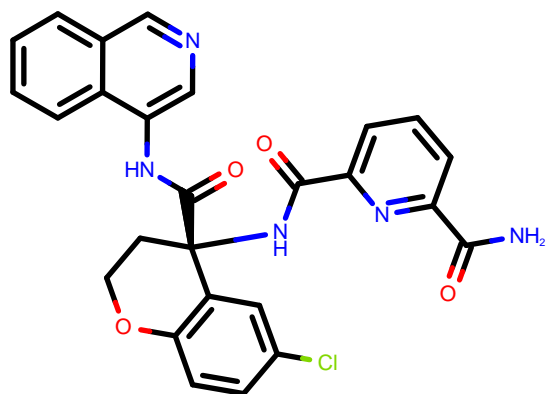
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC[C@@]4H5C(=O)N5

RUN: RUN3517

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.24

EN300-130656_1_1



CID: EN300-130656_1_1

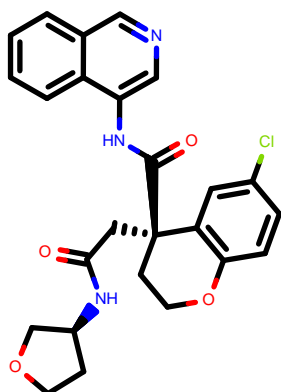
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccc(n5)C(=O)N

RUN: RUN1042

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.21

EN300-171752_1_2



CID: EN300-171752_1_2

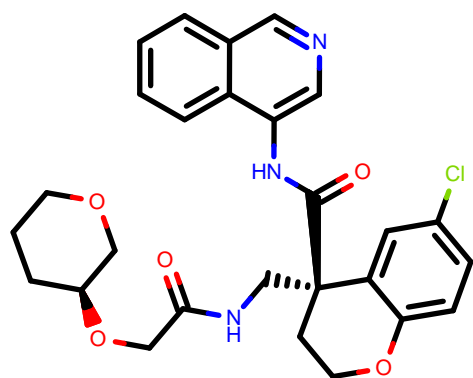
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@]4H5C(=O)N5

RUN: RUN11471

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.21

EN300-1627945_2_2



CID: EN300-1627945_2_2

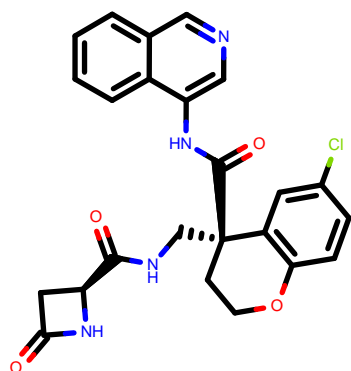
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CO[C@@H]5CCOC5

RUN: RUN5971

DDG (kcal/mol): -0.05

dDDG (kcal/mol): 0.26

EN300-103219_2_1



CID: EN300-103219_2_1

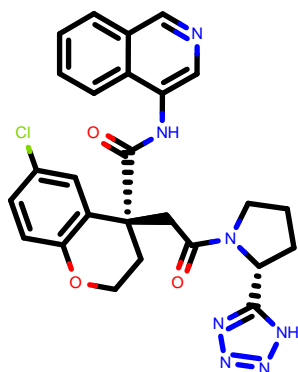
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC(=O)N5

RUN: RUN6505

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.20

EN300-195173_1_1



CID: EN300-195173_1_1

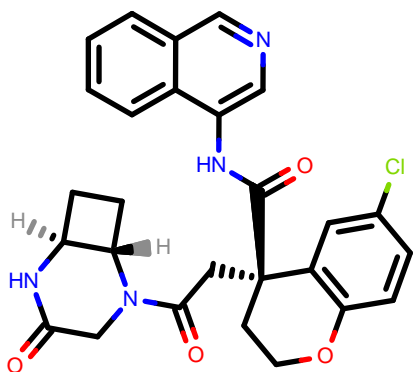
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5c6n[n-]n6

RUN: RUN4977

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.28

EN300-6499164_1_4



CID: EN300-6499164_1_4

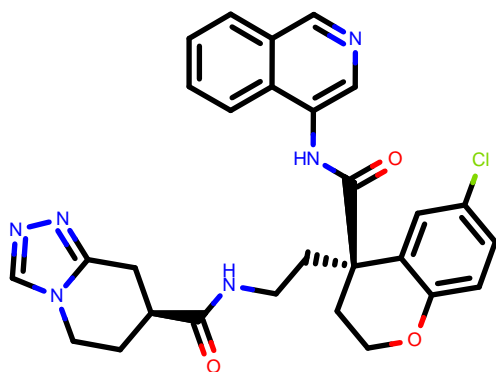
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)N[C@@H]5C[C@@H]5C6

RUN: RUN11793

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.25

EN300-6474341_3_1



CID: EN300-6474341_3_1

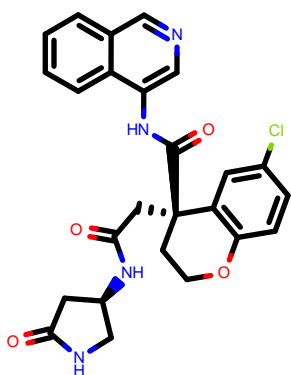
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCN6cnc6C5

