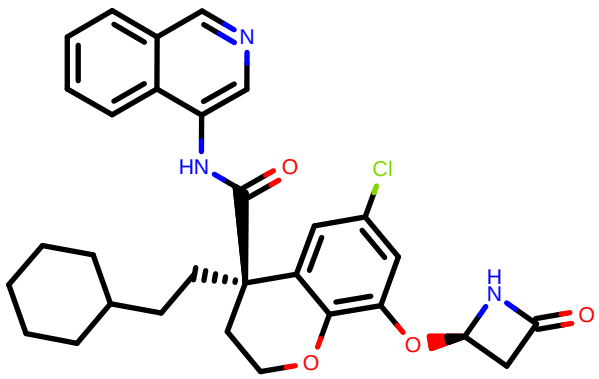
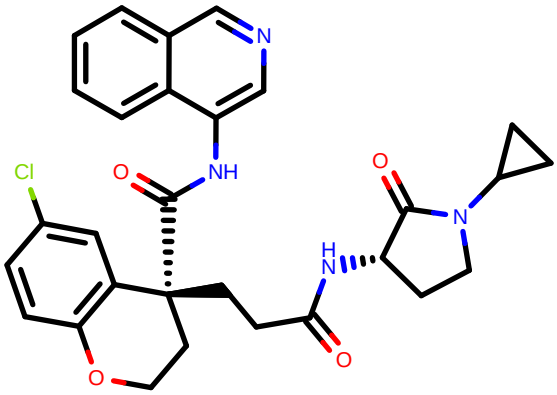
VLA-UCB-50c39ae8-9_1



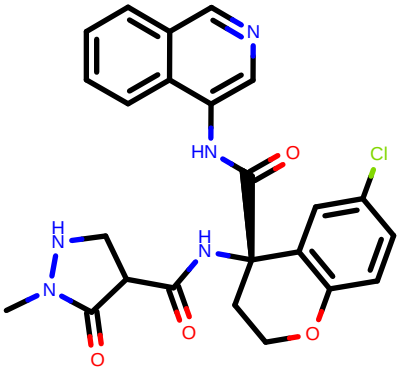
CID:	VLA-UCB-50c39ae8-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN121
DDG (kcal/mol):	-6.04
dDDG (kcal/mol):	0.52

EN300-77438_2_2



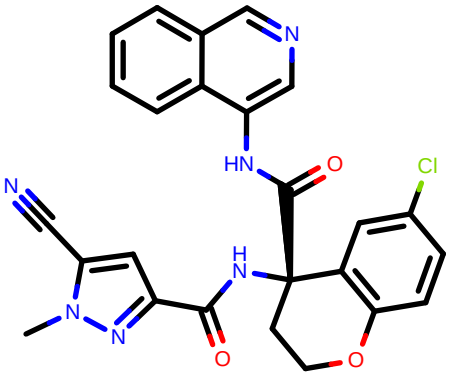
CID:	EN300-77438_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCN(C5=O)C6CC6
RUN:	RUN4348
DDG (kcal/mol):	-5.18
dDDG (kcal/mol):	0.28

EN300-7437779_1_1



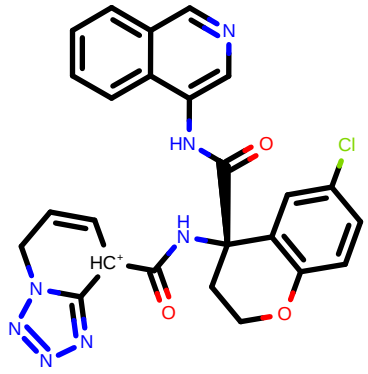
CID:	EN300-7437779_1_1
SMILES:	Cn1c(=O)c(c[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7222
DDG (kcal/mol):	-4.81
dDDG (kcal/mol):	0.22

EN300-248982_1_1



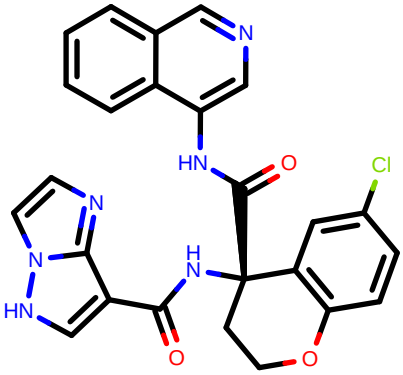
CID:	EN300-248982_1_1
SMILES:	Cn1c(cc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN8718
DDG (kcal/mol):	-4.72
dDDG (kcal/mol):	0.21

EN300-305984_1_1



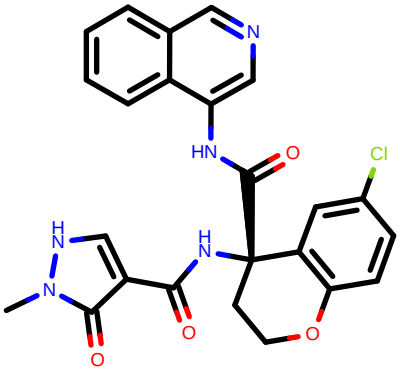
CID:	EN300-305984_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6c5nnn6
RUN:	RUN6395
DDG (kcal/mol):	-4.72
dDDG (kcal/mol):	0.25

EN300-135238_1_1



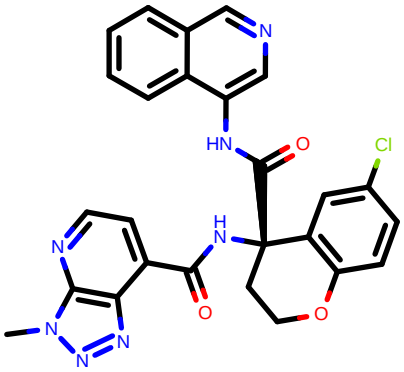
CID:	EN300-135238_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5[nH]cc6
RUN:	RUN7582
DDG (kcal/mol):	-4.68
dDDG (kcal/mol):	0.20

EN300-7437779_1_1



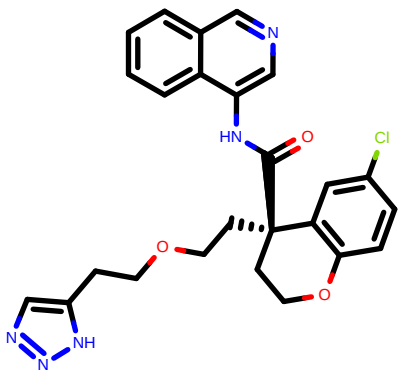
CID:	EN300-7437779_1_1
SMILES:	Cn1c(=O)c(c[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7218
DDG (kcal/mol):	-4.66
dDDG (kcal/mol):	0.22

EN300-202106_1_1



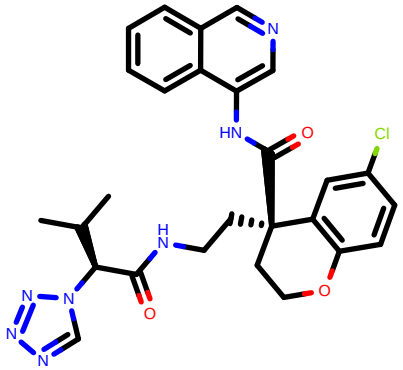
CID:	EN300-202106_1_1
SMILES:	Cn1c2c(c(ccn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)nn1
RUN:	RUN7766
DDG (kcal/mol):	-4.46
dDDG (kcal/mol):	0.22

EN300-222357_3_1



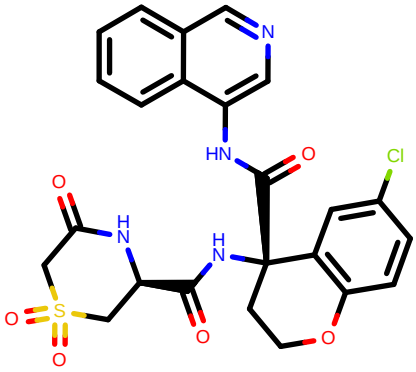
CID:	EN300-222357_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5c[nH]nn5
RUN:	RUN1971
DDG (kcal/mol):	-4.41
dDDG (kcal/mol):	0.23

EN300-297561_3_1



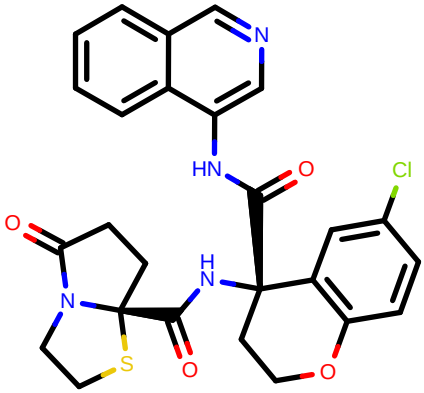
CID:	EN300-297561_3_1
SMILES:	CC(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnnn5
RUN:	RUN2185
DDG (kcal/mol):	-4.40
dDDG (kcal/mol):	0.31

EN300-702756_1_2



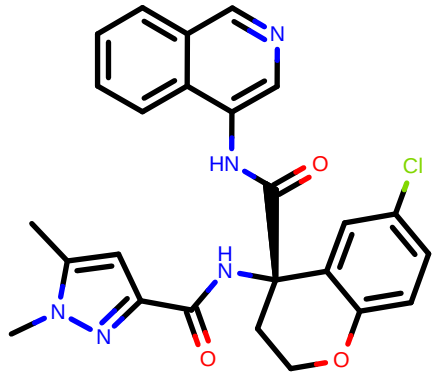
CID:	EN300-702756_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CS(=O)(=O)CC(=O)N5
RUN:	RUN5640
DDG (kcal/mol):	-4.24
dDDG (kcal/mol):	0.27

EN300-10334_1_2



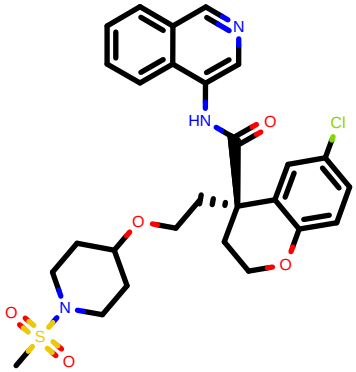
CID:	EN300-10334_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]56CCC(=O)N5CCS6
RUN:	RUN4629
DDG (kcal/mol):	-4.23
dDDG (kcal/mol):	0.31

EN300-1600312_1_1



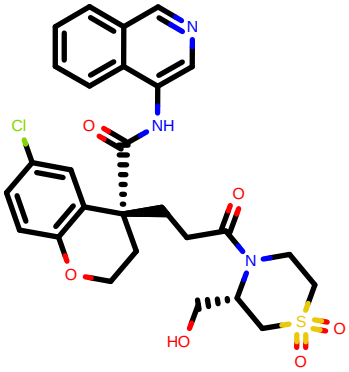
CID:	EN300-1600312_1_1
SMILES:	Cc1cc(nn1C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4977
DDG (kcal/mol):	-4.22
dDDG (kcal/mol):	0.22

EN300-301416_3_1



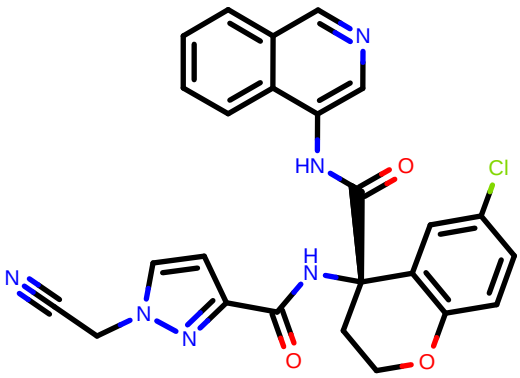
CID:	EN300-301416_3_1
SMILES:	CS(=O)(=O)N1CCC(CC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2489
DDG (kcal/mol):	-4.20
dDDG (kcal/mol):	0.34

EN300-157541_2_1



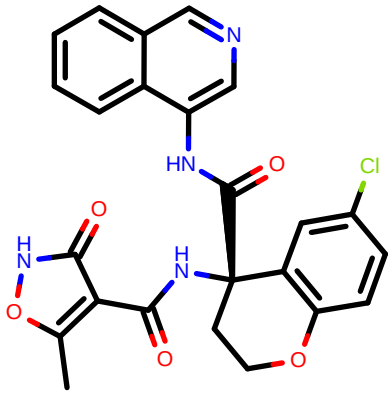
CID:	EN300-157541_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCS(=O)(=O)C[C@@H]5CO
RUN:	RUN7097
DDG (kcal/mol):	-4.18
dDDG (kcal/mol):	0.36

EN300-1251424_1_1



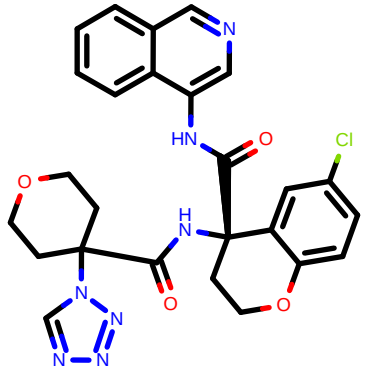
CID:	EN300-1251424_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(n5)CC#N
RUN:	RUN3941
DDG (kcal/mol):	-4.14
dDDG (kcal/mol):	0.25

EN300-110423_1_1



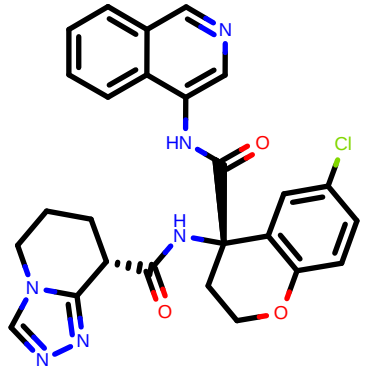
CID:	EN300-110423_1_1
SMILES:	Cc1c(c(=O)[nH]o1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7110
DDG (kcal/mol):	-4.14
dDDG (kcal/mol):	0.26

EN300-254908_1_1



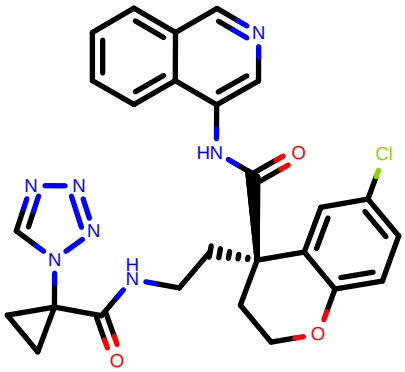
CID:	EN300-254908_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)n6cnnn6
RUN:	RUN7342
DDG (kcal/mol):	-4.04
dDDG (kcal/mol):	0.28

EN300-748981_1_2



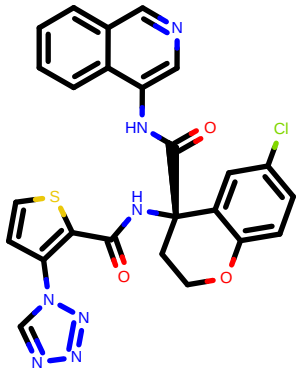
CID:	EN300-748981_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCn6c5nnc6
RUN:	RUN6299
DDG (kcal/mol):	-4.03
dDDG (kcal/mol):	0.28

EN300-263085_3_1



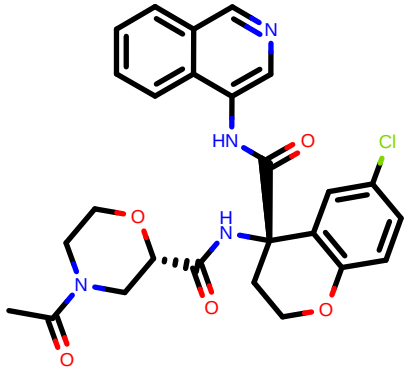
CID:	EN300-263085_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)n6cnnn6
RUN:	RUN479
DDG (kcal/mol):	-3.96
dDDG (kcal/mol):	0.31

EN300-36731_1_1



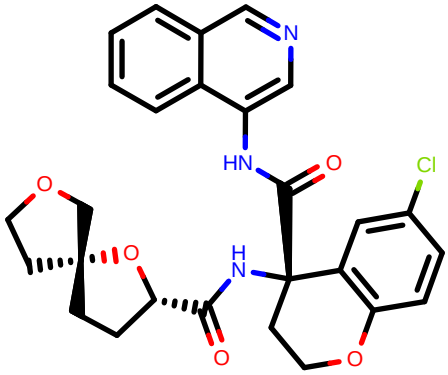
CID:	EN300-36731_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(ccs5)n6cnnn6
RUN:	RUN7814
DDG (kcal/mol):	-3.94
dDDG (kcal/mol):	0.23

EN300-100689_1_1



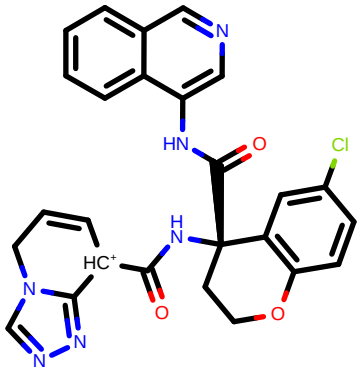
CID:	EN300-100689_1_1
SMILES:	CC(=O)N1CCO[C@@H](C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8882
DDG (kcal/mol):	-3.93
dDDG (kcal/mol):	0.36

EN300-3031933_1_1



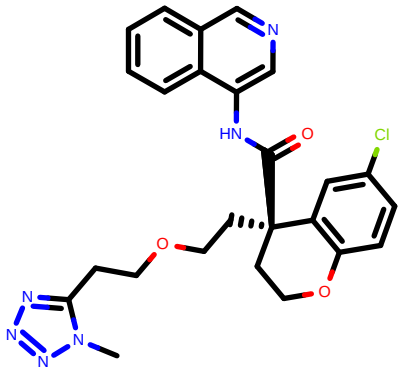
CID:	EN300-3031933_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCC6(O5)CCOC6
RUN:	RUN8098
DDG (kcal/mol):	-3.91
dDDG (kcal/mol):	0.37

EN300-1726153_1_1



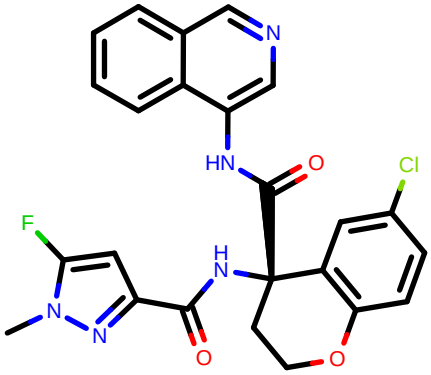
CID:	EN300-1726153_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6c5nnc6
RUN:	RUN6455
DDG (kcal/mol):	-3.88
dDDG (kcal/mol):	0.26

EN300-365398_3_1



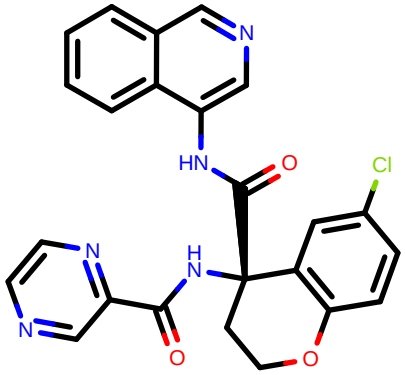
CID:	EN300-365398_3_1
SMILES:	Cn1c(nnn1)CCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN624
DDG (kcal/mol):	-3.86
dDDG (kcal/mol):	0.26

EN300-243465_1_1



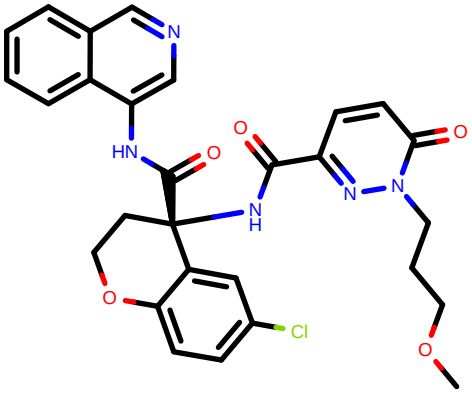
CID:	EN300-243465_1_1
SMILES:	Cn1c(cc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F
RUN:	RUN4565
DDG (kcal/mol):	-3.82
dDDG (kcal/mol):	0.22

EN300-19900_1_1



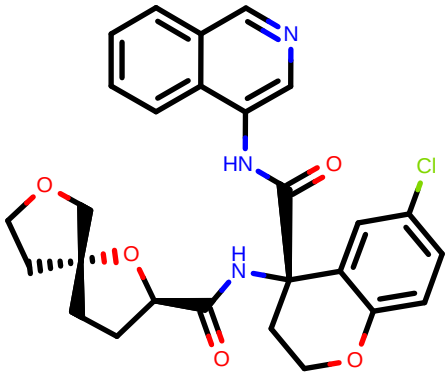
CID:	EN300-19900_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnccn5
RUN:	RUN5680
DDG (kcal/mol):	-3.82
dDDG (kcal/mol):	0.18

EN300-297872_1_1



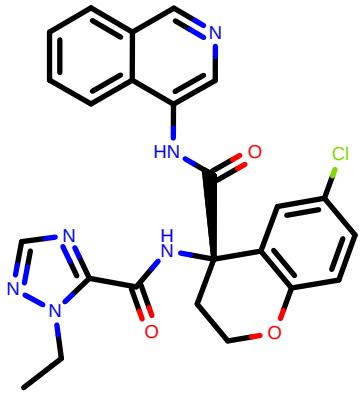
CID:	EN300-297872_1_1
SMILES:	COCCCn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3286
DDG (kcal/mol):	-3.79
dDDG (kcal/mol):	0.33

EN300-3031933_1_2



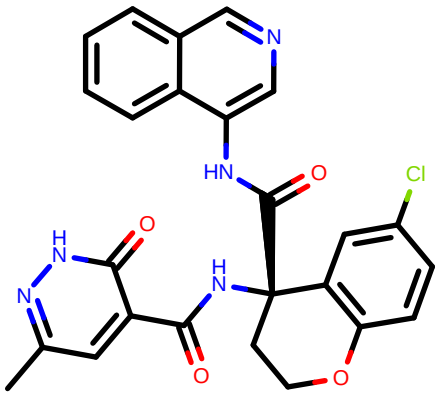
CID:	EN300-3031933_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCC6(O5)CCOC6
RUN:	RUN6583
DDG (kcal/mol):	-3.77
dDDG (kcal/mol):	0.31

EN300-6494693_1_1



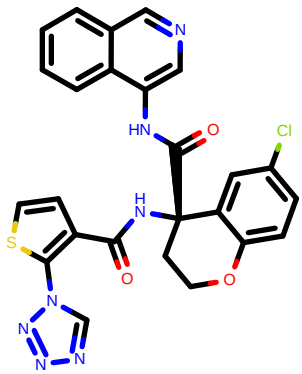
CID:	EN300-6494693_1_1
SMILES:	CCn1c(ncn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5001
DDG (kcal/mol):	-3.77
dDDG (kcal/mol):	0.24

EN300-147499_1_1



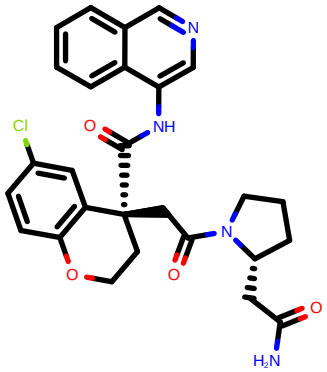
CID:	EN300-147499_1_1
SMILES:	Cc1cc(c(=O)[nH]n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7438
DDG (kcal/mol):	-3.74
dDDG (kcal/mol):	0.25

EN300-6744029_1_1



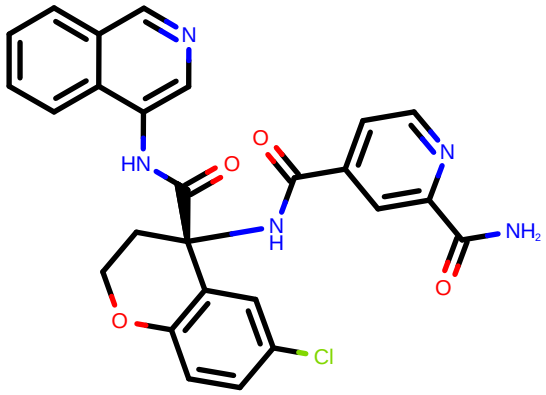
CID:	EN300-6744029_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccsc5n6cnnn6
RUN:	RUN7262
DDG (kcal/mol):	-3.73
dDDG (kcal/mol):	0.29

EN300-124652_1_1



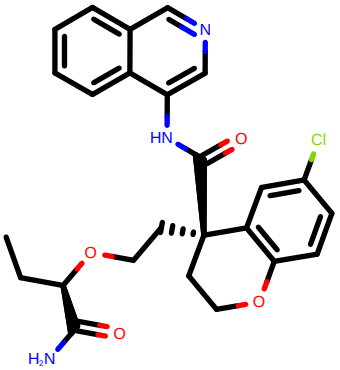
CID:	EN300-124652_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CC(=O)N
RUN:	RUN2904
DDG (kcal/mol):	-3.71
dDDG (kcal/mol):	0.32

EN300-102071_1_1



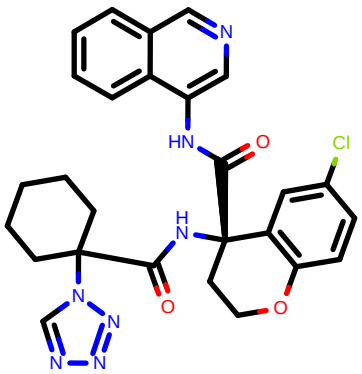
CID:	EN300-102071_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)C(=O)N
RUN:	RUN5081
DDG (kcal/mol):	-3.69
dDDG (kcal/mol):	0.27

EN300-65839_3_2



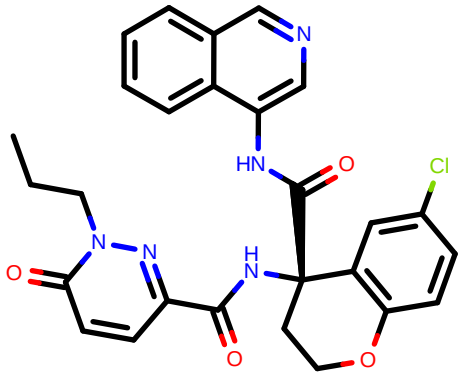
CID:	EN300-65839_3_2
SMILES:	CC[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1699
DDG (kcal/mol):	-3.69
dDDG (kcal/mol):	0.32

EN300-186536_1_1



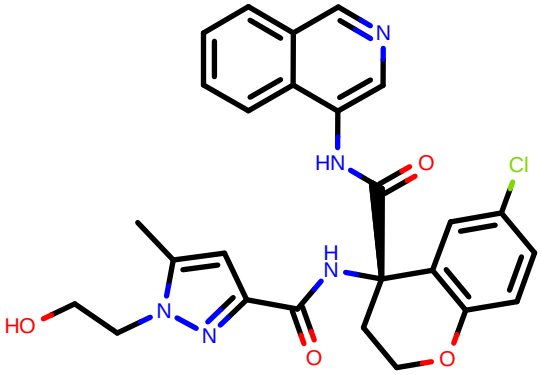
CID:	EN300-186536_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCCC5)n6cnnn6
RUN:	RUN7150
DDG (kcal/mol):	-3.69
dDDG (kcal/mol):	0.33

EN300-09334_1_1



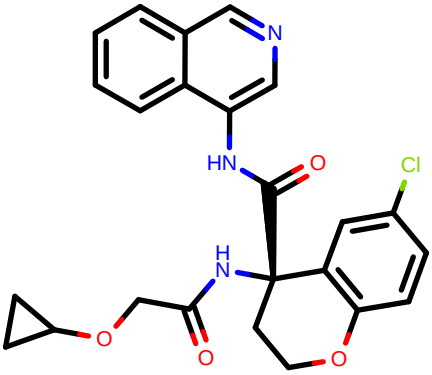
CID:	EN300-09334_1_1
SMILES:	CCCn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5688
DDG (kcal/mol):	-3.68
dDDG (kcal/mol):	0.29

EN300-6739934_1_1



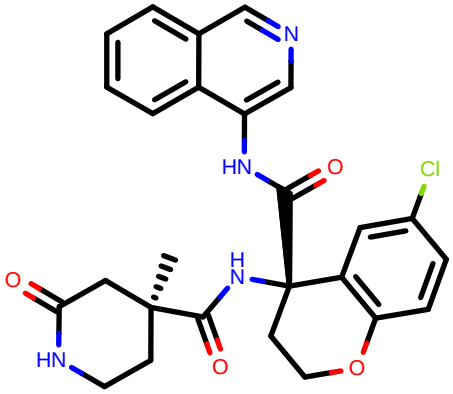
CID:	EN300-6739934_1_1
SMILES:	Cc1cc(nn1CCO)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5149
DDG (kcal/mol):	-3.66
dDDG (kcal/mol):	0.25

EN300-378373_1_1



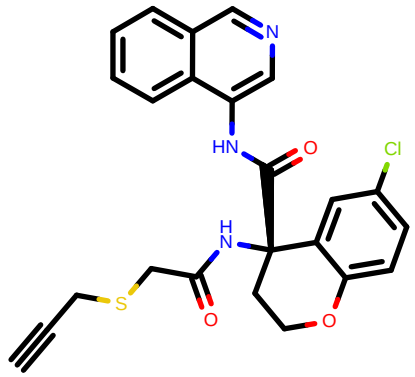
CID:	EN300-378373_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC5CC5
RUN:	RUN2862
DDG (kcal/mol):	-3.65
dDDG (kcal/mol):	0.22

EN300-315854_1_1



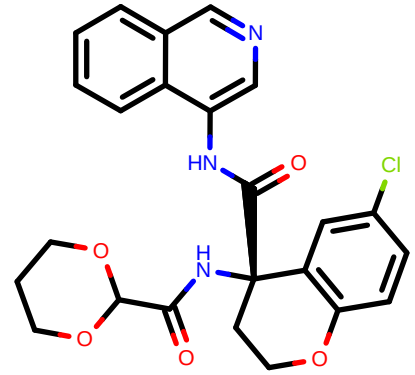
CID:	EN300-315854_1_1
SMILES:	C[C@@]1(CCNC(=O)C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3829
DDG (kcal/mol):	-3.63
dDDG (kcal/mol):	0.34

EN300-86878_1_1



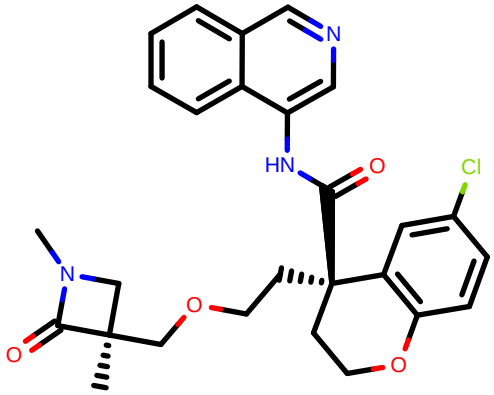
CID:	EN300-86878_1_1
SMILES:	C#CCSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN585
DDG (kcal/mol):	-3.55
dDDG (kcal/mol):	0.20

EN300-170985_1_1



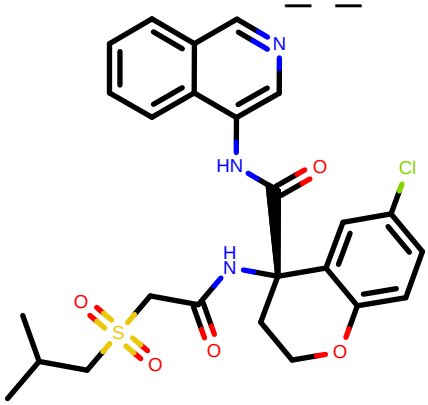
CID:	EN300-170985_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCCO5
RUN:	RUN3438
DDG (kcal/mol):	-3.54
dDDG (kcal/mol):	0.24

EN300-1273362_3_2



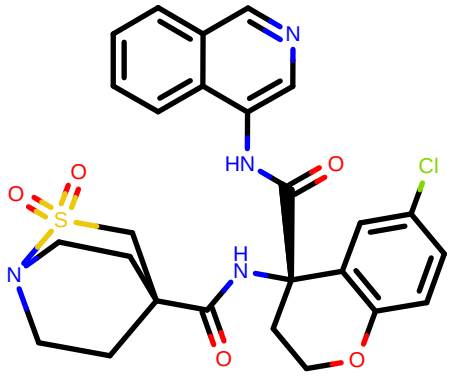
CID:	EN300-1273362_3_2
SMILES:	C[C@]1(CN(C1=O)C)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN305
DDG (kcal/mol):	-3.53
dDDG (kcal/mol):	0.34

EN300-42243_1_1



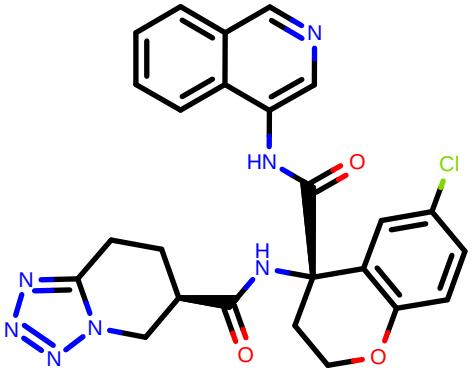
CID:	EN300-42243_1_1
SMILES:	CC(C)CS(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN798
DDG (kcal/mol):	-3.52
dDDG (kcal/mol):	0.31

EN300-6731334_1_1



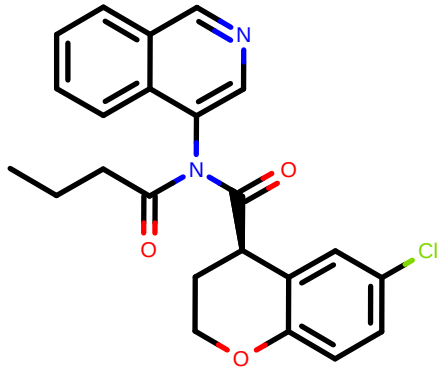
CID:	EN300-6731334_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CCN(CC5)S(=O)(=O)C6
RUN:	RUN7258
DDG (kcal/mol):	-3.48
dDDG (kcal/mol):	0.38

EN300-269453_1_1



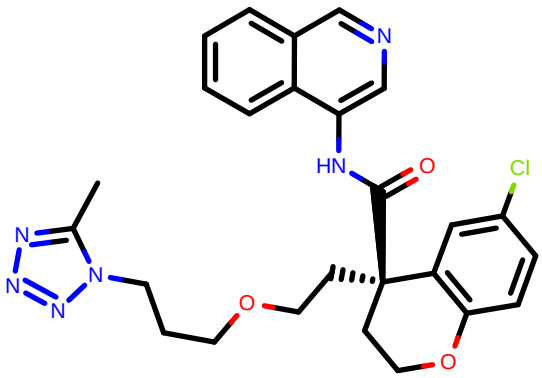
CID:	EN300-269453_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCc6nnnn6C5
RUN:	RUN8198
DDG (kcal/mol):	-3.48
dDDG (kcal/mol):	0.29

DAR-DIA-5ff57136-11_1



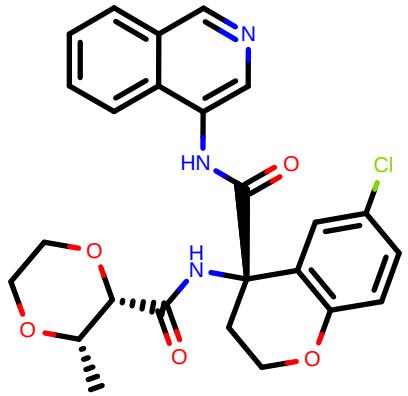
CID:	DAR-DIA-5ff57136-11_1
SMILES:	C=C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN221
DDG (kcal/mol):	-3.47
dDDG (kcal/mol):	0.27

EN300-197715_3_1



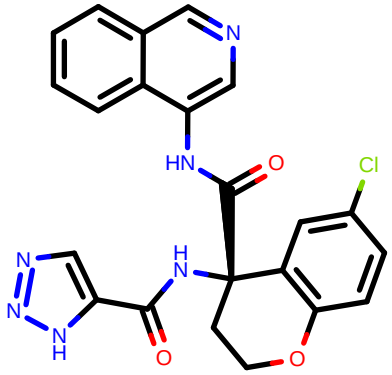
CID:	EN300-197715_3_1
SMILES:	Cc1nnnn1CCCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN805
DDG (kcal/mol):	-3.46
dDDG (kcal/mol):	0.30

EN300-299215_1_1



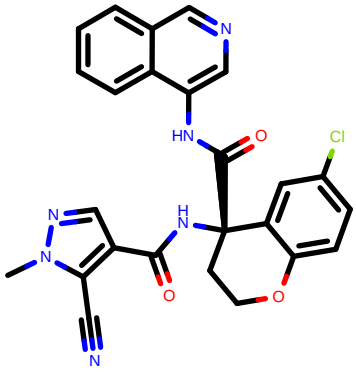
CID:	EN300-299215_1_1
SMILES:	C[C@H]1[C@H](OCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5856
DDG (kcal/mol):	-3.45
dDDG (kcal/mol):	0.28

EN300-31998_1_1



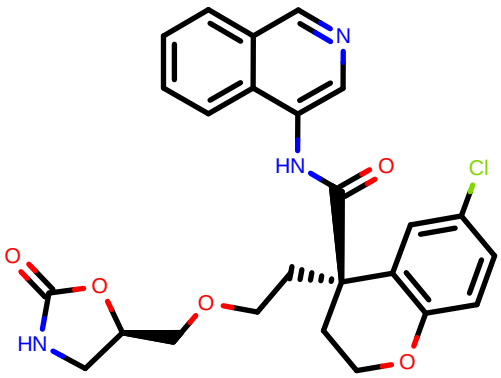
CID:	EN300-31998_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]nn5
RUN:	RUN4525
DDG (kcal/mol):	-3.45
dDDG (kcal/mol):	0.17

EN300-140837_1_1



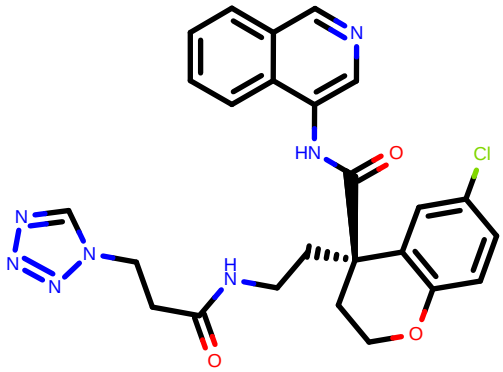
CID:	EN300-140837_1_1
SMILES:	Cn1c(c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN7490
DDG (kcal/mol):	-3.44
dDDG (kcal/mol):	0.25

EN300-203293_3_2



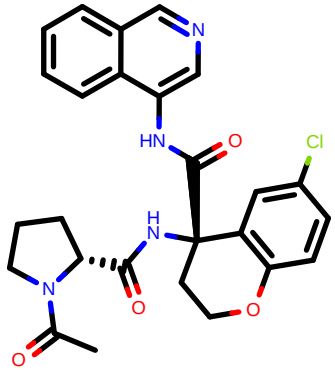
CID:	EN300-203293_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CNC(=O)O5
RUN:	RUN742
DDG (kcal/mol):	-3.43
dDDG (kcal/mol):	0.28

EN300-191904_3_1



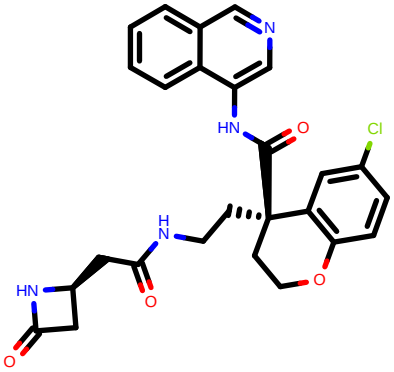
CID:	EN300-191904_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cnnn5
RUN:	RUN5594
DDG (kcal/mol):	-3.42
dDDG (kcal/mol):	0.24

EN300-12587_1_1



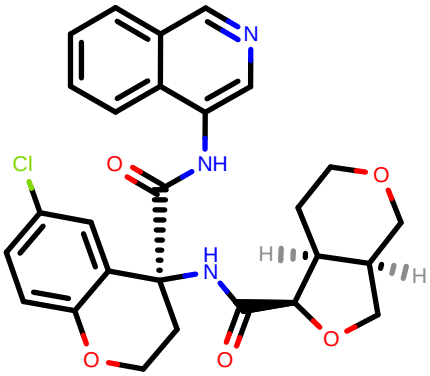
CID:	EN300-12587_1_1
SMILES:	CC(=O)N1CCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5660
DDG (kcal/mol):	-3.40
dDDG (kcal/mol):	0.35

EN300-250593_3_2



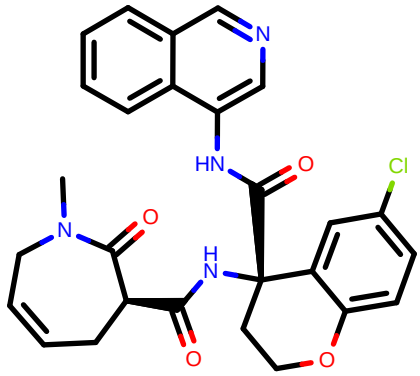
CID:	EN300-250593_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CC(=O)N5
RUN:	RUN11232
DDG (kcal/mol):	-3.39
dDDG (kcal/mol):	0.24

EN300-746830_1_1



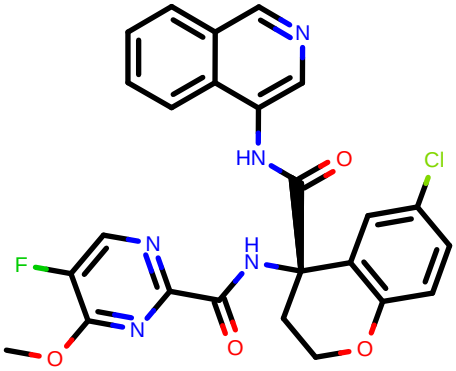
CID:	EN300-746830_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5[C@H]6CCOC[C@H]6CO5
RUN:	RUN3022
DDG (kcal/mol):	-3.38
dDDG (kcal/mol):	0.24

EN300-304695_1_1



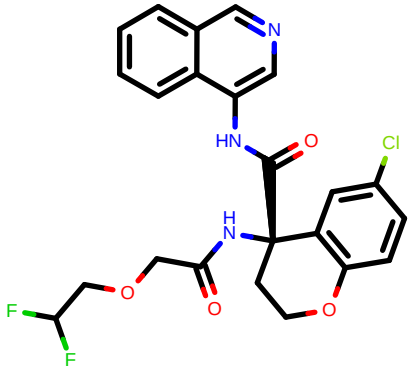
CID:	EN300-304695_1_1
SMILES:	CN1CCCC[C@@H](C1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7234
DDG (kcal/mol):	-3.38
dDDG (kcal/mol):	0.30

EN300-1703711_1_1



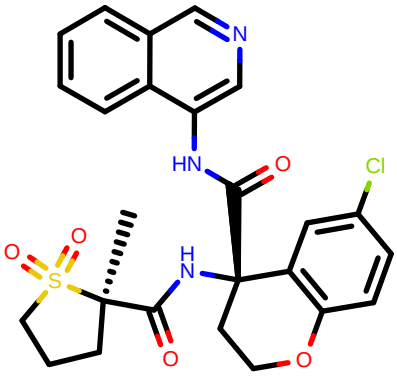
CID:	EN300-1703711_1_1
SMILES:	COc1c(cnc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F
RUN:	RUN4509
DDG (kcal/mol):	-3.35
dDDG (kcal/mol):	0.25

EN300-315792_1_1



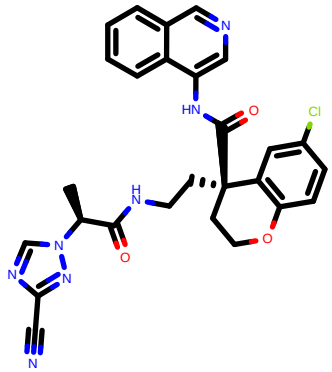
CID:	EN300-315792_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COCC(F)F
RUN:	RUN521
DDG (kcal/mol):	-3.34
dDDG (kcal/mol):	0.24

EN300-373476_1_1



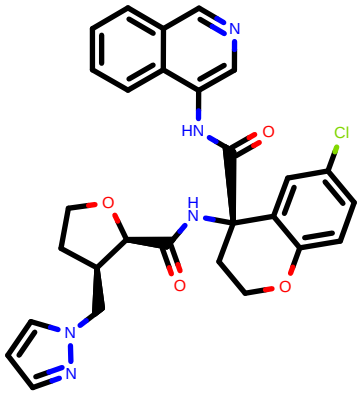
CID:	EN300-373476_1_1
SMILES:	C[C@@]1(CCCS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3825
DDG (kcal/mol):	-3.34
dDDG (kcal/mol):	0.38

EN300-198515_3_1



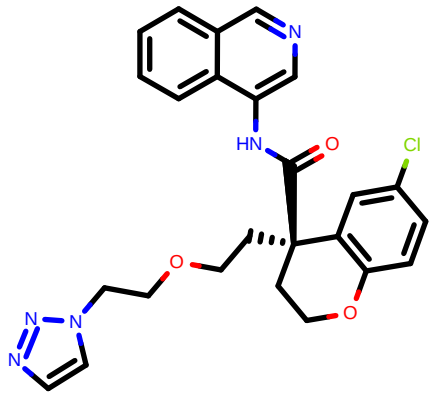
CID:	EN300-198515_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnc(n5)C#N
RUN:	RUN2121
DDG (kcal/mol):	-3.30
dDDG (kcal/mol):	0.33

EN300-304627_1_1



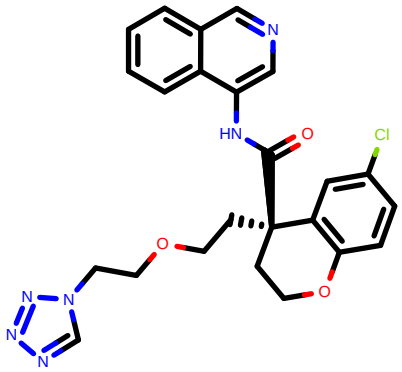
CID:	EN300-304627_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5[C@H](CCO5)Cn6cccn6
RUN:	RUN3174
DDG (kcal/mol):	-3.29
dDDG (kcal/mol):	0.32

EN300-1715993_3_1



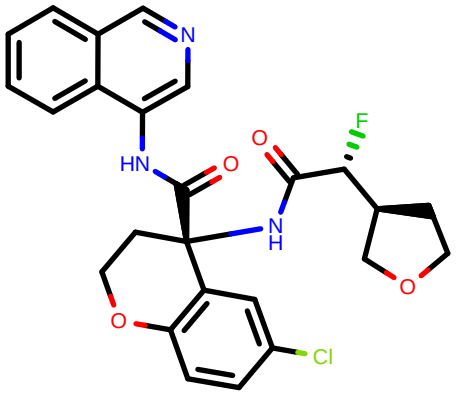
CID:	EN300-1715993_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5ccnn5
RUN:	RUN1396
DDG (kcal/mol):	-3.28
dDDG (kcal/mol):	0.31

EN300-364679_3_1



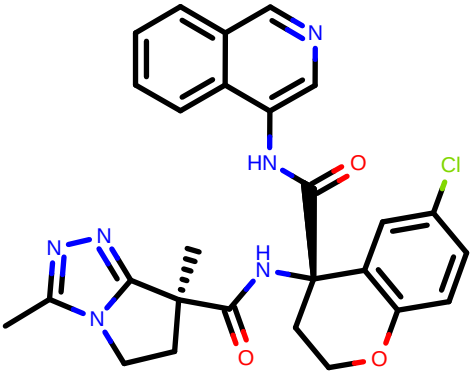
CID:	EN300-364679_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCn5cnnn5
RUN:	RUN297
DDG (kcal/mol):	-3.27
dDDG (kcal/mol):	0.25

EN300-783124_1_3



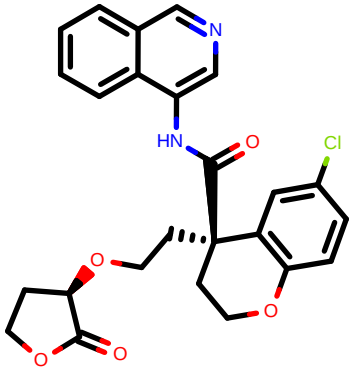
CID:	EN300-783124_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]([C@H]5CCOC5)F
RUN:	RUN1285
DDG (kcal/mol):	-3.27
dDDG (kcal/mol):	0.26

EN300-7431629_1_2



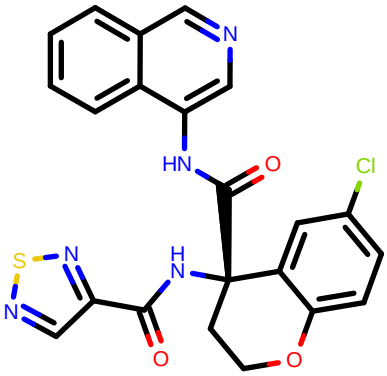
CID:	EN300-7431629_1_2
SMILES:	Cc1nnc2n1CC[C@]2(C)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7402
DDG (kcal/mol):	-3.27
dDDG (kcal/mol):	0.39

EN300-20496_3_1



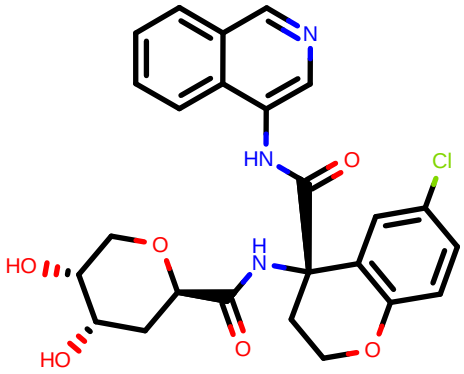
CID:	EN300-20496_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCOC5=O
RUN:	RUN1851
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.23

EN300-42270_1_1



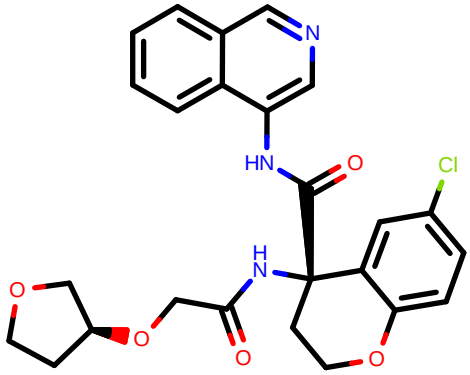
CID:	EN300-42270_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnsn5
RUN:	RUN3478
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.18

EN300-7352736_1_1



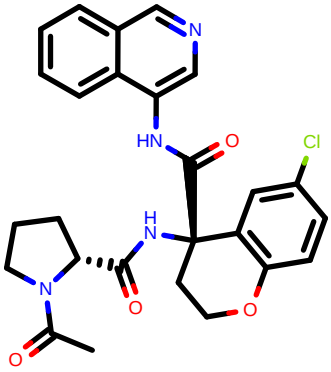
CID:	EN300-7352736_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H]([C@@H](CO5)O)O
RUN:	RUN3006
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.26

EN300-99391_1_2



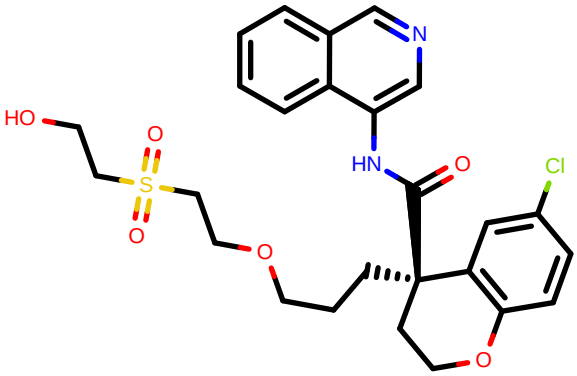
CID:	EN300-99391_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@H]5CCOC5
RUN:	RUN2378
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.23