RUN: RUN15387

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

EN300-127487_1_1



CID: EN300-127487_1_1

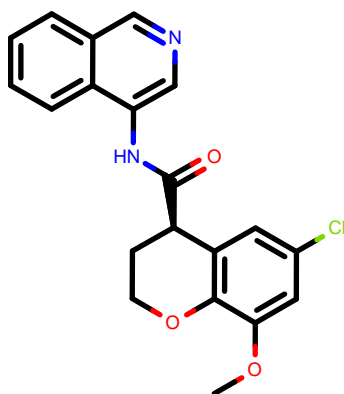
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC(=O)NCS

RUN: RUN12642

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.21

DAR-DIA-6a508060-4_1



CID: DAR-DIA-6a508060-4_1

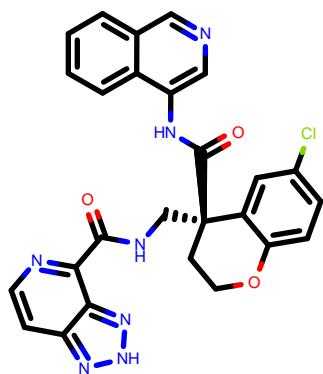
SMILES: COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cnc4c3cccc4)Cl

RUN: RUN148

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.13

EN300-7426383_2_1



CID: EN300-7426383_2_1

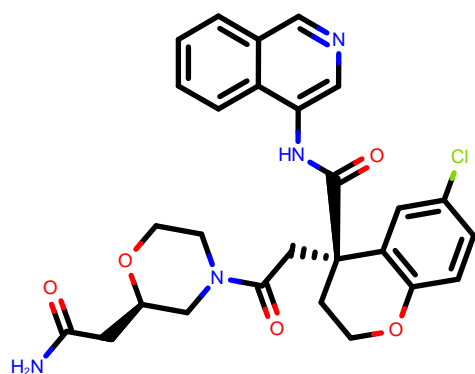
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c6c(cnc5)n[nH]6

RUN: RUN3367

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.25

EN300-321558_1_1



CID: EN300-321558_1_1

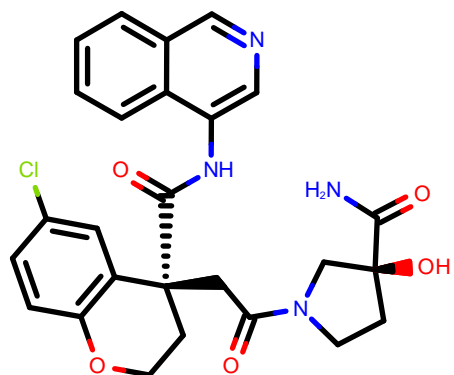
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CC(=O)N

RUN: RUN10217

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.21

EN300-172481_1_2



CID: EN300-172481_1_2

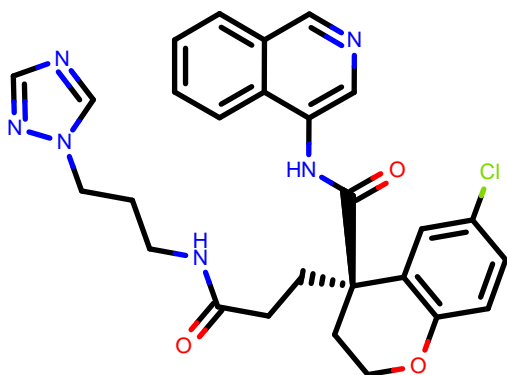
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)(C(=O)N)O

RUN: RUN5985

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.31

EN300-270328_2_1



CID: EN300-270328_2_1

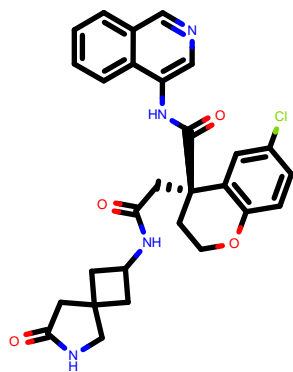
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCN5enon5

RUN: RUN11514

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.24

EN300-1440100_1_1



CID: EN300-1440100_1_1

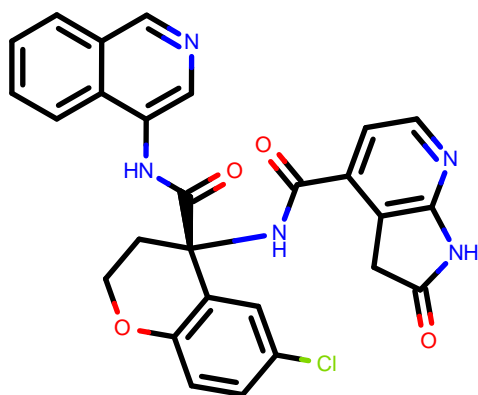
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC6(C5)CC(=O)NC6

RUN: RUN4469

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.25

EN300-269863_1_1



CID: EN300-269863_1_1

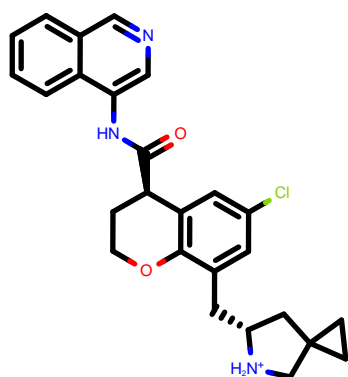
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6c5CC(=O)N6

RUN: RUN8136

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.23

DAR-DIA-23e5a6a0-9_2



CID: DAR-DIA-23e5a6a0-9_2

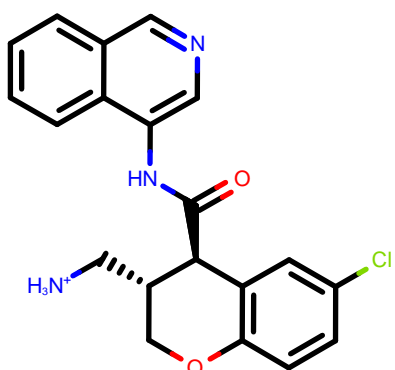
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC[C@H]5CC6(CC6)C[NH2+]5Cl

RUN: RUN187

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.38

MAK-UNK-8be7dca9-3_3



CID: MAK-UNK-8be7dca9-3_3

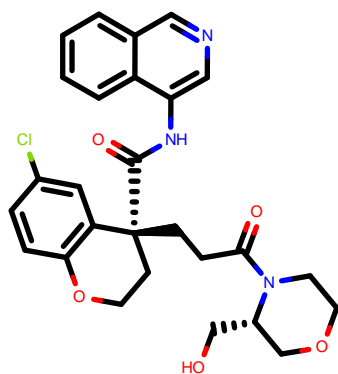
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC[C@H]3C[NH3+]Cl

RUN: RUN96

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.10

EN300-154201_2_1



CID: EN300-154201_2_1

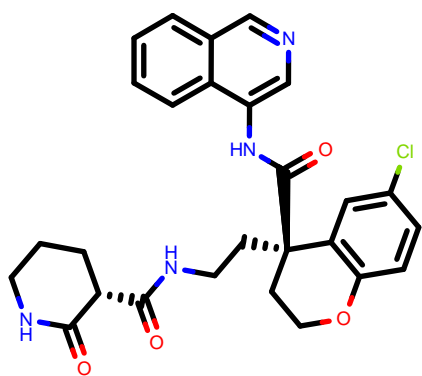
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@@]3H5CO

RUN: RUN2013

DDG (kcal/mol): -0.04

dDDG (kcal/mol): 0.25

EN300-82616_3_2



CID: EN300-82616_3_2

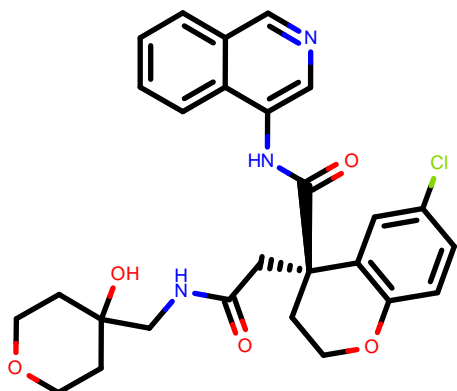
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H]5CCCCNS=O

RUN: RUN13812

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.30

EN300-141942_1_1



CID: EN300-141942_1_1

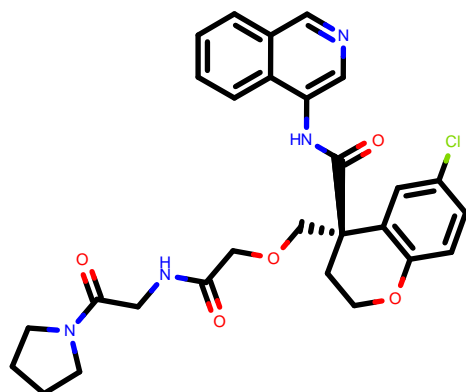
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(COCCO5)O

RUN: RUN13200

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.25

EN300-28340_2_1



CID: EN300-28340_2_1

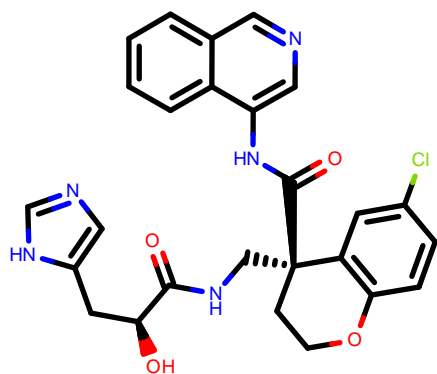
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCC(=O)N5CCCC5

RUN: RUN2160

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.27

EN300-6503811_2_1



CID: EN300-6503811_2_1

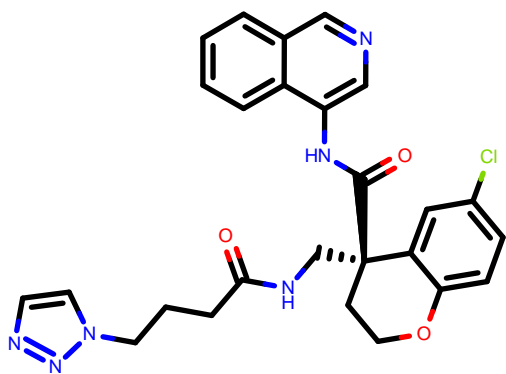
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](Cc5nc[nH]5)O