EN300-211777_1_1



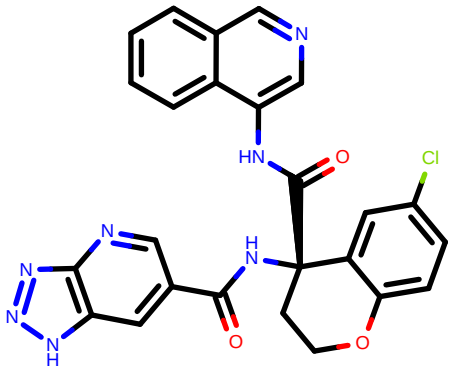
CID:	EN300-211777_1_1
SMILES:	CC(=O)N1CCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5664
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.28

EN300-7463171_4_1



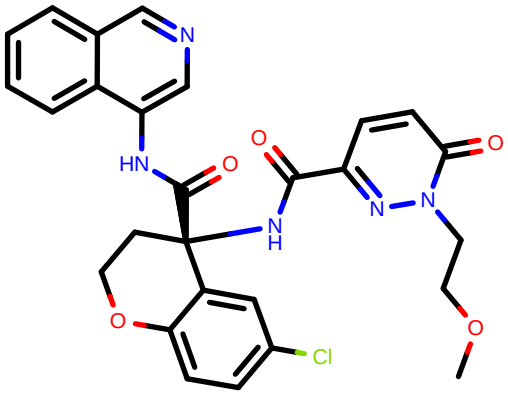
CID:	EN300-7463171_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCS(=O)(=O)CCO
RUN:	RUN1535
DDG (kcal/mol):	-3.25
dDDG (kcal/mol):	0.75

EN300-124555_1_1



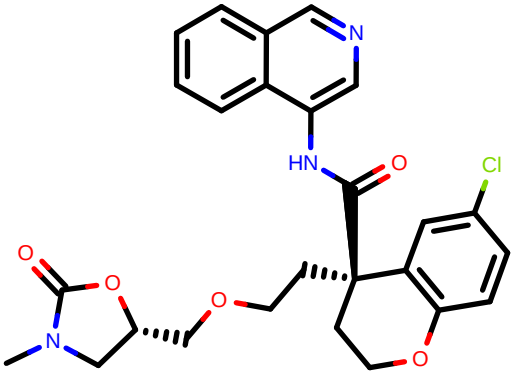
CID:	EN300-124555_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(nc5)n[nH]n6
RUN:	RUN8806
DDG (kcal/mol):	-3.24
dDDG (kcal/mol):	0.23

EN300-23417_1_1



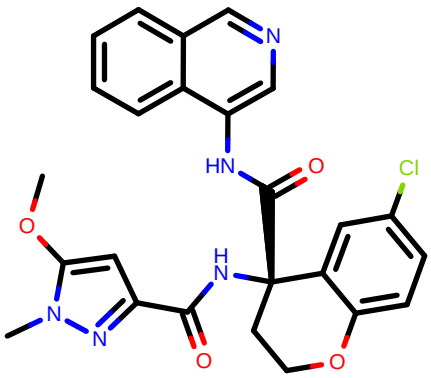
CID:	EN300-23417_1_1
SMILES:	COCCn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4021
DDG (kcal/mol):	-3.24
dDDG (kcal/mol):	0.39

EN300-222969_3_2



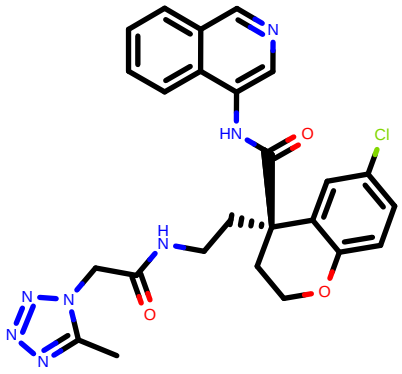
CID:	EN300-222969_3_2
SMILES:	CN1C[C@H](OC1=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN457
DDG (kcal/mol):	-3.24
dDDG (kcal/mol):	0.30

EN300-142240_1_1



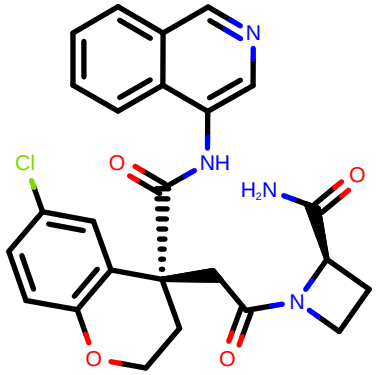
CID:	EN300-142240_1_1
SMILES:	Cn1c(cc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN4157
DDG (kcal/mol):	-3.22
dDDG (kcal/mol):	0.27

EN300-1244816_3_1



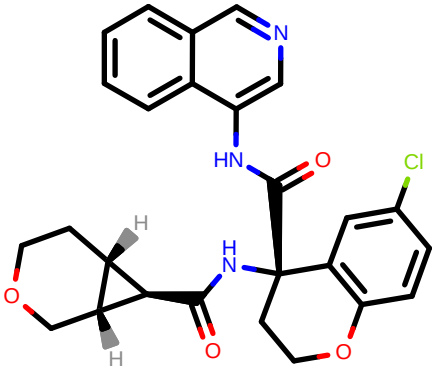
CID:	EN300-1244816_3_1
SMILES:	Cc1nnnn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7052
DDG (kcal/mol):	-3.20
dDDG (kcal/mol):	0.26

EN300-862094_1_1



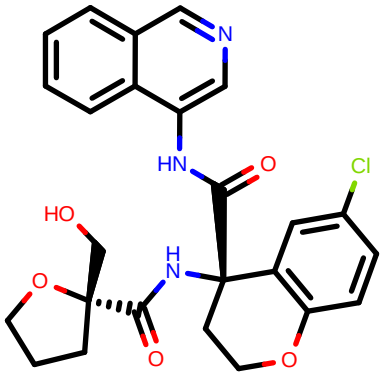
CID:	EN300-862094_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]5C(=O)N
RUN:	RUN9796
DDG (kcal/mol):	-3.20
dDDG (kcal/mol):	0.27

EN300-1644723_1_5



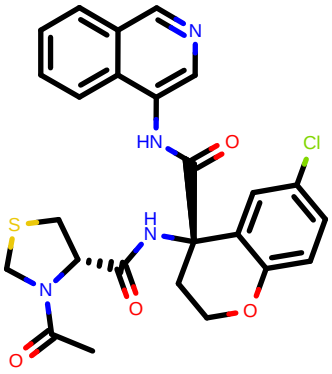
CID:	EN300-1644723_1_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@@H]6[C@H]5COCC6
RUN:	RUN3598
DDG (kcal/mol):	-3.20
dDDG (kcal/mol):	0.23

EN300-1425677_1_1



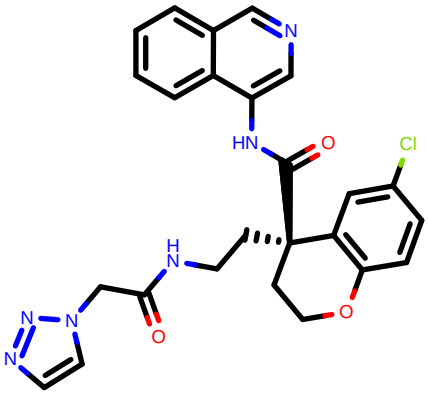
CID:	EN300-1425677_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCO5)CO
RUN:	RUN4881
DDG (kcal/mol):	-3.19
dDDG (kcal/mol):	0.29

EN300-56202_1_1



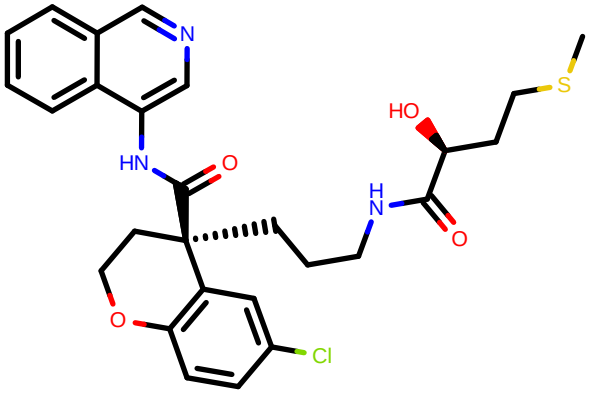
CID:	EN300-56202_1_1
SMILES:	CC(=O)N1CSC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5564
DDG (kcal/mol):	-3.19
dDDG (kcal/mol):	0.37

EN300-100467_3_1



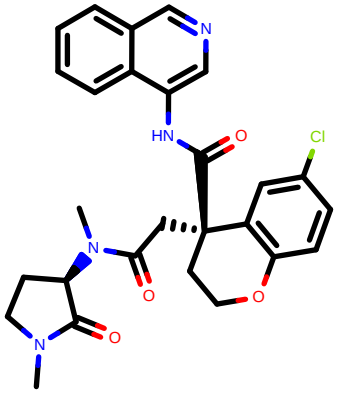
CID:	EN300-100467_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccnn5
RUN:	RUN5095
DDG (kcal/mol):	-3.19
dDDG (kcal/mol):	0.28

EN300-103144_4_1



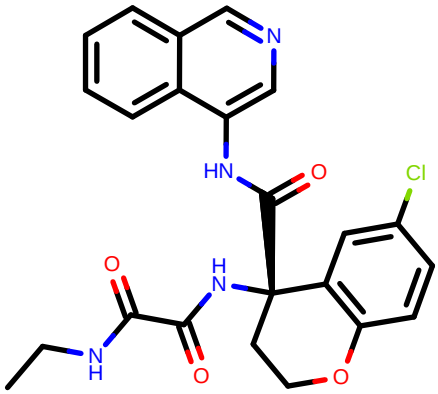
CID:	EN300-103144_4_1
SMILES:	CSCC[C@@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN9831
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.31

EN300-209048_1_2



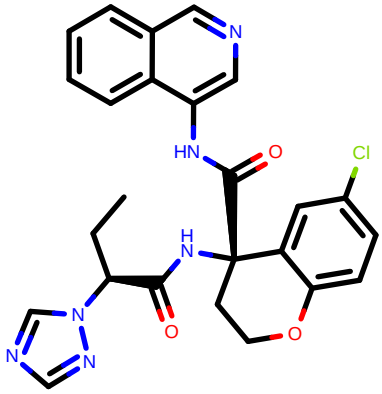
CID:	EN300-209048_1_2
SMILES:	CN1CC[C@H](C1=O)N(C)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11012
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.30

EN300-1262608_1_1



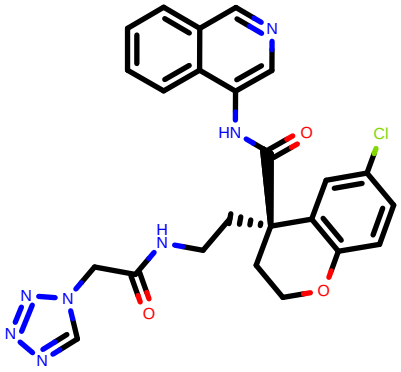
CID:	EN300-1262608_1_1
SMILES:	CCNC(=O)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5069
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.21

EN300-651307_1_1



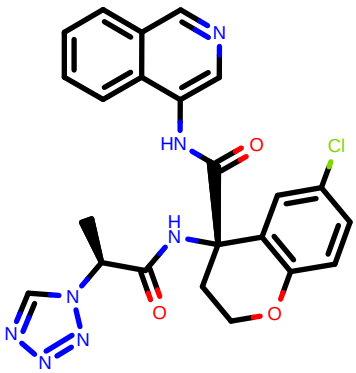
CID:	EN300-651307_1_1
SMILES:	CC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN4101
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.30

EN300-20980_3_1



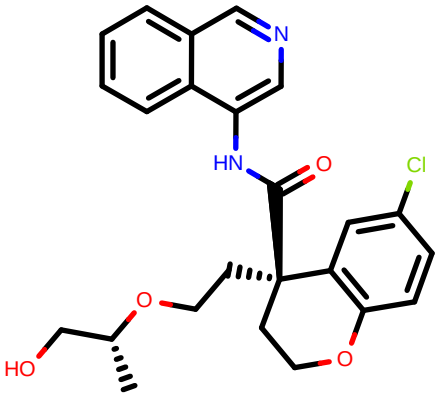
CID:	EN300-20980_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnnn5
RUN:	RUN3060
DDG (kcal/mol):	-3.16
dDDG (kcal/mol):	0.21

EN300-191915_1_1



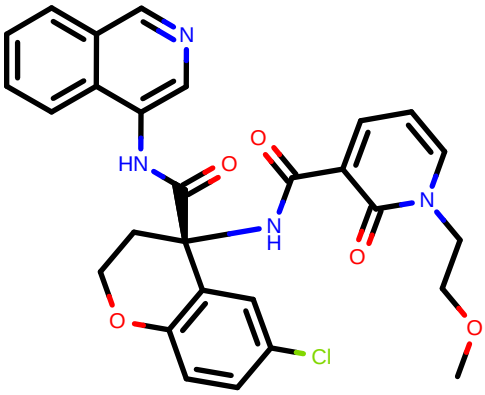
CID:	EN300-191915_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnnn5
RUN:	RUN4397
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.27

EN300-175186_3_2



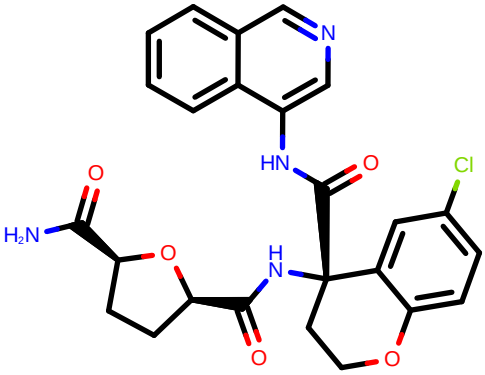
CID:	EN300-175186_3_2
SMILES:	C[C@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1364
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.26

EN300-685077_1_1



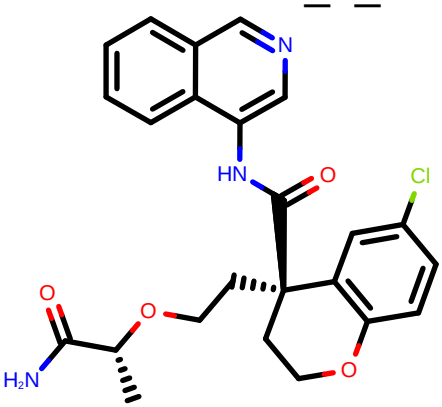
CID:	EN300-685077_1_1
SMILES:	COCCn1cccc(c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8114
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.34

EN300-315238_1_1



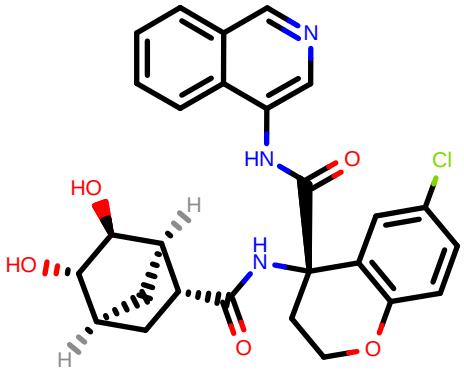
CID:	EN300-315238_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](O5)C(=O)N
RUN:	RUN5872
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.29

EN300-17381_3_2



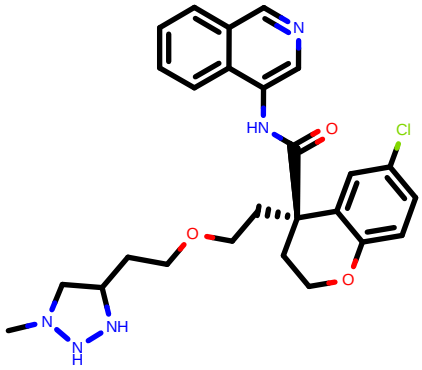
CID:	EN300-17381_3_2
SMILES:	C[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1891
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.22

EN300-6744028_1_5



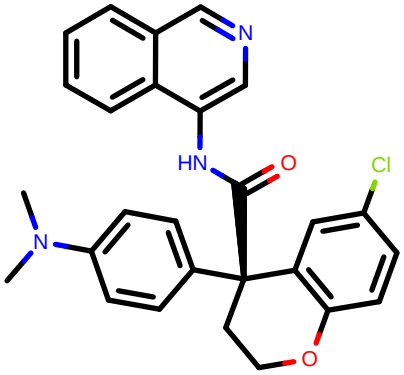
CID:	EN300-6744028_1_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6CC5[C@@H]([C@H]6O)O
RUN:	RUN7510
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.26

EN300-1600786_3_1



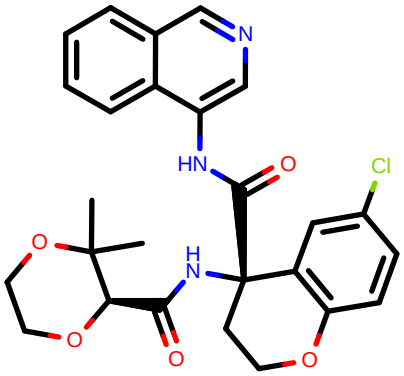
CID:	EN300-1600786_3_1
SMILES:	Cn1cc(nn1)CCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1819
DDG (kcal/mol):	-3.11
dDDG (kcal/mol):	0.29

FRA-DIA-13af2da5-2_1



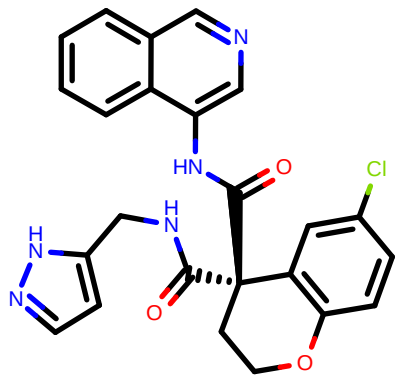
CID:	FRA-DIA-13af2da5-2_1
SMILES:	CN(C)c1ccc(cc1)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN168
DDG (kcal/mol):	-3.10
dDDG (kcal/mol):	0.18

EN300-1601684_1_2



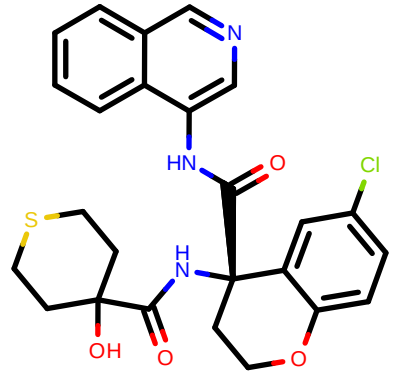
CID:	EN300-1601684_1_2
SMILES:	CC1([C@H](OCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN6775
DDG (kcal/mol):	-3.10
dDDG (kcal/mol):	0.25

VLA-UCB-34f3ed0c-3_1



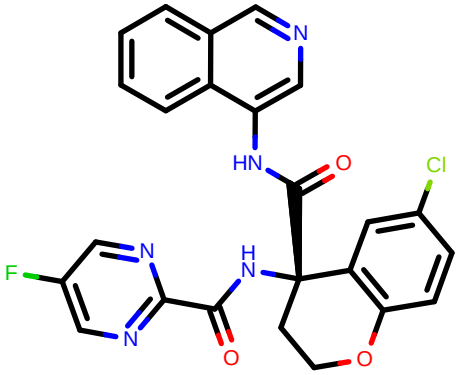
CID:	VLA-UCB-34f3ed0c-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)NCc5cc[nH]n5
RUN:	RUN269
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.25

EN300-122340_1_1



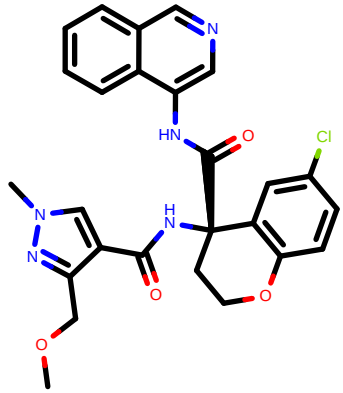
CID:	EN300-122340_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCSCC5)O
RUN:	RUN4401
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.43

EN300-149296_1_1



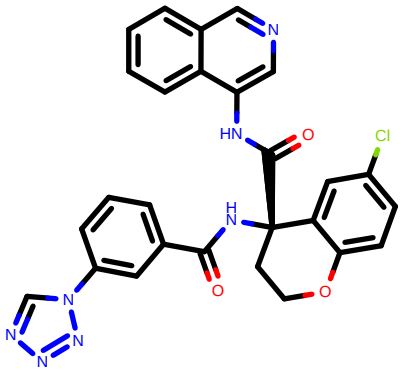
CID:	EN300-149296_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncc(cn5)F
RUN:	RUN4897
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.21

EN300-244148_1_1



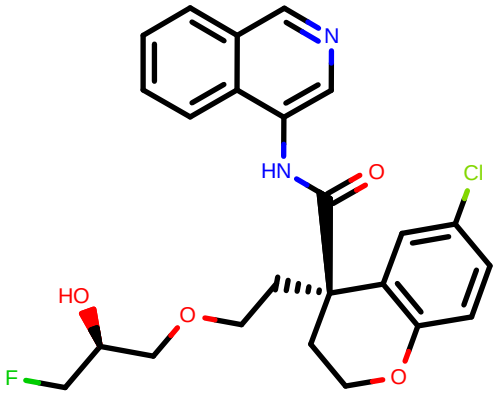
CID:	EN300-244148_1_1
SMILES:	Cn1cc(c(n1)COC)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6271
DDG (kcal/mol):	-3.06
dDDG (kcal/mol):	0.24

EN300-09239_1_1



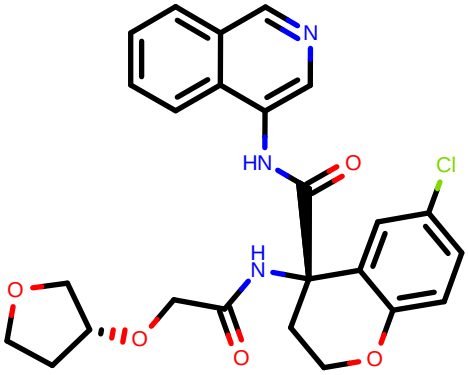
CID:	EN300-09239_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccc(c5)n6cnnn6
RUN:	RUN8990
DDG (kcal/mol):	-3.05
dDDG (kcal/mol):	0.26

EN300-1968342_3_1



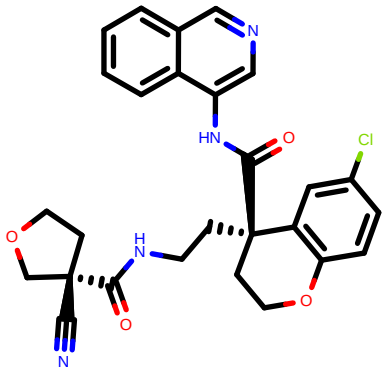
CID:	EN300-1968342_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H](CF)O
RUN:	RUN916
DDG (kcal/mol):	-3.05
dDDG (kcal/mol):	0.32

EN300-99391_1_1



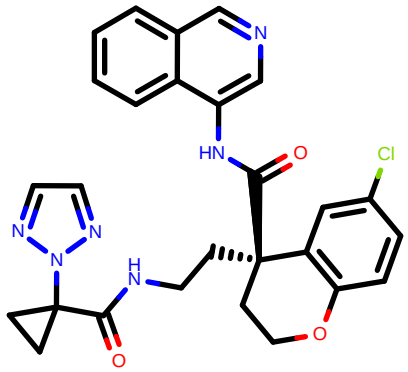
CID:	EN300-99391_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@@H]5CCOC5
RUN:	RUN1764
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.20

EN300-261210_3_2



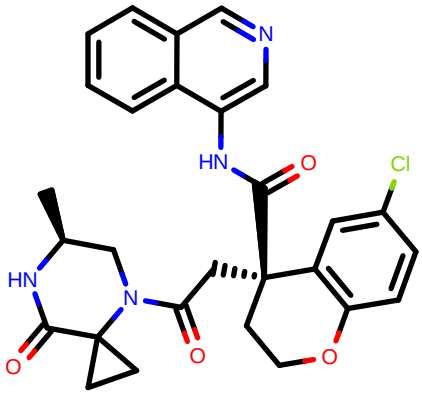
CID:	EN300-261210_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOC5)C#N
RUN:	RUN898
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.31

EN300-1722017_3_1



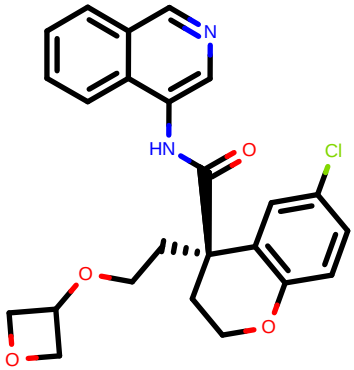
CID:	EN300-1722017_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)n6nccn6
RUN:	RUN6773
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.29

EN300-7542429_1_2



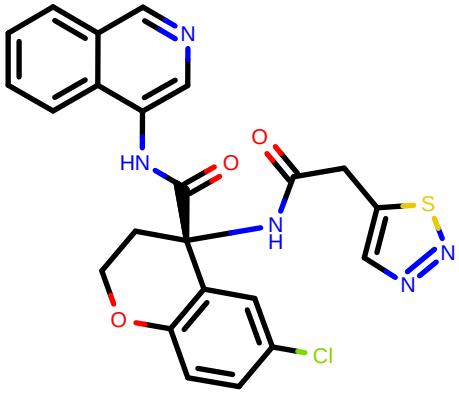
CID:	EN300-7542429_1_2
SMILES:	C[C@H]1CN(C2(CC2)C(=O)N1)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9203
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.36

EN300-317082_3_1



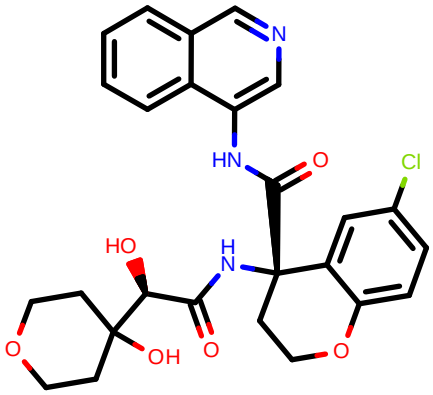
CID:	EN300-317082_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC5COC5
RUN:	RUN1340
DDG (kcal/mol):	-3.02
dDDG (kcal/mol):	0.20

EN300-260152_1_1



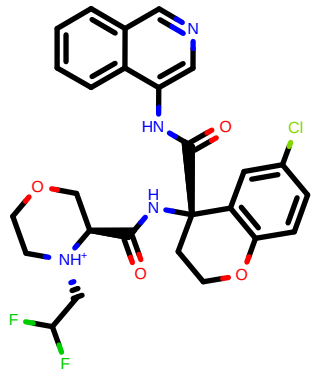
CID:	EN300-260152_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnns5
RUN:	RUN1205
DDG (kcal/mol):	-3.01
dDDG (kcal/mol):	0.24

EN300-749499_1_1



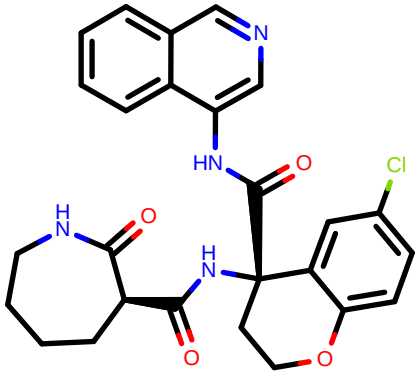
CID:	EN300-749499_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5(CCOCC5)O)O
RUN:	RUN2236
DDG (kcal/mol):	-3.01
dDDG (kcal/mol):	0.29

EN300-140582_1_1



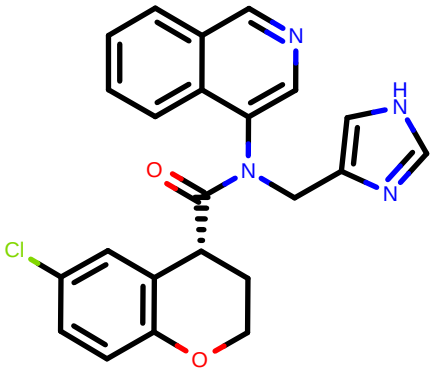
CID:	EN300-140582_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COCCN5CC(F)F
RUN:	RUN4285
DDG (kcal/mol):	-3.01
dDDG (kcal/mol):	0.31

EN300-6737762_1_2



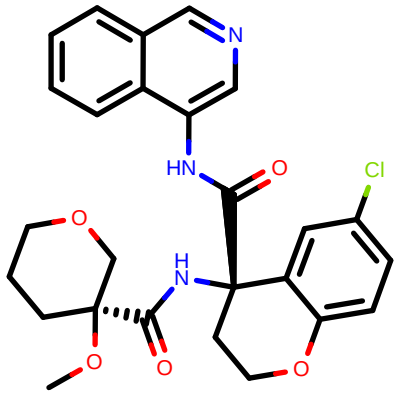
CID:	EN300-6737762_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCCNC5=O
RUN:	RUN6016
DDG (kcal/mol):	-3.00
dDDG (kcal/mol):	0.30

ALP-UNI-44c99a80-2_1



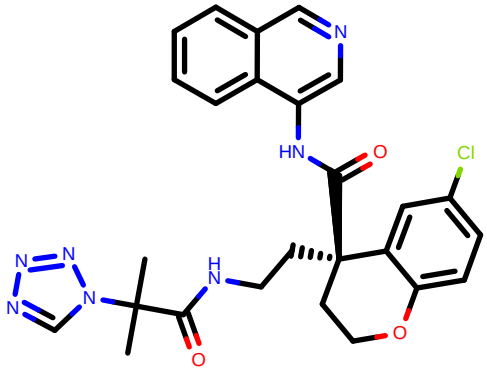
CID:	ALP-UNI-44c99a80-2_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN251
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.19

EN300-1072199_1_2



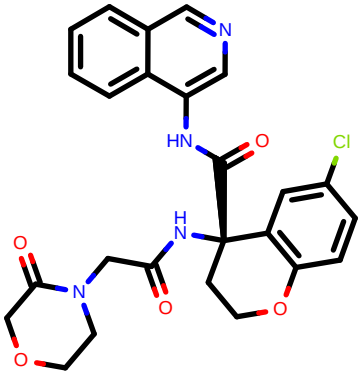
CID:	EN300-1072199_1_2
SMILES:	CO[C@]1(CCCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6136
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.31

EN300-1248064_3_1



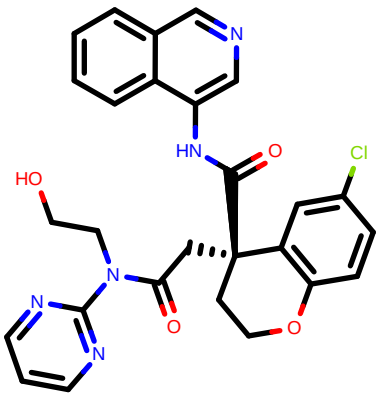
CID:	EN300-1248064_3_1
SMILES:	CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnnn5
RUN:	RUN2153
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.30

EN300-186943_1_1



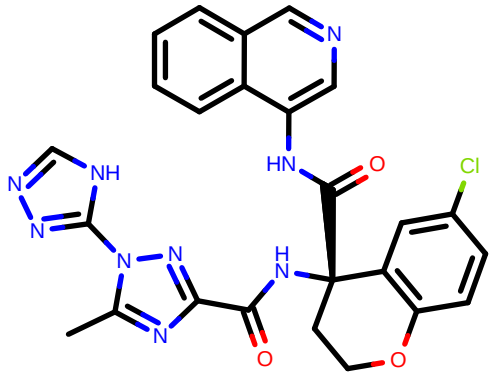
CID:	EN300-186943_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCOCC5=O
RUN:	RUN2922
DDG (kcal/mol):	-2.97
dDDG (kcal/mol):	0.27

EN300-65352_1_1



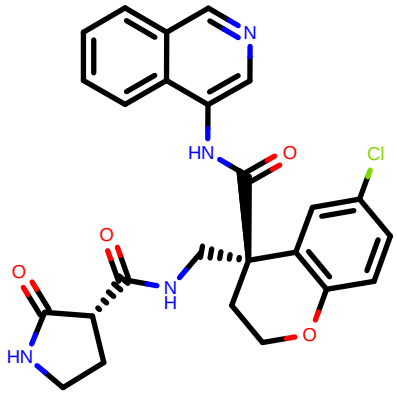
CID:	EN300-65352_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5ncccn5
RUN:	RUN10290
DDG (kcal/mol):	-2.96
dDDG (kcal/mol):	0.38

EN300-26973_1_1



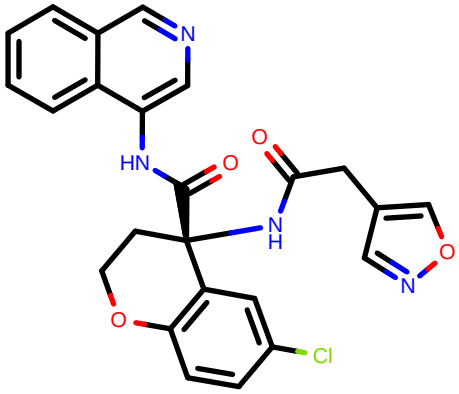
CID:	EN300-26973_1_1
SMILES:	Cc1nc(nn1c2[nH]cnn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8522
DDG (kcal/mol):	-2.96
dDDG (kcal/mol):	0.29

EN300-94945_2_1



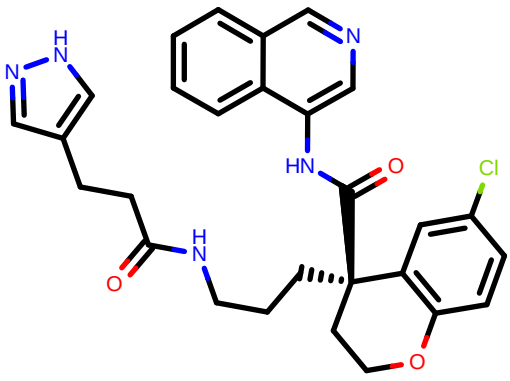
CID:	EN300-94945_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCNC5=O
RUN:	RUN5937
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.24

EN300-315963_1_1



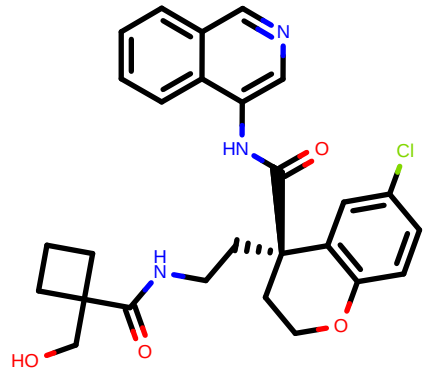
CID:	EN300-315963_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnoc5
RUN:	RUN1077
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.21

EN300-250836_4_1



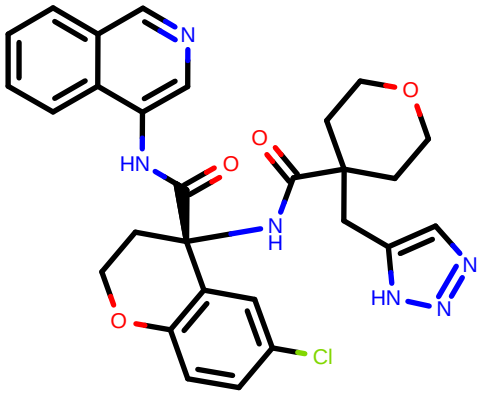
CID:	EN300-250836_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCc5c[nH]nc5
RUN:	RUN9727
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.39

EN300-149975_3_1



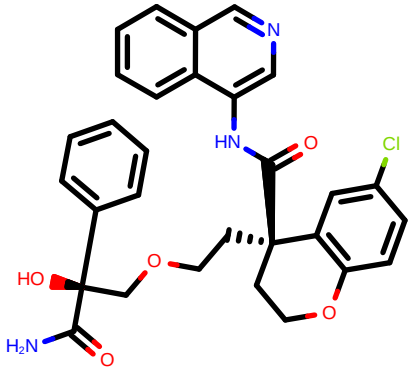
CID:	EN300-149975_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)CO
RUN:	RUN4887
DDG (kcal/mol):	-2.93
dDDG (kcal/mol):	0.33

EN300-1716880_1_1



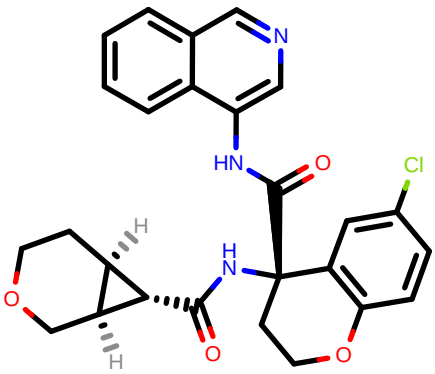
CID:	EN300-1716880_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)Cc6c[nH]nn6
RUN:	RUN6323
DDG (kcal/mol):	-2.92
dDDG (kcal/mol):	0.37

EN300-248526_3_2



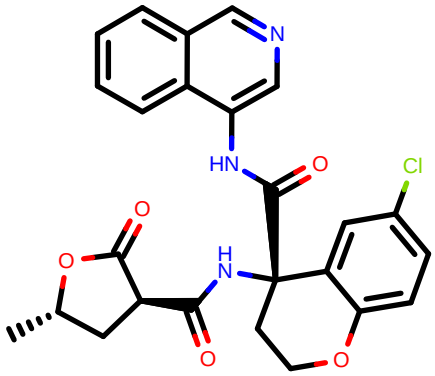
CID:	EN300-248526_3_2
SMILES:	c1ccc(cc1)[C@](COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(C(=O)N)O
RUN:	RUN600
DDG (kcal/mol):	-2.91
dDDG (kcal/mol):	0.47

EN300-1644723_1_4



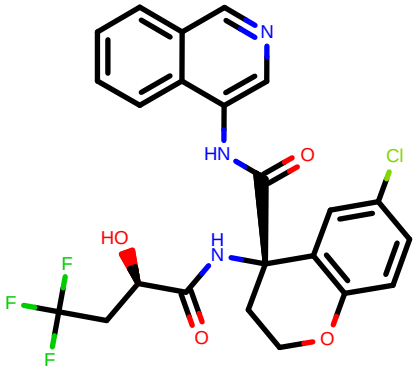
CID:	EN300-1644723_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5[C@H]6[C@@H]5COCC6
RUN:	RUN3354
DDG (kcal/mol):	-2.91
dDDG (kcal/mol):	0.24

EN300-7444533_1_2



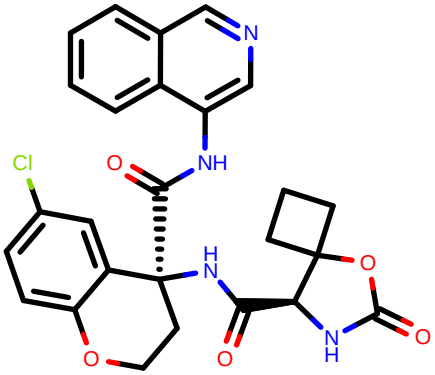
CID:	EN300-7444533_1_2
SMILES:	C[C@H]1C[C@@H](C(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2934
DDG (kcal/mol):	-2.90
dDDG (kcal/mol):	0.27

EN300-1932013_1_1



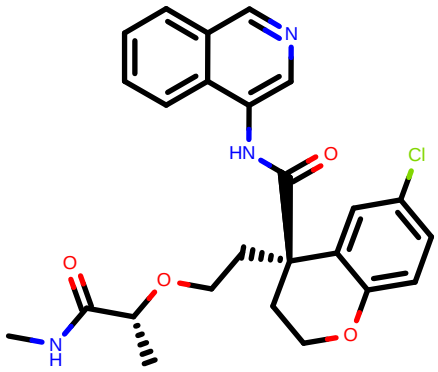
CID:	EN300-1932013_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CC(F)(F)F)O
RUN:	RUN3901
DDG (kcal/mol):	-2.89
dDDG (kcal/mol):	0.33

EN300-7432415_1_2



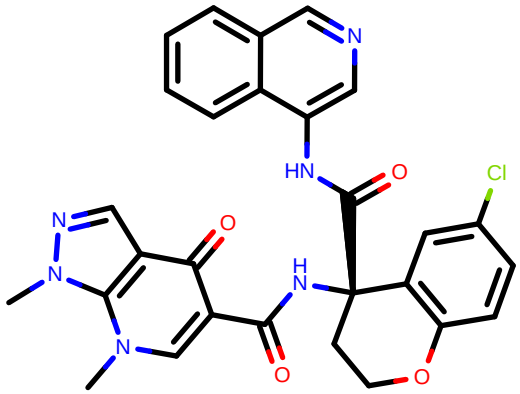
CID:	EN300-7432415_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C6(CCC6)OC(=O)N5
RUN:	RUN4493
DDG (kcal/mol):	-2.88
dDDG (kcal/mol):	0.31

EN300-211482_3_2



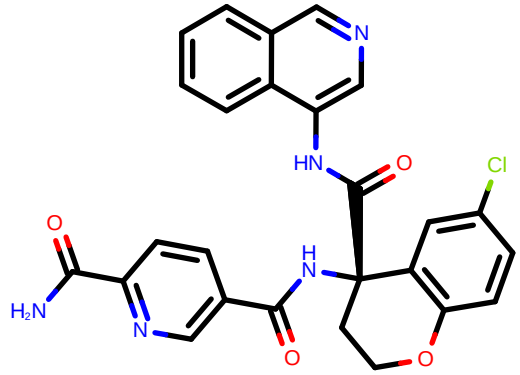
CID:	EN300-211482_3_2
SMILES:	C[C@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1955
DDG (kcal/mol):	-2.88
dDDG (kcal/mol):	0.29

EN300-128324_1_1



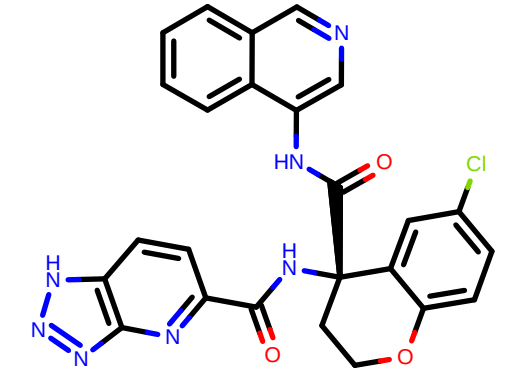
CID:	EN300-128324_1_1
SMILES:	Cn1cc(c(=O)c2c1n(nc2)C)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9116
DDG (kcal/mol):	-2.88
dDDG (kcal/mol):	0.31

EN300-58864_1_1



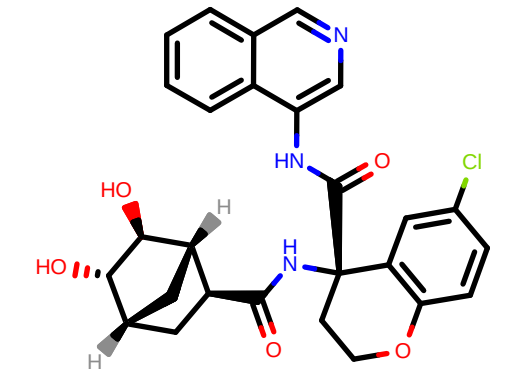
CID:	EN300-58864_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(nc5)C(=O)N
RUN:	RUN8826
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.25

EN300-133058_1_1



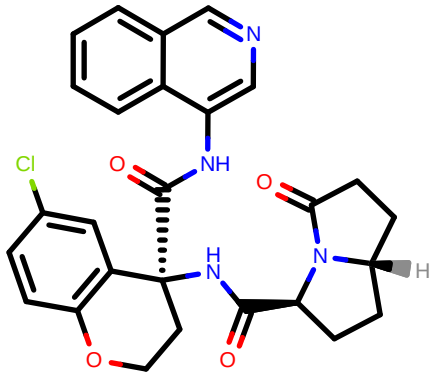
CID:	EN300-133058_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)n[nH]n6
RUN:	RUN4341
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.25

EN300-6744028_1_6



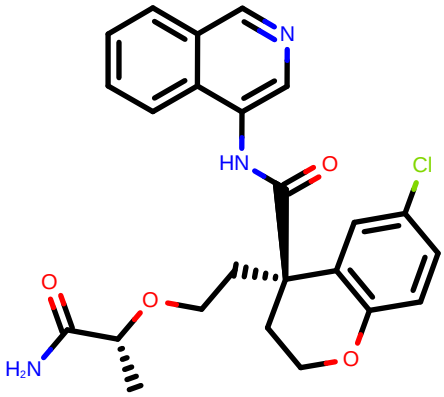
CID:	EN300-6744028_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC6CC5[C@@H]([C@H]6O)O
RUN:	RUN6351
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.35

EN300-6479181_1_1



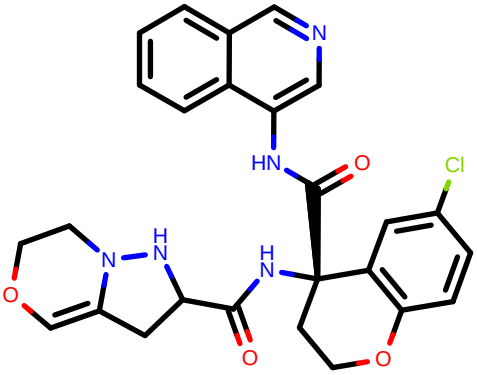
CID:	EN300-6479181_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC[C@@H]6N5C(=O)CC6
RUN:	RUN8066
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.39

EN300-17381_3_2



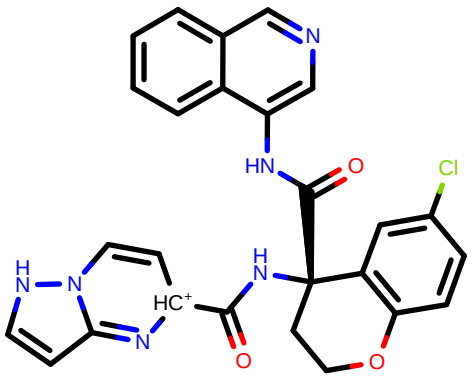
CID:	EN300-17381_3_2
SMILES:	C[C@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1883
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.23

EN300-244278_1_1



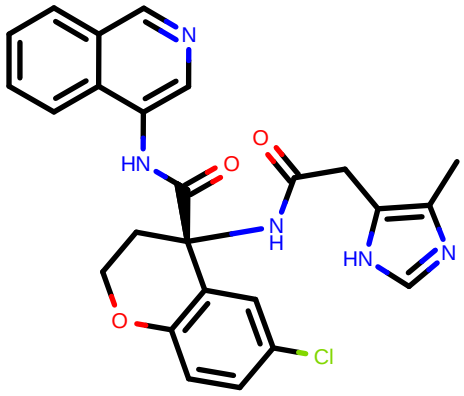
CID:	EN300-244278_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCOC6
RUN:	RUN8852
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.22

EN300-323327_1_1



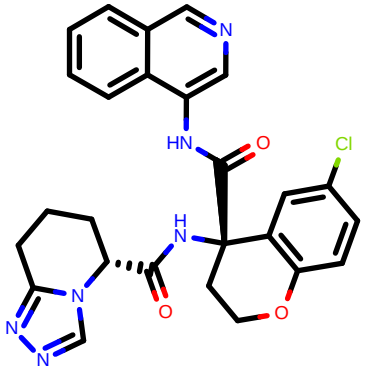
CID:	EN300-323327_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6c(n5)ccn6
RUN:	RUN5492
DDG (kcal/mol):	-2.85
dDDG (kcal/mol):	0.19

EN300-186929_1_1



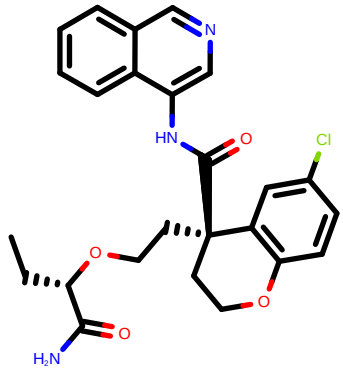
CID:	EN300-186929_1_1
SMILES:	Cc1c(nc[nH]1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5812
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.21

EN300-6478631_1_2



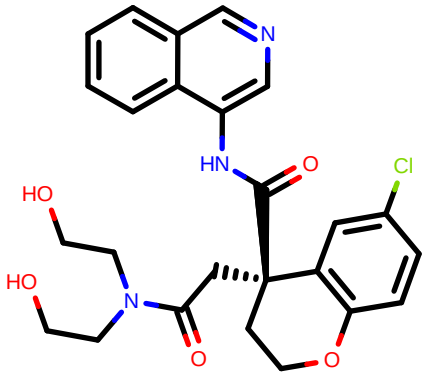
CID:	EN300-6478631_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCc6n5cnn6
RUN:	RUN3206
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.35

EN300-65839_3_1



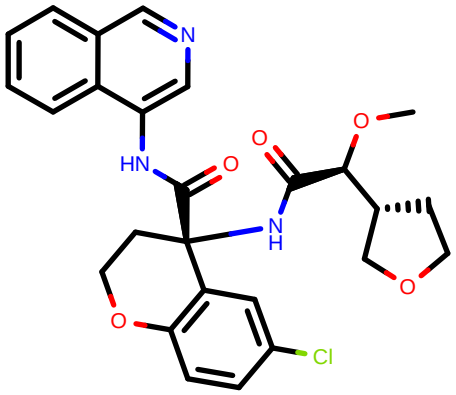
CID:	EN300-65839_3_1
SMILES:	CC[C@@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2155
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.25

EN300-19762_1_1



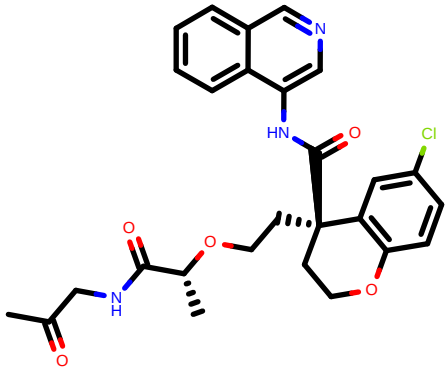
CID:	EN300-19762_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)CCO
RUN:	RUN6681
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.37

EN300-298552_1_1



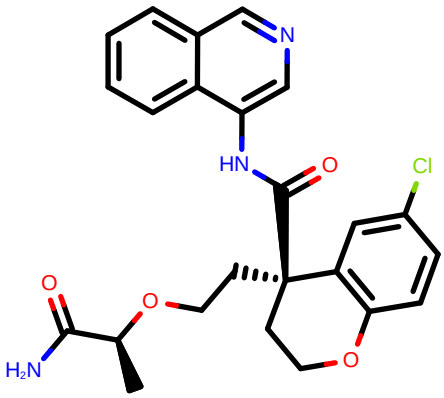
CID:	EN300-298552_1_1
SMILES:	CO[C@@H]([C@@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3402
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.21

EN300-131093_3_2



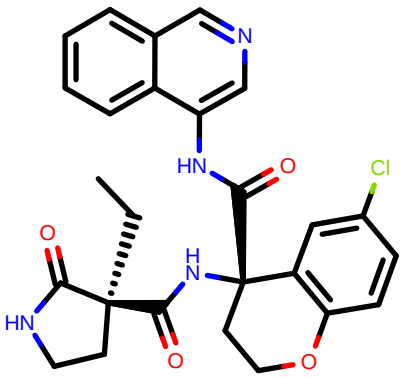
CID:	EN300-131093_3_2
SMILES:	C[C@H](C(=O)NCC(=O)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1691
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.31

EN300-17381_3_1



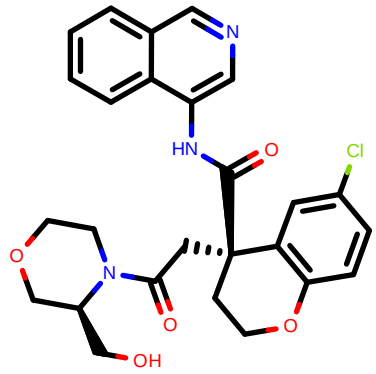
CID:	EN300-17381_3_1
SMILES:	C[C@@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2043
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.24

EN300-304135_1_1



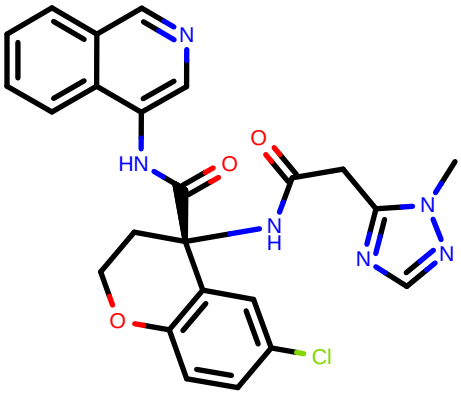
CID:	EN300-304135_1_1
SMILES:	CC[C@@]1(CCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3050
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.29

EN300-154201_1_1



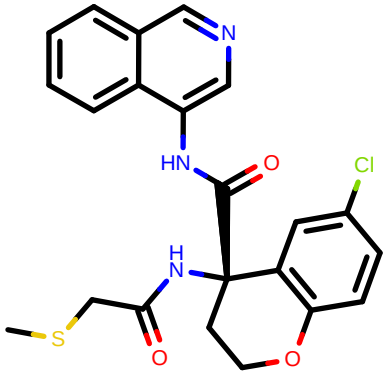
CID:	EN300-154201_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO
RUN:	RUN9780
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.28

EN300-209316_1_1



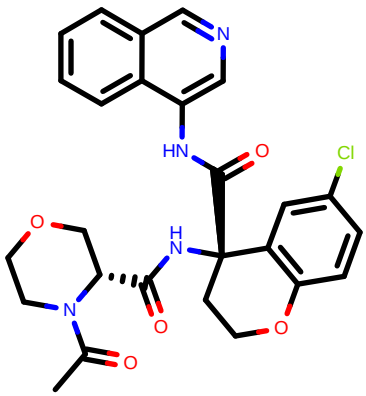
CID:	EN300-209316_1_1
SMILES:	Cn1c(ncn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5061
DDG (kcal/mol):	-2.79
dDDG (kcal/mol):	0.24

EN300-07879_1_1



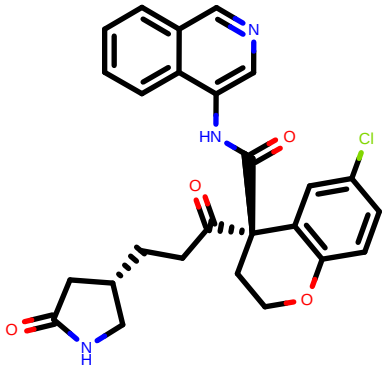
CID:	EN300-07879_1_1
SMILES:	CSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1061
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.21

EN300-116313_1_1



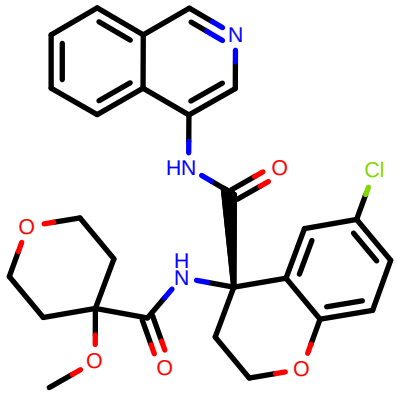
CID:	EN300-116313_1_1
SMILES:	CC(=O)N1CCOC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5568
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.32

VLA-UCB-34f3ed0c-21_2



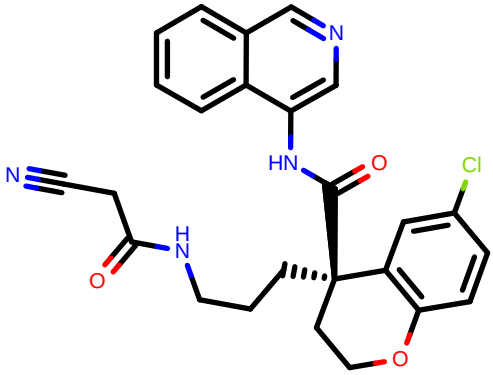
CID:	VLA-UCB-34f3ed0c-21_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NC5
RUN:	RUN0
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.37

EN300-204133_1_1



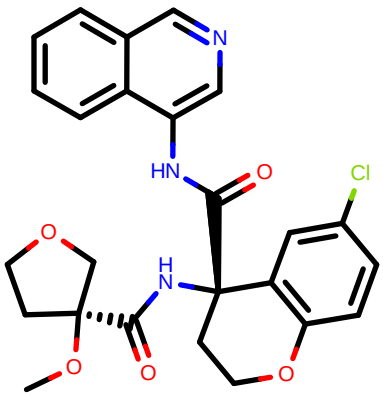
CID:	EN300-204133_1_1
SMILES:	COC1(CCOCC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4141
DDG (kcal/mol):	-2.77
dDDG (kcal/mol):	0.28

EN300-19926_4_1



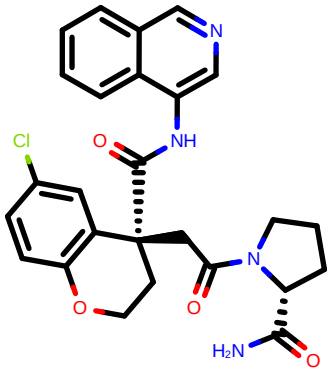
CID:	EN300-19926_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CC#N
RUN:	RUN9939
DDG (kcal/mol):	-2.77
dDDG (kcal/mol):	0.25

EN300-174668_1_2



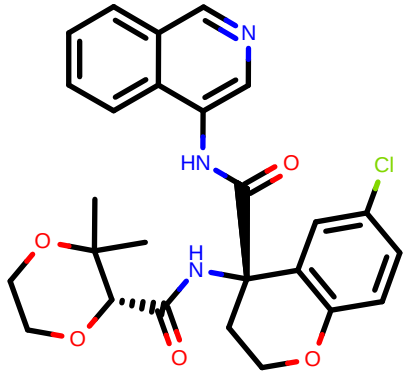
CID:	EN300-174668_1_2
SMILES:	CO[C@]1(CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3718
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.38

EN300-245098_1_1



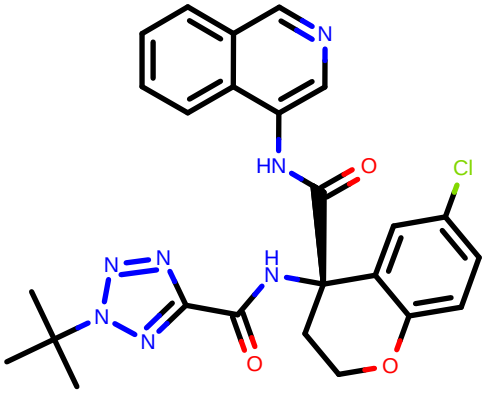
CID:	EN300-245098_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5C(=O)N
RUN:	RUN11090
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.31

EN300-1601684_1_1



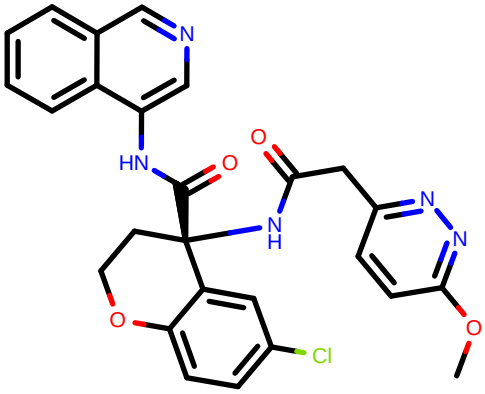
CID:	EN300-1601684_1_1
SMILES:	CC1([C@@H](OCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN7186
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.26

EN300-268087_1_1



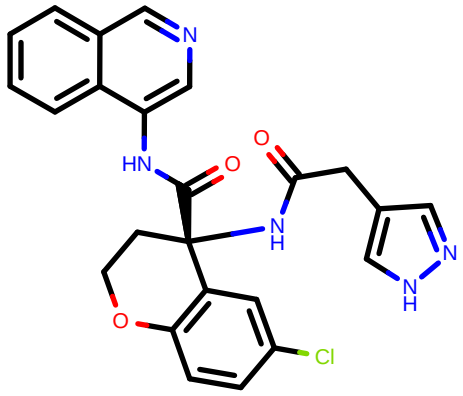
CID:	EN300-268087_1_1
SMILES:	CC(C)(C)n1nc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8879
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.29

EN300-7540889_1_1



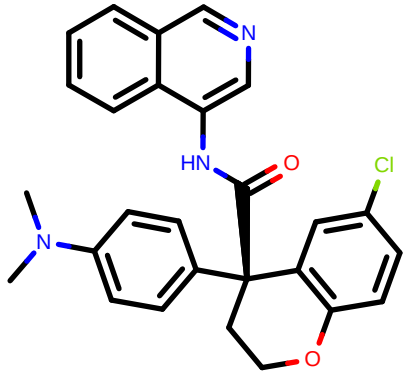
CID:	EN300-7540889_1_1
SMILES:	COc1ccc(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5169
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.23

EN300-1589101_1_1



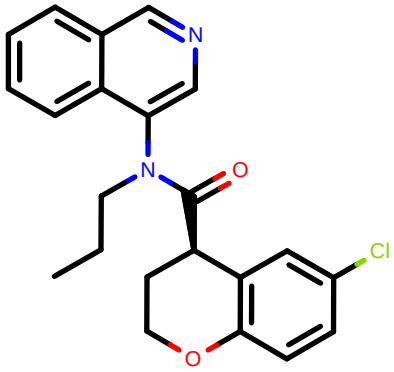
CID:	EN300-1589101_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5c[nH]nc5
RUN:	RUN2172
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.25

VLA-UCB-551c2366-1_1



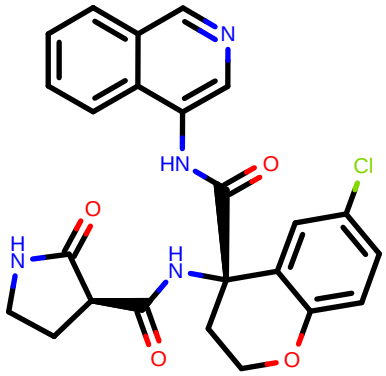
CID:	VLA-UCB-551c2366-1_1
SMILES:	CN(C)c1ccc(cc1)[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN170
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.20

DAR-DIA-5ff57136-13_1



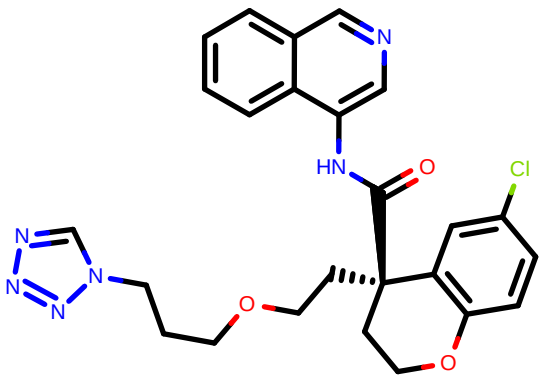
CID:	DAR-DIA-5ff57136-13_1
SMILES:	C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN92
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.13

EN300-94945_1_2



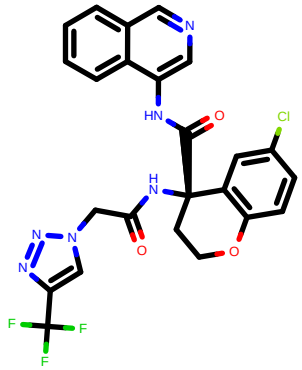
CID:	EN300-94945_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCNC5=O
RUN:	RUN2926
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.21

EN300-1696962_3_1



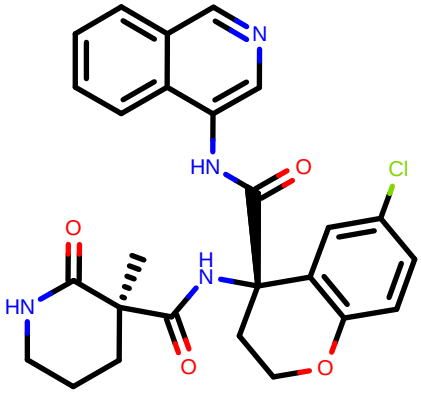
CID:	EN300-1696962_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCn5cnnn5
RUN:	RUN409
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.26

EN300-2910941_1_1



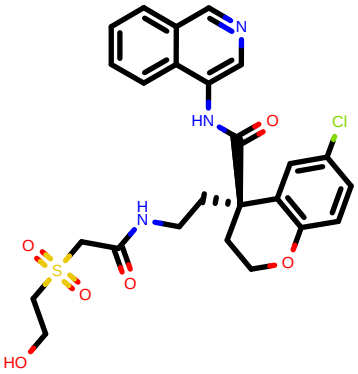
CID:	EN300-2910941_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(nn5)C(F)(F)F
RUN:	RUN7890
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.30

EN300-178876_1_1



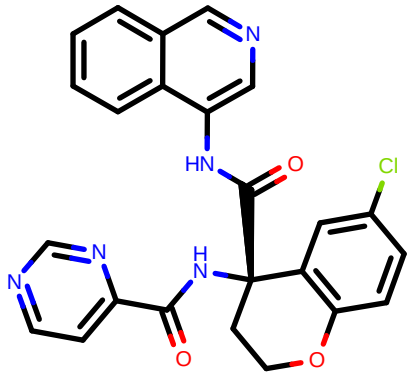
CID:	EN300-178876_1_1
SMILES:	C[C@@]1(CCCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4945
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.40

EN300-4293814_3_1



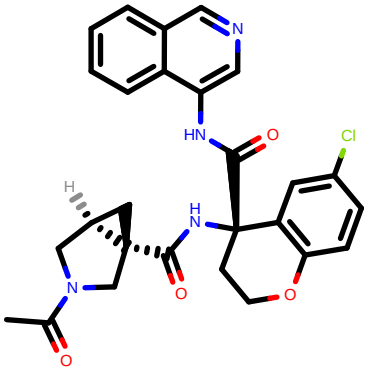
CID:	EN300-4293814_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)CCO
RUN:	RUN4227
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.54

EN300-111006_1_1



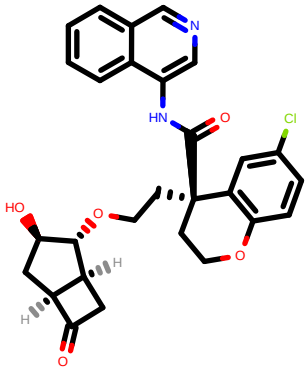
CID:	EN300-111006_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccncn5
RUN:	RUN5528
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.19

EN300-313062_1_4



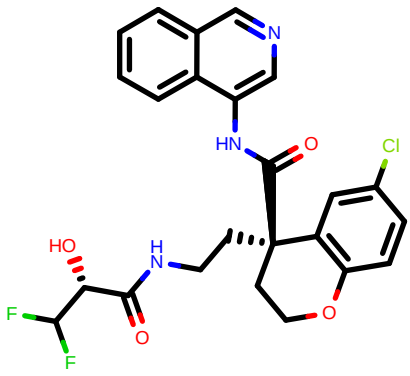
CID:	EN300-313062_1_4
SMILES:	CC(=O)N1C[C@H]2C[C@]2(C1)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7398
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.24

EN300-6481287_3_1



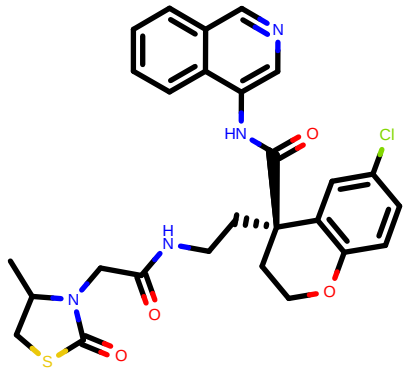
CID:	EN300-6481287_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5[C@@H](C[C@H]6[C@@H]5CC6=O)O
RUN:	RUN2461
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.26

EN300-1932780_3_2



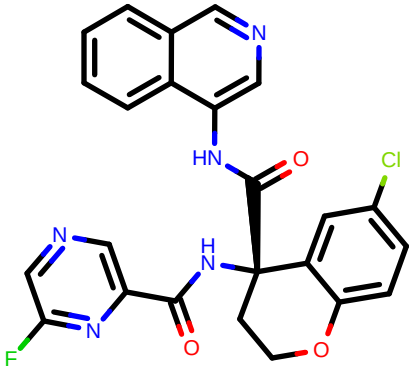
CID:	EN300-1932780_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C(F)F)O
RUN:	RUN7920
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.28

EN300-12067_3_1



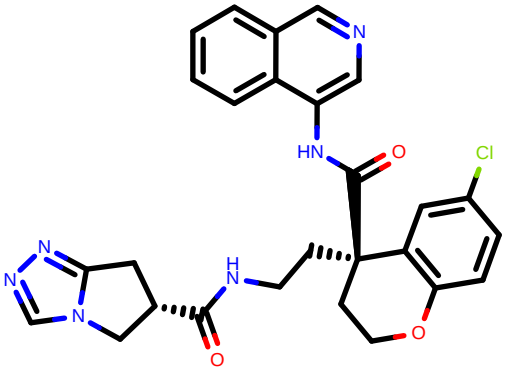
CID:	EN300-12067_3_1
SMILES:	Cc1csc(=O)n1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3548
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.27

EN300-373552_1_1



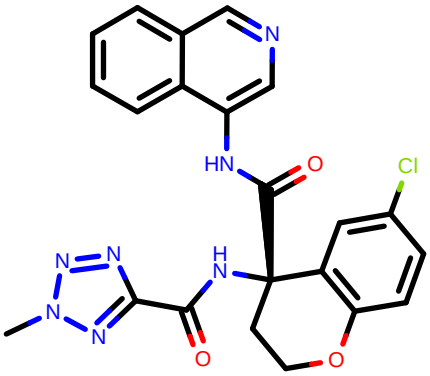
CID:	EN300-373552_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncc(n5)F
RUN:	RUN6667
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.20

EN300-6745453_3_2



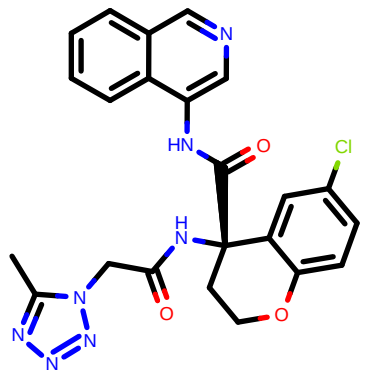
CID:	EN300-6745453_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5Cc6nncn6C5
RUN:	RUN8380
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.29

EN300-216978_1_1



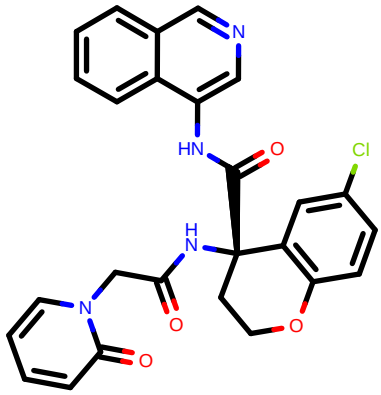
CID:	EN300-216978_1_1
SMILES:	Cn1nc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4161
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.22

EN300-1244816_1_1



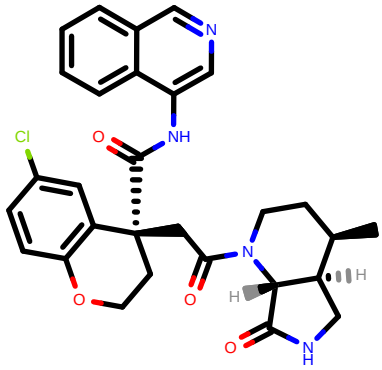
CID:	EN300-1244816_1_1
SMILES:	Cc1nnnn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3710
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.27

EN300-11714_1_1



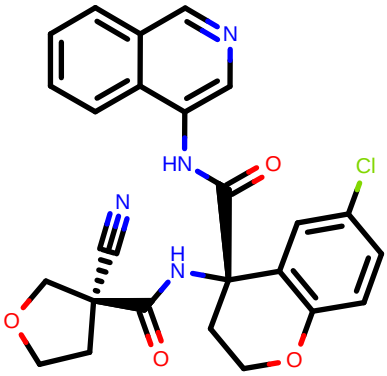
CID:	EN300-11714_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccccc5=O
RUN:	RUN3098
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.26

EN300-6739879_1_1



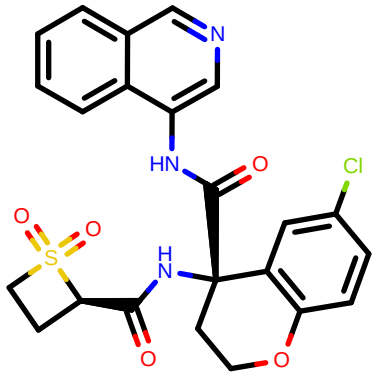
CID:	EN300-6739879_1_1
SMILES:	C[C@@H]1CCN([C@@H]2[C@@H]1CNC2=O)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN11048
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.38

EN300-261210_1_2



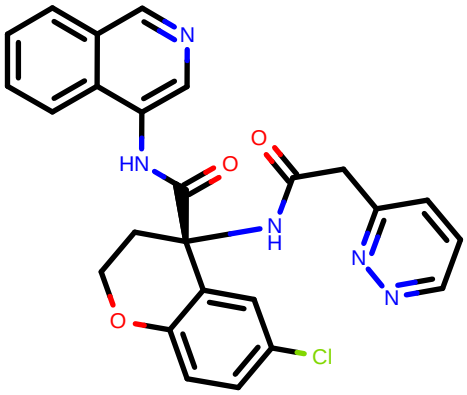
CID:	EN300-261210_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CCOC5)C#N
RUN:	RUN5145
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.28

EN300-1387104_1_2



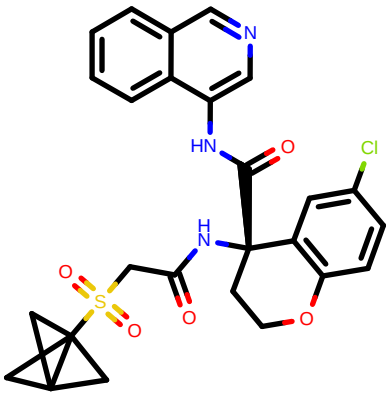
CID:	EN300-1387104_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCS5(=O)=O
RUN:	RUN2287
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.28

EN300-7456948_1_1



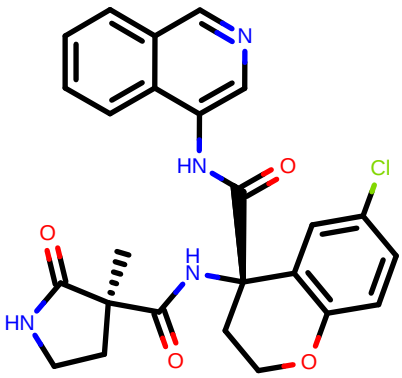
CID:	EN300-7456948_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cccnn5
RUN:	RUN3466
DDG (kcal/mol):	-2.66
dDDG (kcal/mol):	0.23

EN300-6763072_1_1



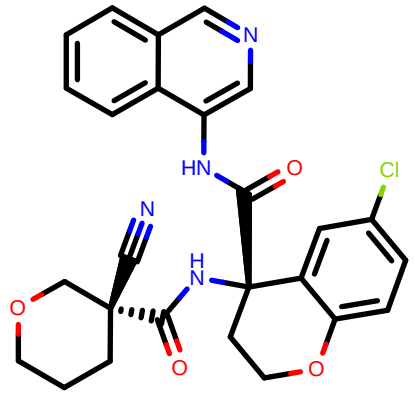
CID:	EN300-6763072_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS(=O)(=O)C56CC(C5)C6
RUN:	RUN7130
DDG (kcal/mol):	-2.66
dDDG (kcal/mol):	0.32

EN300-207959_1_1



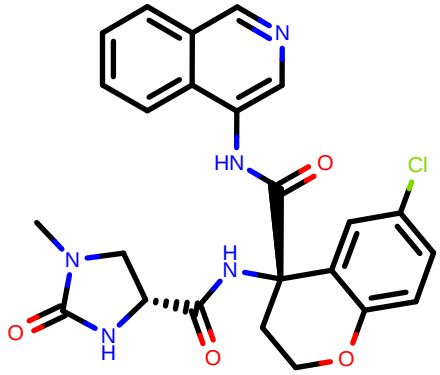
CID:	EN300-207959_1_1
SMILES:	C[C@@]1(CCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4093
DDG (kcal/mol):	-2.65
dDDG (kcal/mol):	0.33

EN300-301925_1_1



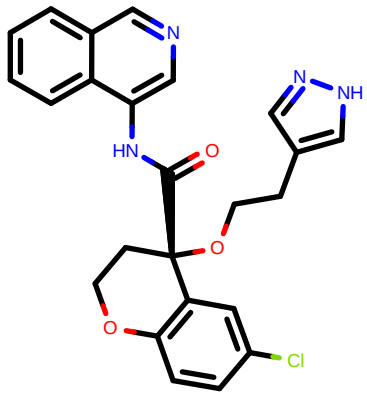
CID:	EN300-301925_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCCOC5)C#N
RUN:	RUN5780
DDG (kcal/mol):	-2.65
dDDG (kcal/mol):	0.36

EN300-255795_1_1



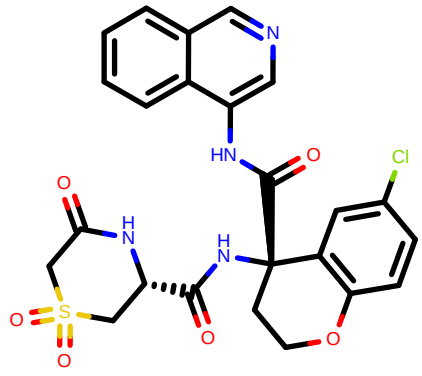
CID:	EN300-255795_1_1
SMILES:	CN1C[C@@H](NC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1868
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.24

EDJ-MED-28ec730d-5_1



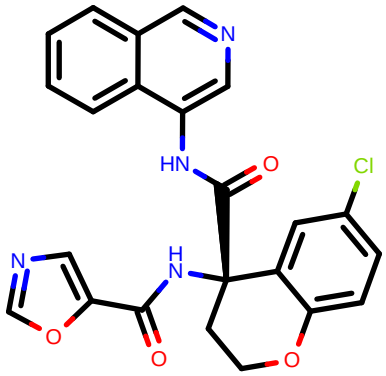
CID:	EDJ-MED-28ec730d-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5
RUN:	RUN31
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.23

EN300-754584_1_1



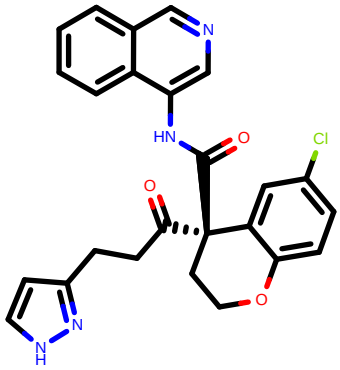
CID:	EN300-754584_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CS(=O)(=O)CC(=O)N5
RUN:	RUN5217
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.23

EN300-25446_1_1



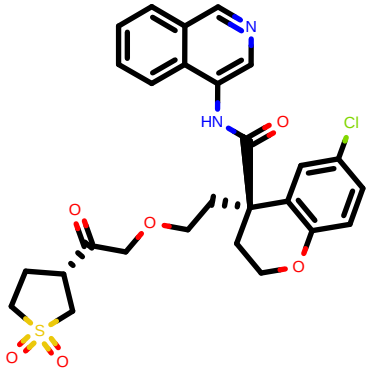
CID:	EN300-25446_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnco5
RUN:	RUN3362
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.16

VLA-UCB-34f3ed0c-8_1



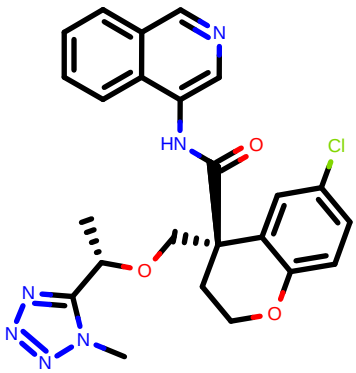
CID:	VLA-UCB-34f3ed0c-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5cc[nH]n5
RUN:	RUN76
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.22

EN300-226314_3_2



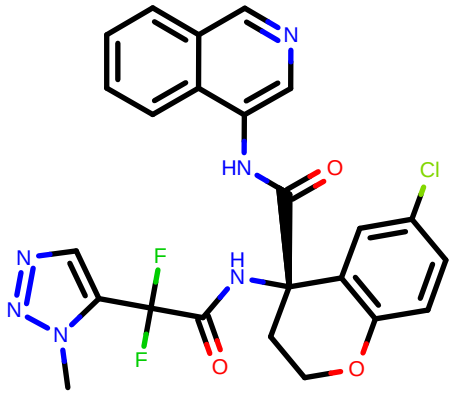
CID:	EN300-226314_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@H]5CCS(=O)(=O)C5
RUN:	RUN1332
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.35

EN300-173006_2_1



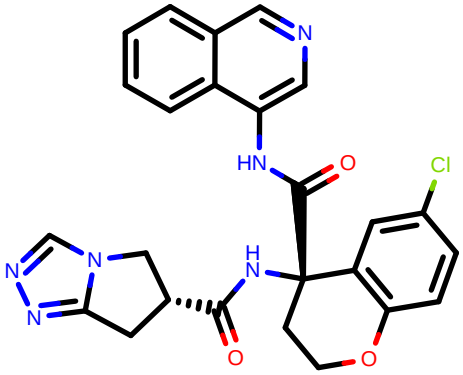
CID:	EN300-173006_2_1
SMILES:	C[C@@H](c1nnnn1C)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2149
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.29

EN300-1726073_1_1



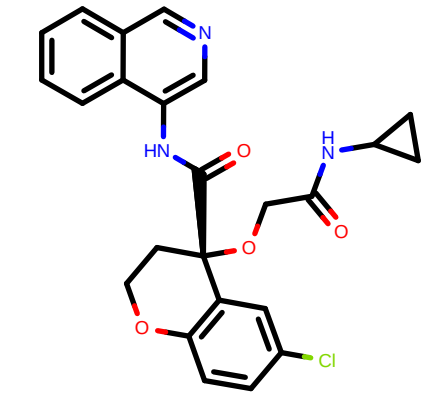
CID:	EN300-1726073_1_1
SMILES:	Cn1c(cnn1)C(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(F)F
RUN:	RUN5596
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.26

EN300-6745453_1_1



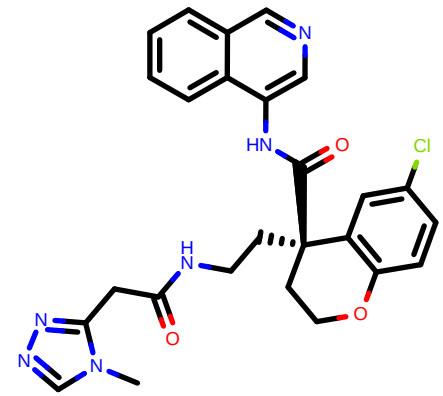
CID:	EN300-6745453_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5Cc6nncn6C5
RUN:	RUN8026
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.23

EN300-1253178_1_1



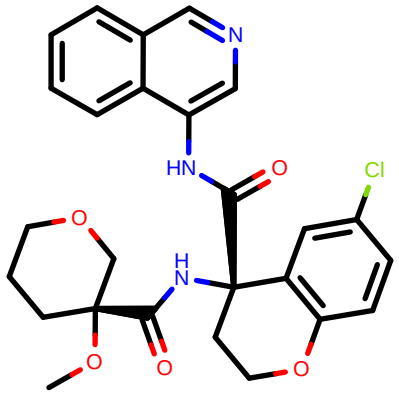
CID:	EN300-1253178_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC5CC5
RUN:	RUN628
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.19

EN300-6494474_3_1



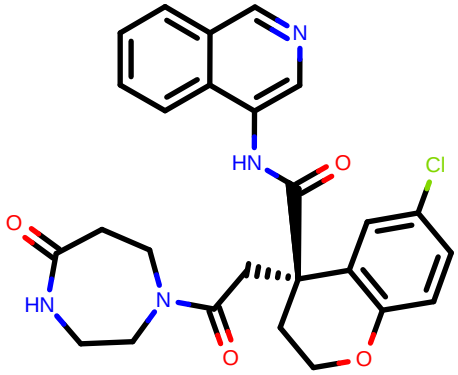
CID:	EN300-6494474_3_1
SMILES:	Cn1cnnc1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6325
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.29

EN300-1072199_1_1



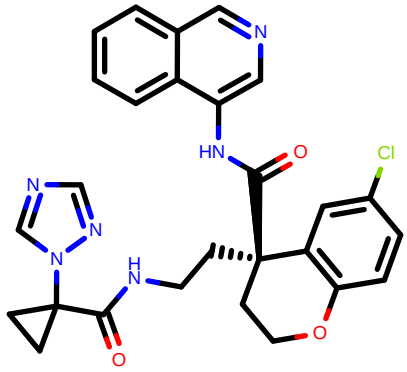
CID:	EN300-1072199_1_1
SMILES:	CO[C@@]1(CCCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5153
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.30

EN300-69107_1_1



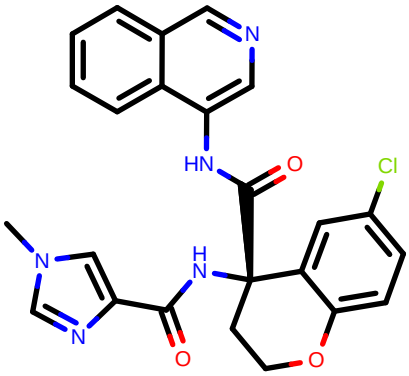
CID:	EN300-69107_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(=O)NCC5
RUN:	RUN2976
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.42

EN300-246440_3_1



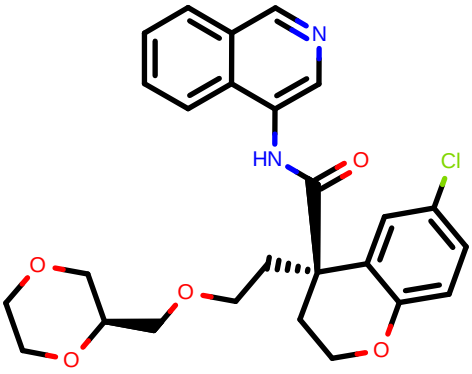
CID:	EN300-246440_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)n6cncn6
RUN:	RUN455
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.32

EN300-97847_1_1



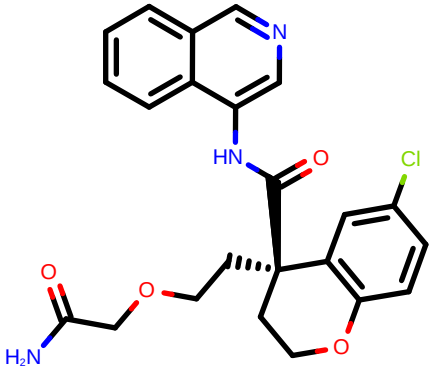
CID:	EN300-97847_1_1
SMILES:	Cn1cc(nc1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3302
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.23

EN300-139167_3_1



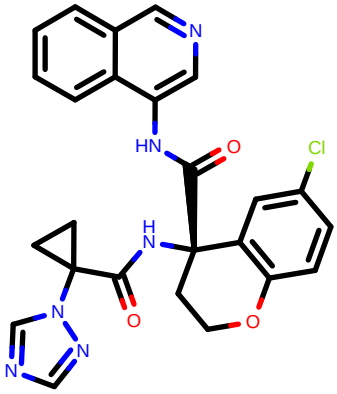
CID:	EN300-139167_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCCO5
RUN:	RUN648
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.28

EN300-18249_3_1



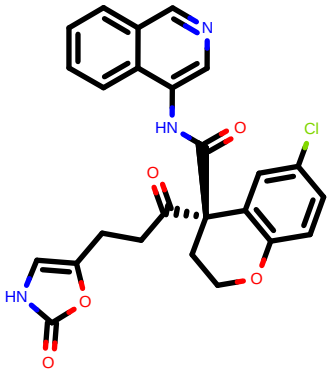
CID:	EN300-18249_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N
RUN:	RUN1564
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.20

EN300-246440_1_1



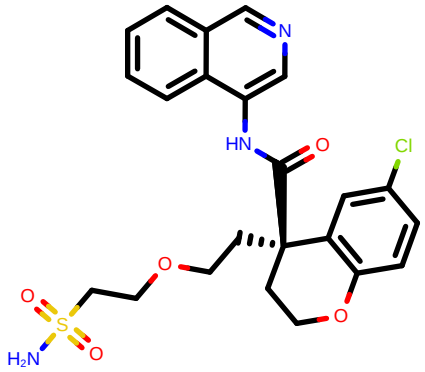
CID:	EN300-246440_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)n6cncn6
RUN:	RUN6511
DDG (kcal/mol):	-2.60
dDDG (kcal/mol):	0.28

VLA-UCB-34f3ed0c-9_1



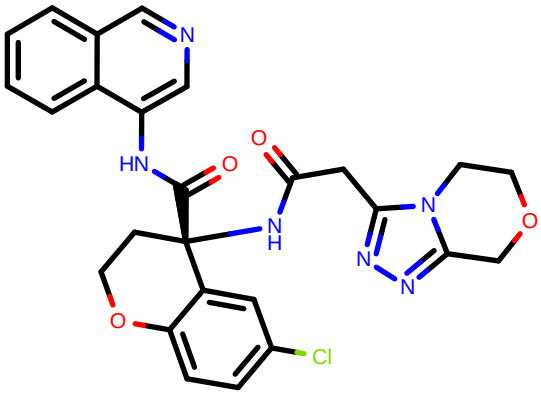
CID:	VLA-UCB-34f3ed0c-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5c[nH]c(=O)o5
RUN:	RUN72
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.27

EN300-270710_3_1



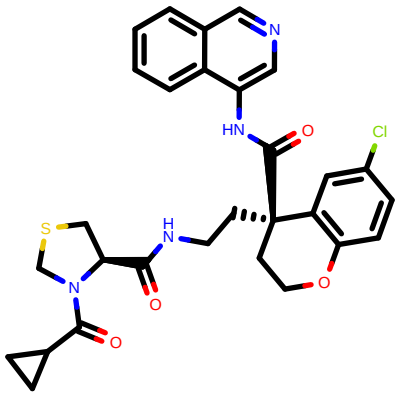
CID:	EN300-270710_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCS(=O)(=O)N
RUN:	RUN1811
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.27

EN300-1718836_1_1



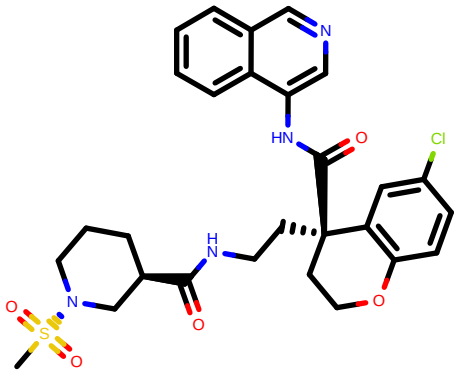
CID:	EN300-1718836_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5nnc6n5CCOC6
RUN:	RUN8162
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.29

EN300-18928_3_1



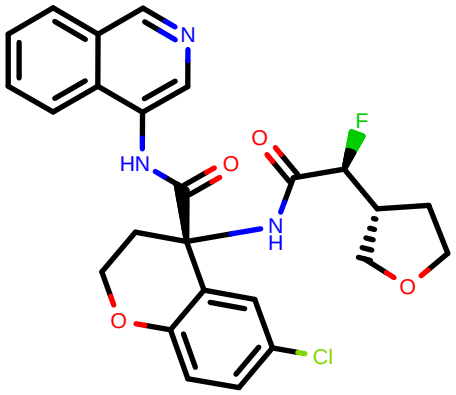
CID:	EN300-18928_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CSCN5C(=O)C6CC6
RUN:	RUN5894
DDG (kcal/mol):	-2.59
dDDG (kcal/mol):	0.40

EN300-27341_3_2



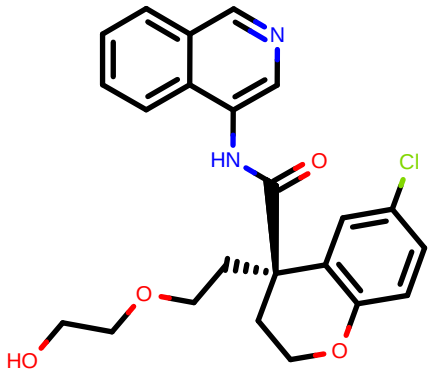
CID:	EN300-27341_3_2
SMILES:	CS(=O)(=O)N1CCC[C@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2677
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.49

EN300-783124_1_2



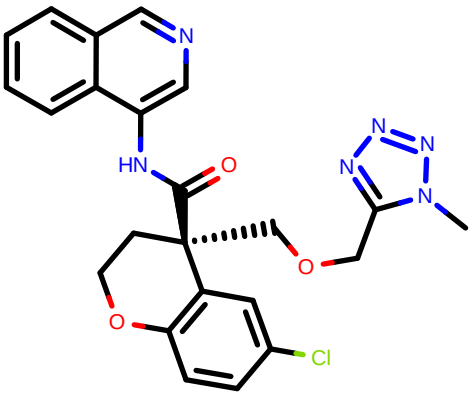
CID:	EN300-783124_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@@H]5CCOC5)F
RUN:	RUN2315
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.20

EN300-21258_3_1



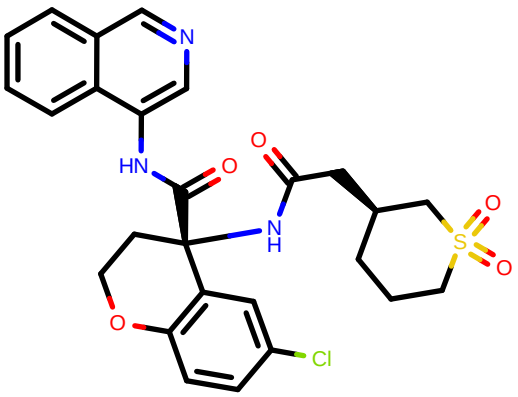
CID:	EN300-21258_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCO
RUN:	RUN1516
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.21

EN300-62574_2_1



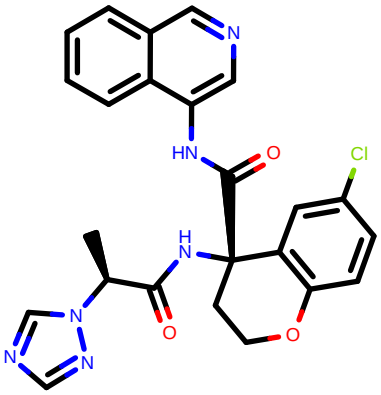
CID:	EN300-62574_2_1
SMILES:	Cn1c(nnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1102
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.21

EN300-220676_1_1



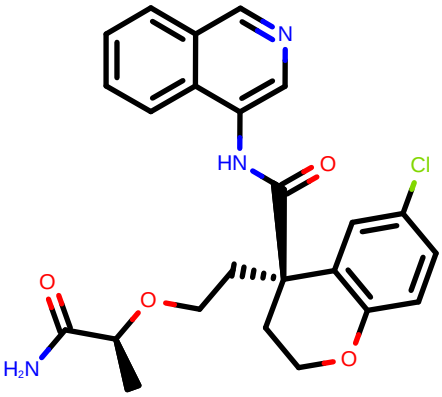
CID:	EN300-220676_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCS(=O)(=O)C5
RUN:	RUN2044
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.32

EN300-30397_1_1



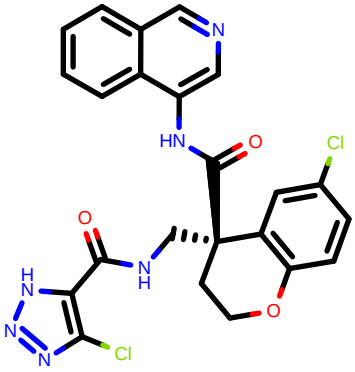
CID:	EN300-30397_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN3813
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.35

EN300-17381_3_1



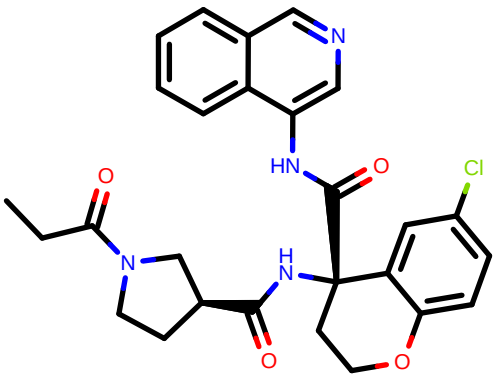
CID:	EN300-17381_3_1
SMILES:	C[C@@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2035
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.26

EN300-149013_2_1



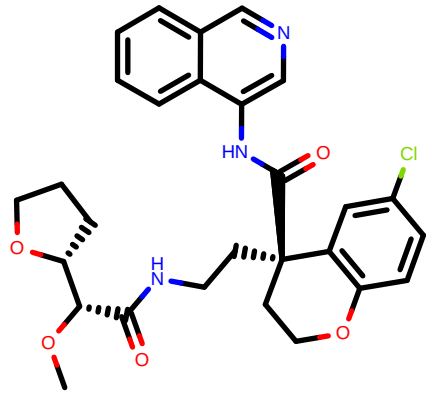
CID:	EN300-149013_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c([nH]nn5)Cl
RUN:	RUN7791
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.21

EN300-114133_1_1



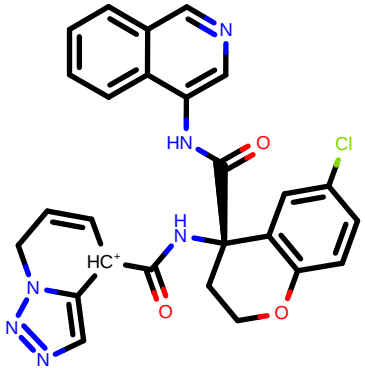
CID:	EN300-114133_1_1
SMILES:	CCC(=O)N1CC[C@@H](C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7042
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.44

EN300-6277108_3_4



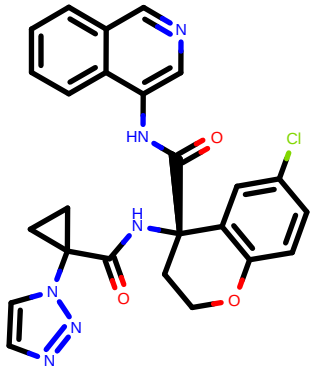
CID:	EN300-6277108_3_4
SMILES:	CO[C@H]([C@H]1CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4335
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.34

EN300-1074262_1_1



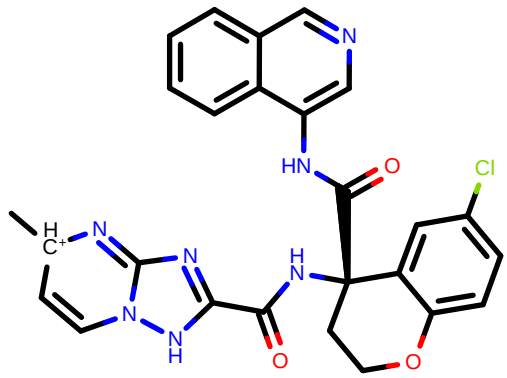
CID:	EN300-1074262_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccn6c5cnn6
RUN:	RUN7098
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.26

EN300-658559_1_1



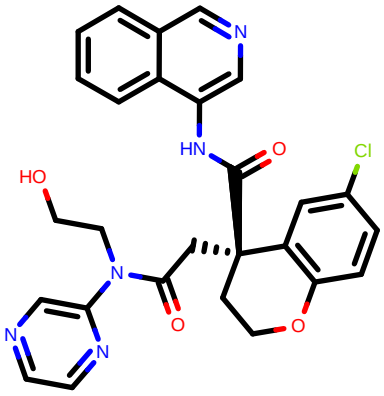
CID:	EN300-658559_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)n6ccnn6
RUN:	RUN6767
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.28

EN300-21221_1_1



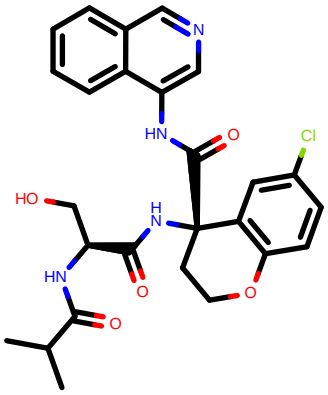
CID:	EN300-21221_1_1
SMILES:	Cc1ccn2c(n1)nc(n2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8888
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.23

EN300-370792_1_1



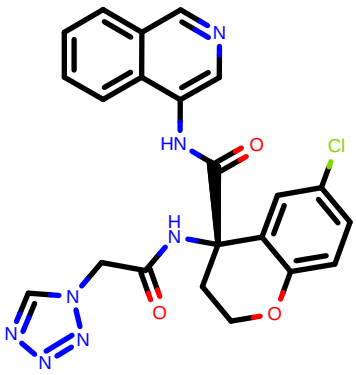
CID:	EN300-370792_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)c5cnccn5
RUN:	RUN6293
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.29

EN300-212266_1_1



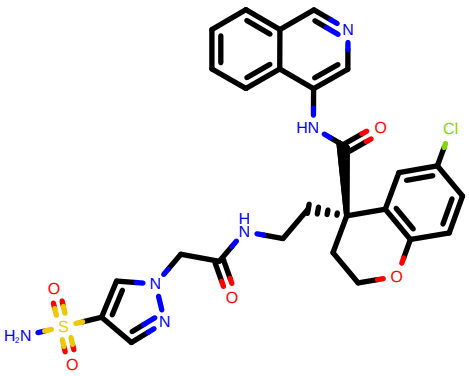
CID:	EN300-212266_1_1
SMILES:	CC(C)C(=O)N[C@@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7314
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.36

EN300-20980_1_1



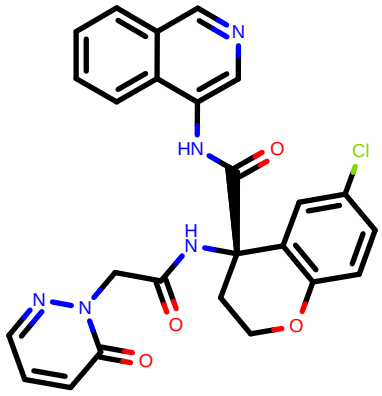
CID:	EN300-20980_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnnn5
RUN:	RUN5380
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.23

EN300-60514_3_1



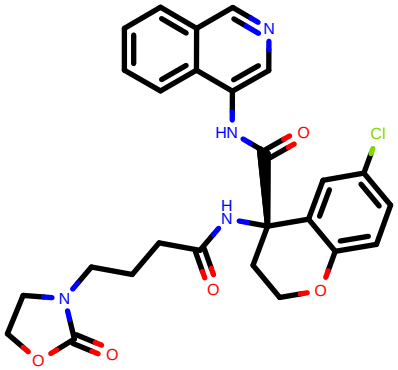
CID:	EN300-60514_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(cn5)S(=O)(=O)N
RUN:	RUN11336
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.38

EN300-237561_1_1



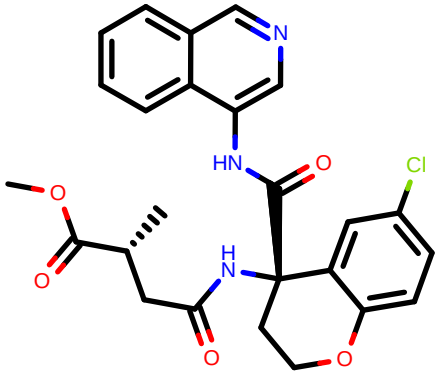
CID:	EN300-237561_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)cccn5
RUN:	RUN3714
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.32

EN300-45182_1_1



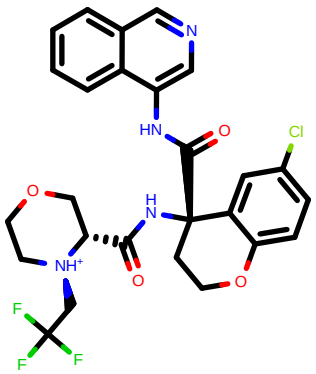
CID:	EN300-45182_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCN5CCOC5=O
RUN:	RUN2755
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.32

EN300-108413_1_2



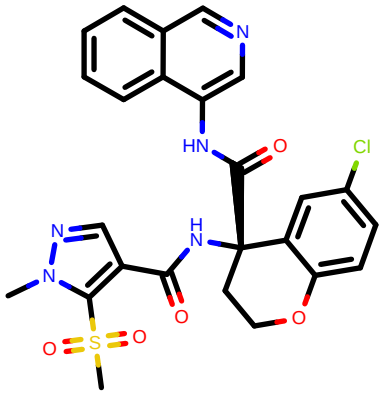
CID:	EN300-108413_1_2
SMILES:	C[C@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN2511
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.24