RUN: RUN8349

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.29

EN300-124301_2_1



CID: EN300-124301_2_1

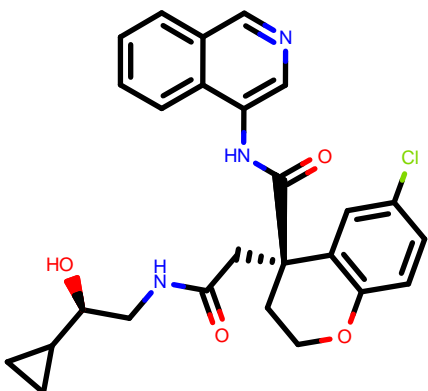
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)C[C@@]5Cn5

RUN: RUN4371

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.26

EN300-67533_1_2



CID: EN300-67533_1_2

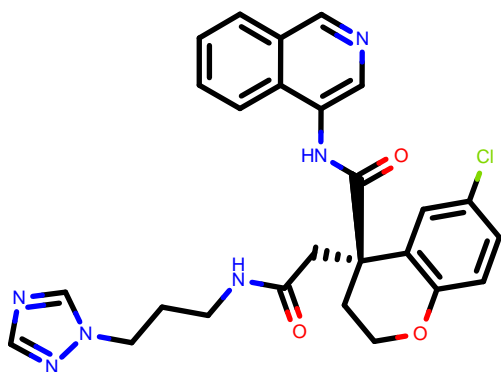
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NC[C@@]5C5O

RUN: RUN3297

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.27

EN300-270328_1_1



CID: EN300-270328_1_1

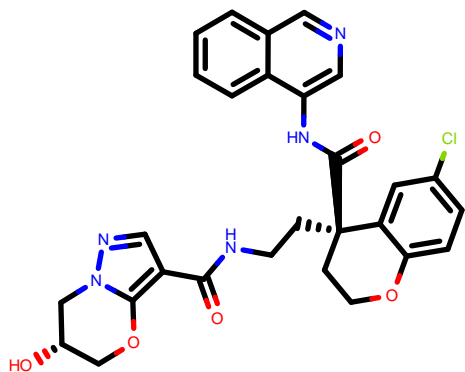
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)NCCn5ncn5

RUN: RUN5273

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.21

EN300-6497444_3_2



CID: EN300-6497444_3_2

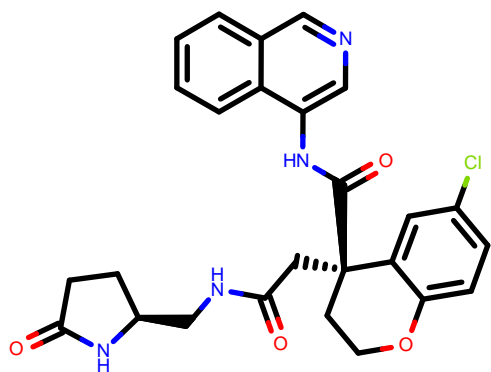
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CNC(=O)c5cnc6c5OC[C@@]7H7

RUN: RUN5041

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.29

EN300-75030_1_2



CID: EN300-75030_1_2

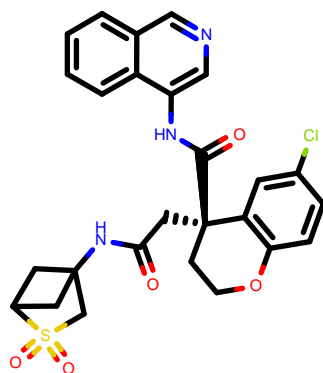
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]H5CCCC(=O)N5

RUN: RUN7239

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.22

EN300-7493768_1_1



CID: EN300-7493768_1_1

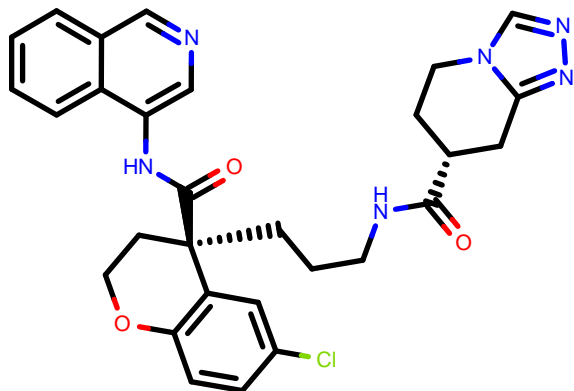
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC56CC(C5)S(=O)(=O)C6

RUN: RUN14610

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.23

EN300-6474341_4_2



CID: EN300-6474341_4_2

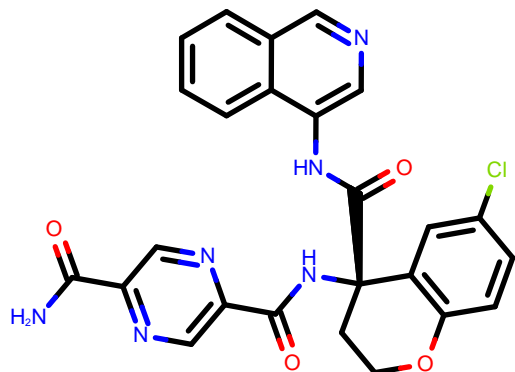
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]H5CCN6N6C5