EN300-201551_1_2



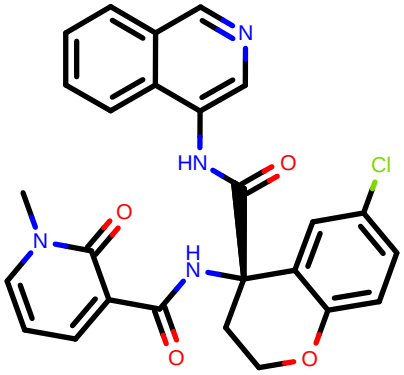
CID:	EN300-201551_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COCCN5CC(F)(F)F
RUN:	RUN7690
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.35

EN300-180069_1_1



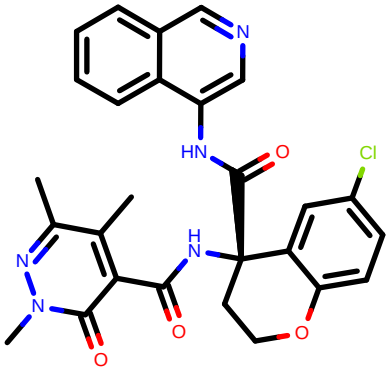
CID:	EN300-180069_1_1
SMILES:	Cn1c(c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN8086
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.31

EN300-69811_1_1



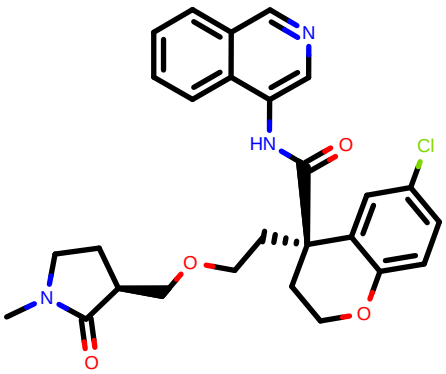
CID:	EN300-69811_1_1
SMILES:	Cn1cccc(c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6339
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.27

EN300-28894_1_1



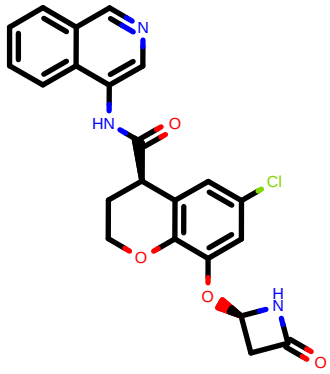
CID:	EN300-28894_1_1
SMILES:	Cc1c(nn(c(=O)c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C)C
RUN:	RUN8462
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.25

EN300-260816_3_2



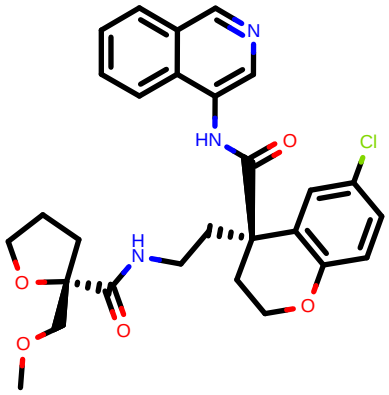
CID:	EN300-260816_3_2
SMILES:	CN1CC[C@H](C1=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1060
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.28

VLA-UCB-50c39ae8-8_1



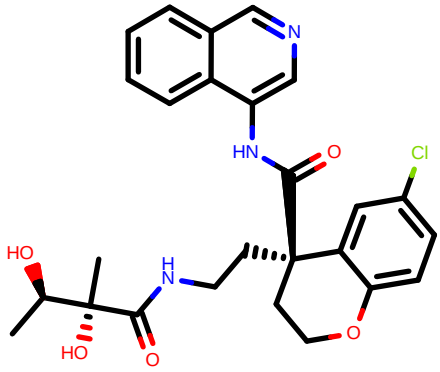
CID:	VLA-UCB-50c39ae8-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl
RUN:	RUN104
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.25

EN300-1301381_3_1



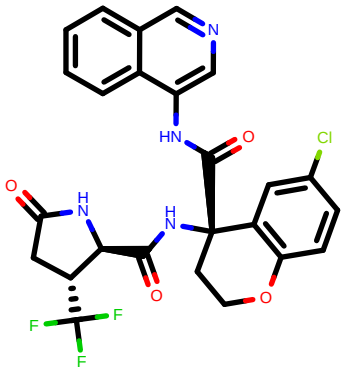
CID:	EN300-1301381_3_1
SMILES:	COC[C@@]1(CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7116
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.31

EN300-202922_3_2



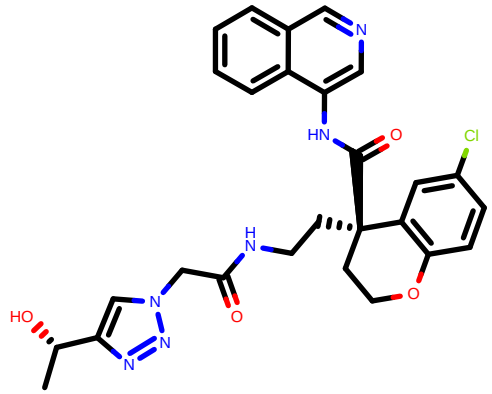
CID:	EN300-202922_3_2
SMILES:	C[C@H]([C@@](C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN1569
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.36

EN300-169955_1_2



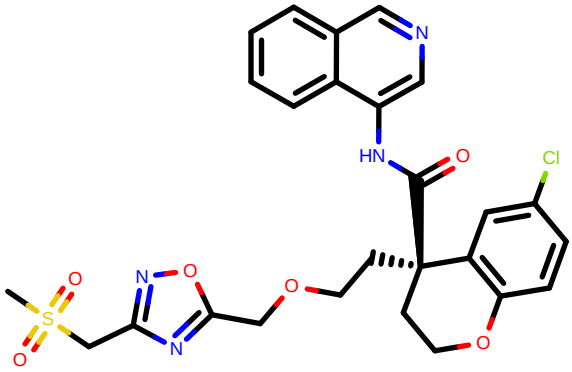
CID:	EN300-169955_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@H]5[C@@H](CC(=O)N5)C(F)(F)F
RUN:	RUN7254
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.34

EN300-109540_3_1



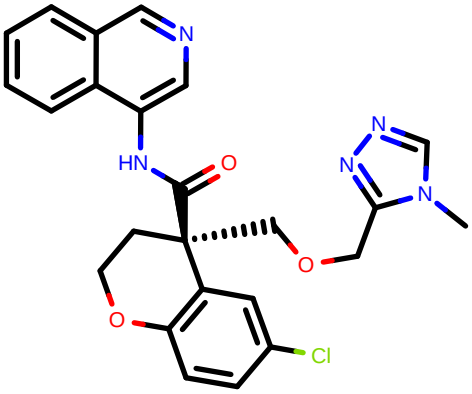
CID:	EN300-109540_3_1
SMILES:	C[C@@H](c1cn(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN8776
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.36

EN300-94900_3_1



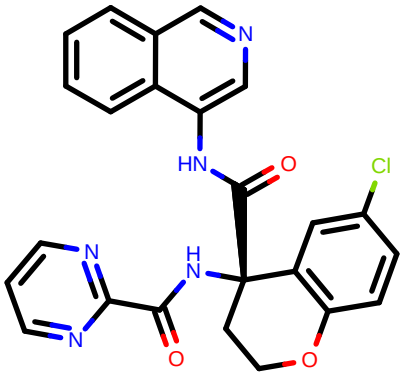
CID:	EN300-94900_3_1
SMILES:	CS(=O)(=O)Cc1nc(on1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2091
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.37

EN300-113112_2_1



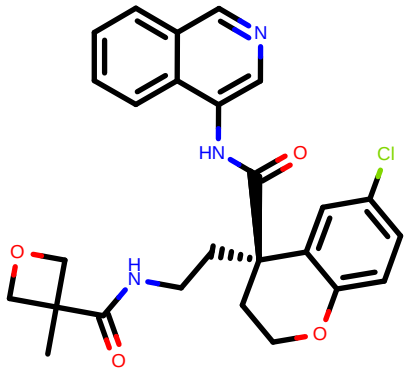
CID:	EN300-113112_2_1
SMILES:	Cn1cnnc1COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1438
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.21

EN300-80230_1_1



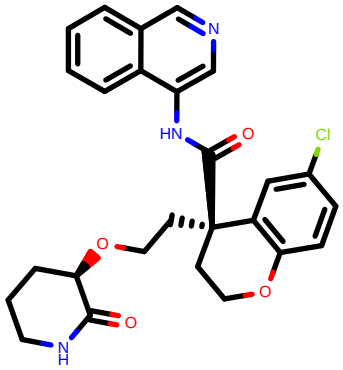
CID:	EN300-80230_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncccn5
RUN:	RUN3973
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.18

EN300-78753_3_1



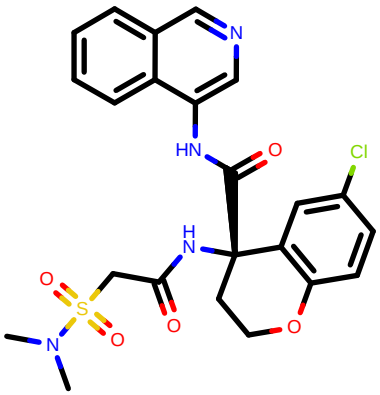
CID:	EN300-78753_3_1
SMILES:	CC1(COC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3915
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.31

EN300-107267_3_1



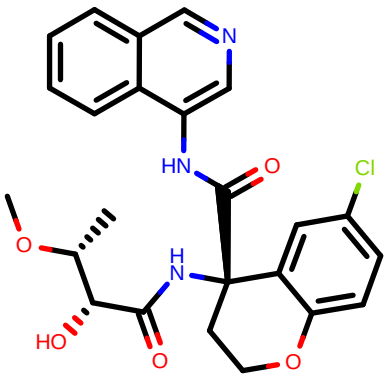
CID:	EN300-107267_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCCNC5=O
RUN:	RUN2335
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.26

EN300-133128_1_1



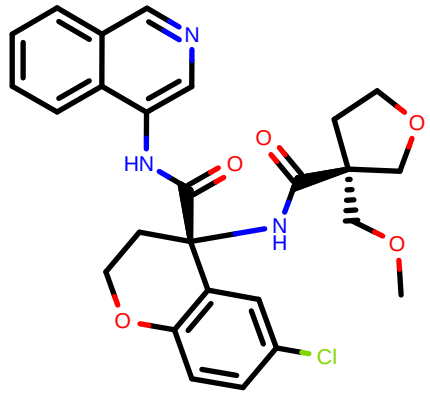
CID:	EN300-133128_1_1
SMILES:	CN(C)S(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4213
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.27

EN300-220194_1_4



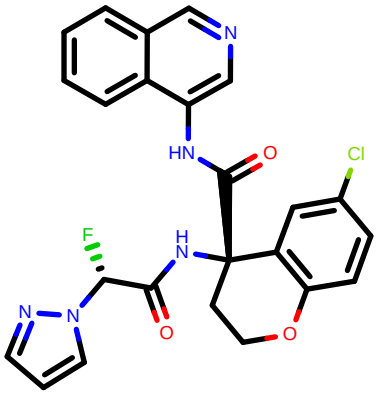
CID:	EN300-220194_1_4
SMILES:	C[C@H]([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN4593
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.23

EN300-248883_1_1



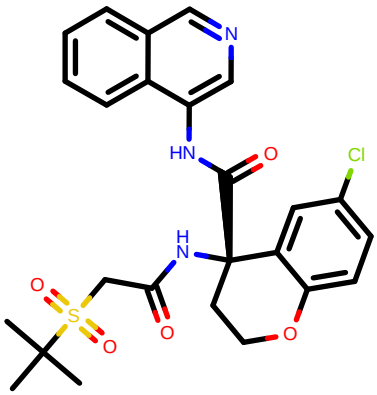
CID:	EN300-248883_1_1
SMILES:	COC[C@@]1(CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6331
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.35

EN300-1726277_1_2



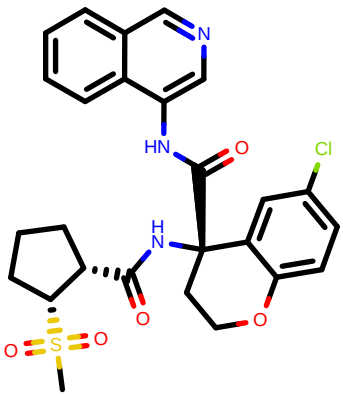
CID:	EN300-1726277_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](n5cccn5)F
RUN:	RUN5868
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.28

EN300-123589_1_1



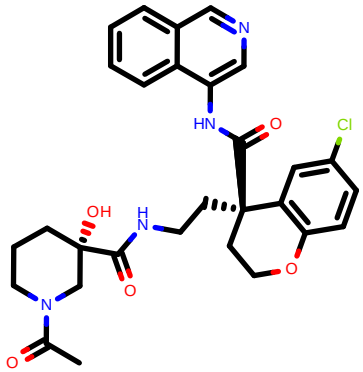
CID:	EN300-123589_1_1
SMILES:	CC(C)(C)S(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6048
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.25

EN300-1387145_1_1



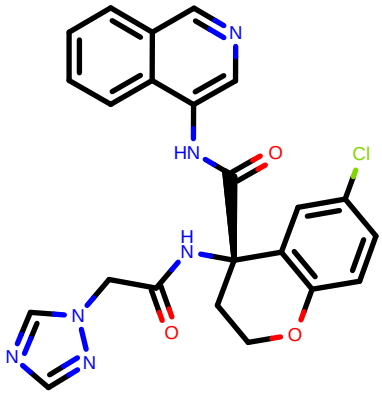
CID:	EN300-1387145_1_1
SMILES:	CS(=O)(=O)[C@@H]1CCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5257
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.27

EN300-210552_3_2



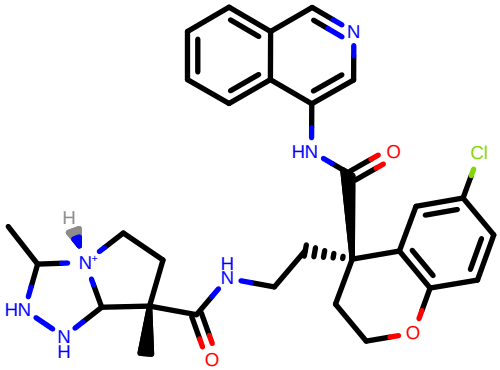
CID:	EN300-210552_3_2
SMILES:	CC(=O)N1CCC[C@](C1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3304
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.52

EN300-06654_1_1



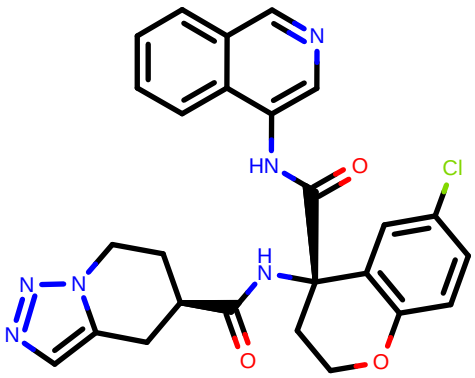
CID:	EN300-06654_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cncn5
RUN:	RUN5704
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.19

EN300-7431629_3_2



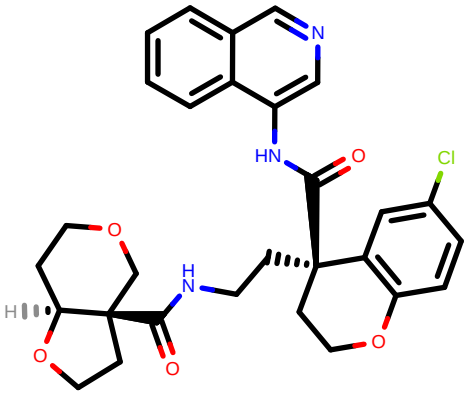
CID:	EN300-7431629_3_2
SMILES:	Cc1nnc2n1CC[C@]2(C)C(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8937
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.33

EN300-7430501_1_1



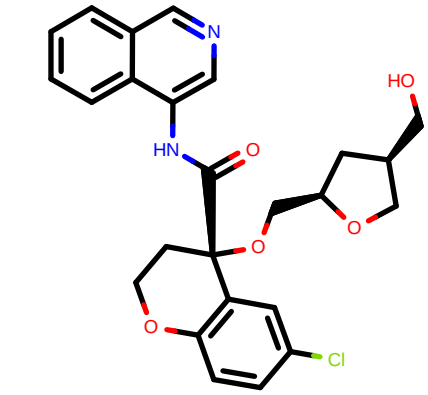
CID:	EN300-7430501_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCn6c(cnn6)C5
RUN:	RUN7710
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.27

EN300-341337_3_3



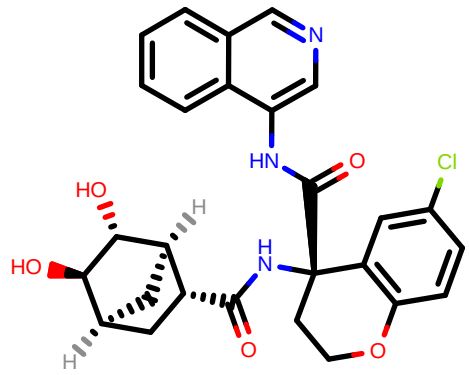
CID:	EN300-341337_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]56CCO[C@H]5CCOC6
RUN:	RUN10348
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.31

EN300-6494158_1_4



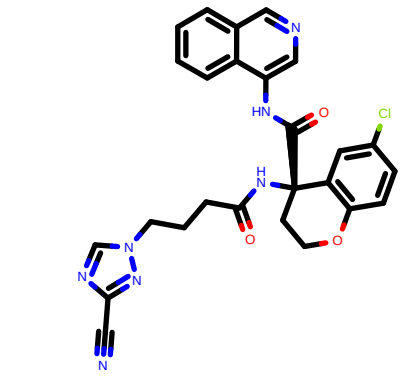
CID:	EN300-6494158_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[C@H](CO5)CO
RUN:	RUN2429
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.29

EN300-6744028_1_3



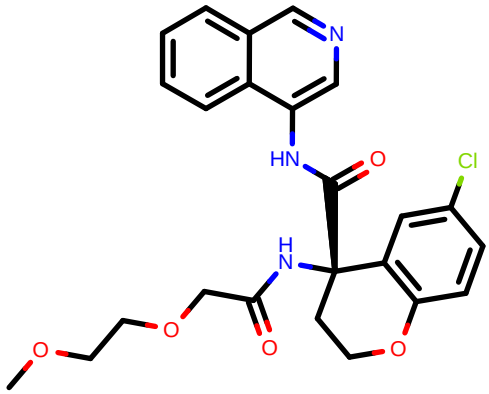
CID:	EN300-6744028_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6CC5[C@H]([C@@H]6O)O
RUN:	RUN7554
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.30

EN300-245265_1_1



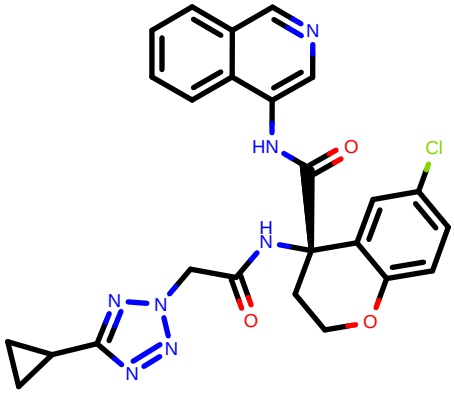
CID:	EN300-245265_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCn5cnc(n5)C#N
RUN:	RUN1477
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.40

EN300-20375_1_1



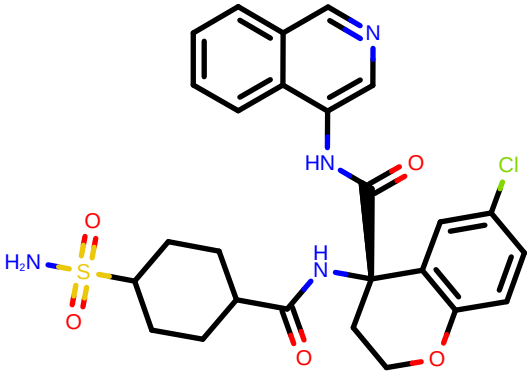
CID:	EN300-20375_1_1
SMILES:	COCCOCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1117
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.22

EN300-1719432_1_1



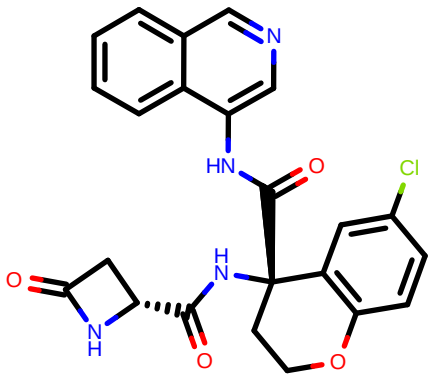
CID:	EN300-1719432_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5nc(nn5)C6CC6
RUN:	RUN6631
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.30

EN300-83864_1_1



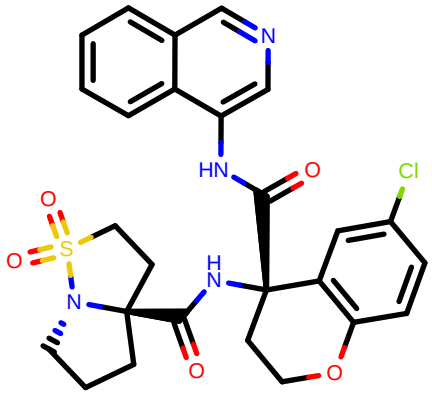
CID:	EN300-83864_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCC(CC5)S(=O)(=O)N
RUN:	RUN9143
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.38

EN300-184266_1_1



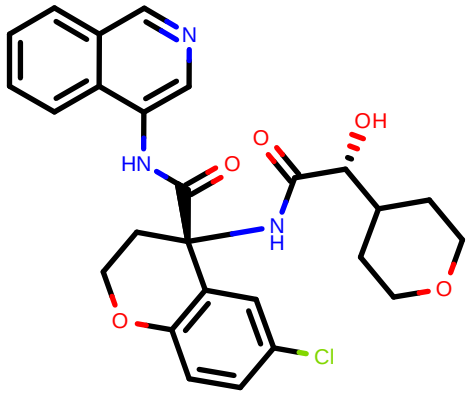
CID:	EN300-184266_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N5
RUN:	RUN1269
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.26

EN300-6733459_1_1



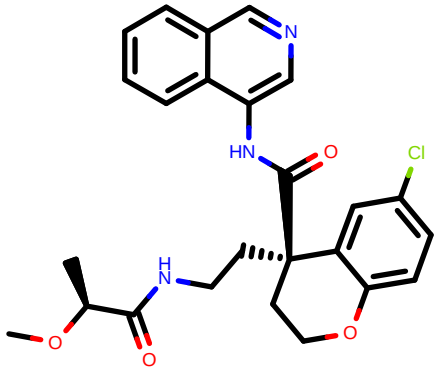
CID:	EN300-6733459_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCCN5S(=O)(=O)CC6
RUN:	RUN6383
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.48

EN300-79180_1_1



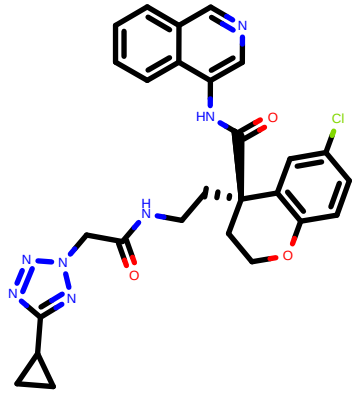
CID:	EN300-79180_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5CCOCC5)O
RUN:	RUN5137
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.35

EN300-258477_3_1



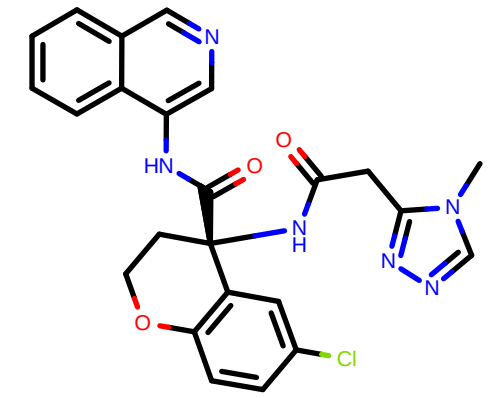
CID:	EN300-258477_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN3236
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.26

EN300-1719432_3_1



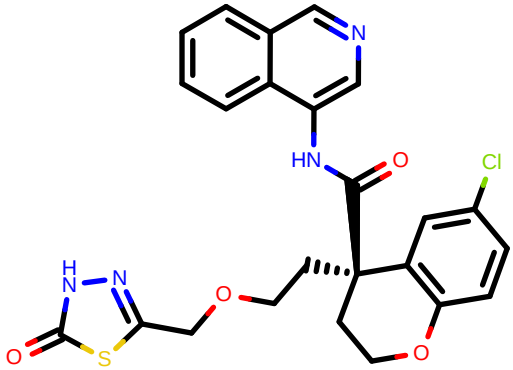
CID:	EN300-1719432_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5nc(nn5)C6CC6
RUN:	RUN10646
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.32

EN300-6494474_1_1



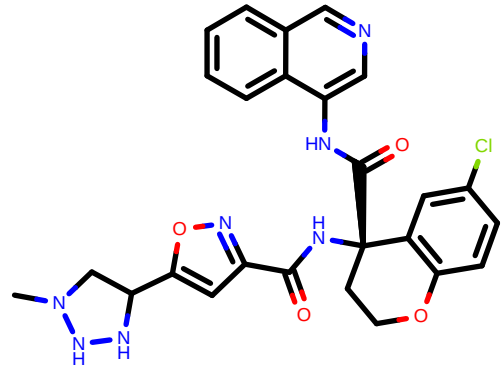
CID:	EN300-6494474_1_1
SMILES:	Cn1cnnc1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5980
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.23

EN300-171766_3_1



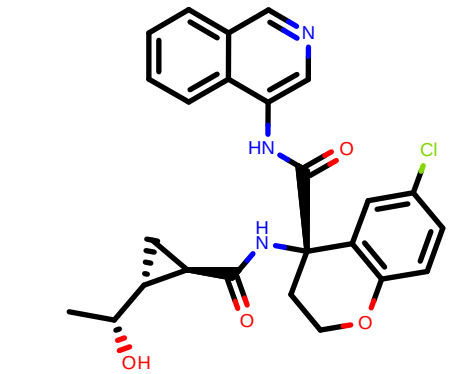
CID:	EN300-171766_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5n[nH]c(=O)s5
RUN:	RUN980
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.27

EN300-1789253_1_1



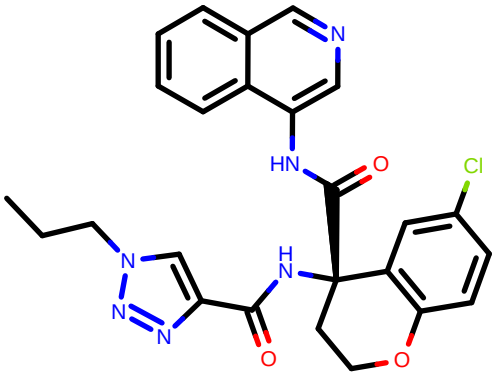
CID:	EN300-1789253_1_1
SMILES:	Cn1cc(nn1)c2cc(no2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9047
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.24

EN300-6729572_1_6



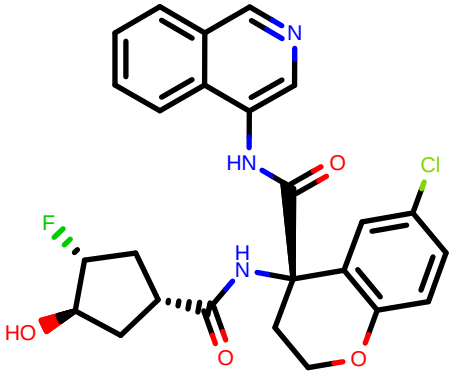
CID:	EN300-6729572_1_6
SMILES:	C[C@H]([C@@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1892
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.24

EN300-123416_1_1



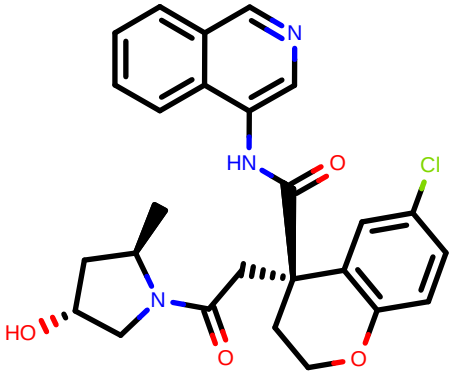
CID:	EN300-123416_1_1
SMILES:	CCCn1cc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7322
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.27

EN300-7461217_1_1



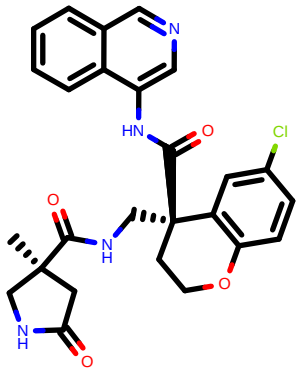
CID:	EN300-7461217_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@H](C@@H](C5)F)O
RUN:	RUN7350
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.27

EN300-173562_1_3



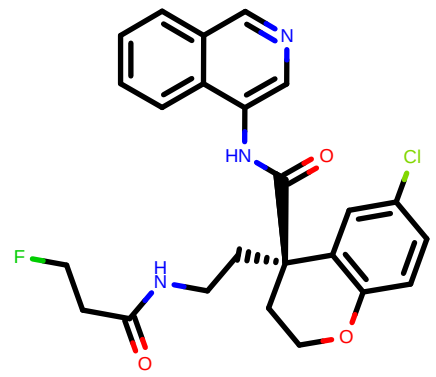
CID:	EN300-173562_1_3
SMILES:	C[C@@H]1C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10522
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.32

EN300-132157_2_1



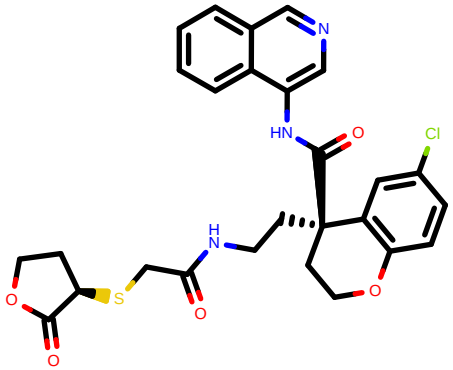
CID:	EN300-132157_2_1
SMILES:	C[C@@]1(CC(=O)NC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4606
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.28

EN300-97758_3_1



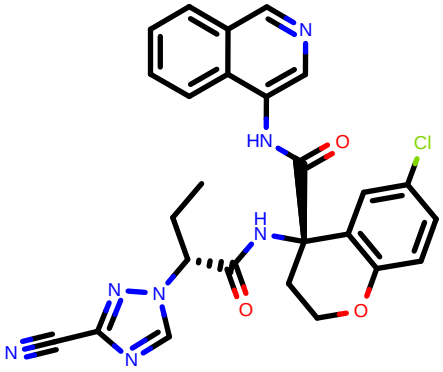
CID:	EN300-97758_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCF
RUN:	RUN3104
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.22

EN300-113218_3_1



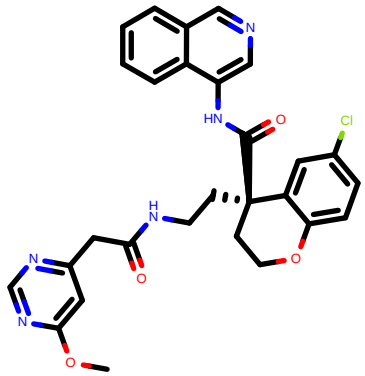
CID:	EN300-113218_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@@H]5CCOC5=O
RUN:	RUN5834
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.34

EN300-245264_1_2



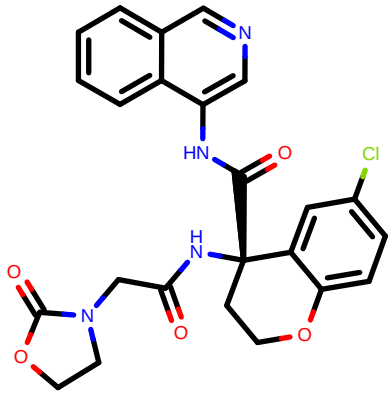
CID:	EN300-245264_1_2
SMILES:	CC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnc(n5)C#N
RUN:	RUN6032
DDG (kcal/mol):	-2.44
dDDG (kcal/mol):	0.27

EN300-7444950_3_1



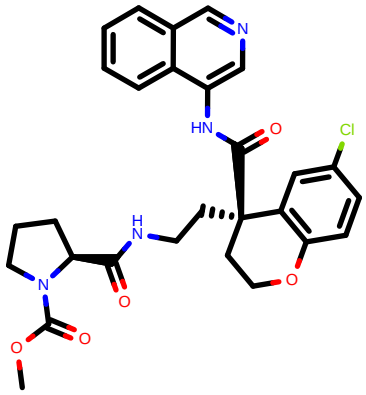
CID:	EN300-7444950_3_1
SMILES:	COc1cc(ncn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9042
DDG (kcal/mol):	-2.44
dDDG (kcal/mol):	0.31

EN300-172179_1_1



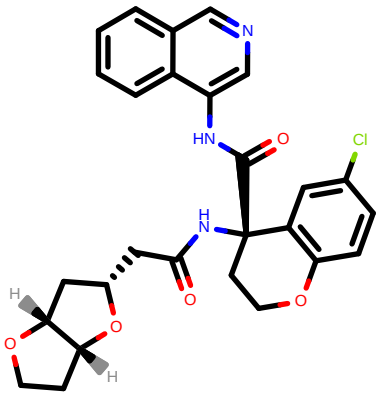
CID:	EN300-172179_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCOC5=O
RUN:	RUN1149
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.30

EN300-66845_3_2



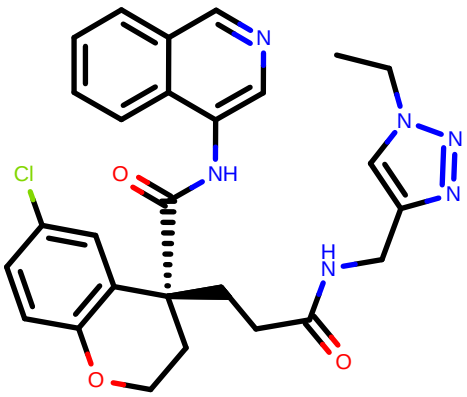
CID:	EN300-66845_3_2
SMILES:	COC(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5742
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.31

EN300-7355519_1_6



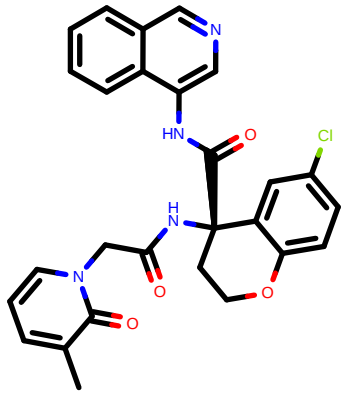
CID:	EN300-7355519_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5C[C@@H]6[C@H](O5)CCO6
RUN:	RUN6878
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.28

EN300-300088_2_1



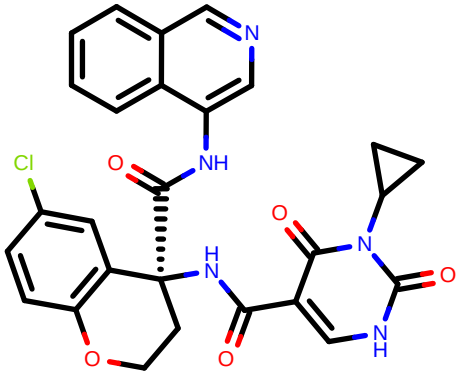
CID:	EN300-300088_2_1
SMILES:	CCn1cc(nn1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9805
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.25

EN300-126104_1_1



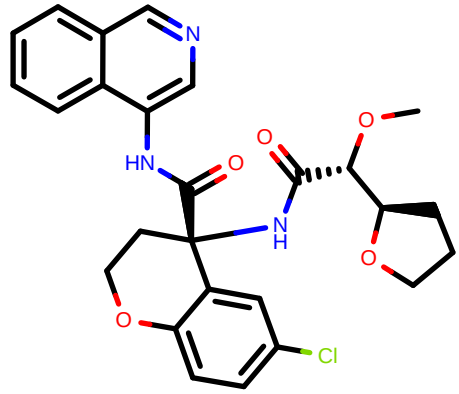
CID:	EN300-126104_1_1
SMILES:	Cc1cccn(c1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2710
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.30

EN300-7433864_1_1



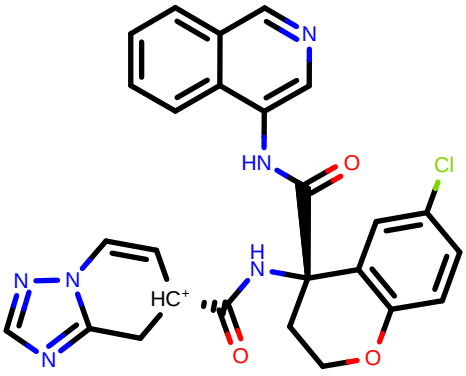
CID:	EN300-7433864_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c(=O)n(c5=O)C6CC6
RUN:	RUN8566
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.39

EN300-6277108_1_4



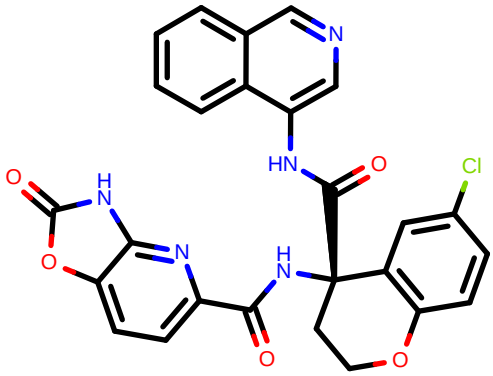
CID:	EN300-6277108_1_4
SMILES:	CO[C@H]([C@H]1CCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5752
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.27

EN300-192893_1_1



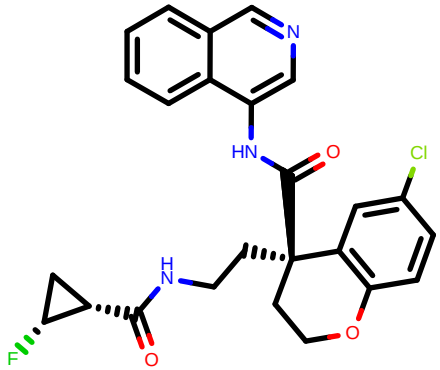
CID:	EN300-192893_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6c(c5)ncn6
RUN:	RUN5233
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.22

EN300-188174_1_1



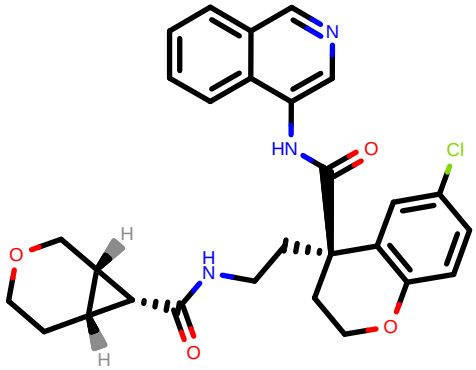
CID:	EN300-188174_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(n5)[nH]c(=O)o6
RUN:	RUN8918
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.25

EN300-97300_3_4



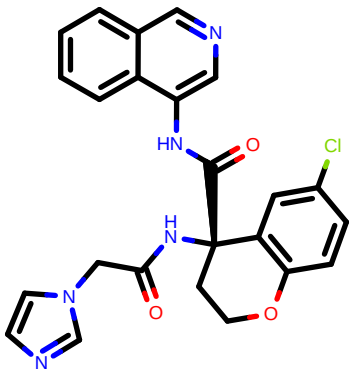
CID:	EN300-97300_3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@H]5F
RUN:	RUN7892
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.23

EN300-1644723_3_3



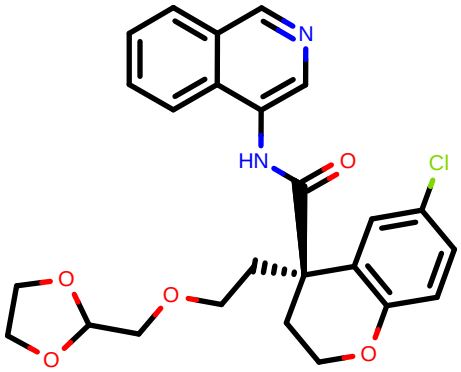
CID:	EN300-1644723_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5[C@H]6[C@@H]5COCC6
RUN:	RUN7224
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.29

EN300-38979_1_1



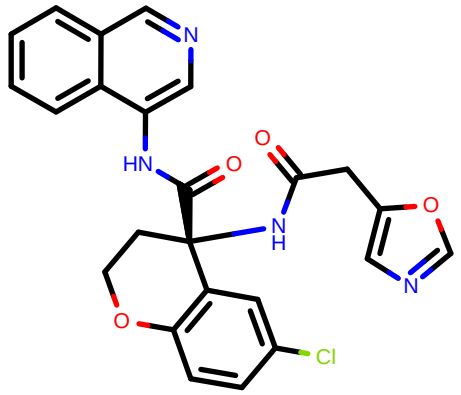
CID:	EN300-38979_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5
RUN:	RUN4569
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.24

EN300-77092_3_1



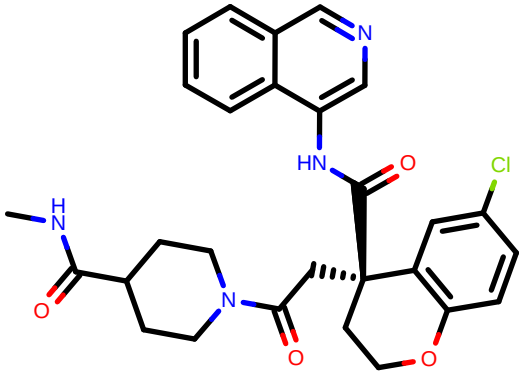
CID:	EN300-77092_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5OCCO5
RUN:	RUN2131
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.32

EN300-6491117_1_1



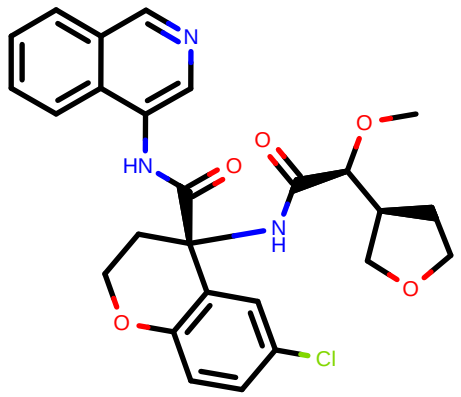
CID:	EN300-6491117_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnco5
RUN:	RUN3530
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.24

EN300-24653_1_1



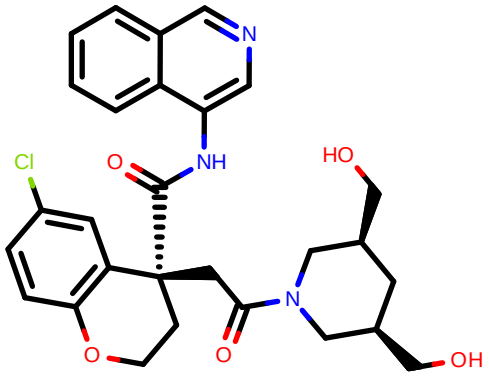
CID:	EN300-24653_1_1
SMILES:	CNC(=O)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9993
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.33

EN300-298552_1_3



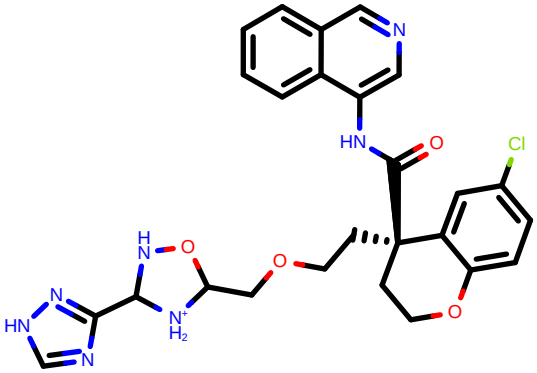
CID:	EN300-298552_1_3
SMILES:	CO[C@@H]([C@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2584
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.27

EN300-2007627_1_1



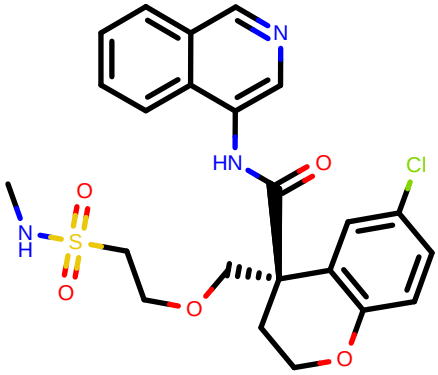
CID:	EN300-2007627_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H](C5)CO)CO
RUN:	RUN4923
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.31

EN300-92031_3_1



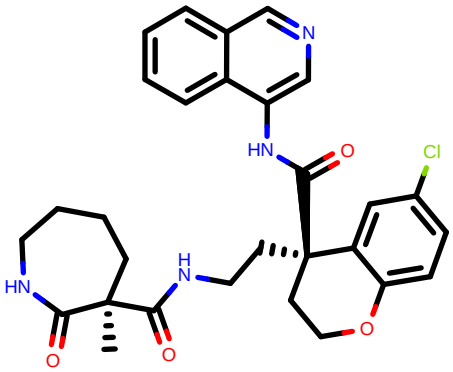
CID:	EN300-92031_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nc(no5)c6[nH]cnn6
RUN:	RUN2537
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.31

EN300-6482967_2_1



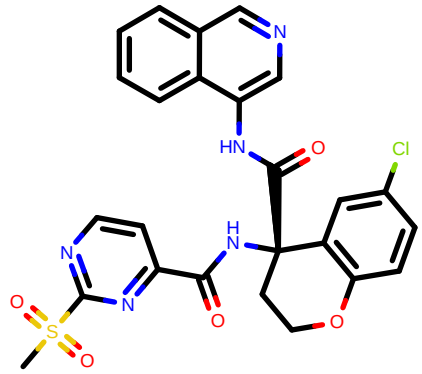
CID:	EN300-6482967_2_1
SMILES:	CNS(=O)(=O)CCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN650
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.33

EN300-6745081_3_2



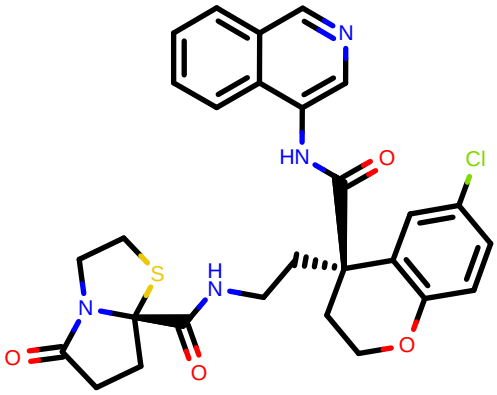
CID:	EN300-6745081_3_2
SMILES:	C[C@]1(CCCCNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2868
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.36

EN300-205622_1_1



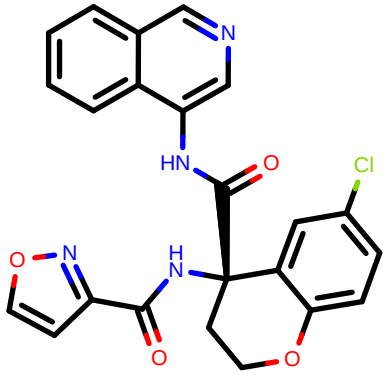
CID:	EN300-205622_1_1
SMILES:	CS(=O)(=O)c1nccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6208
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.37

EN300-10334_3_1



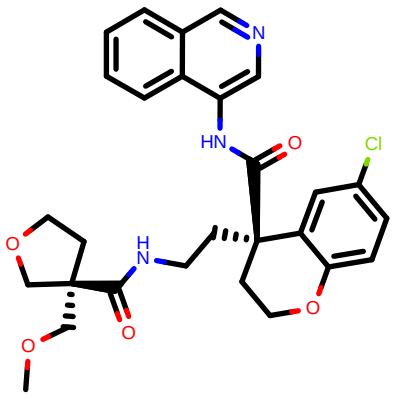
CID:	EN300-10334_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]56CCC(=O)N5CCS6
RUN:	RUN4291
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.31

EN300-22245_1_1



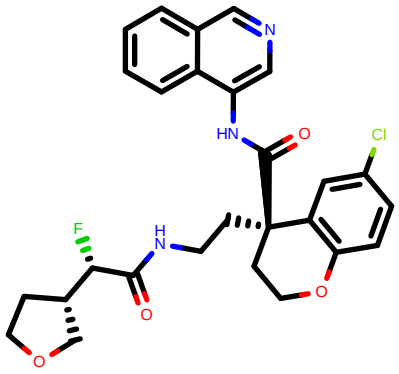
CID:	EN300-22245_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccon5
RUN:	RUN3350
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.20

EN300-248883_3_2



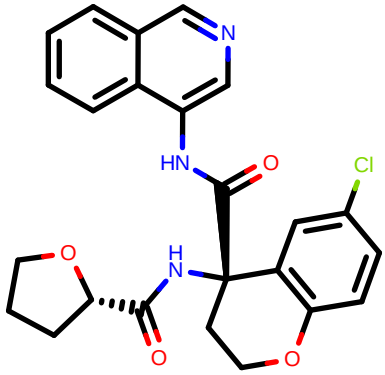
CID:	EN300-248883_3_2
SMILES:	COC[C@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5151
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.32

EN300-783124_3_4



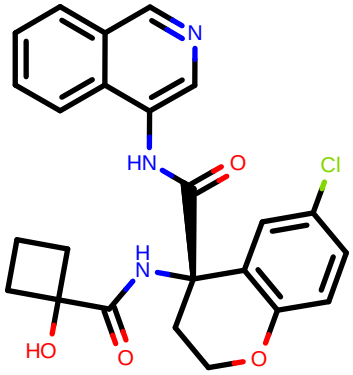
CID:	EN300-783124_3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]([C@H]5CCOC5)F
RUN:	RUN9920
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.29

EN300-21009_1_1



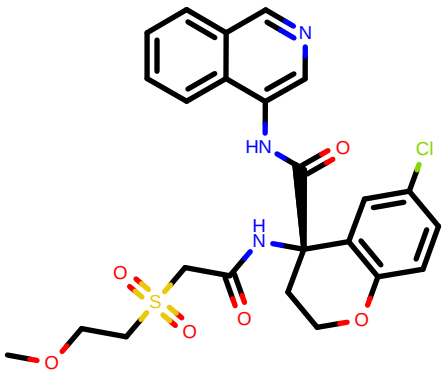
CID:	EN300-21009_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCO5
RUN:	RUN4313
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.23

EN300-52009_1_1



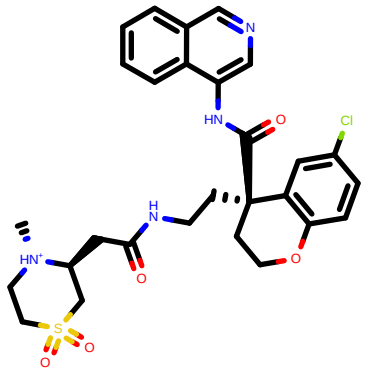
CID:	EN300-52009_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCC5)O
RUN:	RUN3134
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.26

EN300-39501_1_1



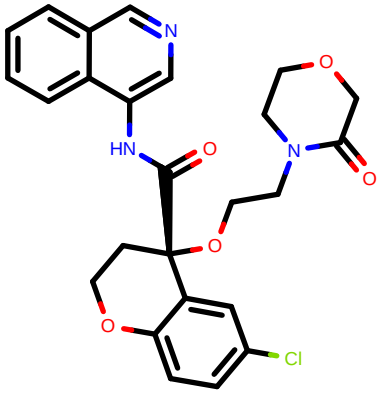
CID:	EN300-39501_1_1
SMILES:	COCCS(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN609
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.35