RUN: RUN11955

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.24

EN300-1273172_1_1



CID: EN300-1273172_1_1

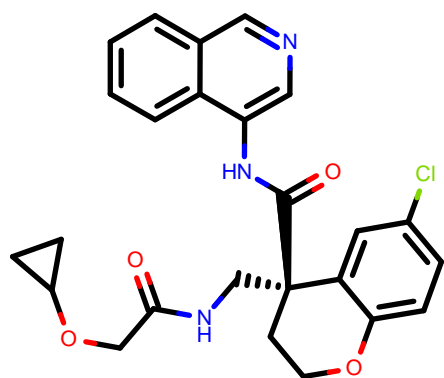
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncnc5C(=O)N

RUN: RUN355

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.19

EN300-378373_2_1



CID: EN300-378373_2_1

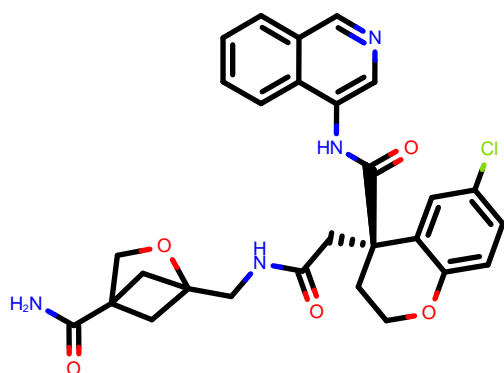
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COC5CC5

RUN: RUN1476

DDG (kcal/mol): -0.03

dDDG (kcal/mol): 0.20

EN300-6733595_1_1



CID: EN300-6733595_1_1

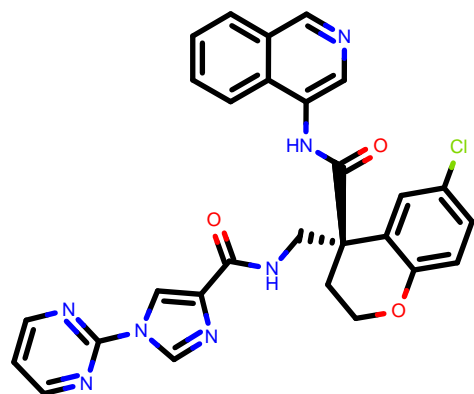
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC56CC(C5)CO6)C(=O)N

RUN: RUN15427

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-261056_2_1



CID: EN300-261056_2_1

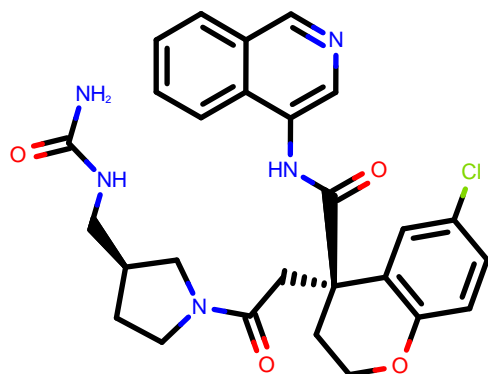
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(cn5)c6nccn6

RUN: RUN2162

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.23

EN300-210256_1_2



CID: EN300-210256_1_2

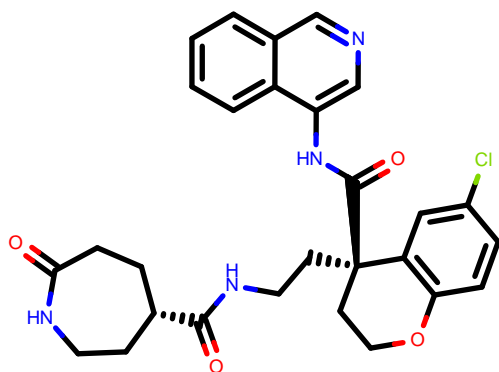
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C@H)(C5)CNC(=O)N

RUN: RUN7799

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-152337_3_2



CID: EN300-152337_3_2

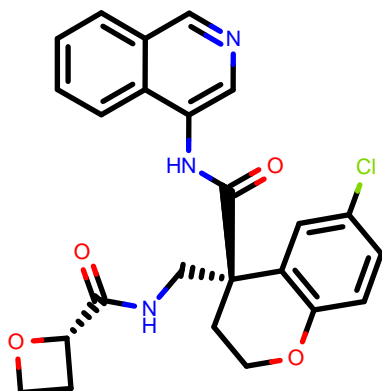
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H]5CCCC(=O)NCC5

RUN: RUN14818

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.24

EN300-85760_2_1



CID: EN300-85760_2_1

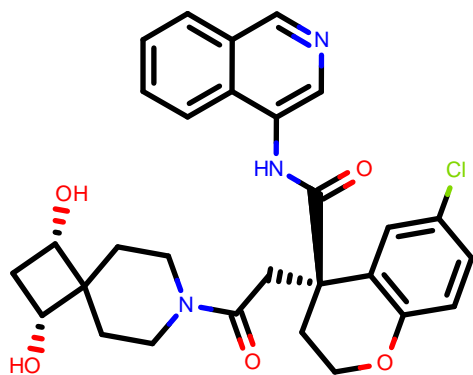
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C@H]5CCO5

RUN: RUN4759

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.19

EN300-7448078_1_1



CID: EN300-7448078_1_1

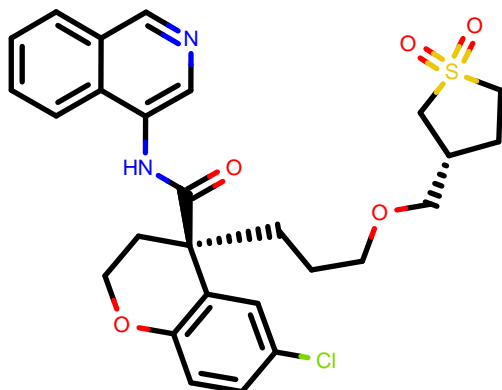
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC(CCS)C@H]1C[C@@H]6O1

RUN: RUN10089

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.25

EN300-1448603_4_2



CID: EN300-1448603_4_2

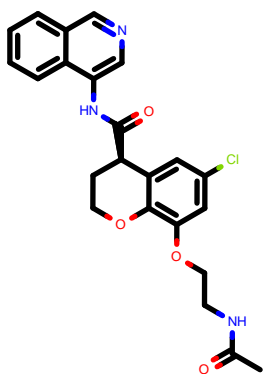
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5SCCS(=O)(=O)C5

RUN: RUN2121

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.28

NAU-LAT-0543f7f2-10_1



CID: NAU-LAT-0543f7f2-10_1

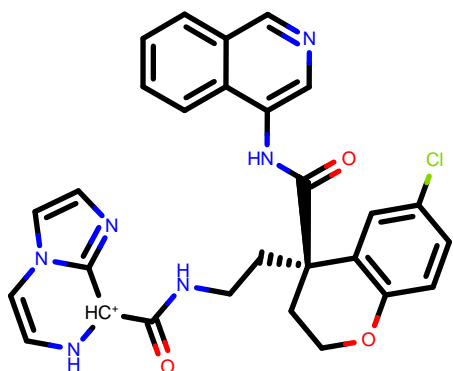
SMILES: CC(=O)NCCOC1cc(cc2c1OCC[C@H]2C(=O)Nc3ncc4c3ccc4)Cl

RUN: RUN157

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-225012_3_1



CID: EN300-225012_3_1

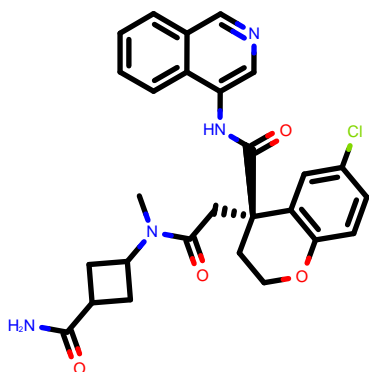
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CNc6ncn6c5

RUN: RUN5021

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.25

EN300-321459_1_1



CID: EN300-321459_1_1

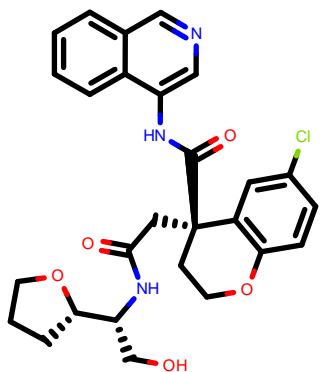
SMILES: CNC(=O)C[C@@]1(c2c(ccc(c2O)OCC1C(=O)Nc3c4c(cnc3cc4)C)C)H5[C@@H](C)Cl=O

RUN: RUN5625

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.26

EN300-190026_1_3



CID: EN300-190026_1_3

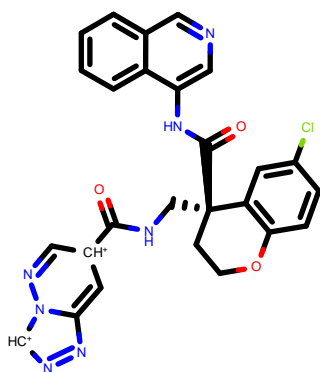
SMILES: c1ccc2c(c1)ncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)[C@@]5H5CCO5

RUN: RUN13448

DDG (kcal/mol): -0.02

dDDG (kcal/mol): 0.39

EN300-7438185_2_1



CID: EN300-7438185_2_1

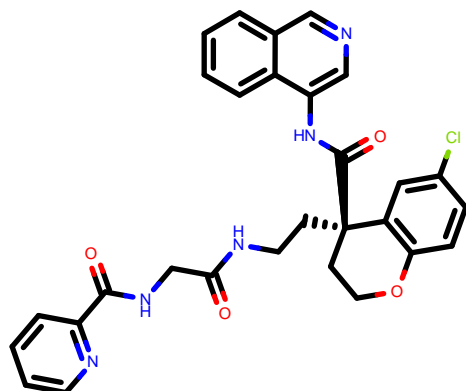
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6nnn6nc5

RUN: RUN9170

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.23

EN300-83280_3_1



CID: EN300-83280_3_1

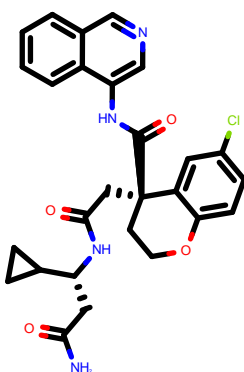
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)c5ccccc5