EN300-300020_3_1



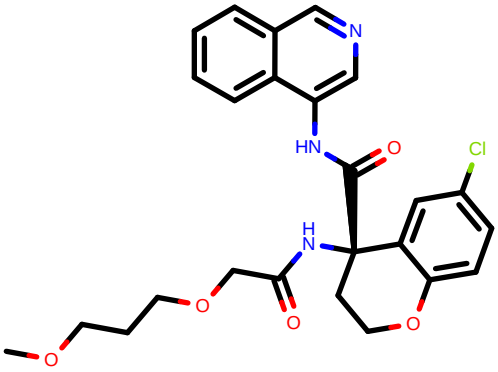
CID:	EN300-300020_3_1
SMILES:	CN1CCS(=O)(=O)C[C@@H]1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9211
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.45

EN300-219330_1_1



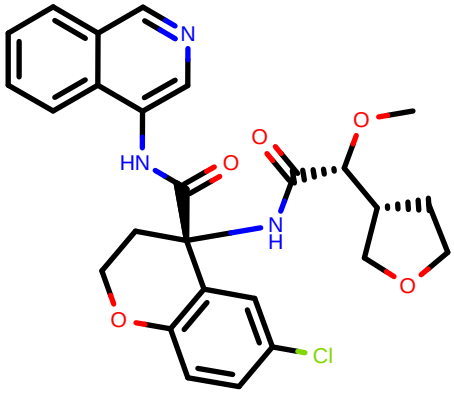
CID:	EN300-219330_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOCC5=O
RUN:	RUN2443
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.25

EN300-125769_1_1



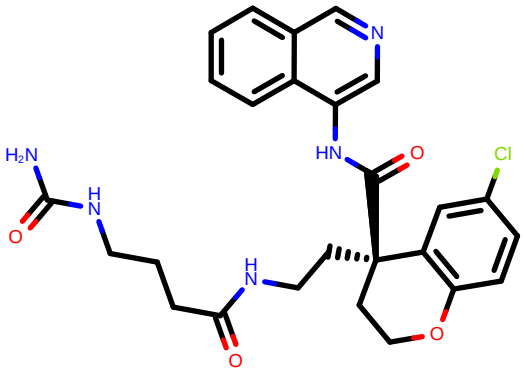
CID:	EN300-125769_1_1
SMILES:	COCCCOCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1365
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.23

EN300-298552_1_2



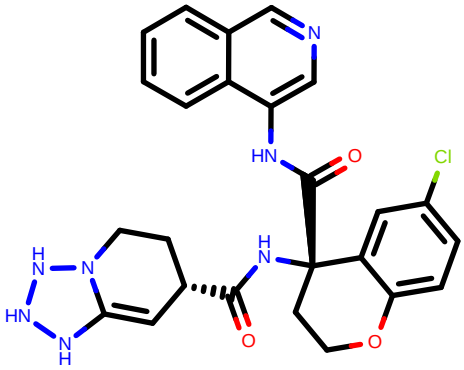
CID:	EN300-298552_1_2
SMILES:	CO[C@H]([C@@H]1CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1373
DDG (kcal/mol):	-2.37
dDDG (kcal/mol):	0.27

EN300-05620_3_1



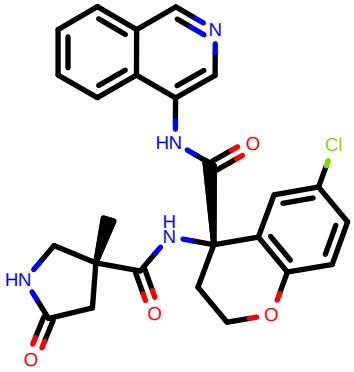
CID:	EN300-05620_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCNC(=O)N
RUN:	RUN9135
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.33

EN300-1653482_1_2



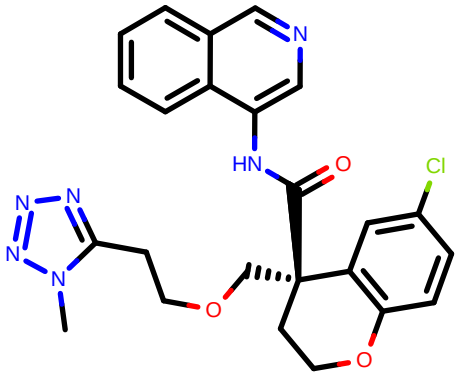
CID:	EN300-1653482_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCn6c(nnn6)C5
RUN:	RUN6307
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.27

EN300-132157_1_2



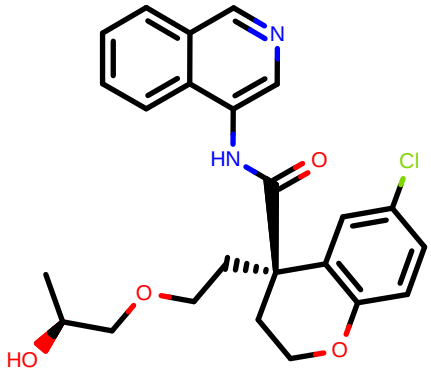
CID:	EN300-132157_1_2
SMILES:	C[C@]1(CC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6994
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.26

EN300-365398_2_1



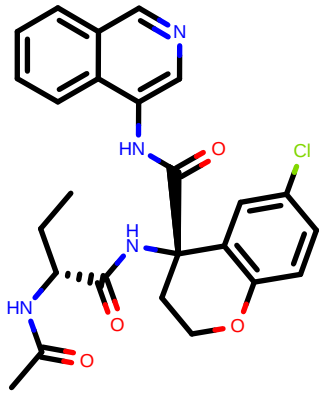
CID:	EN300-365398_2_1
SMILES:	Cn1c(nnn1)CCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1981
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.29

EN300-185378_3_1



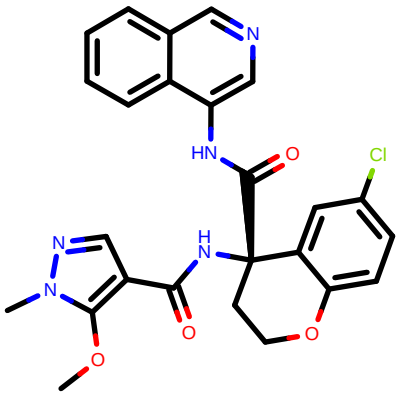
CID:	EN300-185378_3_1
SMILES:	C[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1428
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.26

EN300-332601_1_2



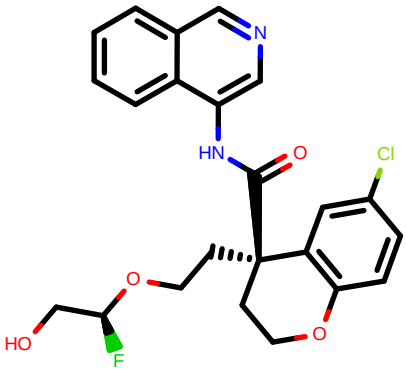
CID:	EN300-332601_1_2
SMILES:	CC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN5237
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.31

EN300-227310_1_1



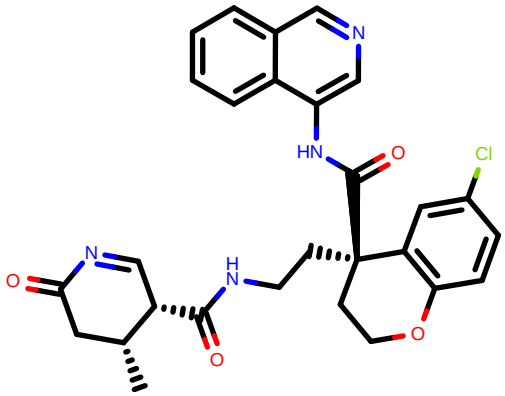
CID:	EN300-227310_1_1
SMILES:	Cn1c(c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN5476
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.28

EN300-861925_3_2



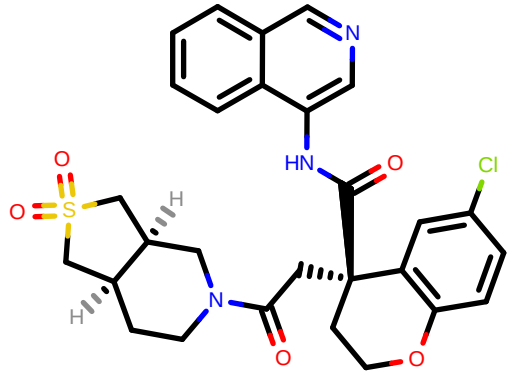
CID:	EN300-861925_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H](CO)F
RUN:	RUN1372
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.27

EN300-95698_3_1



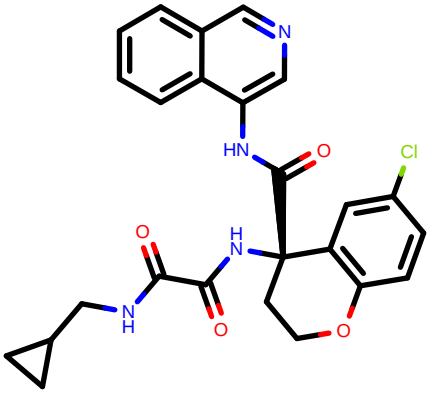
CID:	EN300-95698_3_1
SMILES:	C[C@@H]1CC(=O)NC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10696
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.40

EN300-365993_1_4



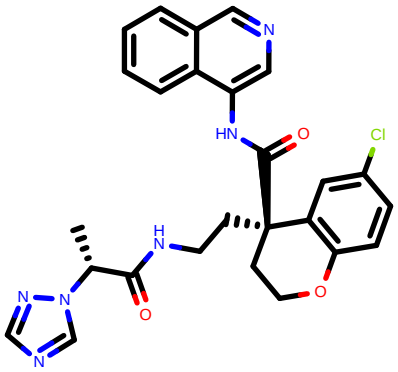
CID:	EN300-365993_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6CS(=O)(=O)C[C@H]6C5
RUN:	RUN842
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.39

EN300-173216_1_1



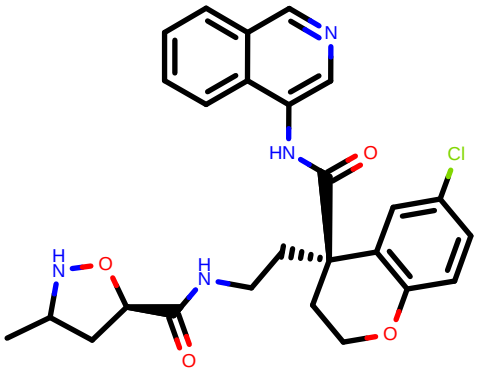
CID:	EN300-173216_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NCC5CC5
RUN:	RUN1716
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.26

EN300-30397_3_2



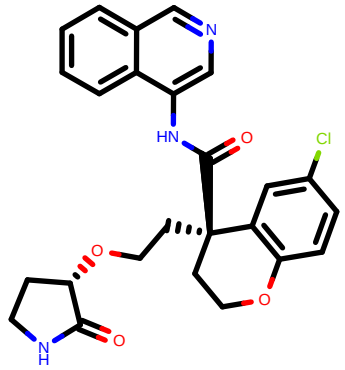
CID:	EN300-30397_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN2768
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.34

EN300-92447_3_2



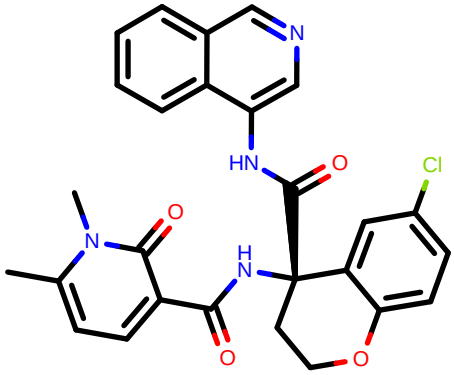
CID:	EN300-92447_3_2
SMILES:	CC1=NO[C@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10638
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.25

EN300-6736413_3_2



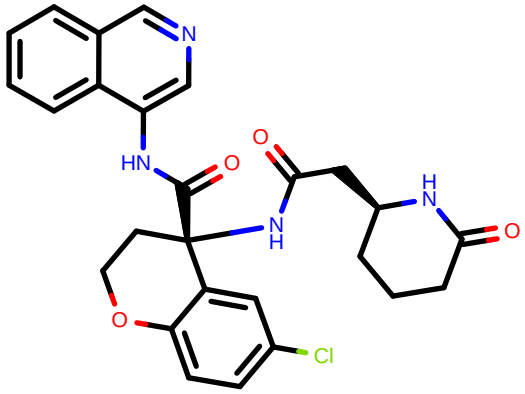
CID:	EN300-6736413_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCNC5=O
RUN:	RUN2349
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.28

EN300-41423_1_1



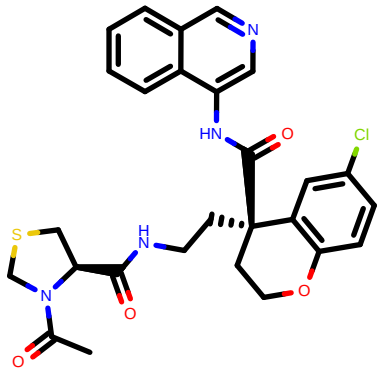
CID:	EN300-41423_1_1
SMILES:	Cc1ccc(c(=O)n1C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8834
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.50

EN300-210084_1_1



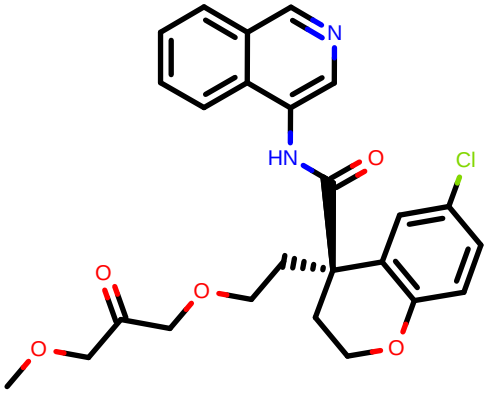
CID:	EN300-210084_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCC(=O)N5
RUN:	RUN3849
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.27

EN300-736749_3_1



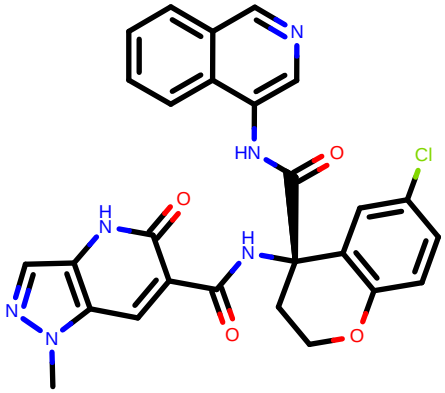
CID:	EN300-736749_3_1
SMILES:	CC(=O)N1CSC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3787
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.28

EN300-125140_3_1



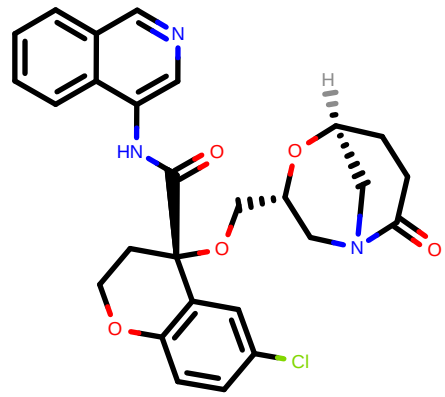
CID:	EN300-125140_3_1
SMILES:	COCC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN735
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.25

EN300-805037_1_1



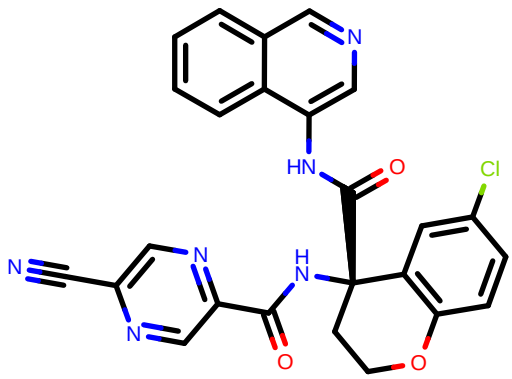
CID:	EN300-805037_1_1
SMILES:	Cn1c2cc(c(=O)[nH]c2cn1)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9029
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.29

EN300-2008102_1_2



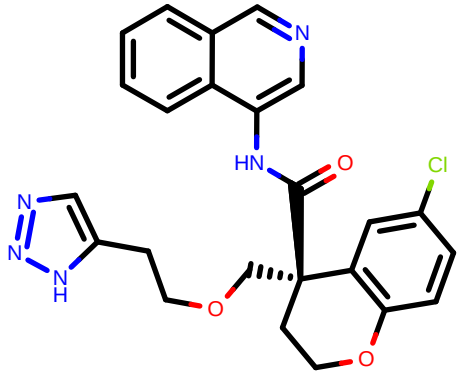
CID:	EN300-2008102_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CN6CC(O5)CCC6=O
RUN:	RUN2520
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.30

EN300-149224_1_1



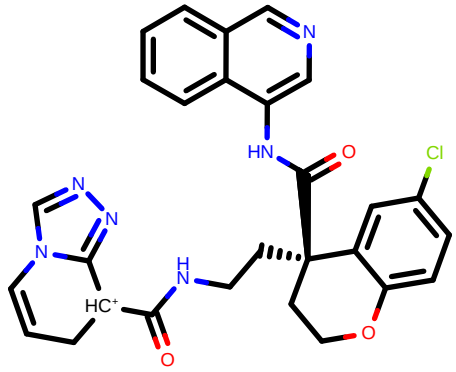
CID:	EN300-149224_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc(cn5)C#N
RUN:	RUN8714
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.21

EN300-222357_2_1



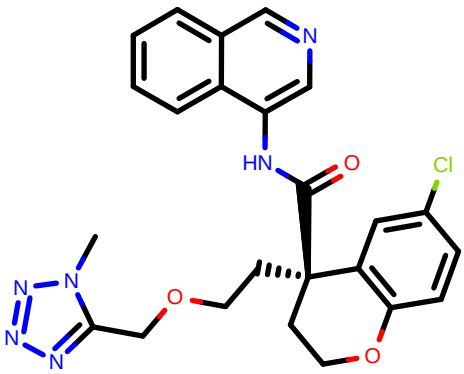
CID:	EN300-222357_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCc5c[nH]nn5
RUN:	RUN990
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.22

EN300-1726153_3_1



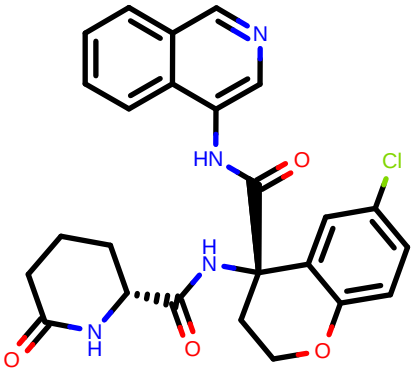
CID:	EN300-1726153_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cccn6c5nnc6
RUN:	RUN7308
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.29

EN300-62574_3_1



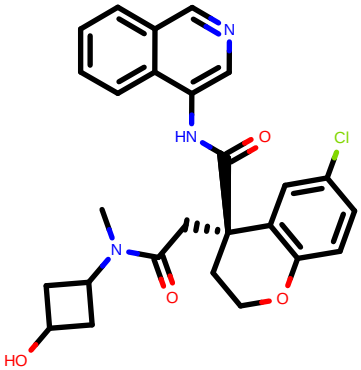
CID:	EN300-62574_3_1
SMILES:	Cn1c(nnn1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1236
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.26

EN300-146491_1_1



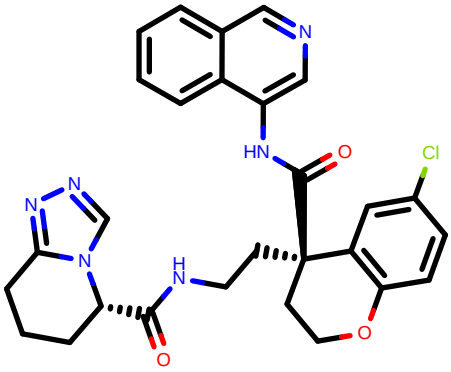
CID:	EN300-146491_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCC(=O)N5
RUN:	RUN3126
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.23

EN300-97697_1_1



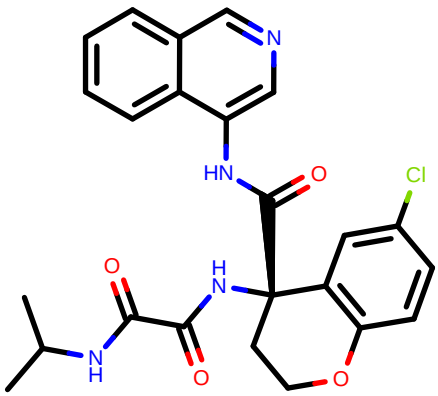
CID:	EN300-97697_1_1
SMILES:	CN(C1CC(C1)O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9000
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.30

EN300-6478631_3_1



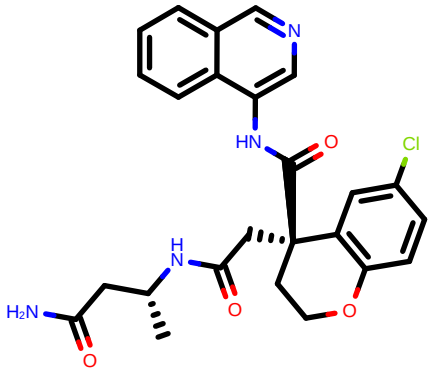
CID:	EN300-6478631_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCc6n5cnn6
RUN:	RUN9949
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.35

EN300-1262640_1_1



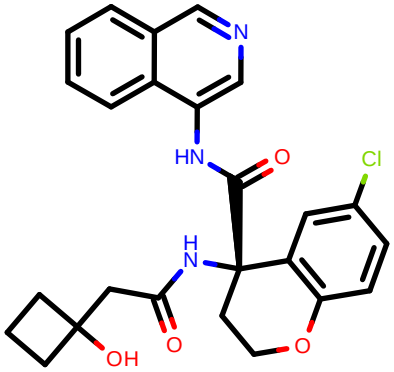
CID:	EN300-1262640_1_1
SMILES:	CC(C)NC(=O)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6064
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.19

EN300-84785_1_2



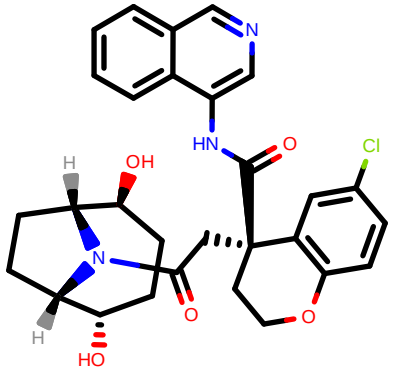
CID:	EN300-84785_1_2
SMILES:	C[C@H](CC(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5922
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.23

EN300-246423_1_1



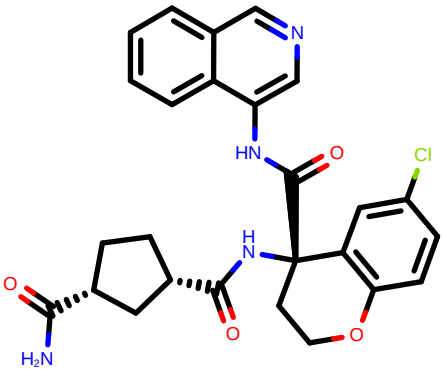
CID:	EN300-246423_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCC5)O
RUN:	RUN545
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.30

EN300-6738887_1_2



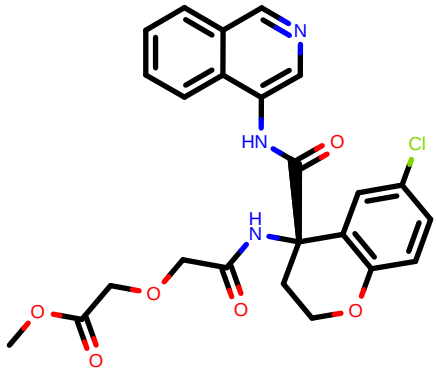
CID:	EN300-6738887_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6CCC5[C@H](CC[C@@H]6O)O
RUN:	RUN9830
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.45

EN300-370753_1_1



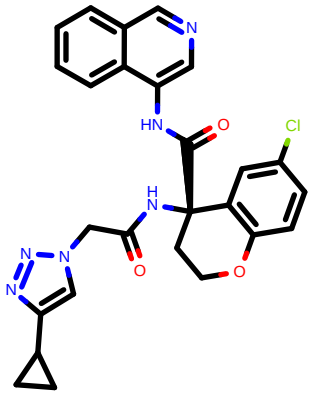
CID:	EN300-370753_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC[C@H](C5)C(=O)N
RUN:	RUN4557
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.43

EN300-205635_1_1



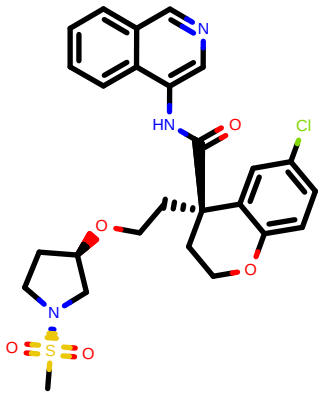
CID:	EN300-205635_1_1
SMILES:	COC(=O)COCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN402
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.25

EN300-107892_1_1



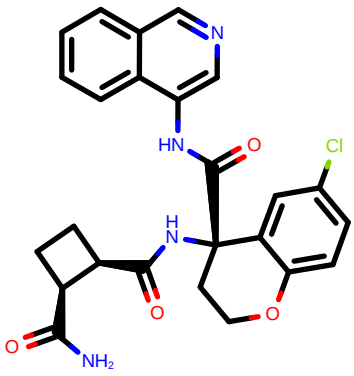
CID:	EN300-107892_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(nn5)C6CC6
RUN:	RUN7298
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.31

EN300-301690_3_2



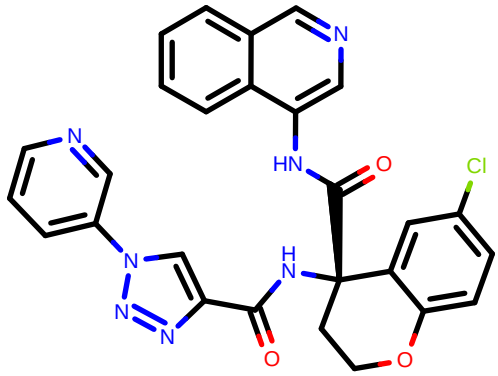
CID:	EN300-301690_3_2
SMILES:	CS(=O)(=O)N1CC[C@H](C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2447
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.31

EN300-217107_1_1



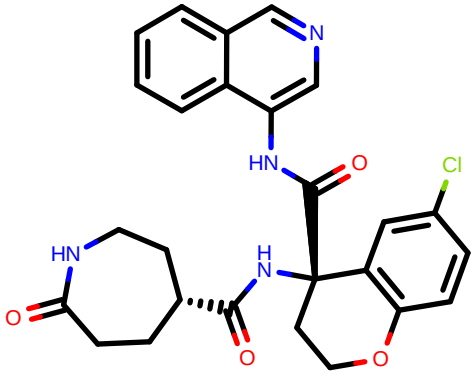
CID:	EN300-217107_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC[C@@H]5C(=O)N
RUN:	RUN6212
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.28

EN300-151330_1_1



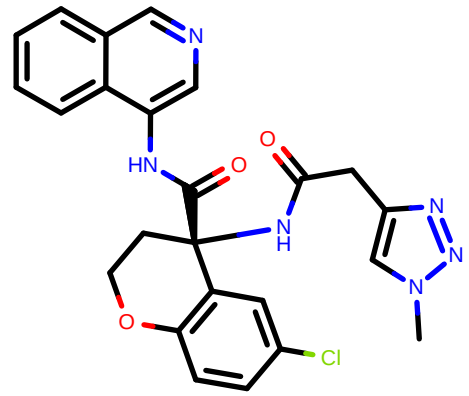
CID:	EN300-151330_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)c6cccnc6
RUN:	RUN8975
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.19

EN300-152337_1_1



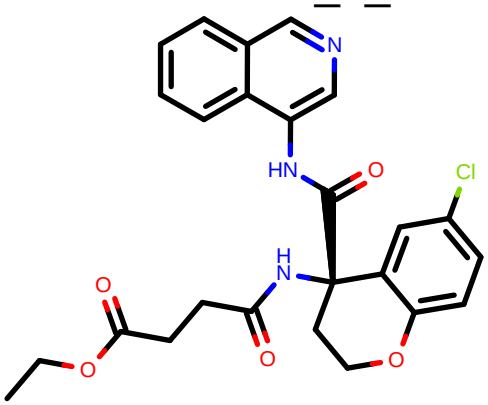
CID:	EN300-152337_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCC(=O)NCC5
RUN:	RUN4269
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.34

EN300-1073264_1_1



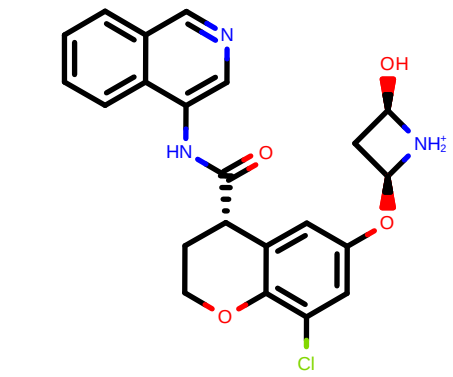
CID:	EN300-1073264_1_1
SMILES:	Cn1cc(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2673
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.21

EN300-17161_1_1



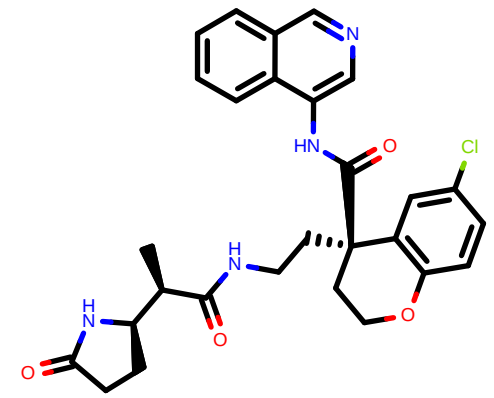
CID:	EN300-17161_1_1
SMILES:	CCOC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1820
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.27

FRA-DIA-b66f7109-3_2



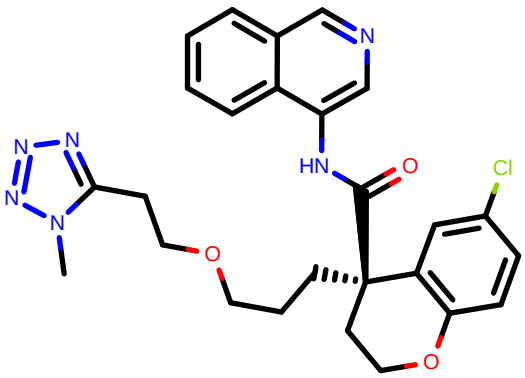
CID:	FRA-DIA-b66f7109-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4Cl)O[C@H]5CC(=O)N5
RUN:	RUN210
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.27

EN300-249421_3_4



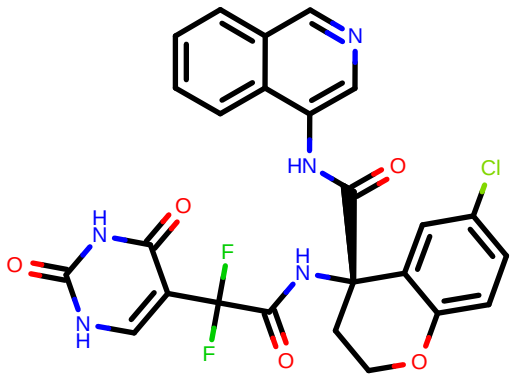
CID:	EN300-249421_3_4
SMILES:	C[C@H]([C@H]1CCC(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4807
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.29

EN300-365398_4_1



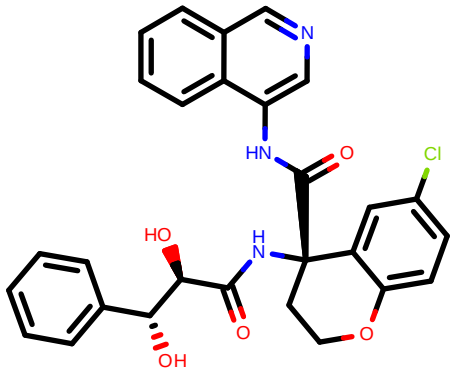
CID:	EN300-365398_4_1
SMILES:	Cn1c(nnn1)CCOCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2022
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.34

EN300-93174_1_1



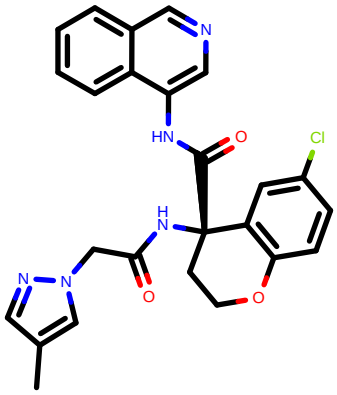
CID:	EN300-93174_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)C(c5c[nH]c(=O)[nH]c5=O)(F)F
RUN:	RUN1916
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.41

EN300-2923949_1_4



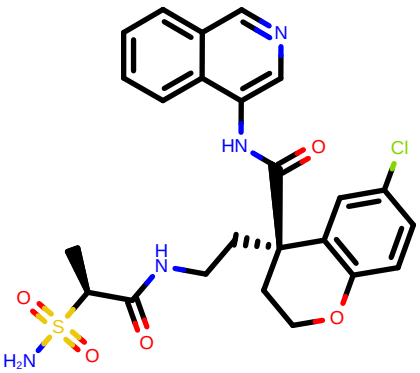
CID:	EN300-2923949_1_4
SMILES:	c1ccc(cc1)[C@H]([C@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O
RUN:	RUN7738
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.31

EN300-51832_1_1



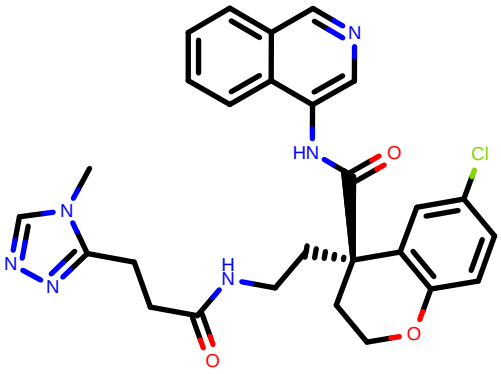
CID:	EN300-51832_1_1
SMILES:	Cc1cnn(c1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7246
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.22

EN300-132615_3_1



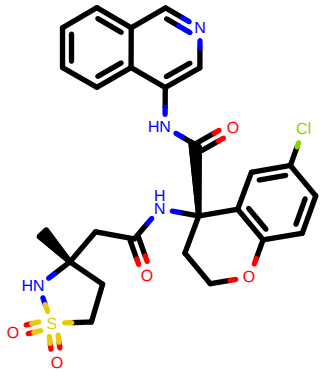
CID:	EN300-132615_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N
RUN:	RUN4267
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.32

EN300-1138792_3_1



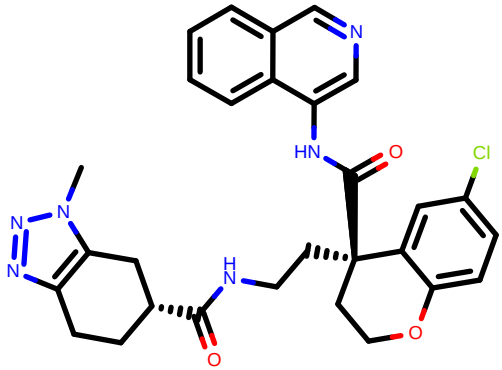
CID:	EN300-1138792_3_1
SMILES:	Cn1cnnc1CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9456
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.30

EN300-385235_1_2



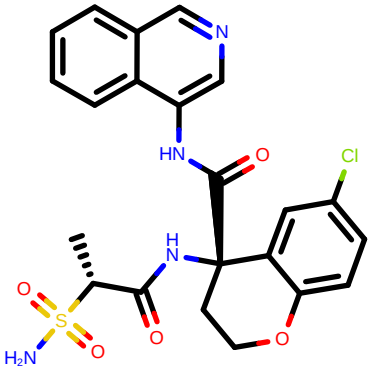
CID:	EN300-385235_1_2
SMILES:	C[C@]1(CCS(=O)(=O)N1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1956
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.39

EN300-217343_3_2



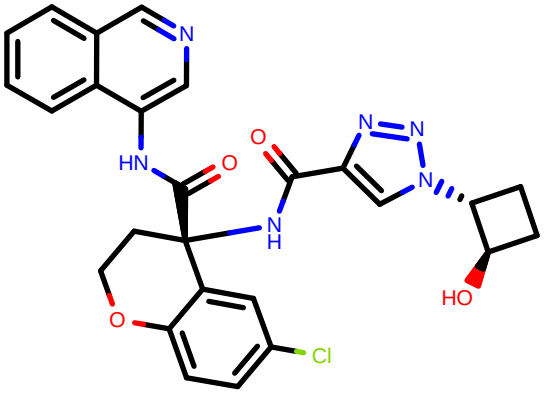
CID:	EN300-217343_3_2
SMILES:	Cn1c2c(nn1)CC[C@H](C2)C(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN10932
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.32

EN300-132615_1_2



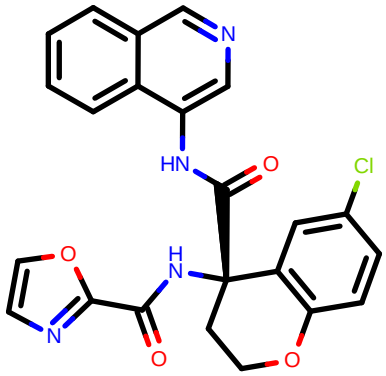
CID:	EN300-132615_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N
RUN:	RUN2805
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.23

EN300-316196_1_1



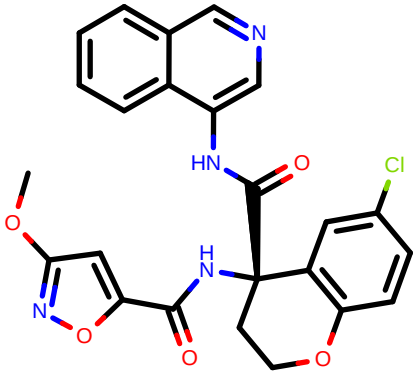
CID:	EN300-316196_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)[C@@H]6CC[C@H]6O
RUN:	RUN7850
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.28

EN300-318344_1_1



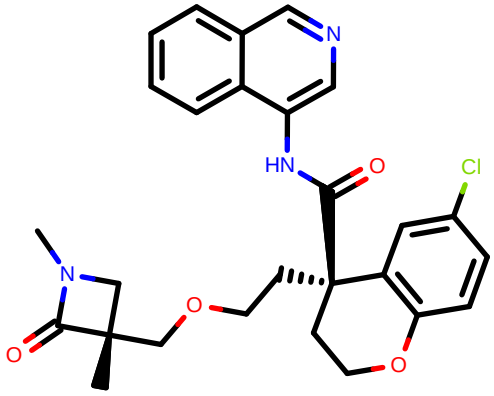
CID:	EN300-318344_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncco5
RUN:	RUN2455
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.19

EN300-131465_1_1



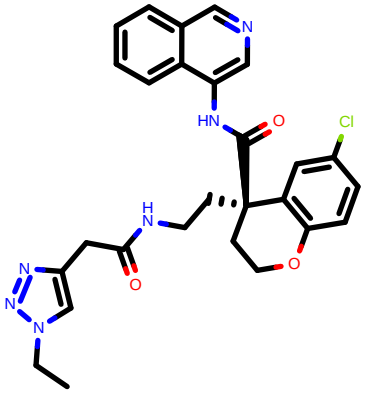
CID:	EN300-131465_1_1
SMILES:	COc1cc(on1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6263
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.24

EN300-1273362_3_1



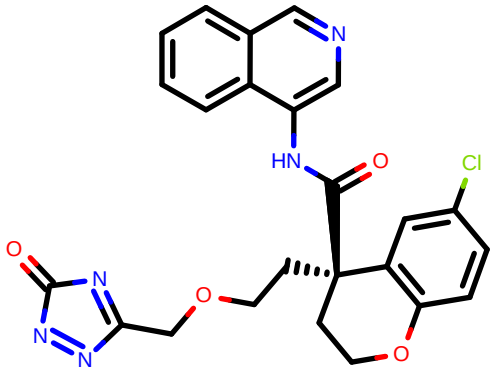
CID:	EN300-1273362_3_1
SMILES:	C[C@@]1(CN(C1=O)C)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN401
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.31

EN300-717276_3_1



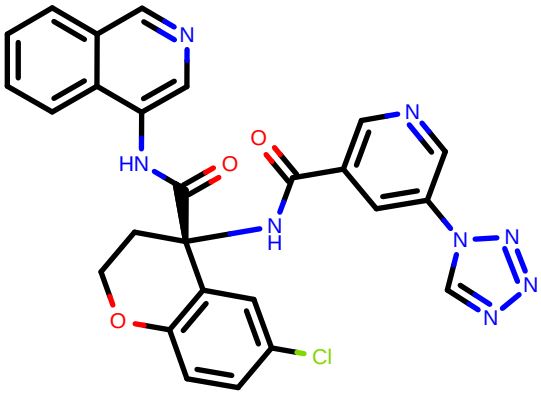
CID:	EN300-717276_3_1
SMILES:	CCn1cc(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7716
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.36

EN300-73772_3_1



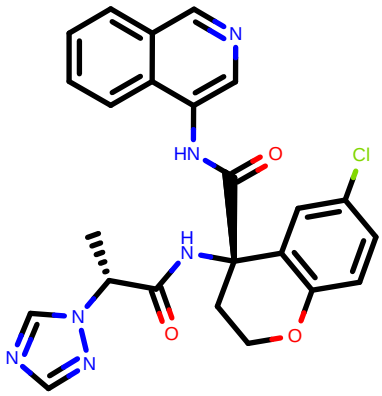
CID:	EN300-73772_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)[nH]n5
RUN:	RUN1308
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.28

EN300-2690393_1_1



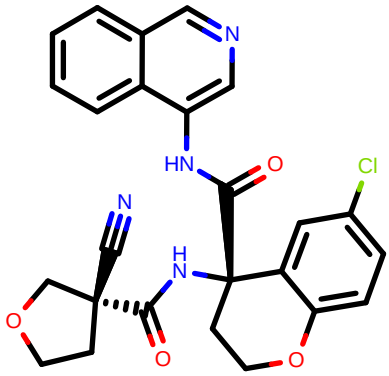
CID:	EN300-2690393_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cnc5)n6cnnn6
RUN:	RUN9008
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.23

EN300-30397_1_2



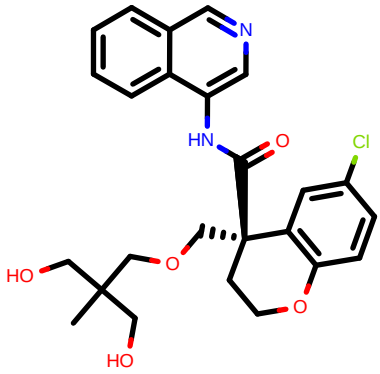
CID:	EN300-30397_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN5157
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.27

EN300-261210_1_1



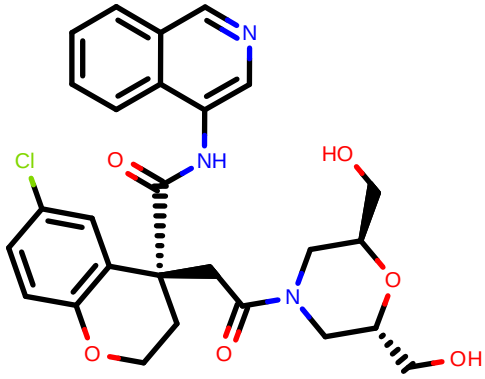
CID:	EN300-261210_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]5(CCOC5)C#N
RUN:	RUN4933
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.27

EN300-218116_2_1



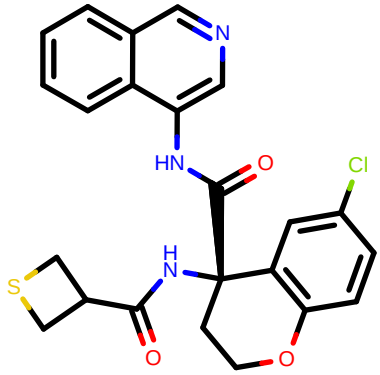
CID:	EN300-218116_2_1
SMILES:	CC(CO)(CO)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1430
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.32

EN300-6735683_1_1



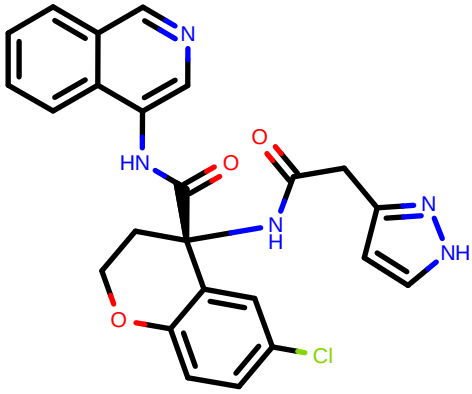
CID:	EN300-6735683_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](O[C@@H](C5)CO)CO
RUN:	RUN3584
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.40

EN300-95094_1_1



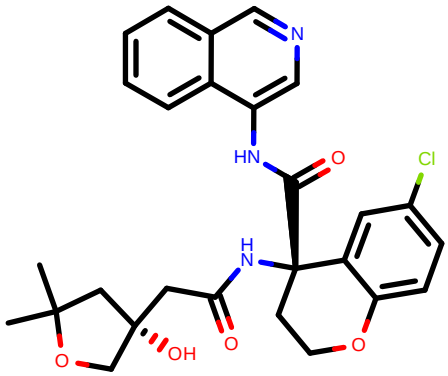
CID:	EN300-95094_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CSC5
RUN:	RUN3146
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.21

EN300-71405_1_1



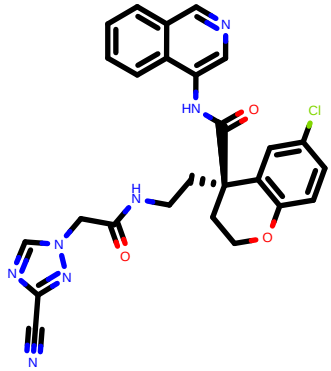
CID:	EN300-71405_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccn[nH]5
RUN:	RUN3730
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.24

EN300-360158_1_2



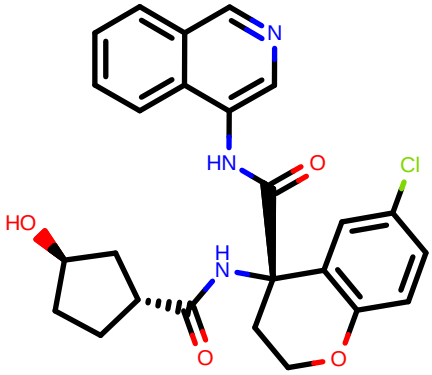
CID:	EN300-360158_1_2
SMILES:	CC1(C[C@](CO1)(CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)C
RUN:	RUN4381
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.28

EN300-111863_3_1



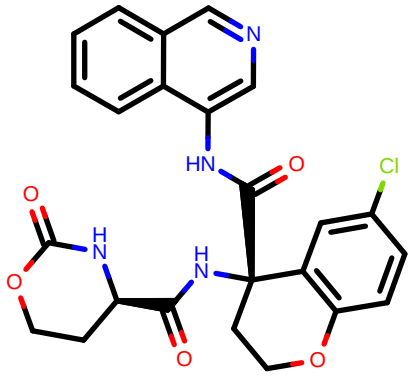
CID:	EN300-111863_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc(n5)C#N
RUN:	RUN5726
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.31

EN300-321597_1_1



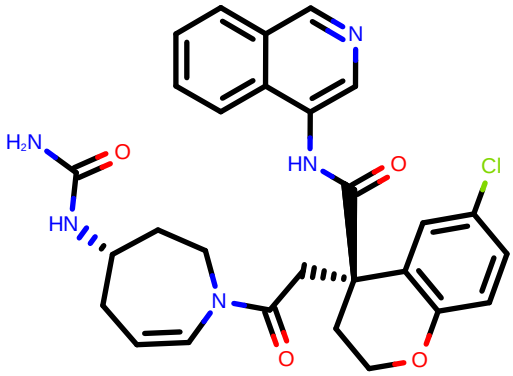
CID:	EN300-321597_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC[C@H](C5)O
RUN:	RUN4333
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.28

EN300-249804_1_2



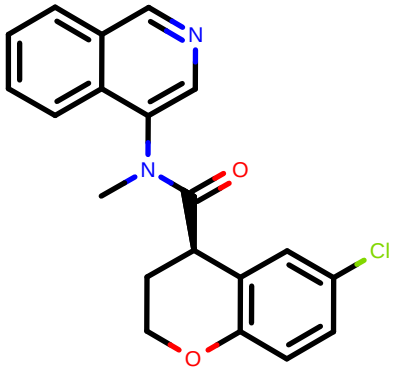
CID:	EN300-249804_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCOC(=O)N5
RUN:	RUN2632
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.22

EN300-6759972_1_1



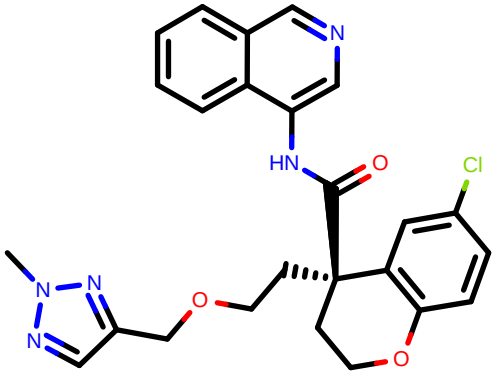
CID:	EN300-6759972_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H](CC5)NC(=O)N
RUN:	RUN10576
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.34

MAK-UNK-3875bbc8-2_1



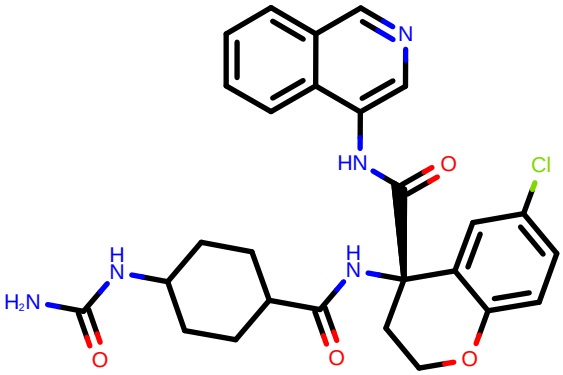
CID:	MAK-UNK-3875bbc8-2_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN49
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.07

EN300-219020_3_1



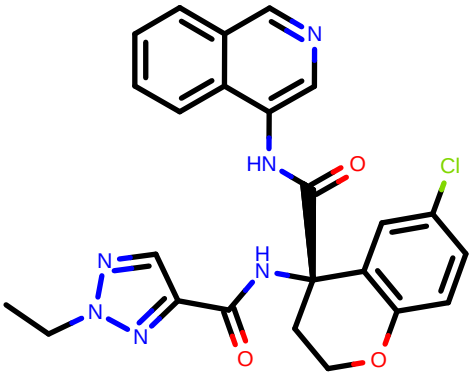
CID:	EN300-219020_3_1
SMILES:	Cn1ncc(n1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1627
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.26

EN300-53591_1_1



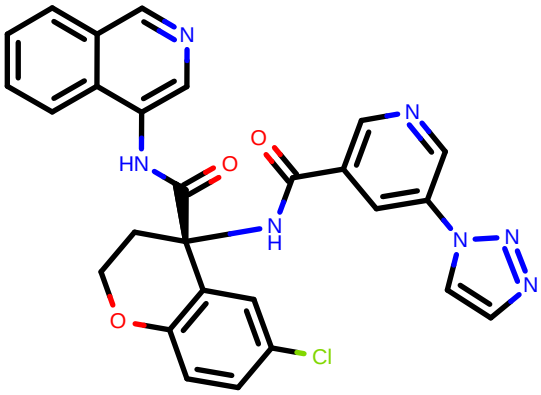
CID:	EN300-53591_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCC(CC5)NC(=O)N
RUN:	RUN8622
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.33

EN300-215465_1_1



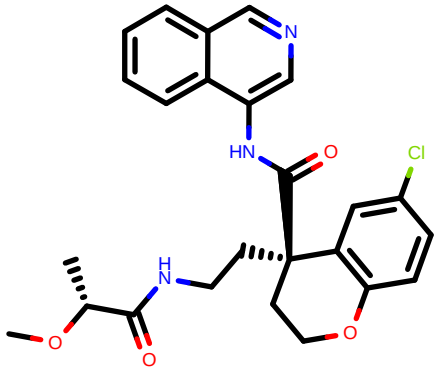
CID:	EN300-215465_1_1
SMILES:	CCn1ncc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4773
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.21

EN300-151298_1_1



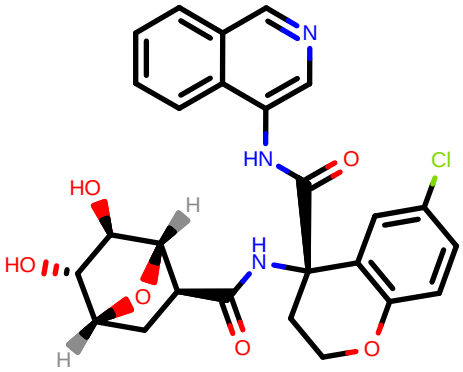
CID:	EN300-151298_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cnc5)n6ccnn6
RUN:	RUN8650
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.31

EN300-247951_3_1



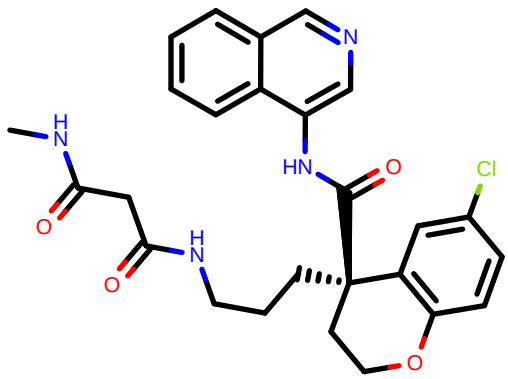
CID:	EN300-247951_3_1
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN2844
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.24

EN300-6764836_1_6



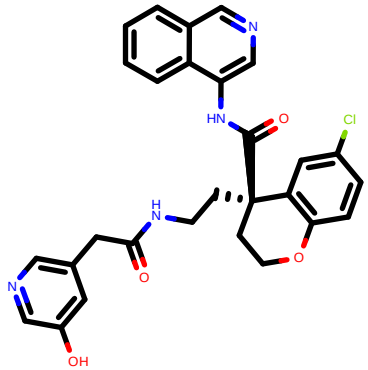
CID:	EN300-6764836_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC6[C@@H]([C@H](CSO6)O)O
RUN:	RUN7078
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.27

EN300-128463_4_1



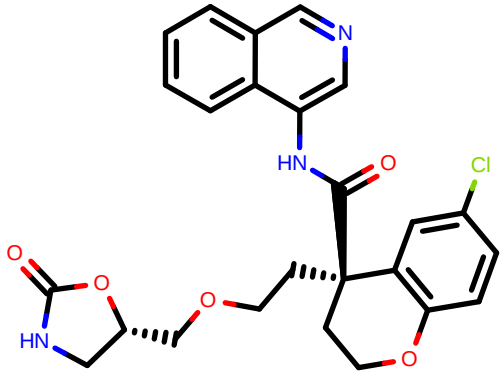
CID:	EN300-128463_4_1
SMILES:	CNC(=O)CC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9974
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.29

EN300-222620_3_1



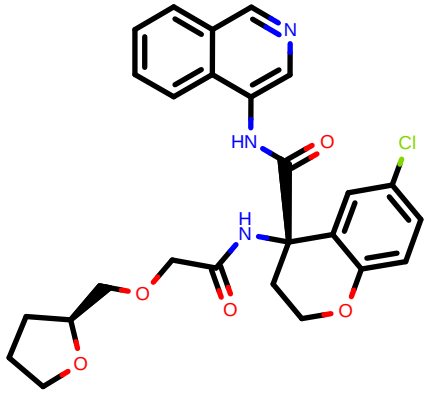
CID:	EN300-222620_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cc(cnc5)O
RUN:	RUN3999
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.38

EN300-203293_3_1



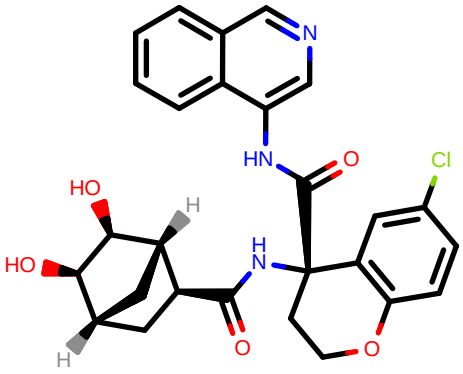
CID:	EN300-203293_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CNC(=O)O5
RUN:	RUN425
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.24

EN300-60033_1_1



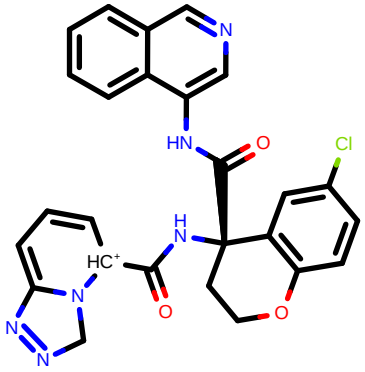
CID:	EN300-60033_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@@H]5CCCO5
RUN:	RUN1541
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.31

EN300-6744028_1_2



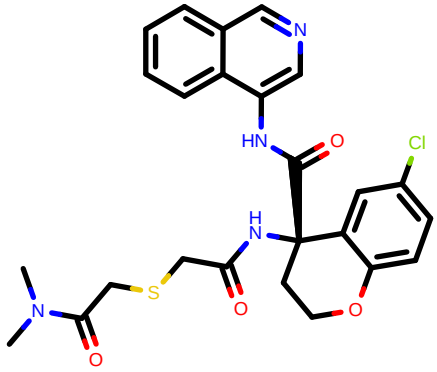
CID:	EN300-6744028_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC6CC5[C@@H]([C@@H]6O)O
RUN:	RUN5017
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.28

EN300-6488157_1_1



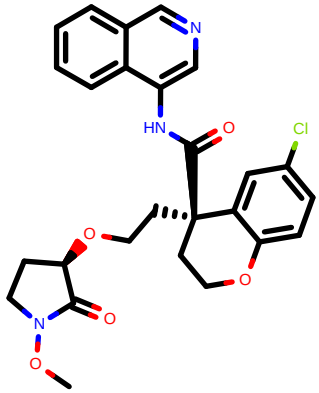
CID:	EN300-6488157_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccc6n5cnn6
RUN:	RUN8058
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.24

EN300-12139_1_1



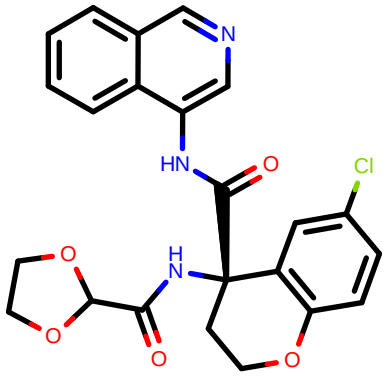
CID:	EN300-12139_1_1
SMILES:	CN(C)C(=O)CSCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN282
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.33

EN300-302058_3_2



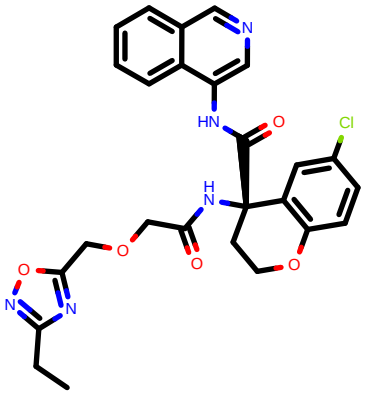
CID:	EN300-302058_3_2
SMILES:	CON1CC[C@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2433
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.26

EN300-154942_1_1



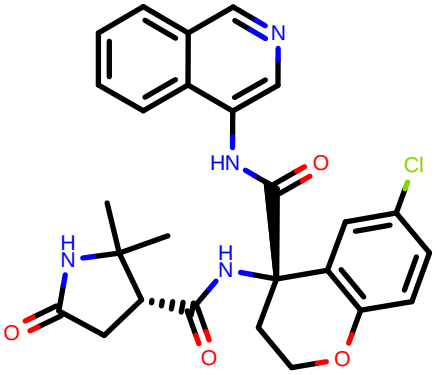
CID:	EN300-154942_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5OCCO5
RUN:	RUN4449
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.22

EN300-702615_1_1



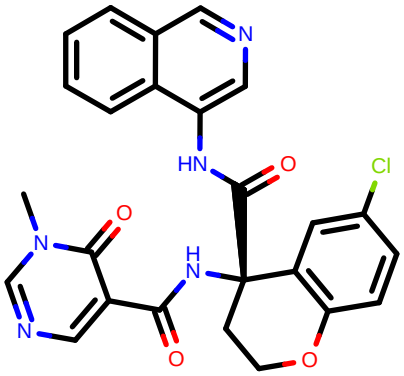
CID:	EN300-702615_1_1
SMILES:	CCc1nc(on1)COCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6998
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.28

EN300-1694056_1_1



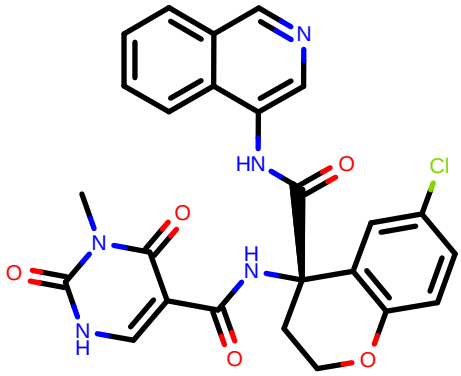
CID:	EN300-1694056_1_1
SMILES:	CC1([C@@H](CC(=O)N1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN3726
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.32

EN300-295132_1_1



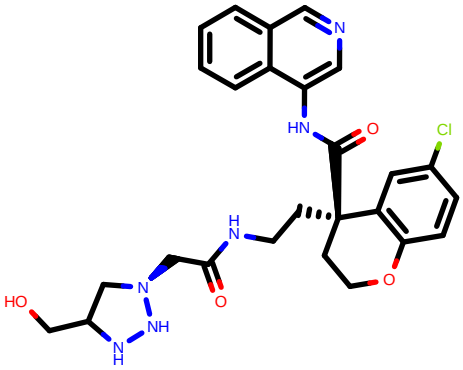
CID:	EN300-295132_1_1
SMILES:	Cn1cncc(c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6966
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.35

EN300-102487_1_1



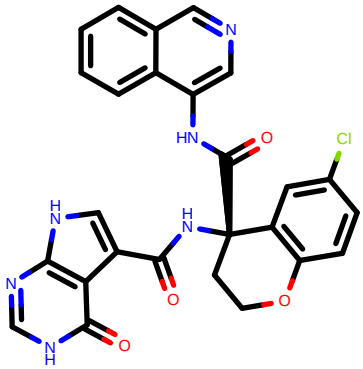
CID:	EN300-102487_1_1
SMILES:	Cn1c(=O)c(c[nH]c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8070
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.26

EN300-108236_3_1



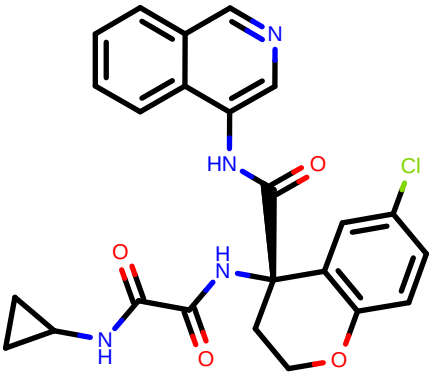
CID:	EN300-108236_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(nn5)CO
RUN:	RUN803
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.32

EN300-746311_1_1



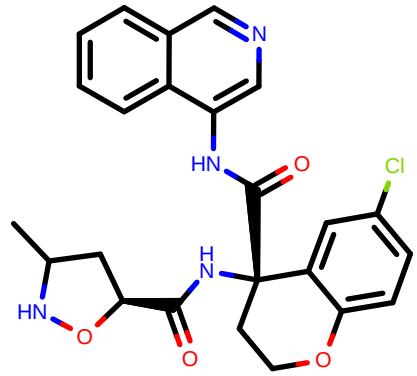
CID:	EN300-746311_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]c6c5c(=O)[nH]cn6
RUN:	RUN8554
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.22

EN300-78135_1_1



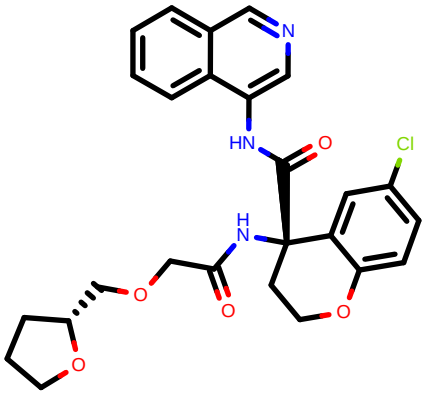
CID:	EN300-78135_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NC5CC5
RUN:	RUN1700
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.21

EN300-92447_1_1



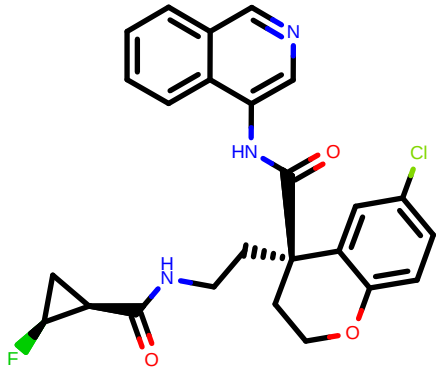
CID:	EN300-92447_1_1
SMILES:	CC1=NO[C@@H](C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4893
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.25

EN300-60033_1_2



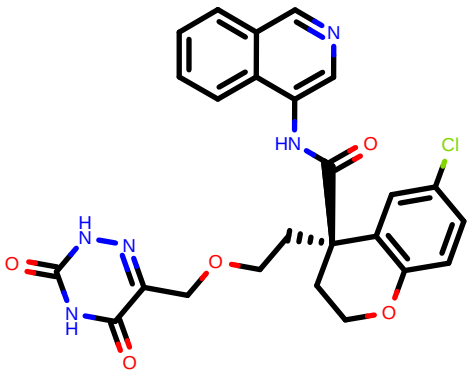
CID:	EN300-60033_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC[C@H]5CCCO5
RUN:	RUN1349
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.32

EN300-1654606_3_1



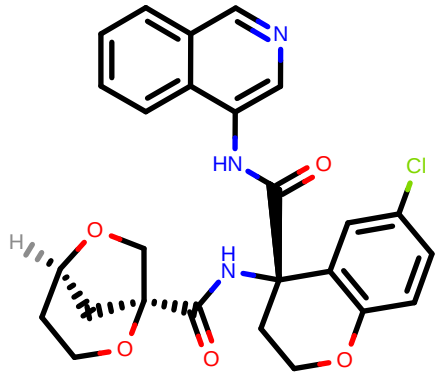
CID:	EN300-1654606_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@@H]5F
RUN:	RUN3839
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.22

EN300-761746_3_1



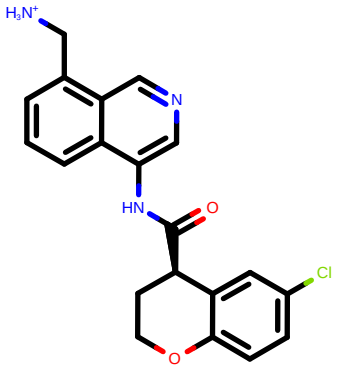
CID:	EN300-761746_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5c(=O)[nH]c(=O)[nH]n5
RUN:	RUN2099
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.29

EN300-6736394_1_1



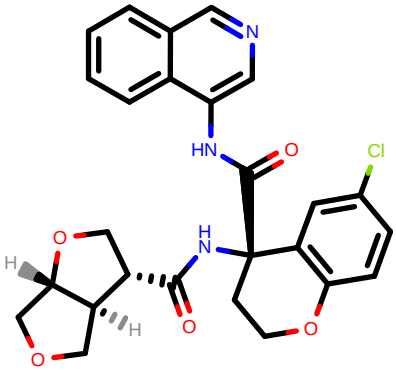
CID:	EN300-6736394_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(CCO5)OC6
RUN:	RUN5121
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.28

NAU-LAT-b7d8c353-8_1



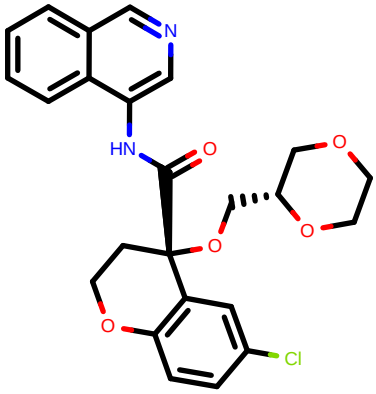
CID:	NAU-LAT-b7d8c353-8_1
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)CN
RUN:	RUN41
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.09

EN300-6482296_1_2



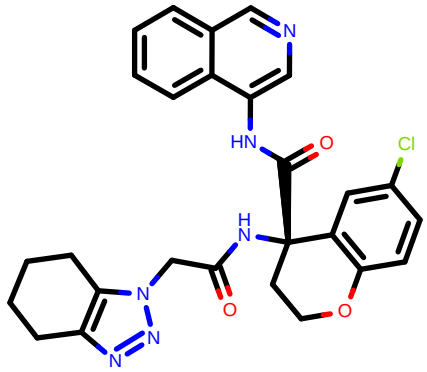
CID:	EN300-6482296_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CO[C@@H]6[C@@H]5COC6
RUN:	RUN3981
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.25

EN300-139167_1_1



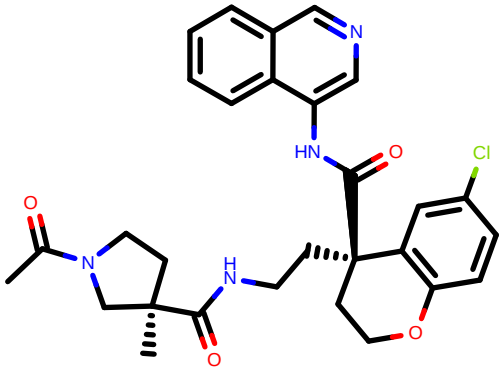
CID:	EN300-139167_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCCO5
RUN:	RUN2231
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.29

EN300-223187_1_1



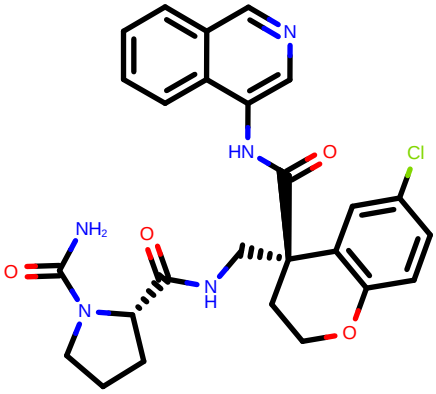
CID:	EN300-223187_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c6c(nn5)CCCC6
RUN:	RUN4649
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.31

EN300-98018_3_1



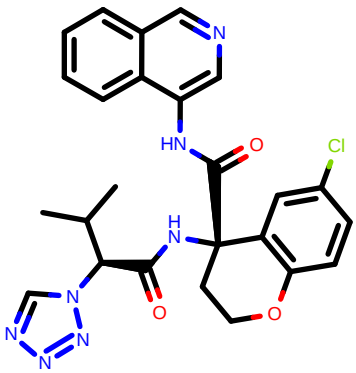
CID:	EN300-98018_3_1
SMILES:	CC(=O)N1CC[C@@](C1)(C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN319
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.33

EN300-87536_2_1



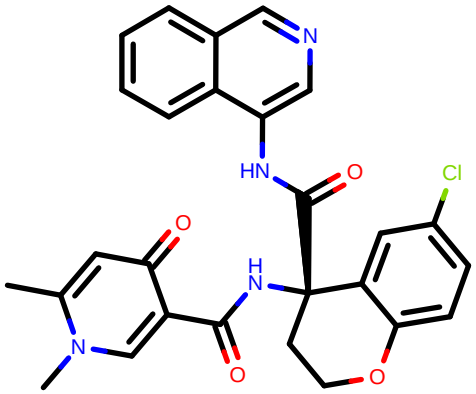
CID:	EN300-87536_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCCN5C(=O)N
RUN:	RUN5741
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.25

EN300-297561_1_1



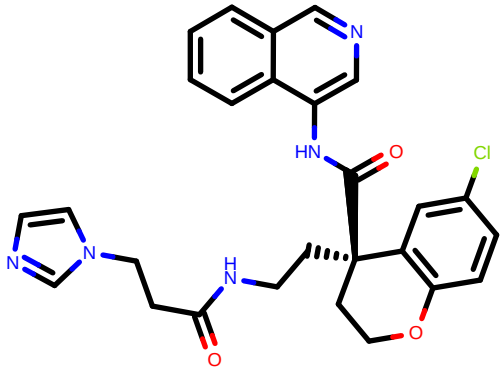
CID:	EN300-297561_1_1
SMILES:	CC(C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnnn5
RUN:	RUN6563
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.30

EN300-199991_1_1



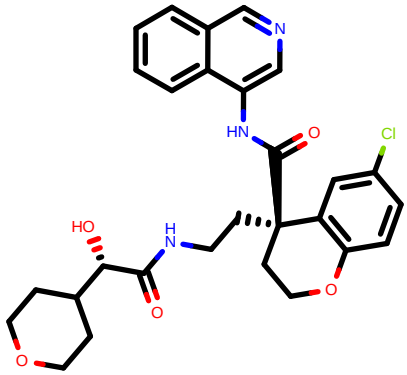
CID:	EN300-199991_1_1
SMILES:	Cc1cc(=O)c(cn1C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8837
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.33

EN300-75342_3_1



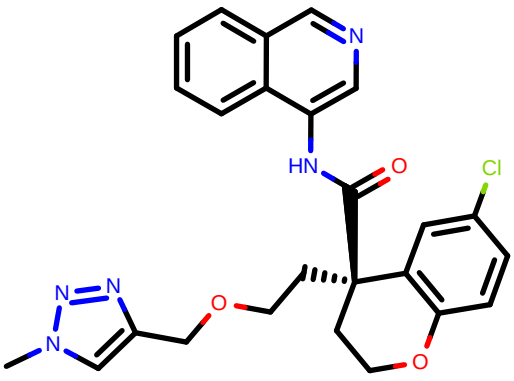
CID:	EN300-75342_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5ccnc5
RUN:	RUN8628
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.32

EN300-79180_3_2



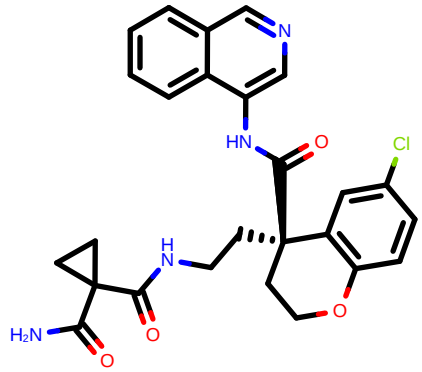
CID:	EN300-79180_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CCOCC5)O
RUN:	RUN5646
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.36

EN300-120282_3_1



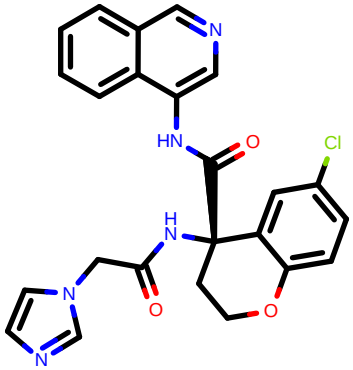
CID:	EN300-120282_3_1
SMILES:	Cn1cc(nn1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1324
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.25

EN300-69070_3_1



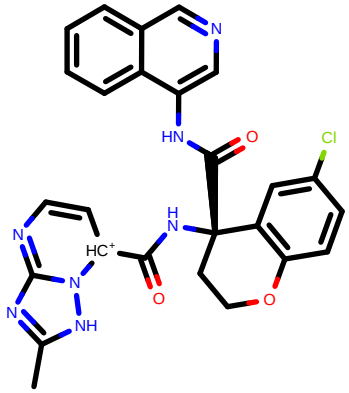
CID:	EN300-69070_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)C(=O)N
RUN:	RUN890
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.30

EN300-38979_1_1



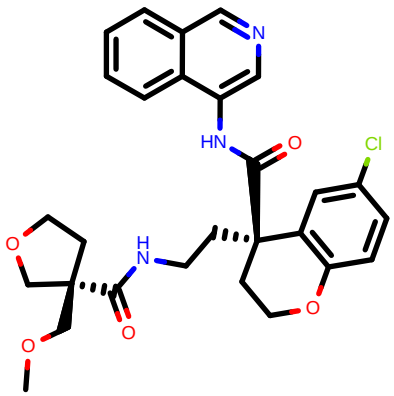
CID:	EN300-38979_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5ccnc5
RUN:	RUN4573
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.24

EN300-131799_1_1



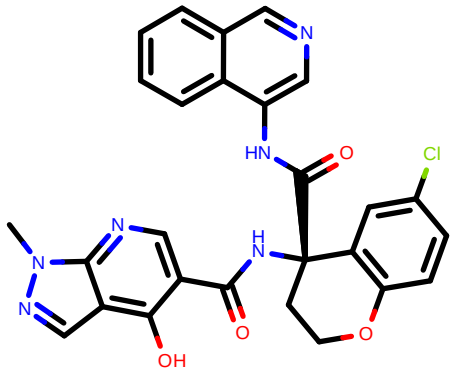
CID:	EN300-131799_1_1
SMILES:	Cc1nc2nccc(n2n1)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8478
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.23

EN300-248883_3_1



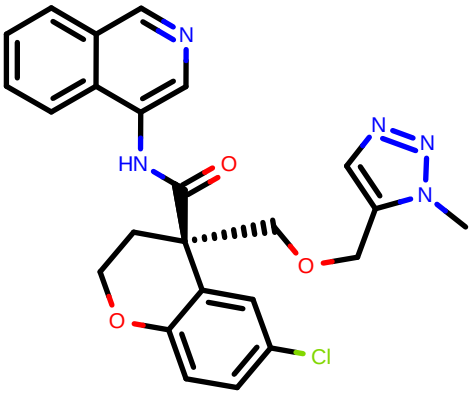
CID:	EN300-248883_3_1
SMILES:	COC[C@@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5702
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.32

EN300-124384_1_1



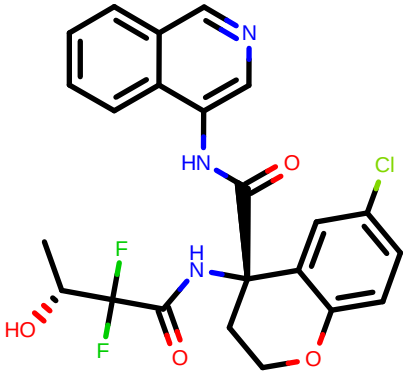
CID:	EN300-124384_1_1
SMILES:	Cn1c2c(cn1)c(c(cn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)O
RUN:	RUN9032
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.28

EN300-216673_2_1



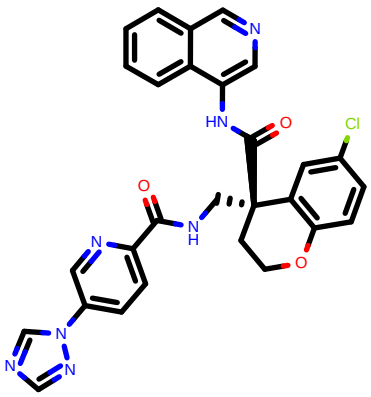
CID:	EN300-216673_2_1
SMILES:	Cn1c(cnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1350
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.24

EN300-185398_1_2



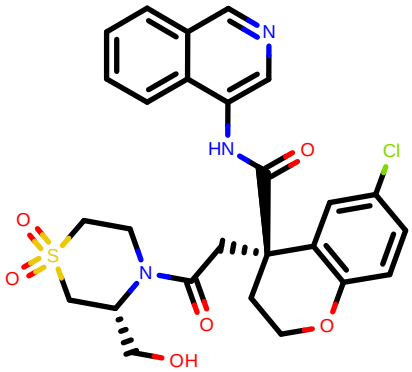
CID:	EN300-185398_1_2
SMILES:	C[C@H](C(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F)O
RUN:	RUN2140
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.20

EN300-195855_2_1



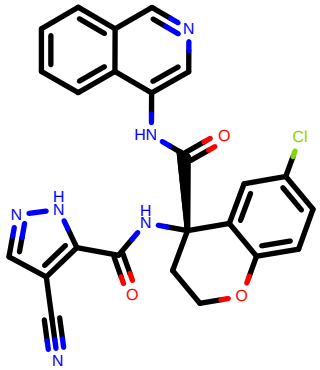
CID:	EN300-195855_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cn5)n6cncn6
RUN:	RUN8767
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.30

EN300-157541_1_2



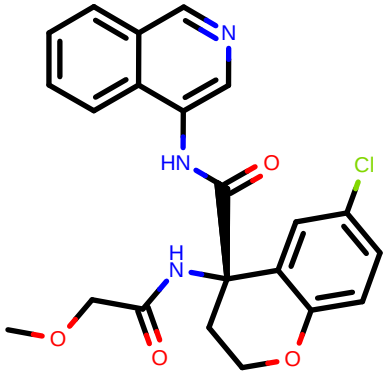
CID:	EN300-157541_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)C[C@H]5CO
RUN:	RUN10942
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.47

EN300-1267109_1_1



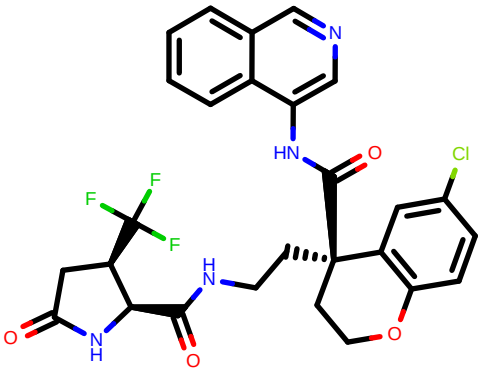
CID:	EN300-1267109_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(cn[nH]5)C#N
RUN:	RUN7450
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.29

EN300-20233_1_1



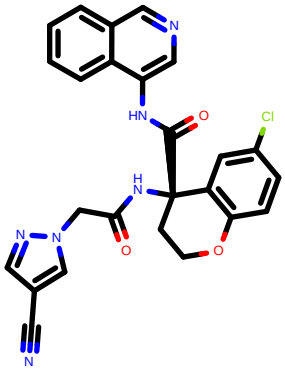
CID:	EN300-20233_1_1
SMILES:	COCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1908
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.20

EN300-169955_3_1



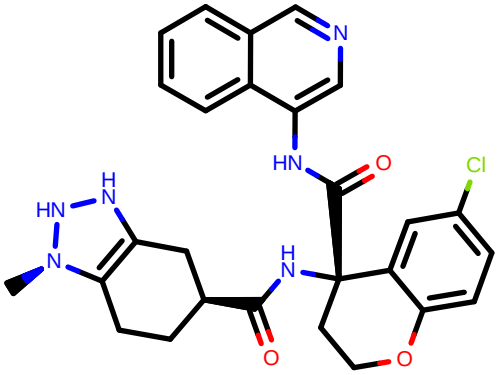
CID:	EN300-169955_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5[C@@H](CC(=O)N5)C(F)(F)F
RUN:	RUN5470
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.31

EN300-1590388_1_1



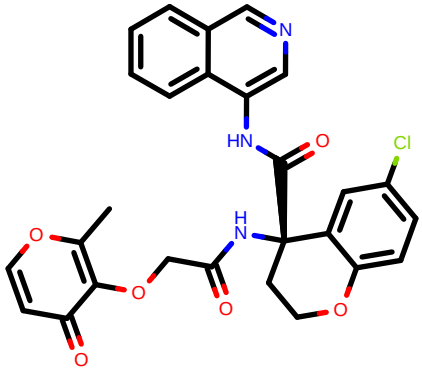
CID:	EN300-1590388_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(cn5)C#N
RUN:	RUN7910
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.26

EN300-185727_1_2



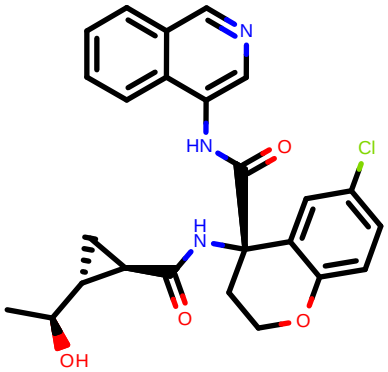
CID:	EN300-185727_1_2
SMILES:	Cn1c2c(nn1)C[C@H](CC2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7878
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.33

EN300-702714_1_1



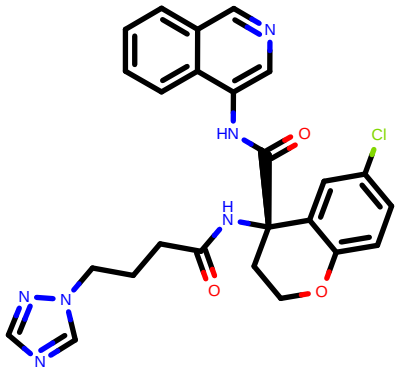
CID:	EN300-702714_1_1
SMILES:	Cc1c(c(=O)cco1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1341
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.32

EN300-6729572_1_5



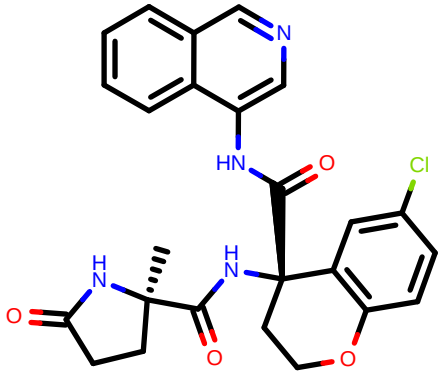
CID:	EN300-6729572_1_5
SMILES:	C[C@@H]([C@@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3094
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.28

EN300-316216_1_1



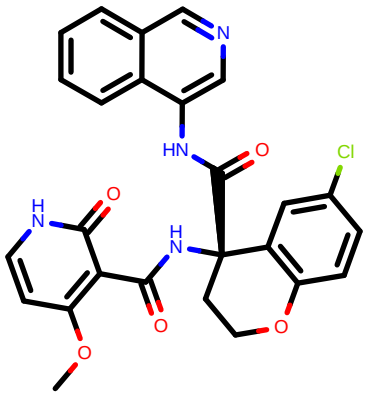
CID:	EN300-316216_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCn5cncn5
RUN:	RUN1748
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.28

EN300-177118_1_1



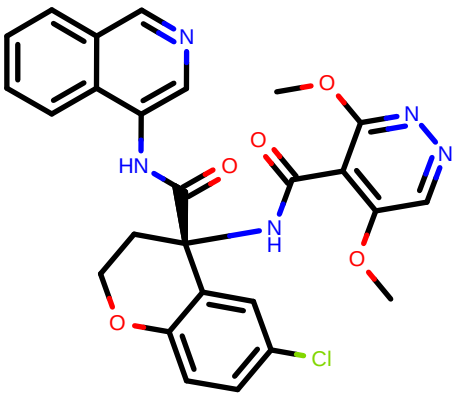
CID:	EN300-177118_1_1
SMILES:	C[C@@]1(CCC(=O)N1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2668
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.29

EN300-156318_1_1



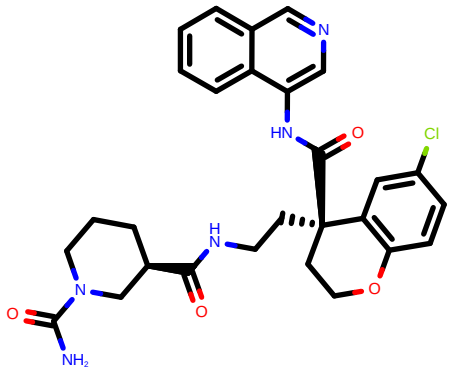
CID:	EN300-156318_1_1
SMILES:	COc1cc[nH]c(=O)c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8166
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.30

EN300-366931_1_1



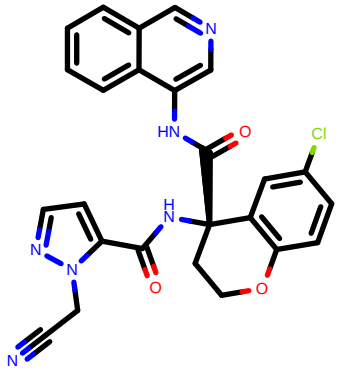
CID:	EN300-366931_1_1
SMILES:	COc1cnnc(c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN7666
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.40

EN300-14767_3_1



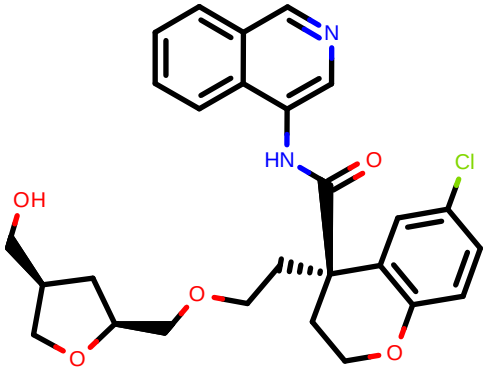
CID:	EN300-14767_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCN(C5)C(=O)N
RUN:	RUN2073
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.36

EN300-373791_1_1



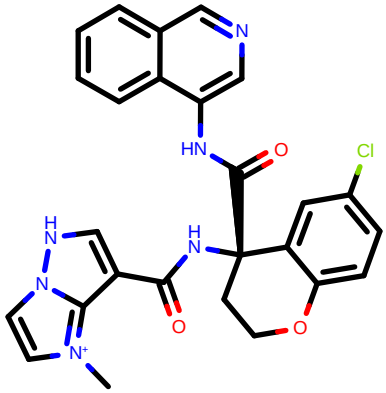
CID:	EN300-373791_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnn5CC#N
RUN:	RUN4677
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.20

EN300-6494158_3_1



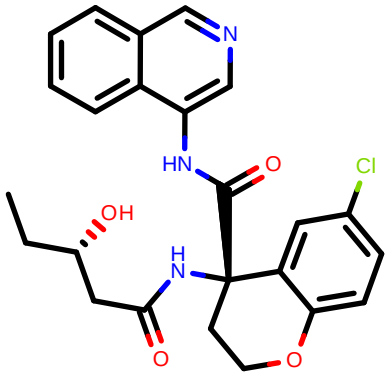
CID:	EN300-6494158_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C[C@@H](CO5)CO
RUN:	RUN528
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.32

EN300-4254263_1_1



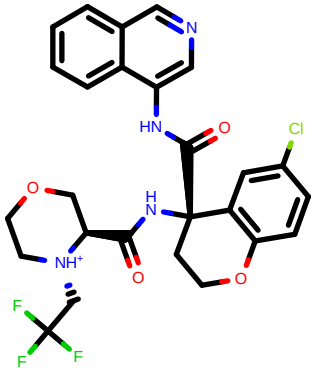
CID:	EN300-4254263_1_1
SMILES:	Cn1ccn2c1c(cn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7142
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.24

EN300-224741_1_1



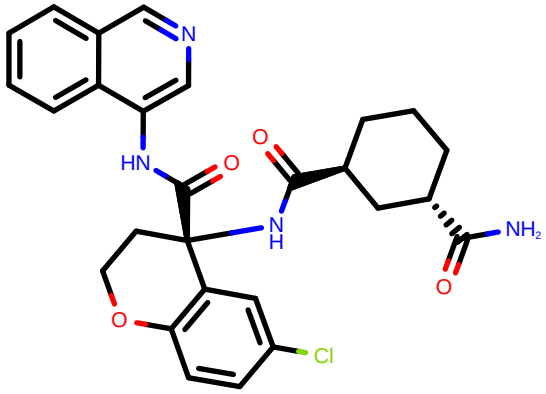
CID:	EN300-224741_1_1
SMILES:	CC[C@@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1125
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.23

EN300-201551_1_1



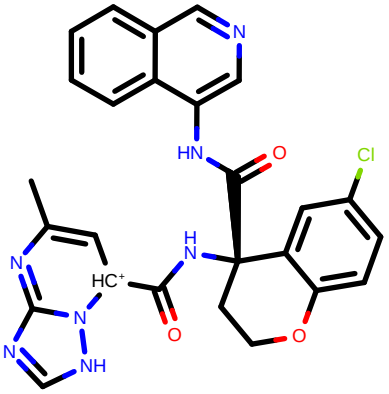
CID:	EN300-201551_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COCCN5CC(F)(F)F
RUN:	RUN8326
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.28

EN300-90142_1_2



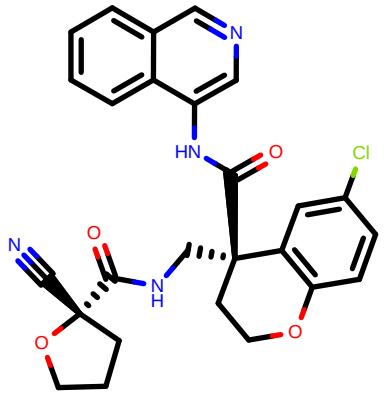
CID:	EN300-90142_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCC[C@@H](C5)C(=O)N
RUN:	RUN5013
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.26

EN300-1666501_1_1



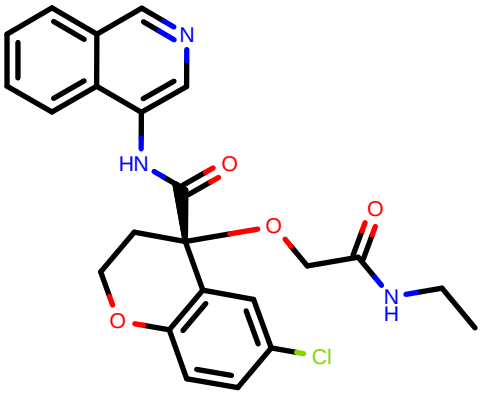
CID:	EN300-1666501_1_1
SMILES:	Cc1cc(n2c(n1)ncn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8282
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.32

EN300-3710141_2_1



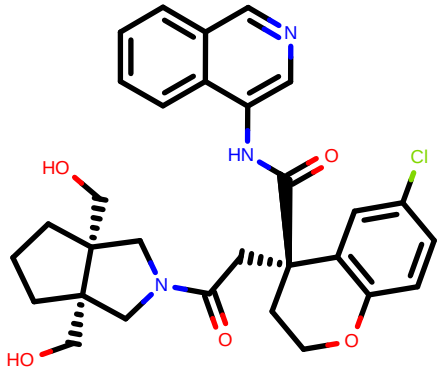
CID:	EN300-3710141_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCCO5)C#N
RUN:	RUN5637
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.33

EN300-7003350_1_1



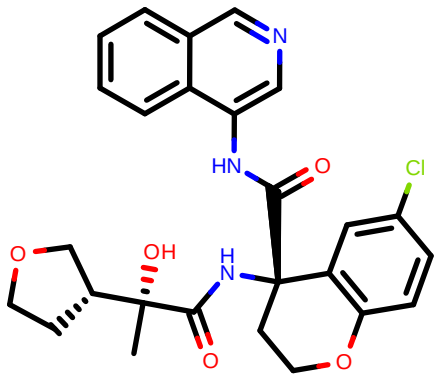
CID:	EN300-7003350_1_1
SMILES:	CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN731
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.19

EN300-1718428_1_1



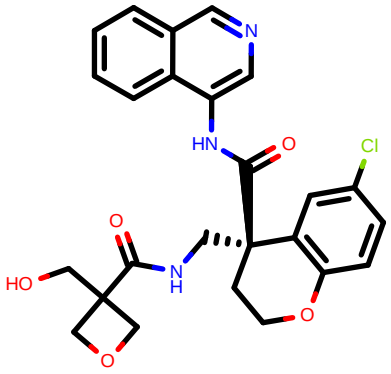
CID:	EN300-1718428_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]6(CCC[C@]6(C5)CO)CO
RUN:	RUN2225
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.37

EN300-217494_1_1



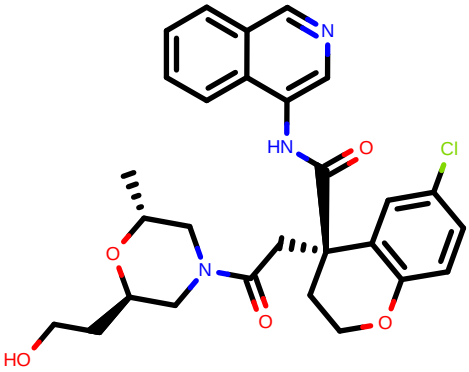
CID:	EN300-217494_1_1
SMILES:	C[C@@]([C@@H]1CCOC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3793
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.27

EN300-105693_2_1



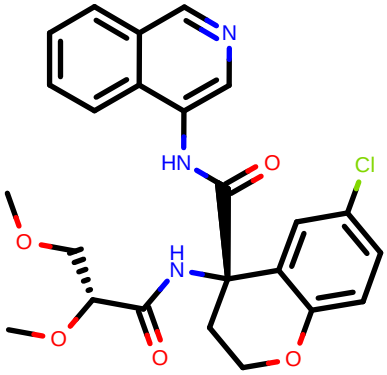
CID:	EN300-105693_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COC5)CO
RUN:	RUN3966
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.31

EN300-212814_1_3



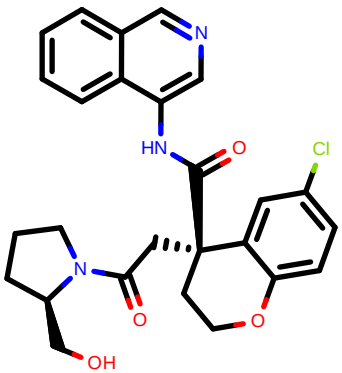
CID:	EN300-212814_1_3
SMILES:	C[C@@H]1CN(C[C@H](O1)CCO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11226
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.34

EN300-305282_1_2



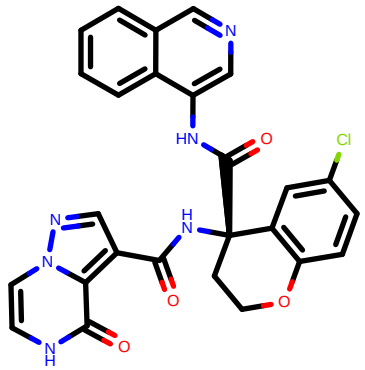
CID:	EN300-305282_1_2
SMILES:	COC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN4097
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.36

EN300-54891_1_1



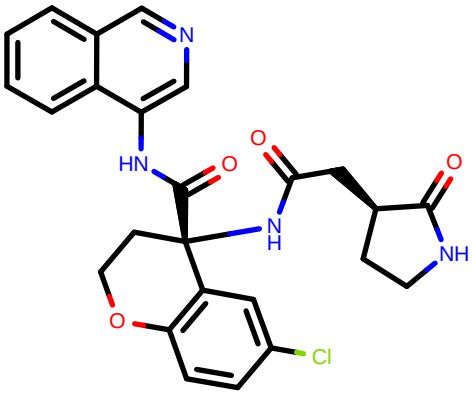
CID:	EN300-54891_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CO
RUN:	RUN10372
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.29

EN300-7463176_1_1



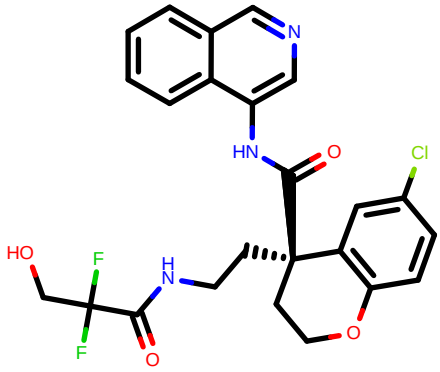
CID:	EN300-7463176_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5c(=O)[nH]cc6
RUN:	RUN8506
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.26

EN300-343474_1_1



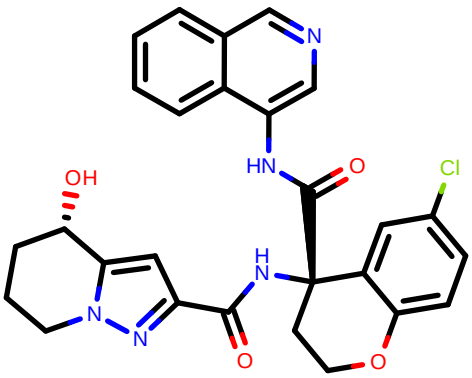
CID:	EN300-343474_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCNC5=O
RUN:	RUN673
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.29

EN300-123489_3_1



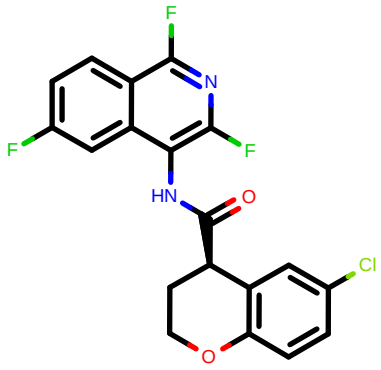
CID:	EN300-123489_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C(CO)(F)F
RUN:	RUN3668
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.23

EN300-399606_1_1



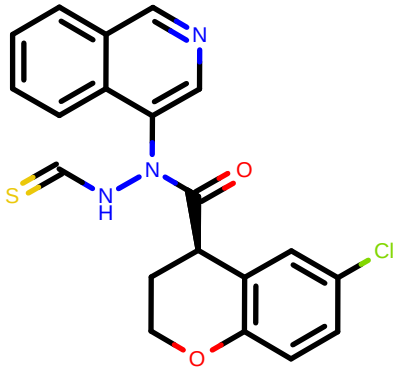
CID:	EN300-399606_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCC[C@@H]6O
RUN:	RUN8942
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.24

JOH-SUS-a69c159d-7_1



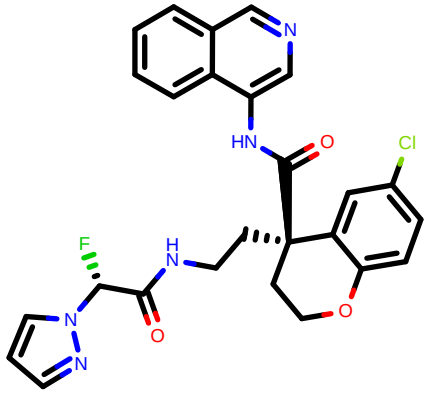
CID:	JOH-SUS-a69c159d-7_1
SMILES:	c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN71
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.05

DAR-DIA-5ff57136-18_1



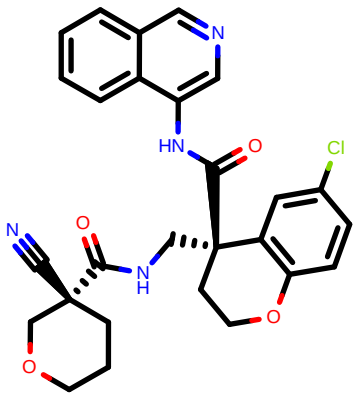
CID:	DAR-DIA-5ff57136-18_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOc4c3cc(cc4)Cl)N=C=S
RUN:	RUN101
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.12

EN300-1726277_3_2



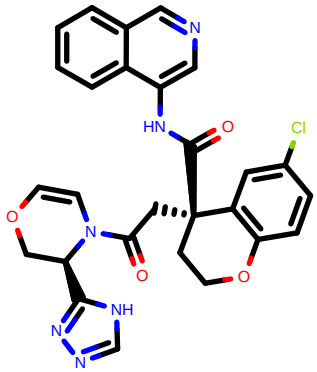
CID:	EN300-1726277_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](n5cccn5)F
RUN:	RUN10710
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.32