RUN: RUN11206

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.24

EN300-85413_1_1



CID: EN300-85413_1_1

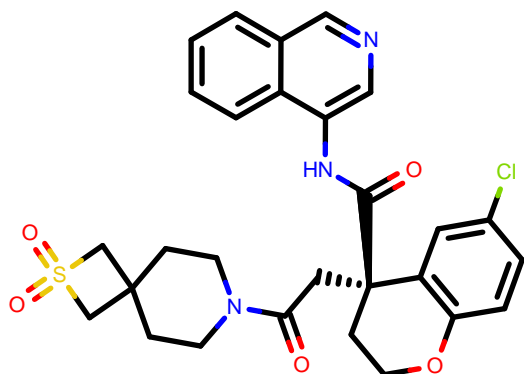
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CC(=O)N)C5CC5

RUN: RUN2363

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.28

EN300-1609249_1_1



CID: EN300-1609249_1_1

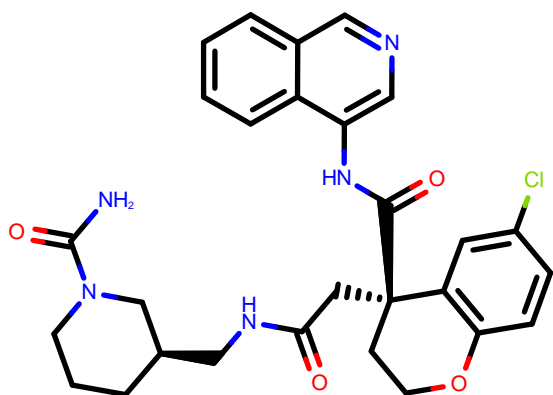
SMILES: c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC6(CC5)CS(=O)(=O)C6

RUN: RUN12624

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.29

EN300-212381_1_2



CID: EN300-212381_1_2

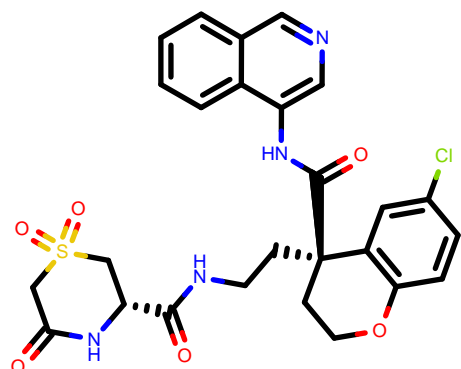
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCN(C5)C(=O)N

RUN: RUN873

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.28

EN300-702756_3_2



CID: EN300-702756_3_2

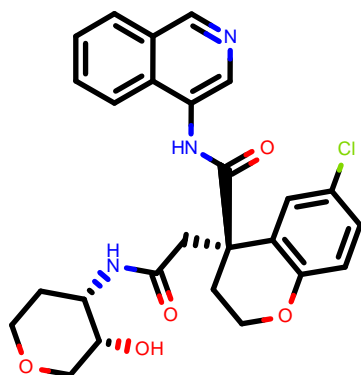
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCN(S(=O)(=O)O)C(=O)N

RUN: RUN15005

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.25

EN300-321053_1_2



CID: EN300-321053_1_2

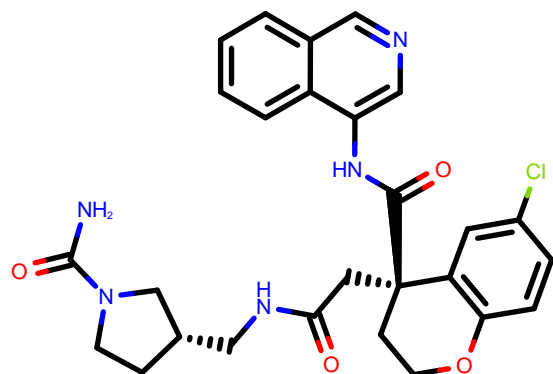
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC[C@@H]5O

RUN: RUN11020

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.26

EN300-210933_1_1



CID: EN300-210933_1_1

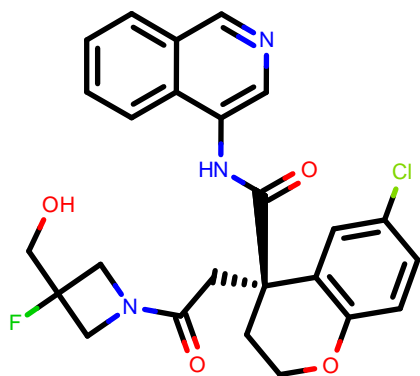
SMILES: c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCN(C5)C(=O)N

RUN: RUN10775

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.23

EN300-204507_1_1



CID: EN300-204507_1_1

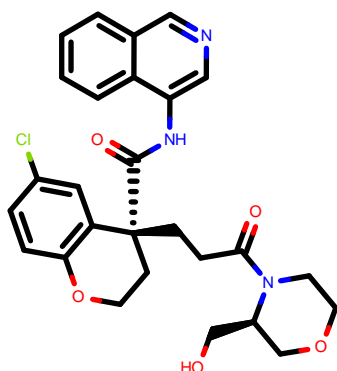
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)(CO)F

RUN: RUN11749

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.25

EN300-173903_2_1



CID: EN300-173903_2_1

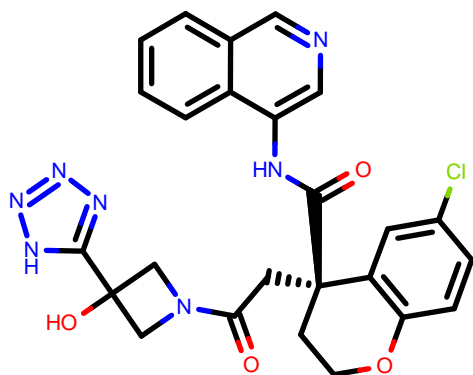
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCC(=O)N5CCOC[C@H]5CO