EN300-301925_2_1



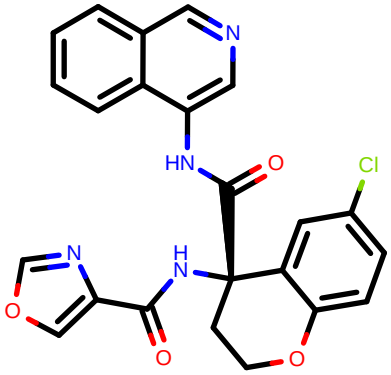
CID:	EN300-301925_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCCOC5)C#N
RUN:	RUN2875
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.29

EN300-205616_1_1



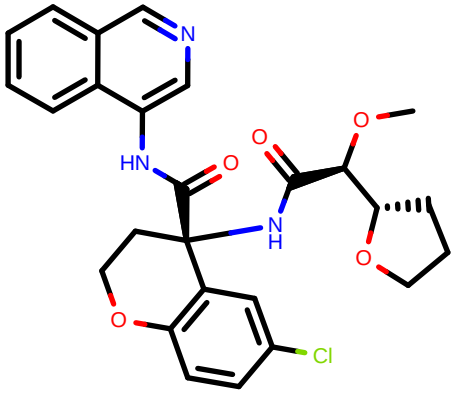
CID:	EN300-205616_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5c6[nH]cnn6
RUN:	RUN7664
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.29

EN300-68618_1_1



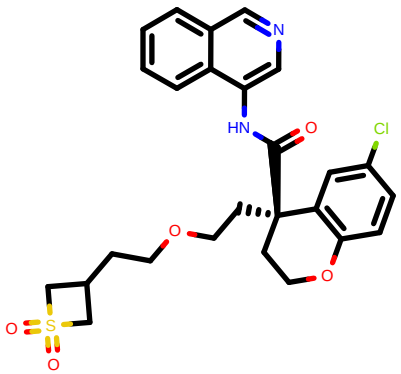
CID:	EN300-68618_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cocn5
RUN:	RUN3058
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.19

EN300-6277108_1_1



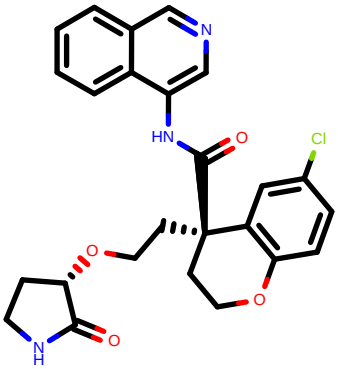
CID:	EN300-6277108_1_1
SMILES:	CO[C@@H]([C@@H]1CCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4725
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.28

EN300-189563_3_1



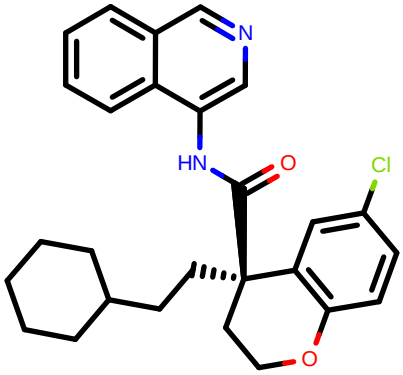
CID:	EN300-189563_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCC5CS(=O)(=O)C5
RUN:	RUN2391
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.31

EN300-6736413_3_2



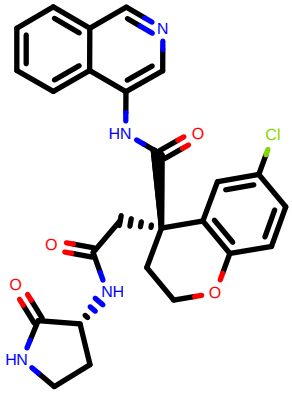
CID:	EN300-6736413_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCNC5=O
RUN:	RUN2342
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.28

VLA-UCB-50c39ae8-10_1



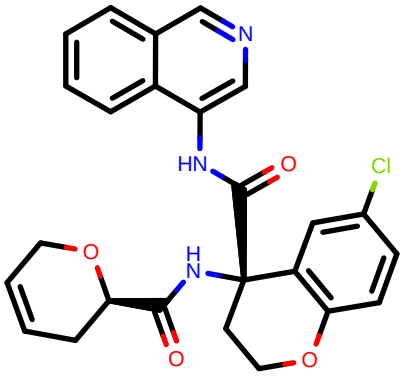
CID:	VLA-UCB-50c39ae8-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN141
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.25

EN300-298184_1_1



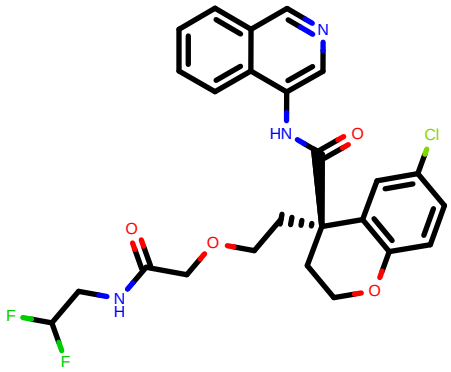
CID:	EN300-298184_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCNC5=O
RUN:	RUN11260
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.27

EN300-378044_1_2



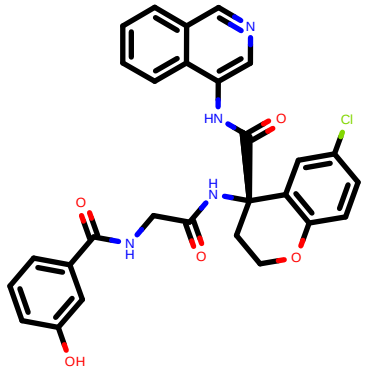
CID:	EN300-378044_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC=CCO5
RUN:	RUN6579
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.25

EN300-120586_3_1



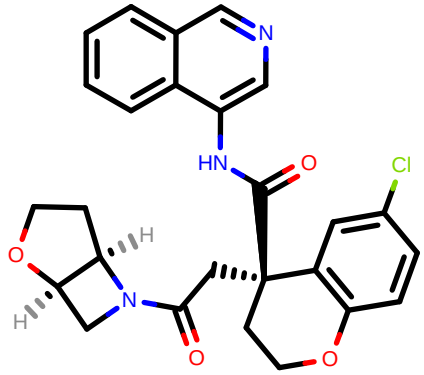
CID:	EN300-120586_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NCC(F)F
RUN:	RUN369
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.31

EN300-54417_1_1



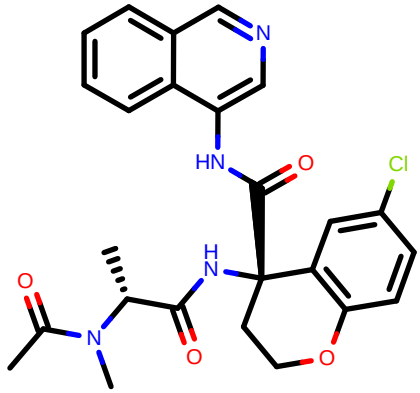
CID:	EN300-54417_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5cccc(c5)O
RUN:	RUN5532
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.33

EN300-651665_1_1



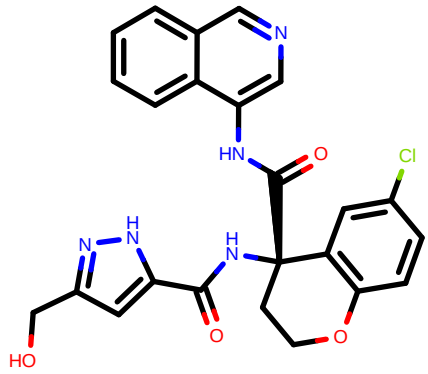
CID:	EN300-651665_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@H]5CCO6
RUN:	RUN6138
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.27

EN300-863933_1_2



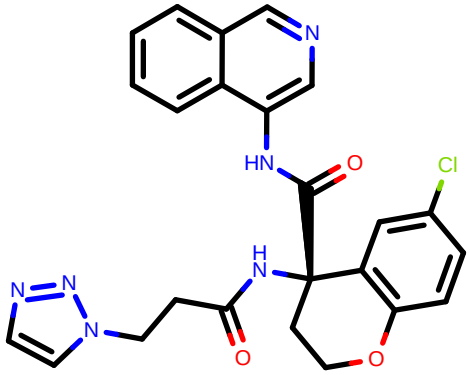
CID:	EN300-863933_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C)C(=O)C
RUN:	RUN3378
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.28

EN300-658865_1_1



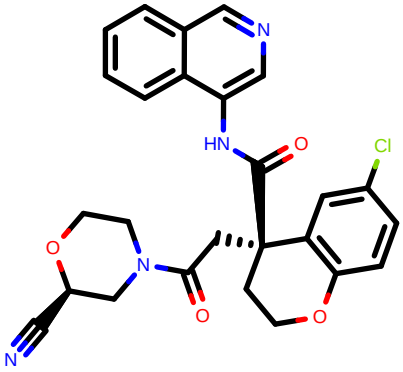
CID:	EN300-658865_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc([nH]n5)CO
RUN:	RUN5788
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.27

EN300-28871_1_1



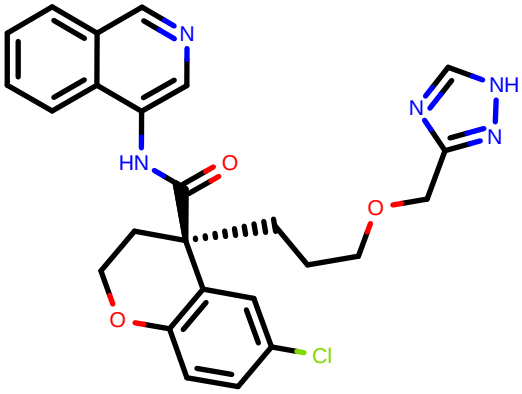
CID:	EN300-28871_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5ccnn5
RUN:	RUN5269
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.21

EN300-70489_1_1



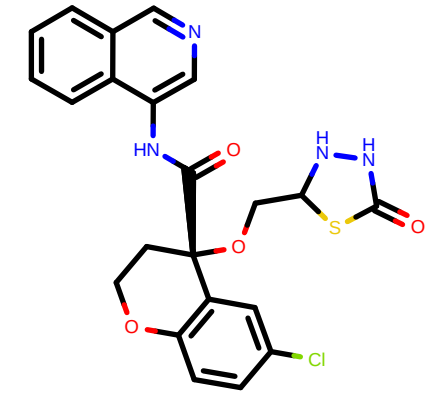
CID:	EN300-70489_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)C#N
RUN:	RUN2828
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.31

EN300-306316_4_1



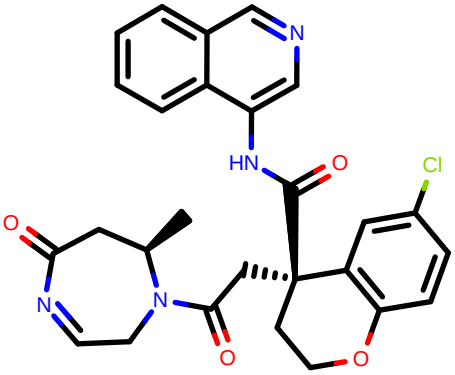
CID:	EN300-306316_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCc5[nH]cnn5
RUN:	RUN284
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.27

EN300-171766_1_1



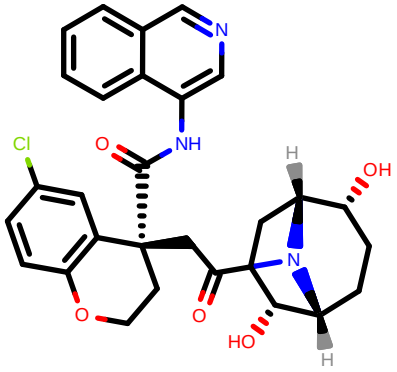
CID:	EN300-171766_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5n[nH]c(=O)s5
RUN:	RUN636
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.20

EN300-74029_1_1



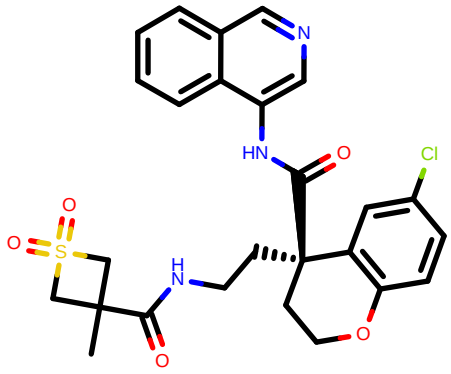
CID:	EN300-74029_1_1
SMILES:	C[C@@H]1CC(=O)NCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3324
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.32

EN300-6760290_1_1



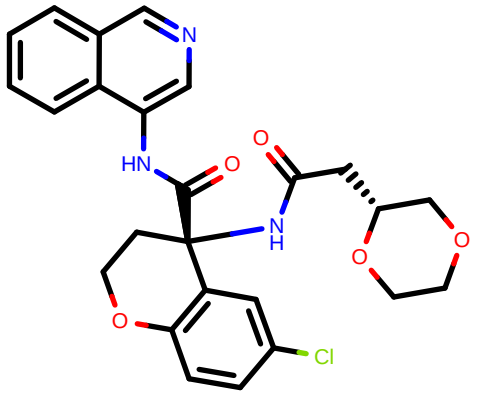
CID:	EN300-6760290_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5[C@@H]6CC[C@H][C@H]5CC[C@H]6O)O
RUN:	RUN11266
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.34

EN300-1718364_3_1



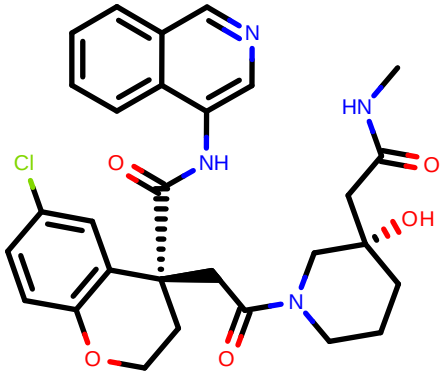
CID:	EN300-1718364_3_1
SMILES:	CC1(CS(=O)(=O)C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10624
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.32

EN300-731622_1_1



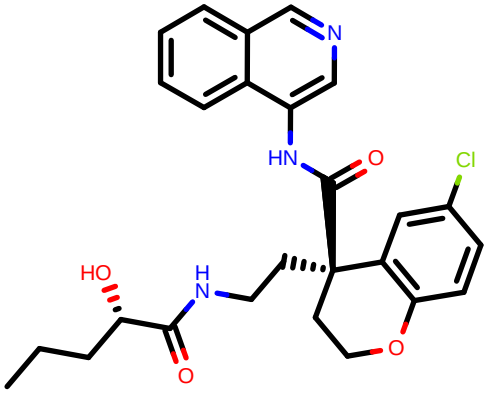
CID:	EN300-731622_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5COCCO5
RUN:	RUN2413
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.25

EN300-259062_1_2



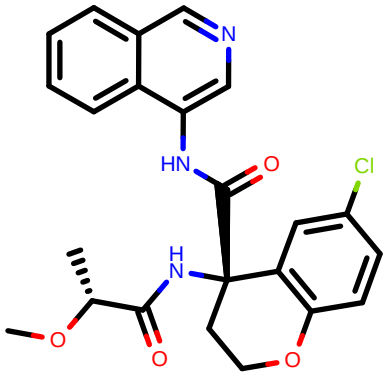
CID:	EN300-259062_1_2
SMILES:	CNC(=O)C[C@]1(CCCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1058
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.36

EN300-219531_3_1



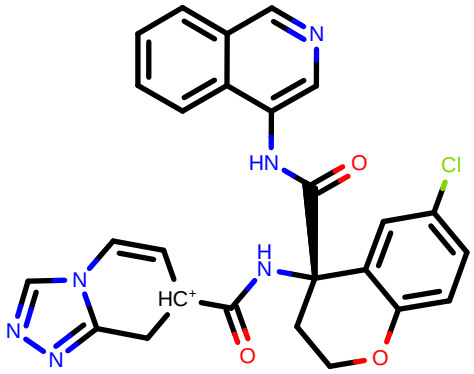
CID:	EN300-219531_3_1
SMILES:	CCC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2758
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.35

EN300-51257_1_2



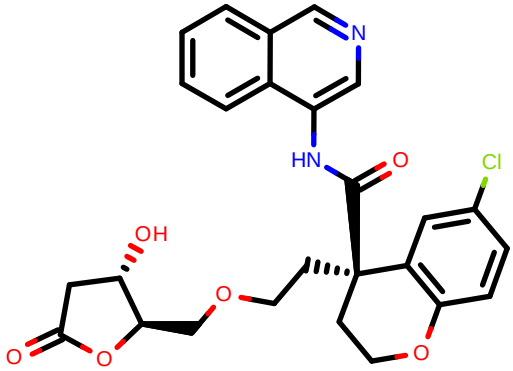
CID:	EN300-51257_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN2188
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.22

EN300-7537194_1_1



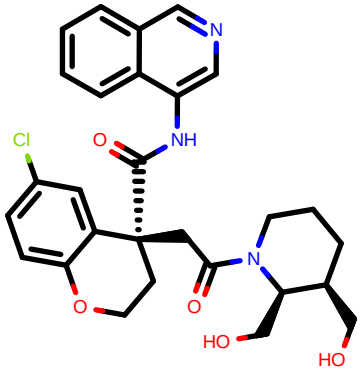
CID:	EN300-7537194_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6cnnc6c5
RUN:	RUN8774
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.21

EN300-6487407_3_1



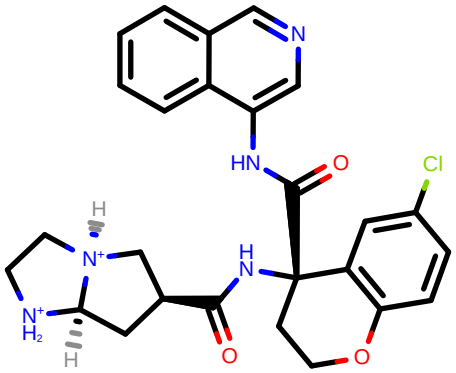
CID:	EN300-6487407_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5[C@H](CC(=O)O5)O
RUN:	RUN433
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.33

EN300-343562_1_1



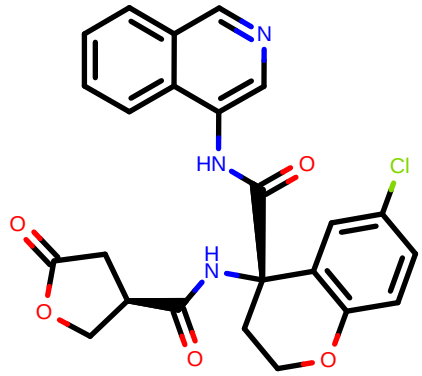
CID:	EN300-343562_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]([C@H]5CO)CO
RUN:	RUN3724
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.39

EN300-7385329_1_2



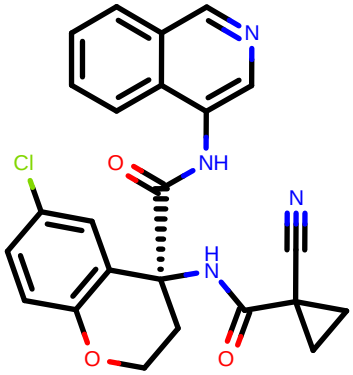
CID:	EN300-7385329_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5Cc6nccn6C5
RUN:	RUN8134
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.32

EN300-113234_1_1



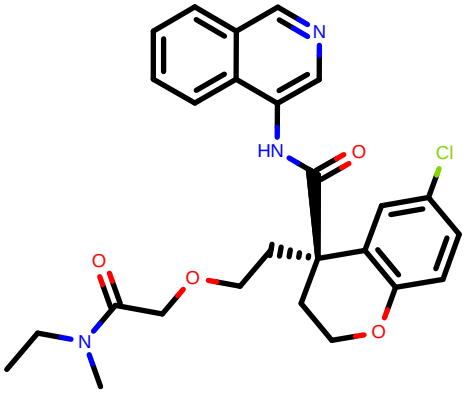
CID:	EN300-113234_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC(=O)OC5
RUN:	RUN4181
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.25

EN300-114082_1_1



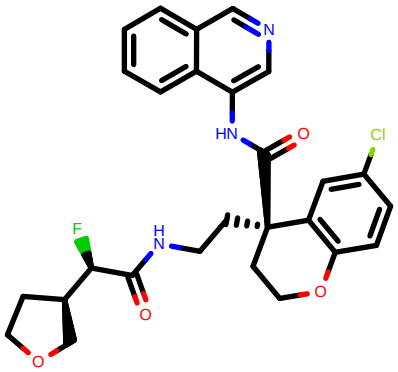
CID:	EN300-114082_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)C#N
RUN:	RUN3222
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.24

EN300-1253122_3_1



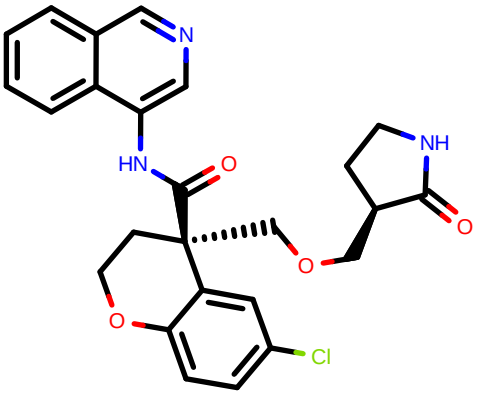
CID:	EN300-1253122_3_1
SMILES:	CCN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN584
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.26

EN300-783124_3_1



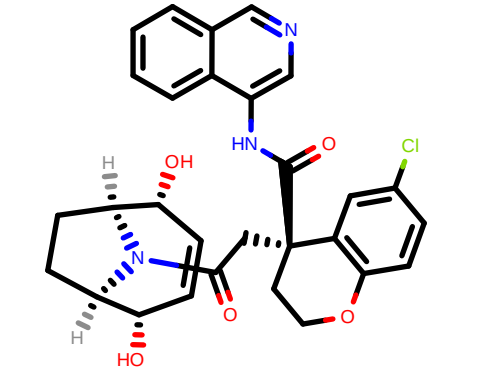
CID:	EN300-783124_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]([C@@H]5CCOC5)F
RUN:	RUN9366
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.22

EN300-246248_2_2



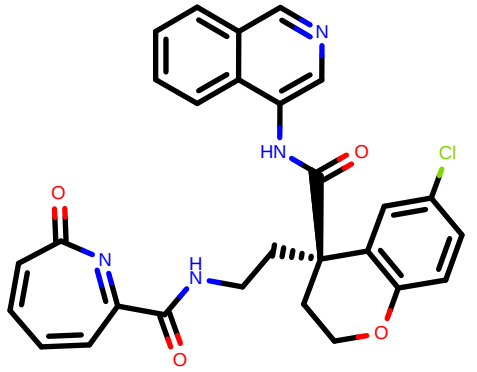
CID:	EN300-246248_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNC5=O
RUN:	RUN998
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.27

EN300-6738887_1_1



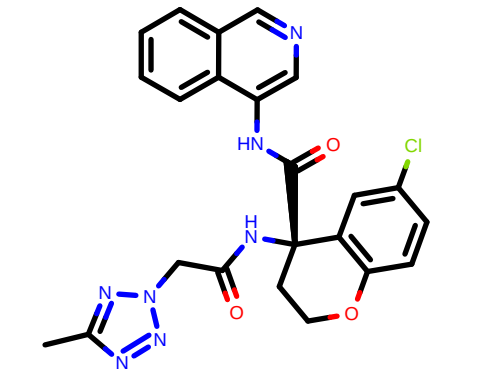
CID:	EN300-6738887_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6CCC5[C@H](CC[C@H]6O)O
RUN:	RUN11046
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.34

EN300-80083_3_1



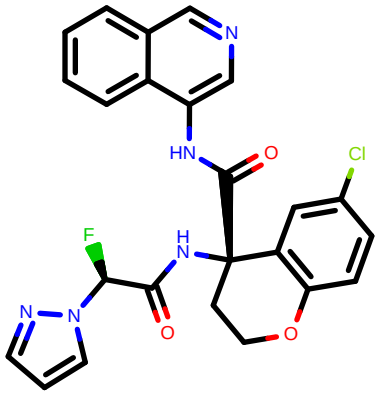
CID:	EN300-80083_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCCC(=O)N5
RUN:	RUN4179
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.31

EN300-6487680_1_1



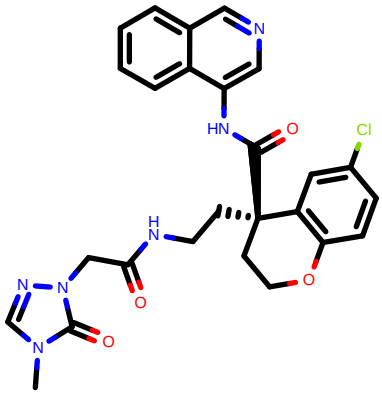
CID:	EN300-6487680_1_1
SMILES:	Cc1nnn(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6699
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.26

EN300-1726277_1_1



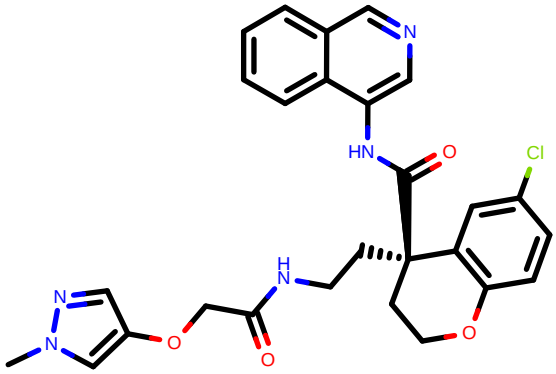
CID:	EN300-1726277_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](n5cccn5)F
RUN:	RUN3342
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.24

EN300-120436_3_1



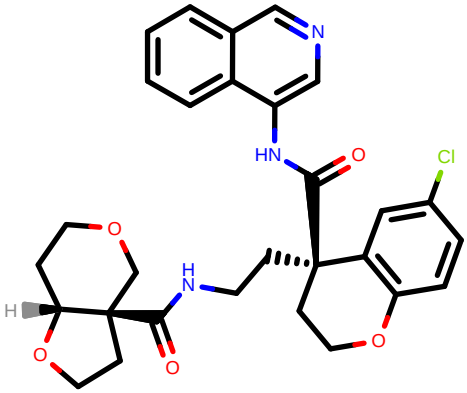
CID:	EN300-120436_3_1
SMILES:	Cn1cnn(c1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11026
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.31

EN300-201553_3_1



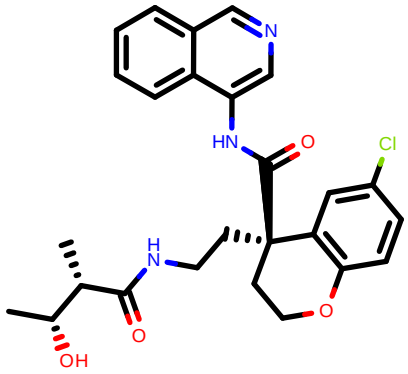
CID:	EN300-201553_3_1
SMILES:	Cn1cc(cn1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9746
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.35

EN300-341337_3_1



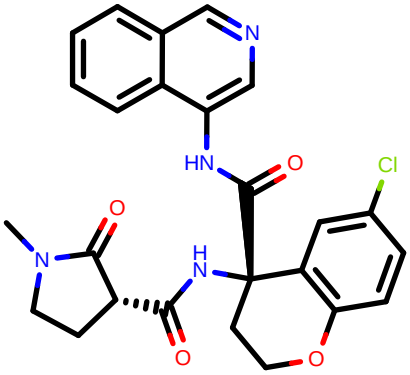
CID:	EN300-341337_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]56CCO[C@@H]5CCOC6
RUN:	RUN5087
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.34

EN300-7089802_3_1



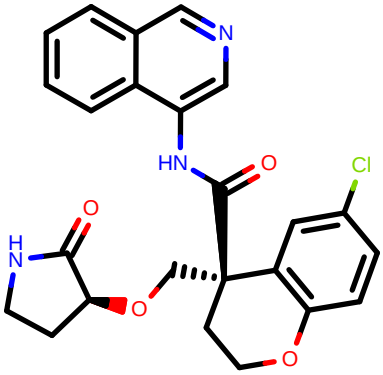
CID:	EN300-7089802_3_1
SMILES:	C[C@@H]([C@@H](C)O)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3016
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.31

EN300-141695_1_2



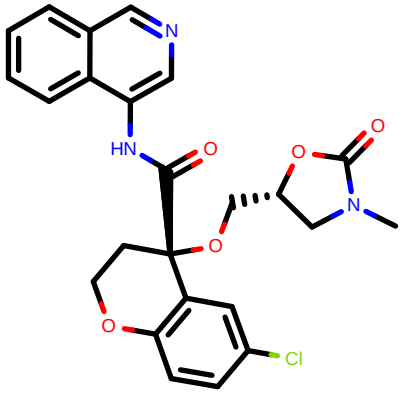
CID:	EN300-141695_1_2
SMILES:	CN1CC[C@H](C1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7086
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.25

EN300-6736413_2_2



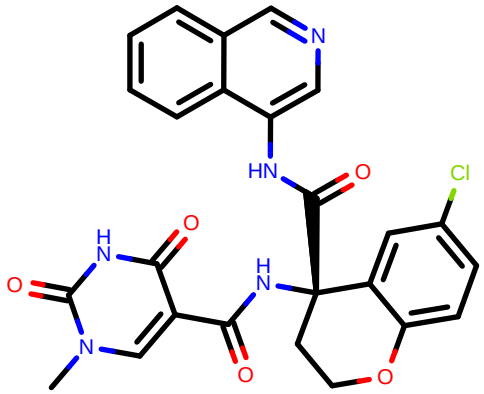
CID:	EN300-6736413_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O
RUN:	RUN1182
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.25

EN300-222969_1_1



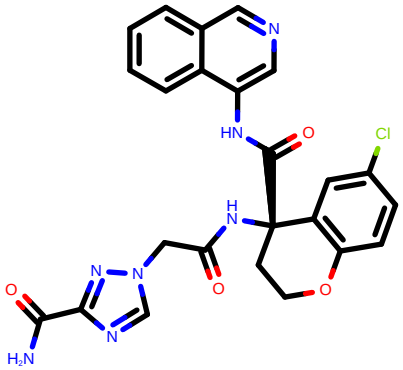
CID:	EN300-222969_1_1
SMILES:	CN1C[C@@H](OC1=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2598
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.36

EN300-37123_1_1



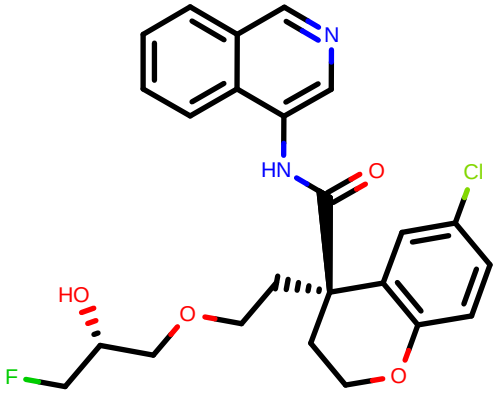
CID:	EN300-37123_1_1
SMILES:	Cn1cc(c(=O)[nH]c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7842
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.28

EN300-262604_1_1



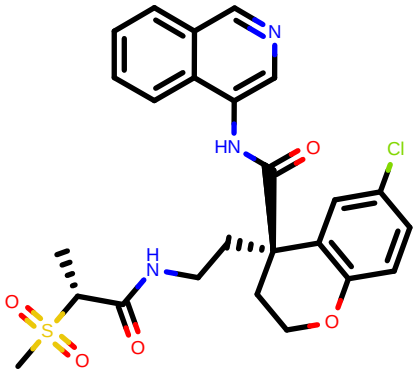
CID:	EN300-262604_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc(n5)C(=O)N
RUN:	RUN6471
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.29

EN300-1968342_3_2



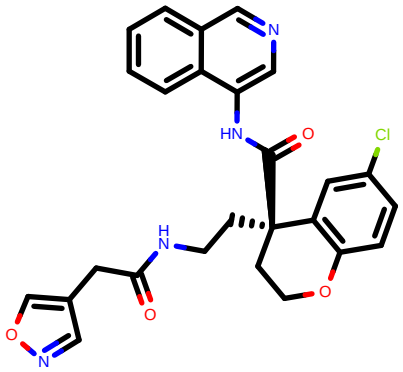
CID:	EN300-1968342_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CF)O
RUN:	RUN1548
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.35

EN300-39405_3_2



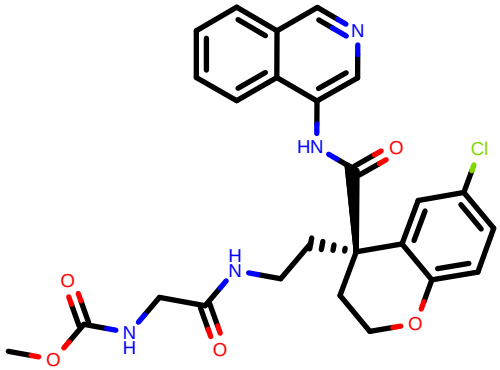
CID:	EN300-39405_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN2703
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.36

EN300-315963_3_1



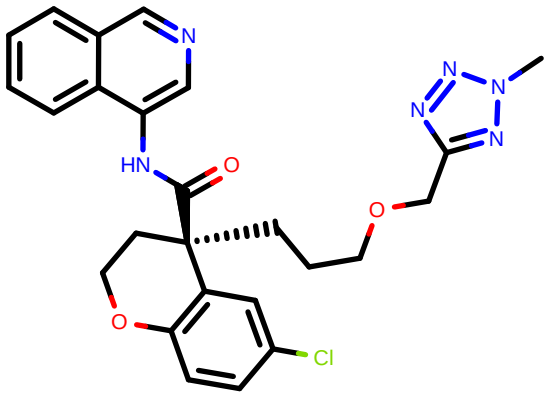
CID:	EN300-315963_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cnoc5
RUN:	RUN2683
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.31

EN300-50009_3_1



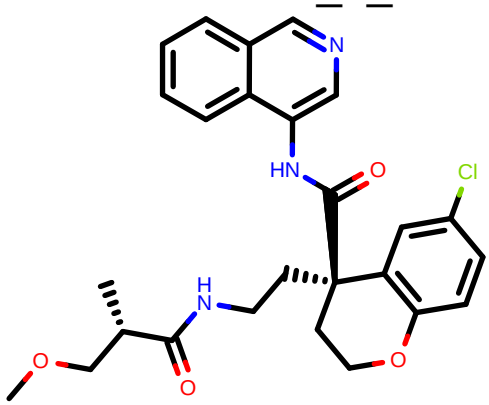
CID:	EN300-50009_3_1
SMILES:	COC(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6888
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.27

EN300-90225_4_1



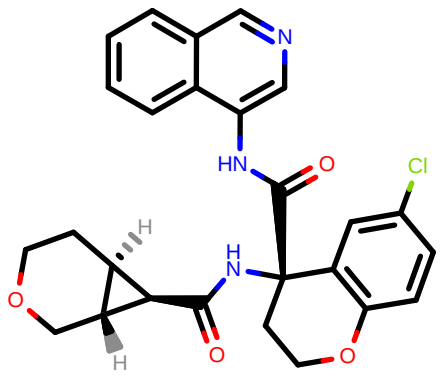
CID:	EN300-90225_4_1
SMILES:	Cn1nc(nn1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN587
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.31

EN300-69162_3_1



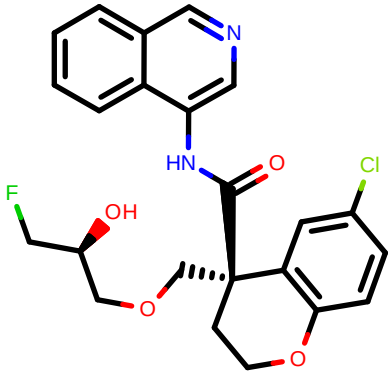
CID:	EN300-69162_3_1
SMILES:	C[C@@H](COC)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6202
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.33

EN300-1644723_1_7



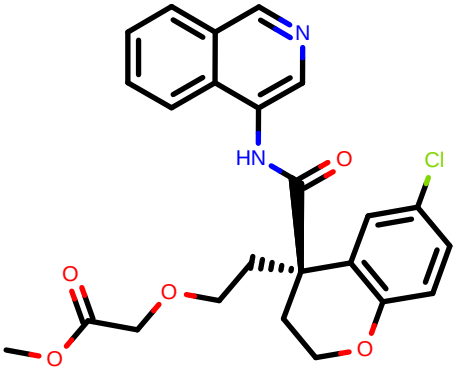
CID:	EN300-1644723_1_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@H]6[C@H]5COCC6
RUN:	RUN3662
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.25

EN300-1968342_2_1



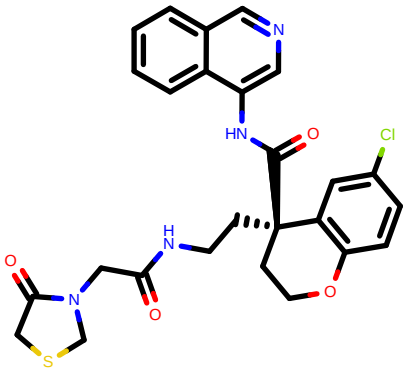
CID:	EN300-1968342_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O
RUN:	RUN483
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.36

EN300-19700_3_1



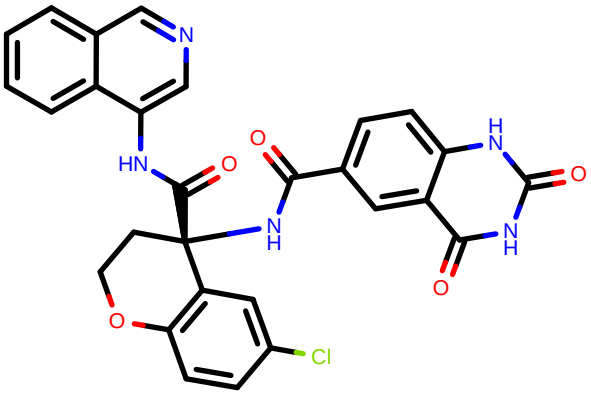
CID:	EN300-19700_3_1
SMILES:	COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1587
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.22

EN300-10747_3_1



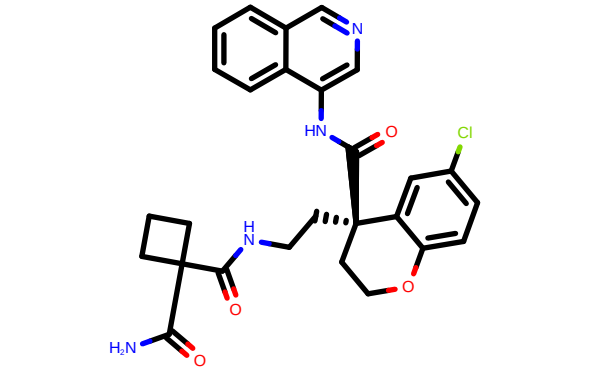
CID:	EN300-10747_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CSCC5=O
RUN:	RUN6230
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.28

EN300-1723214_1_1



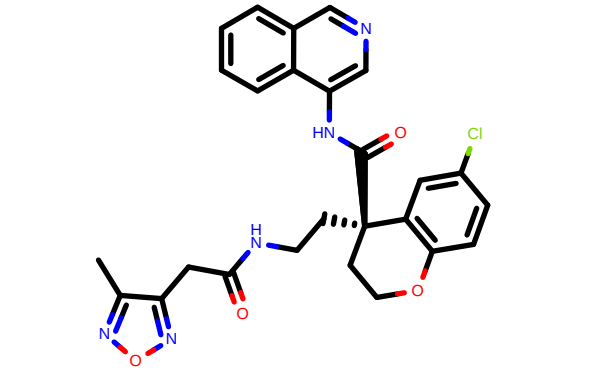
CID:	EN300-1723214_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6c(c5)c(=O)[nH]c(=O)[nH]6
RUN:	RUN9107
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.37

EN300-68747_3_1



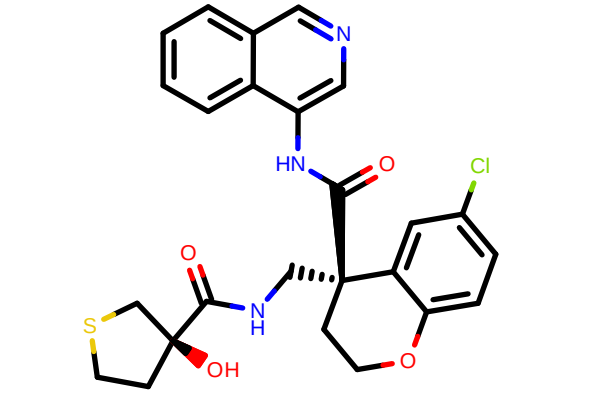
CID:	EN300-68747_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCC5)C(=O)N
RUN:	RUN1330
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.33

EN300-254883_3_1



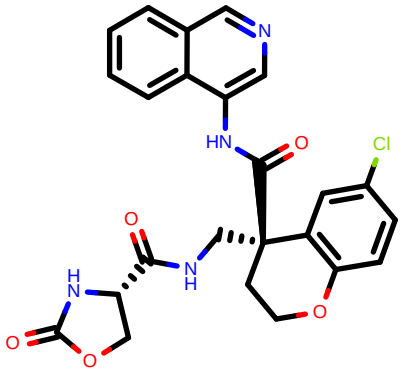
CID:	EN300-254883_3_1
SMILES:	Cc1c(non1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8420
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.28

EN300-122656_2_1



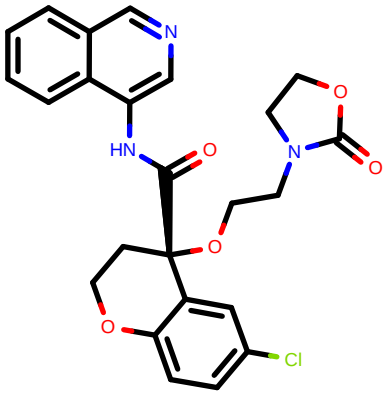
CID:	EN300-122656_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCSC5)O
RUN:	RUN3267
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.39

EN300-201346_2_1



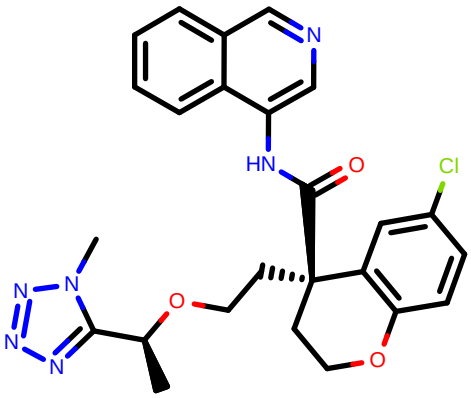
CID:	EN300-201346_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COC(=O)N5
RUN:	RUN4874
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.25

EN300-370967_1_1



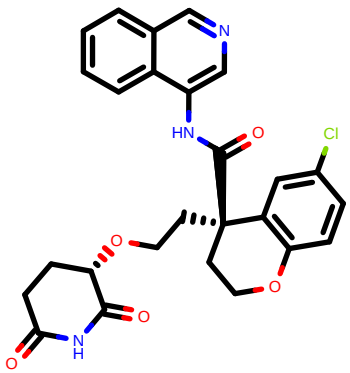
CID:	EN300-370967_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOC5=O
RUN:	RUN1647
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.23

EN300-173006_3_1



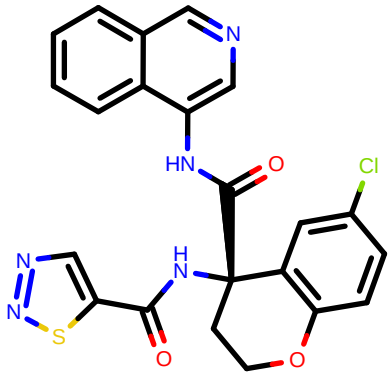
CID:	EN300-173006_3_1
SMILES:	C[C@@H](c1nnnn1C)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1124
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.29

EN300-120920_3_2



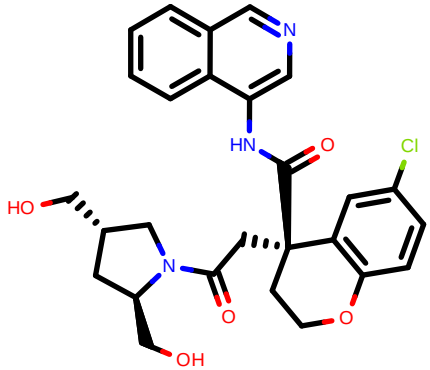
CID:	EN300-120920_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCC(=O)NC5=O
RUN:	RUN2454
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.26

EN300-42269_1_1



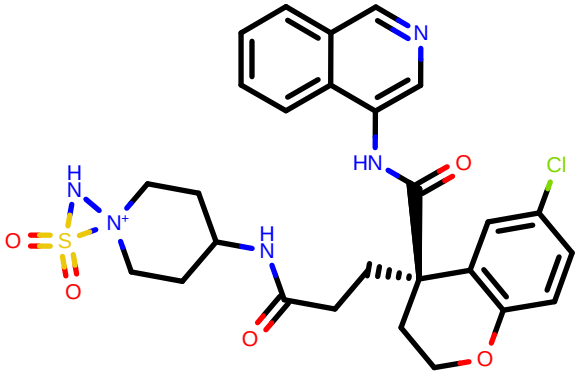
CID:	EN300-42269_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnns5
RUN:	RUN3638
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.22

EN300-1212400_1_2



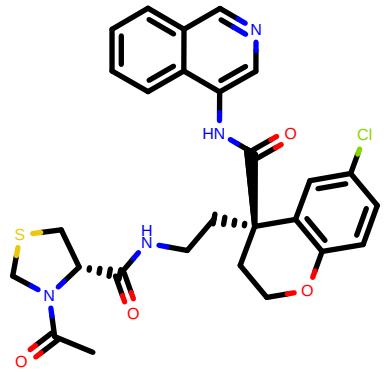
CID:	EN300-1212400_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C[C@@H]5CO)CO
RUN:	RUN5219
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.29

EN300-310398_2_1



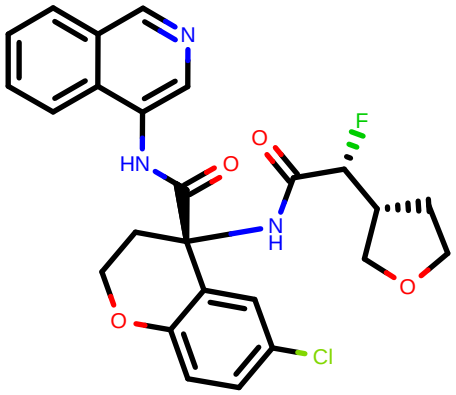
CID:	EN300-310398_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5CCN(CC5)S(=O)(=O)N
RUN:	RUN875
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.29

EN300-761220_3_1



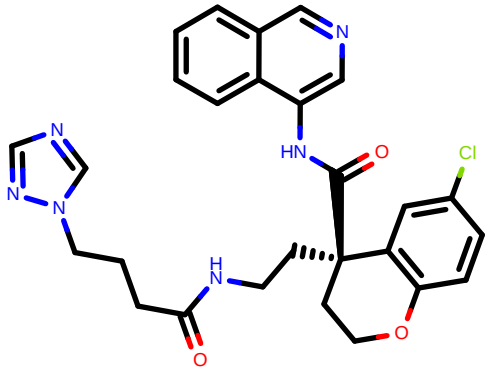
CID:	EN300-761220_3_1
SMILES:	CC(=O)N1CSC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4167
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.29

EN300-783124_1_1



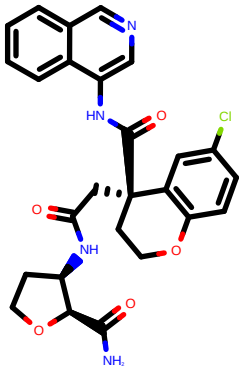
CID:	EN300-783124_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]([C@@H]5CCOC5)F
RUN:	RUN1469
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.23

EN300-316216_3_1



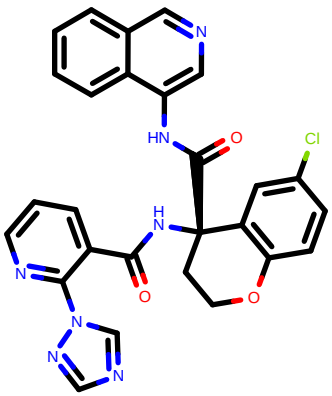
CID:	EN300-316216_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCn5cncn5
RUN:	RUN748
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.31

EN300-7435545_1_1



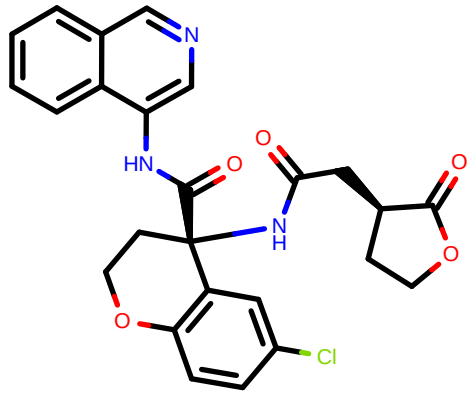
CID:	EN300-7435545_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCO[C@@H]5C(=O)N
RUN:	RUN7056
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.38

EN300-28571_1_1



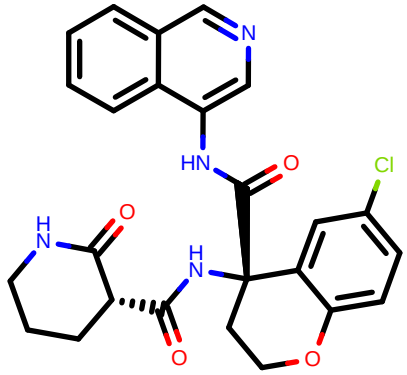
CID:	EN300-28571_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccnc5n6cncn6
RUN:	RUN7966
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.27

EN300-1072972_1_1



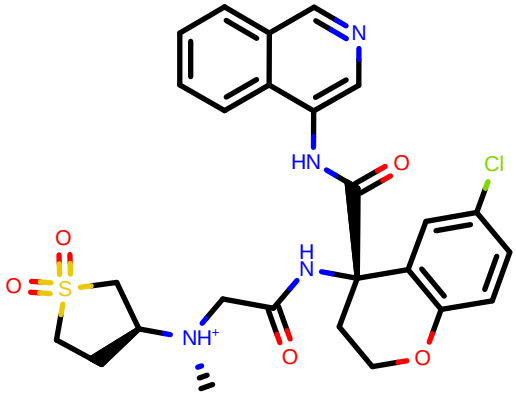
CID:	EN300-1072972_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCOC5=O
RUN:	RUN1133
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.27

EN300-82616_1_1



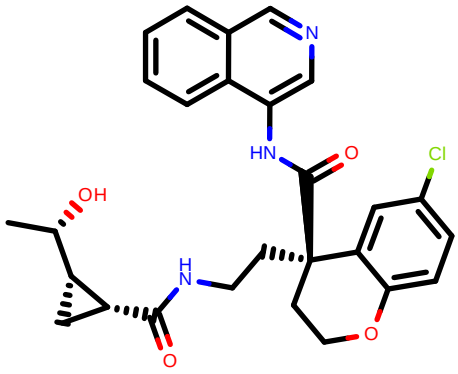
CID:	EN300-82616_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCNC5=O
RUN:	RUN7122
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.32

EN300-14628_1_2



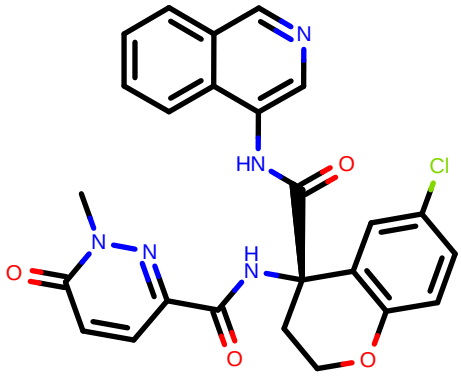
CID:	EN300-14628_1_2
SMILES:	CN(CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)[C@H]5CCS(=O)(=O)C5
RUN:	RUN3853
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.48