RUN: RUN8791

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.32

EN300-344563_1_1



CID: EN300-344563_1_1

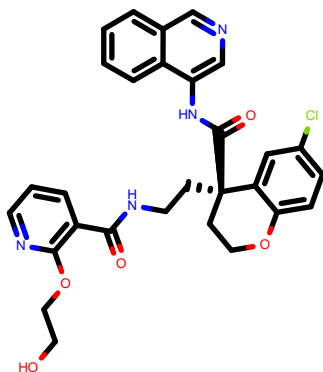
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CC(=O)N5CC(C5)(c6n[nH]n6)O

RUN: RUN10369

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.24

EN300-85043_3_1



CID: EN300-85043_3_1

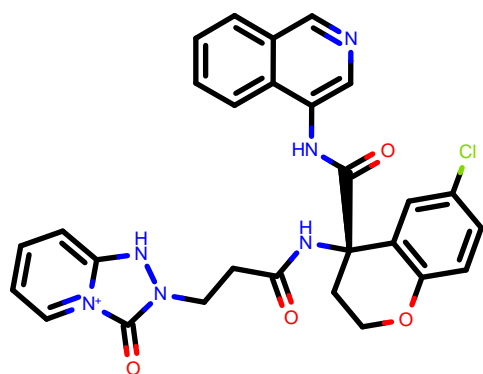
SMILES: c1ccc2c(c1)cnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)C)CCNC(=O)c5ccncc5OCCO

RUN: RUN14550

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.34

EN300-72946_1_1



CID: EN300-72946_1_1

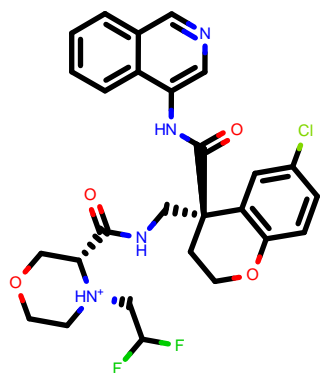
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)NC(=O)CCn5c(=O)n6ccccc6n5

RUN: RUN4566

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.29

EN300-140582_2_2



CID: EN300-140582_2_2

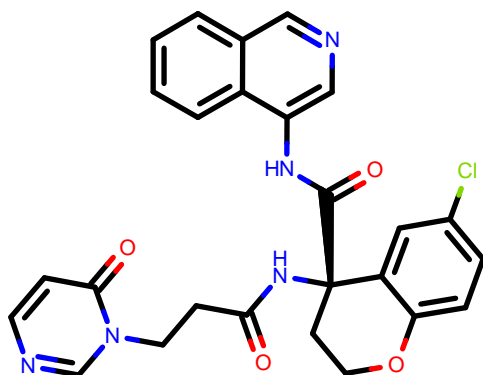
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)CNC(=O)[C@H]5COCCN@]5CC(F)F

RUN: RUN1843

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.30

EN300-219609_1_1



CID: EN300-219609_1_1

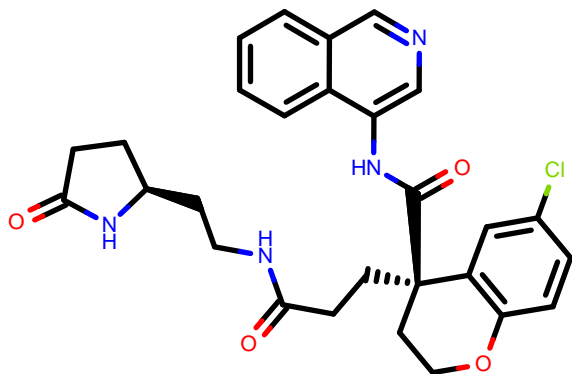
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)NC(=O)CCn5cccc5=O

RUN: RUN4042

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.26

EN300-205779_2_2



CID: EN300-205779_2_2

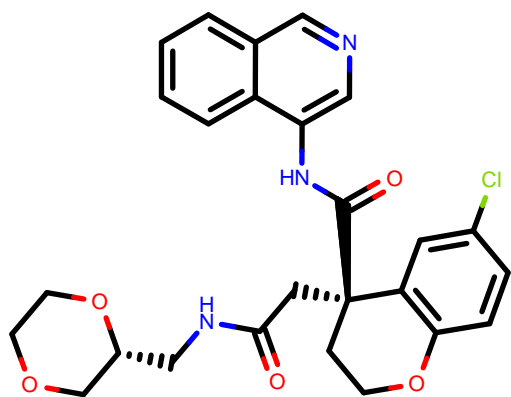
SMILES: c1ccc2c(c1)ncoc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C)CCC(=O)NCC[C@@]4H5COC(=O)N5

RUN: RUN9191

DDG (kcal/mol): -0.01

dDDG (kcal/mol): 0.25

EN300-1699492_1_1



CID:	EN300-1699492_1_1
SMILES:	<chem>c1ccc2c(c1)ncnc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5COCOC5</chem>
RUN:	RUN11934
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.29