EN300-6729572_3_7



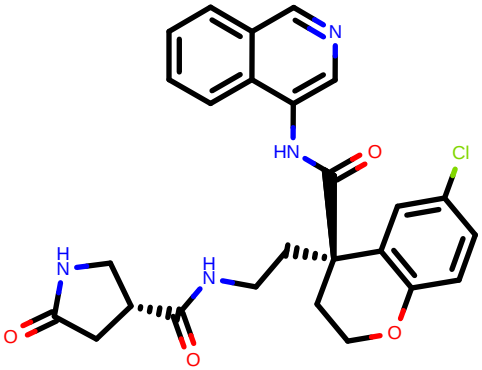
CID:	EN300-6729572_3_7
SMILES:	C[C@@H]([C@H]1C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5678
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.27

EN300-05798_1_1



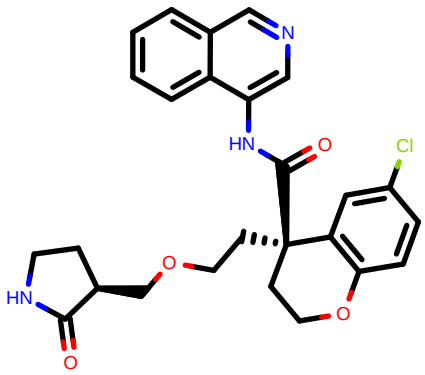
CID:	EN300-05798_1_1
SMILES:	Cn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5584
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.24

EN300-59487_3_1



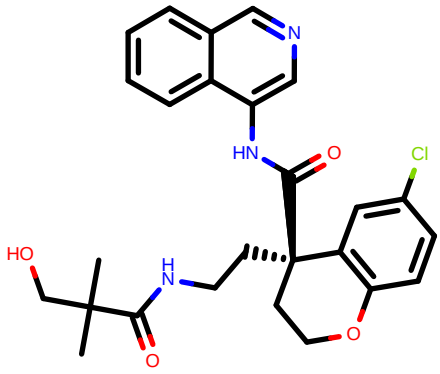
CID:	EN300-59487_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)NC5
RUN:	RUN9051
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.24

EN300-246248_3_1



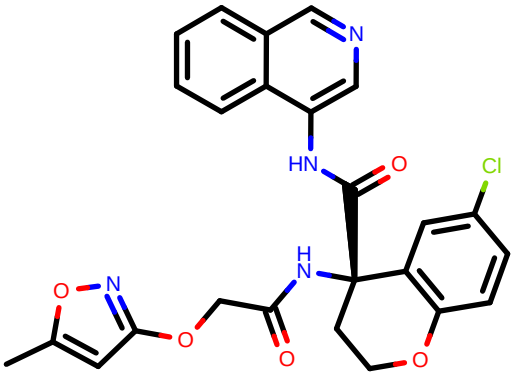
CID:	EN300-246248_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCNC5=O
RUN:	RUN2211
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.27

EN300-65050_3_1



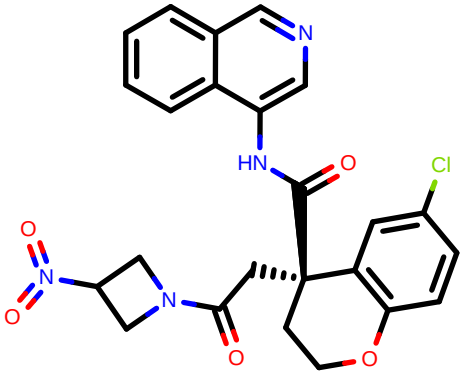
CID:	EN300-65050_3_1
SMILES:	CC(C)(CO)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3252
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.32

EN300-12929_1_1



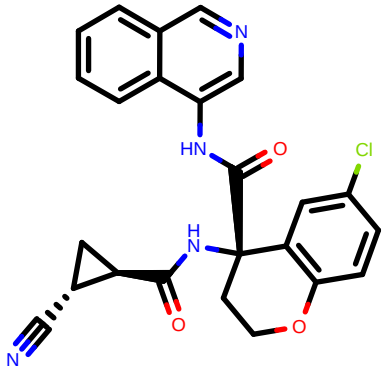
CID:	EN300-12929_1_1
SMILES:	Cc1cc(no1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1445
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.29

EN300-7461023_1_1



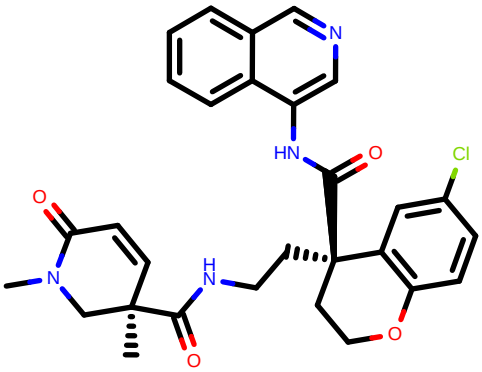
CID:	EN300-7461023_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)N(=O)=O
RUN:	RUN4051
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.20

EN300-1600363_1_1



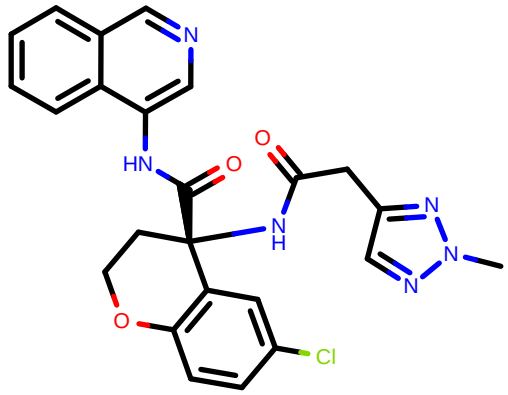
CID:	EN300-1600363_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@H]5C#N
RUN:	RUN2441
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.21

EN300-6734171_3_2



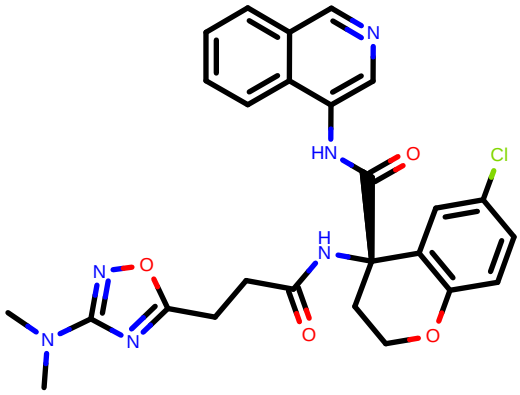
CID:	EN300-6734171_3_2
SMILES:	C[C@]1(CCC(=O)N(C1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2241
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.36

EN300-755161_1_1



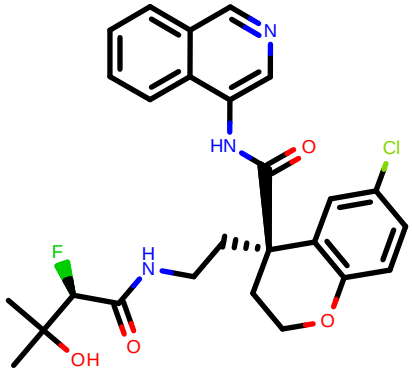
CID:	EN300-755161_1_1
SMILES:	Cn1ncc(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3602
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.23

EN300-152913_1_1



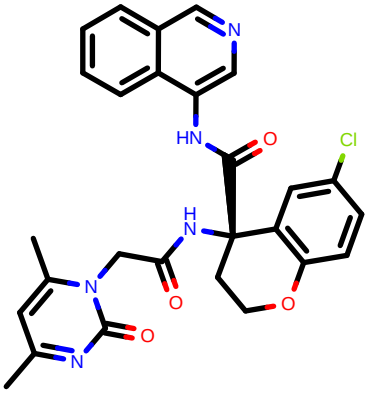
CID:	EN300-152913_1_1
SMILES:	CN(C)c1nc(on1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5021
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.24

EN300-264744_3_2



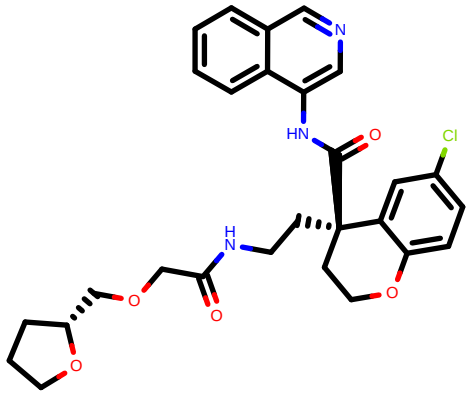
CID:	EN300-264744_3_2
SMILES:	CC(C)([C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)F)O
RUN:	RUN1338
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.29

EN300-137191_1_1



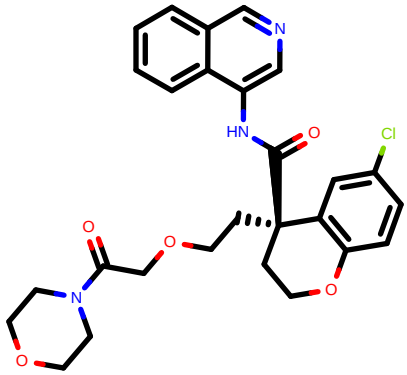
CID:	EN300-137191_1_1
SMILES:	Cc1cc(n(c(=O)n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN7486
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.28

EN300-60033_3_2



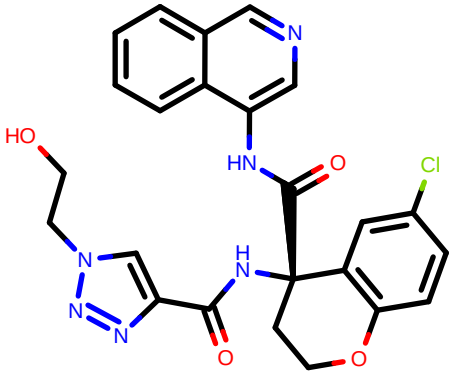
CID:	EN300-60033_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC[C@H]5CCCO5
RUN:	RUN10532
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.44

EN300-1241327_3_1



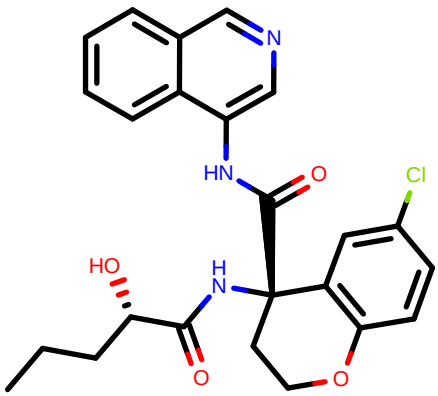
CID:	EN300-1241327_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5
RUN:	RUN829
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.43

EN300-52193_1_1



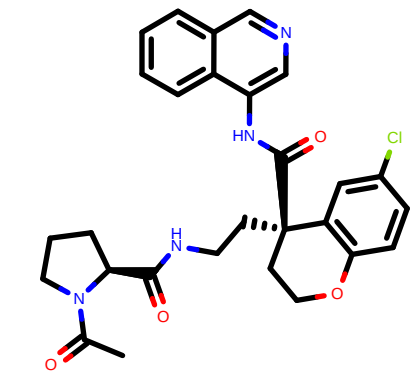
CID:	EN300-52193_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)CCO
RUN:	RUN6571
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.28

EN300-219531_1_1



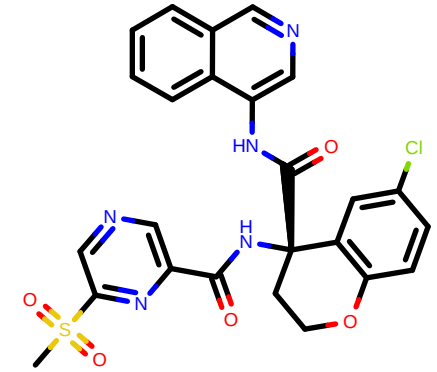
CID:	EN300-219531_1_1
SMILES:	CCC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3066
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.31

EN300-211779_3_1



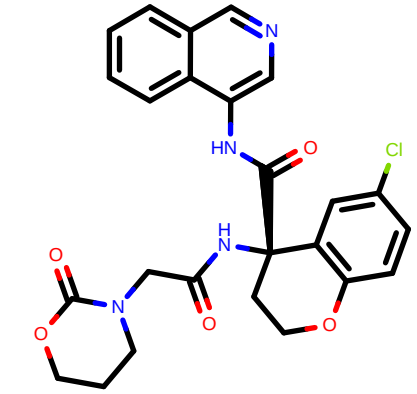
CID:	EN300-211779_3_1
SMILES:	CC(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3456
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.33

EN300-206646_1_1



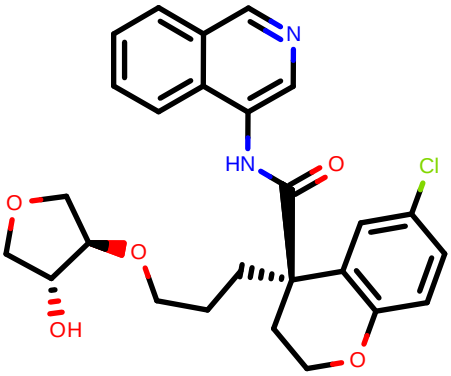
CID:	EN300-206646_1_1
SMILES:	CS(=O)(=O)c1cncc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6347
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.25

EN300-103638_1_1



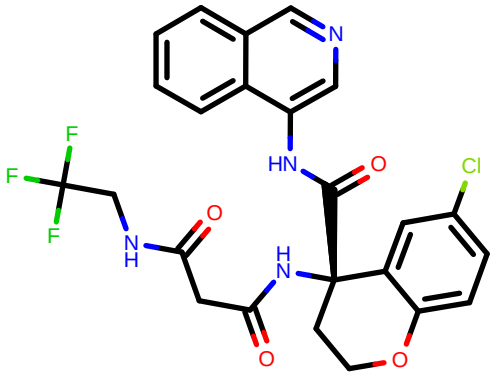
CID:	EN300-103638_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCOC5=O
RUN:	RUN7646
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.28

EN300-331828_4_1



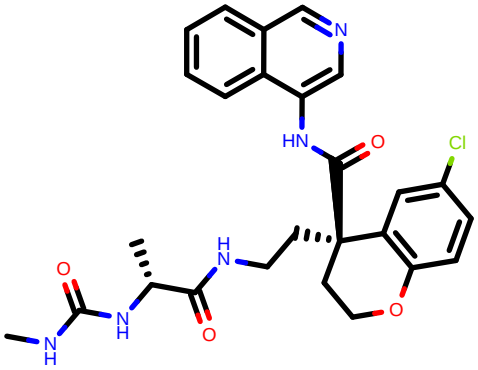
CID:	EN300-331828_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5COC[C@H]5O
RUN:	RUN1447
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.28

EN300-128715_1_1



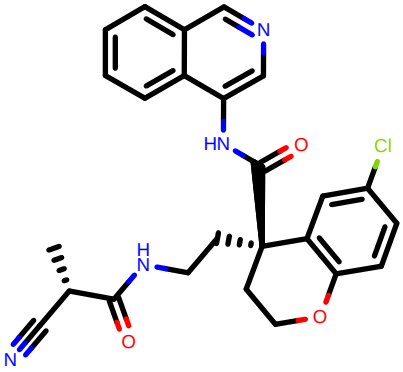
CID:	EN300-128715_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)NCC(F)(F)F
RUN:	RUN5249
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.28

EN300-1258964_3_2



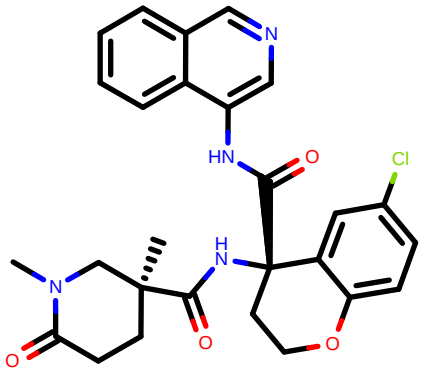
CID:	EN300-1258964_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)NC
RUN:	RUN1026
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.36

EN300-72730_3_1



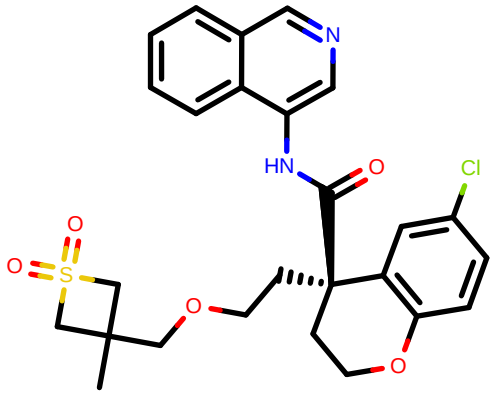
CID:	EN300-72730_3_1
SMILES:	C[C@@H](C#N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2798
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.23

EN300-6734171_1_1



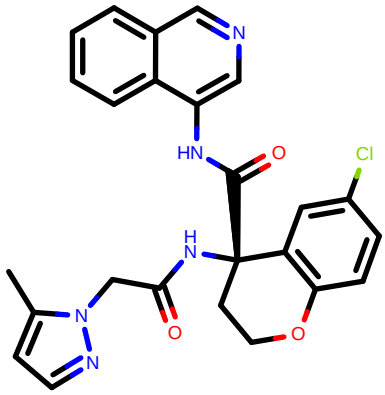
CID:	EN300-6734171_1_1
SMILES:	C[C@@]1(CCC(=O)N(C1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7678
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.33

EN300-1705754_3_1



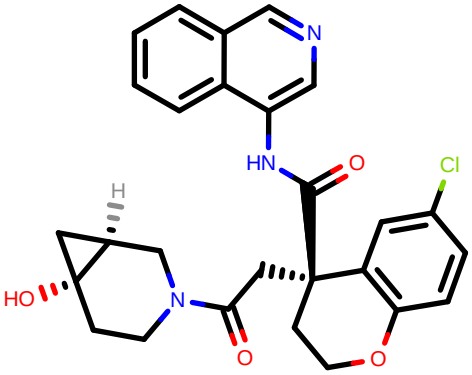
CID:	EN300-1705754_3_1
SMILES:	CC1(CS(=O)(=O)C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN417
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.27

EN300-83558_1_1



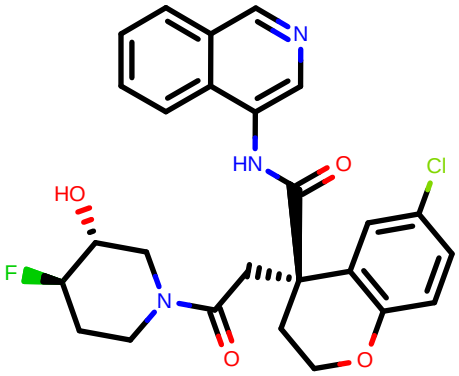
CID:	EN300-83558_1_1
SMILES:	Cc1ccnn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6287
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.23

EN300-303908_1_1



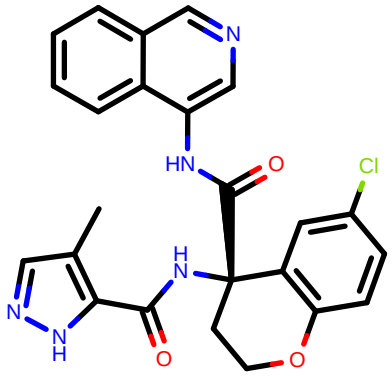
CID:	EN300-303908_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@]6(C[C@H]6C5)O
RUN:	RUN827
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.24

EN300-1655797_1_1



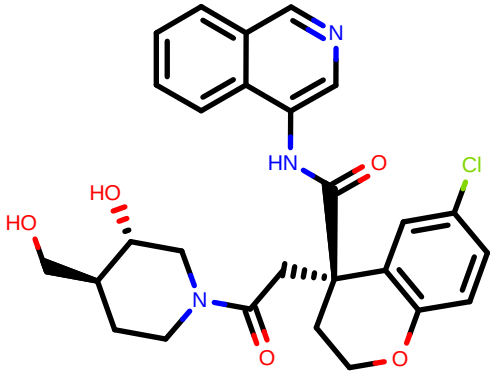
CID:	EN300-1655797_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@@H](C5)O)F
RUN:	RUN2284
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.30

EN300-248178_1_1



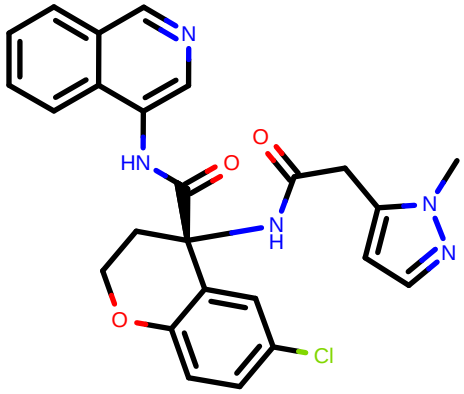
CID:	EN300-248178_1_1
SMILES:	Cc1cn[nH]c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2906
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.28

EN300-95639_1_2



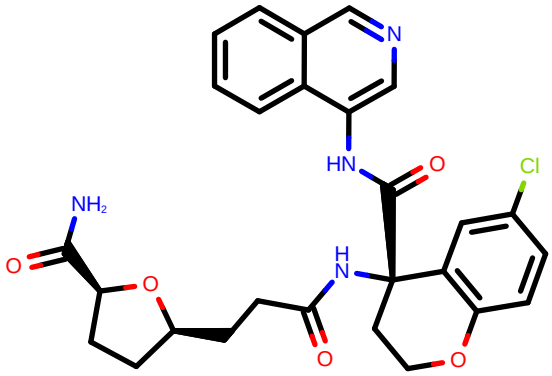
CID:	EN300-95639_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@@H](C5)O)CO
RUN:	RUN343
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.38

EN300-114805_1_1



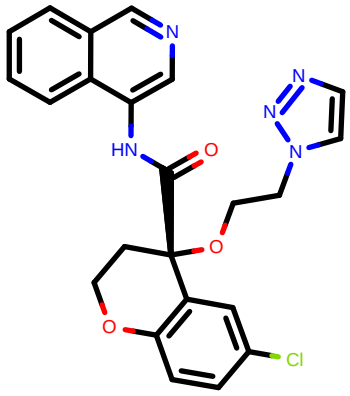
CID:	EN300-114805_1_1
SMILES:	Cn1c(ccn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3997
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.27

EN300-364992_1_1



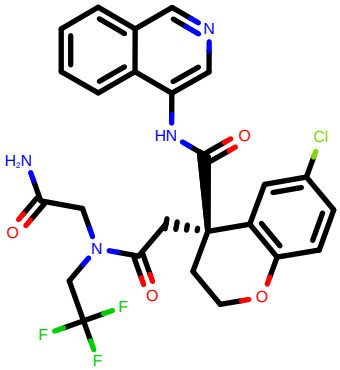
CID:	EN300-364992_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H]5CC[C@H](O5)C(=O)N
RUN:	RUN696
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.33

EN300-1715993_1_1



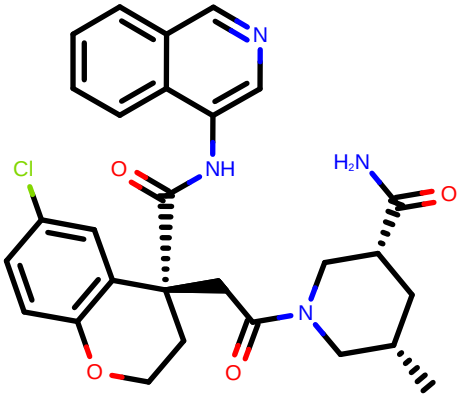
CID:	EN300-1715993_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5ccnn5
RUN:	RUN1424
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.23

EN300-138676_1_1



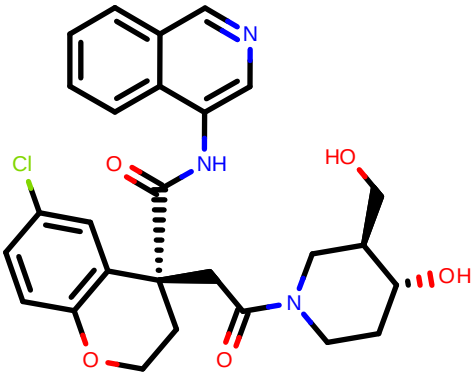
CID:	EN300-138676_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC(=O)N)CC(F)(F)F
RUN:	RUN10085
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.30

EN300-1724086_1_4



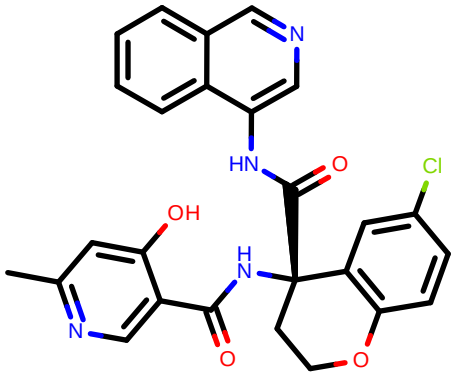
CID:	EN300-1724086_1_4
SMILES:	C[C@H]1C[C@H](CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN7980
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.33

EN300-233678_1_2



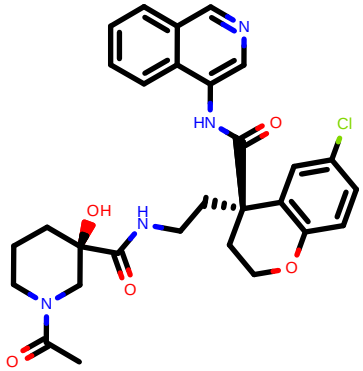
CID:	EN300-233678_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@@H](C5)CO)O
RUN:	RUN3720
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.30

EN300-85853_1_1



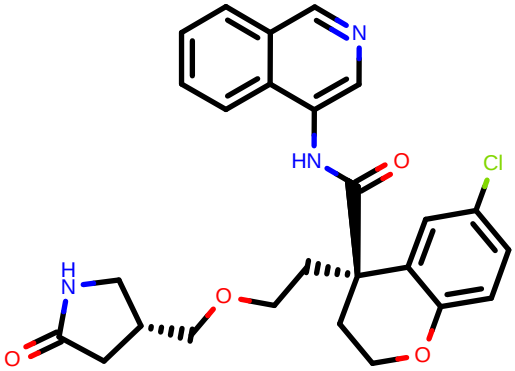
CID:	EN300-85853_1_1
SMILES:	Cc1cc(=O)c(c[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8734
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.27

EN300-210552_3_1



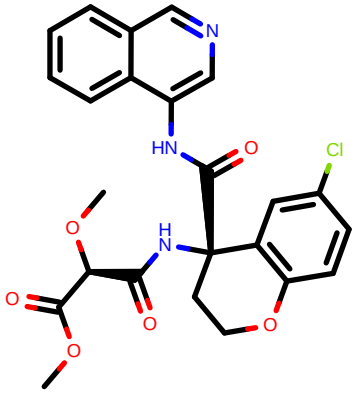
CID:	EN300-210552_3_1
SMILES:	CC(=O)N1CCC[C@@](C1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN9063
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.41

EN300-246747_3_1



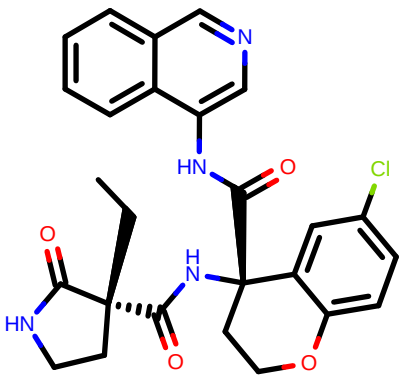
CID:	EN300-246747_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CC(=O)NC5
RUN:	RUN1212
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.28

EN300-1718194_1_1



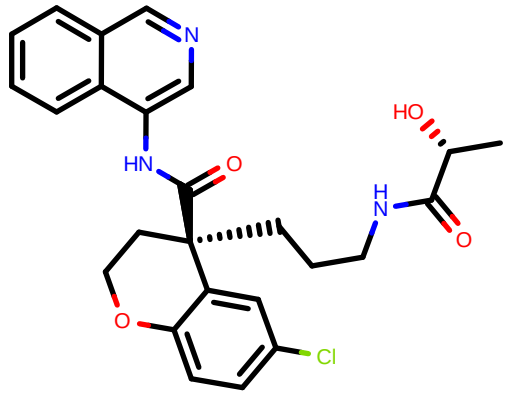
CID:	EN300-1718194_1_1
SMILES:	CO[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN6507
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.37

EN300-304135_1_2



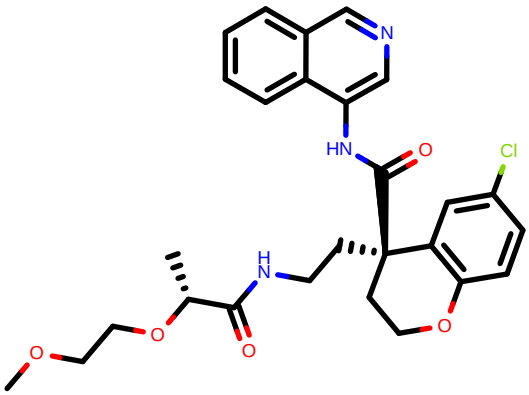
CID:	EN300-304135_1_2
SMILES:	CC[C@]1(CCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6267
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.29

EN300-19542_4_2



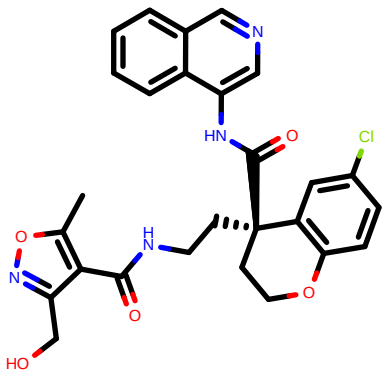
CID:	EN300-19542_4_2
SMILES:	C[C@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN10082
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.34

EN300-77359_3_2



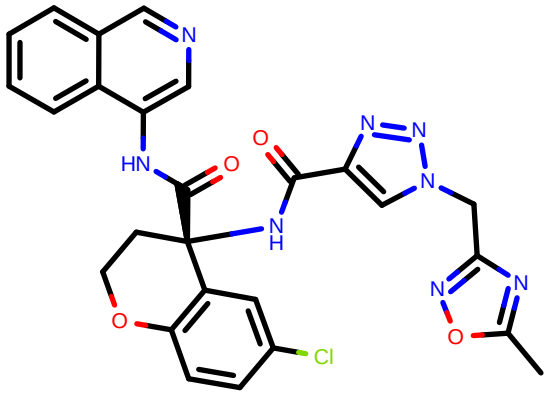
CID:	EN300-77359_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OCCOC
RUN:	RUN10029
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.54

EN300-215799_3_1



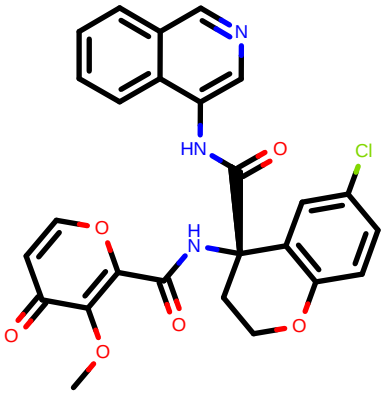
CID:	EN300-215799_3_1
SMILES:	Cc1c(c(no1)CO)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11002
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.31

EN300-182758_1_1



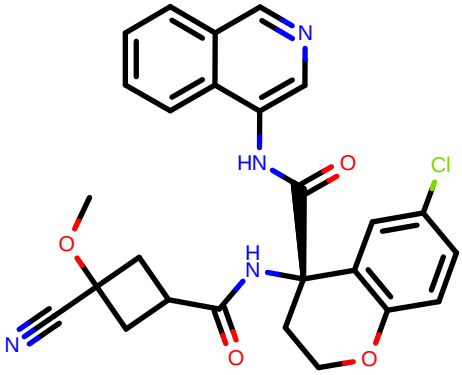
CID:	EN300-182758_1_1
SMILES:	Cc1nc(no1)Cn2cc(nn2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8202
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.24

EN300-7465954_1_1



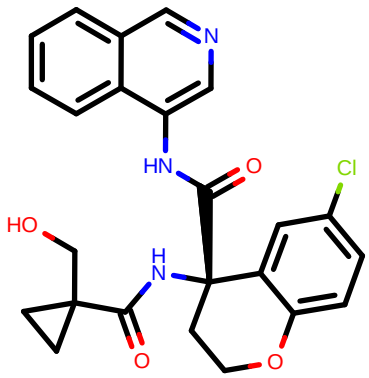
CID:	EN300-7465954_1_1
SMILES:	COc1c(=O)ccoc1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7466
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.26

EN300-1073533_1_1



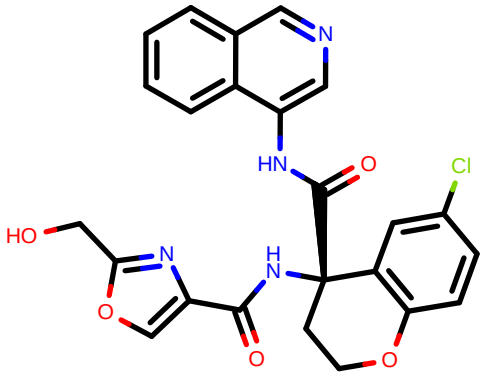
CID:	EN300-1073533_1_1
SMILES:	COC1(CC(C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN7698
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.29

EN300-146174_1_1



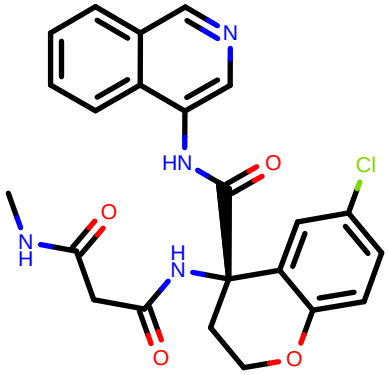
CID:	EN300-146174_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)CO
RUN:	RUN2854
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.25

EN300-7549555_1_1



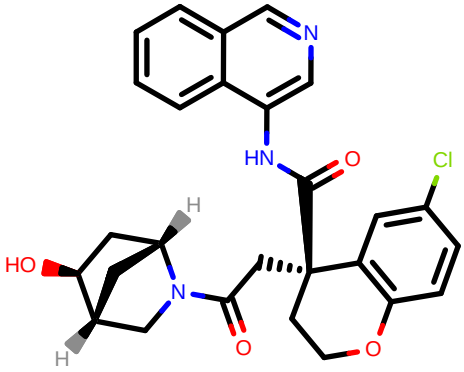
CID:	EN300-7549555_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5coc(n5)CO
RUN:	RUN4037
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.23

EN300-128463_1_1



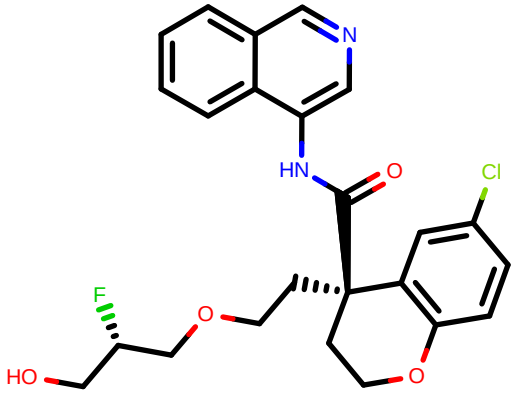
CID:	EN300-128463_1_1
SMILES:	CNC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3785
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.26

EN300-307084_1_1



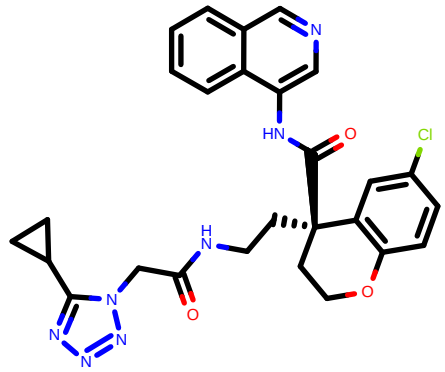
CID:	EN300-307084_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6CC5C[C@@H]6O
RUN:	RUN3512
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.27

EN300-1600517_3_2



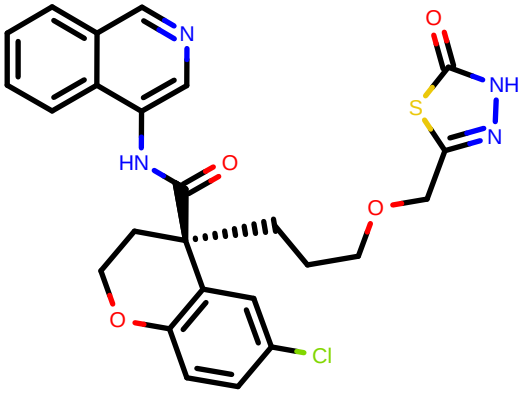
CID:	EN300-1600517_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H](CO)F
RUN:	RUN1228
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.28

EN300-872798_3_1



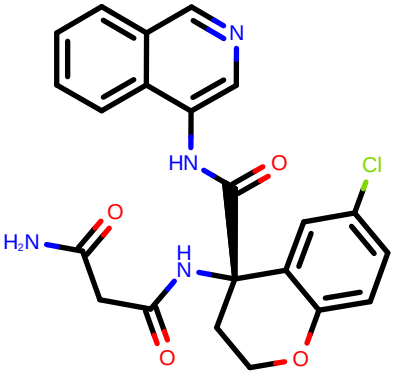
CID:	EN300-872798_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5c(nnn5)C6CC6
RUN:	RUN9161
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.51

EN300-171766_4_1



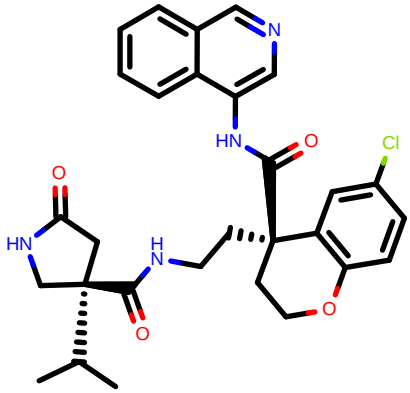
CID:	EN300-171766_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCc5n[nH]c(=O)s5
RUN:	RUN292
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.26

EN300-82179_1_1



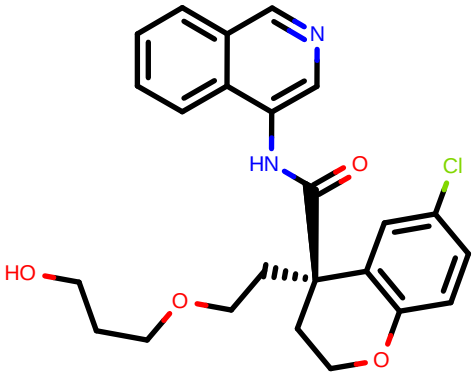
CID:	EN300-82179_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)N
RUN:	RUN2100
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.18

EN300-211203_3_2



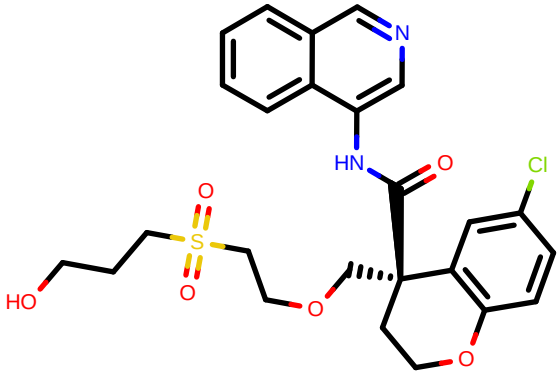
CID:	EN300-211203_3_2
SMILES:	CC(C)[C@]1(CC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7904
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.40

EN300-221518_3_1



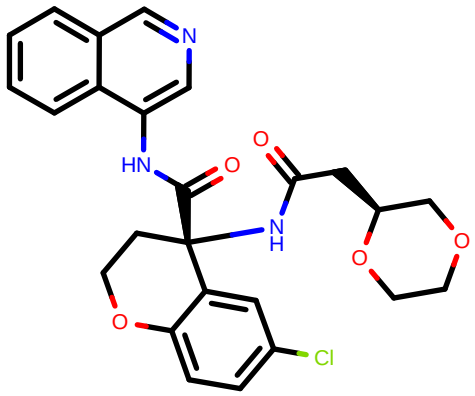
CID:	EN300-221518_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO
RUN:	RUN1420
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.20

EN300-7456499_2_1



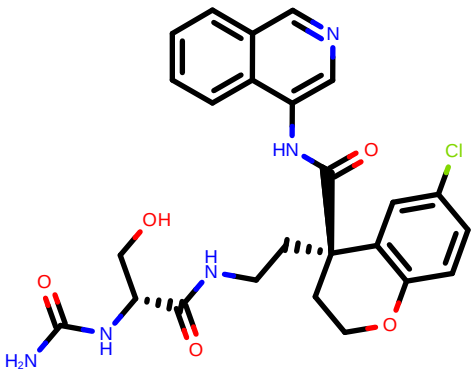
CID:	EN300-7456499_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCS(=O)(=O)CCCO
RUN:	RUN682
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.42

EN300-731622_1_2



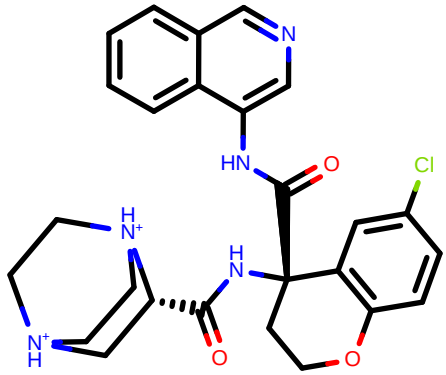
CID:	EN300-731622_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5COCCO5
RUN:	RUN4665
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.27

EN300-10170_3_1



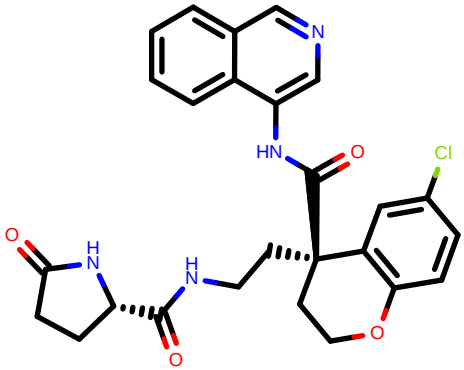
CID:	EN300-10170_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](CO)NC(=O)N
RUN:	RUN1066
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.30

EN300-1605566_1_1



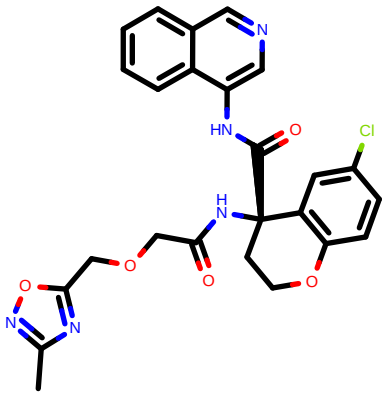
CID:	EN300-1605566_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CN6CCN5CC6
RUN:	RUN4441
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.27

EN300-19515_3_1



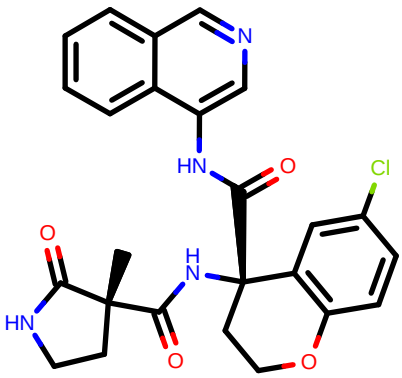
CID:	EN300-19515_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCC(=O)N5
RUN:	RUN7756
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.30

EN300-77006_1_1



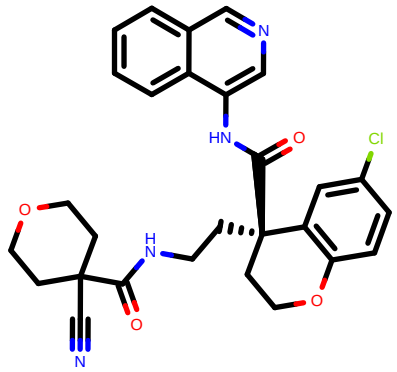
CID:	EN300-77006_1_1
SMILES:	Cc1nc(on1)COCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN965
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.28

EN300-207959_1_2



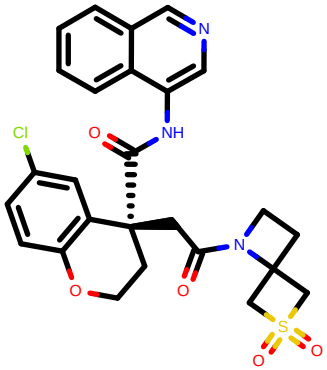
CID:	EN300-207959_1_2
SMILES:	C[C@]1(CCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6379
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.32

EN300-74089_3_1



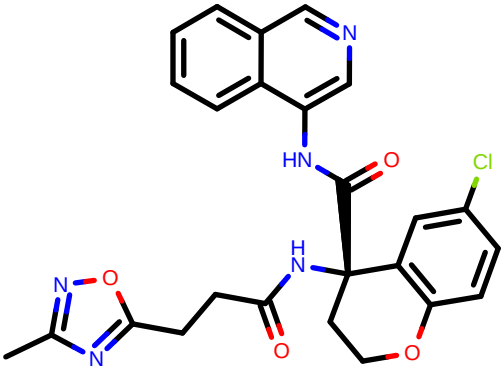
CID:	EN300-74089_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCOCC5)C#N
RUN:	RUN439
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.36

EN300-1717443_1_1



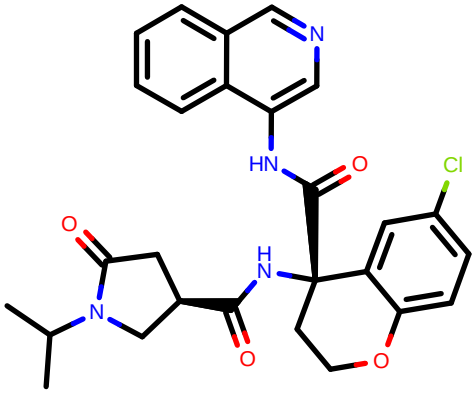
CID:	EN300-1717443_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC56CS(=O)(=O)C6
RUN:	RUN11110
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.32

EN300-27268_1_1



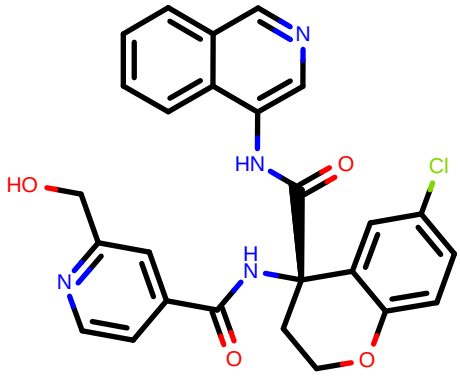
CID:	EN300-27268_1_1
SMILES:	Cc1nc(on1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6639
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.28

EN300-33398_1_1



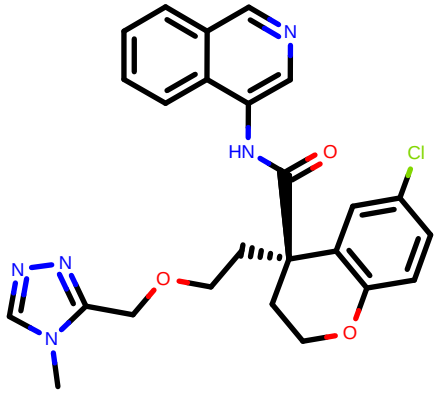
CID:	EN300-33398_1_1
SMILES:	CC(C)N1C[C@@H](CC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7102
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.29

EN300-396748_1_1



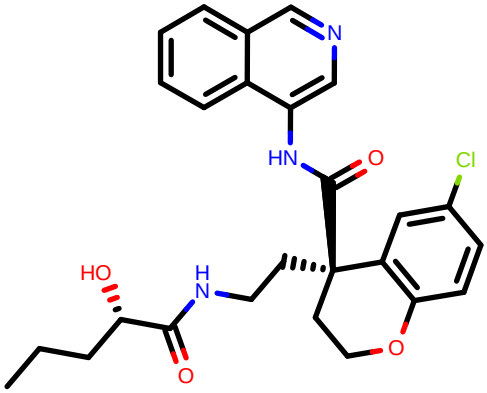
CID:	EN300-396748_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)CO
RUN:	RUN4065
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.28

EN300-113112_3_1



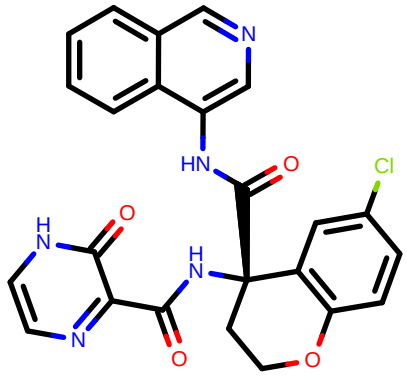
CID:	EN300-113112_3_1
SMILES:	Cn1cnnc1COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1723
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.26

EN300-300217_3_1



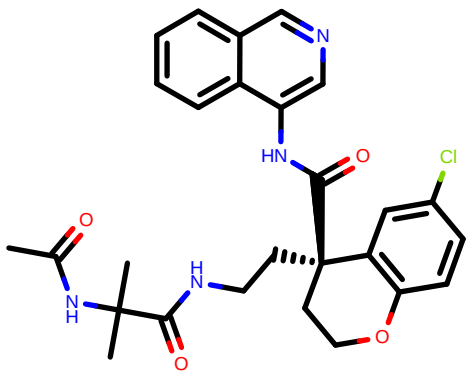
CID:	EN300-300217_3_1
SMILES:	C/C=C\[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5251
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.30

EN300-97055_1_1



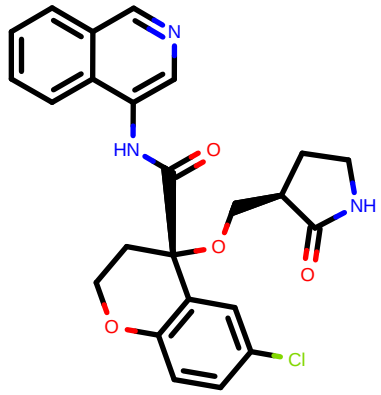
CID:	EN300-97055_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(=O)[nH]ccn5
RUN:	RUN7498
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.25

EN300-65414_3_1



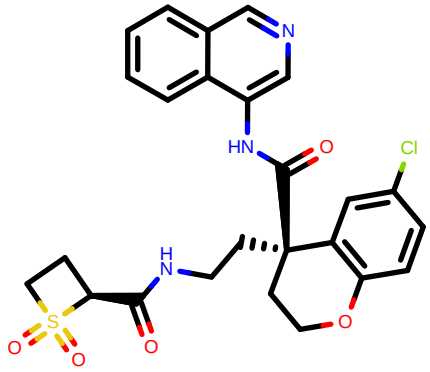
CID:	EN300-65414_3_1
SMILES:	CC(=O)NC(C)(C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4195
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.31

EN300-246248_1_2



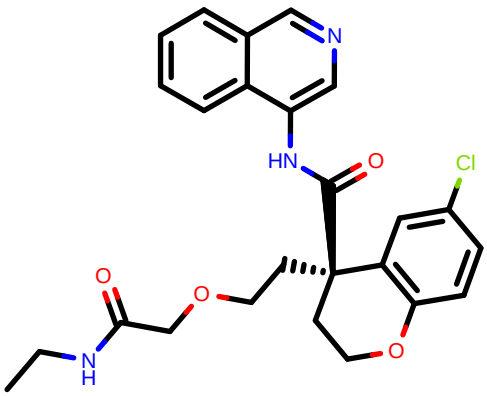
CID:	EN300-246248_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCNC5=O
RUN:	RUN1919
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.26

EN300-1387104_3_1



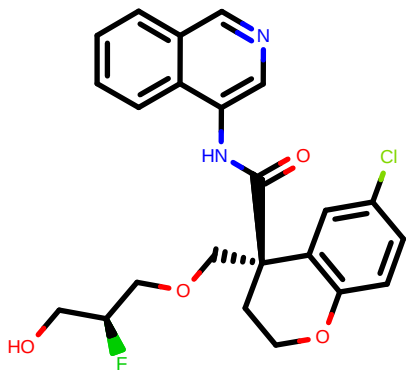
CID:	EN300-1387104_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCS5(=O)=O
RUN:	RUN10268
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.31

EN300-7003350_3_1



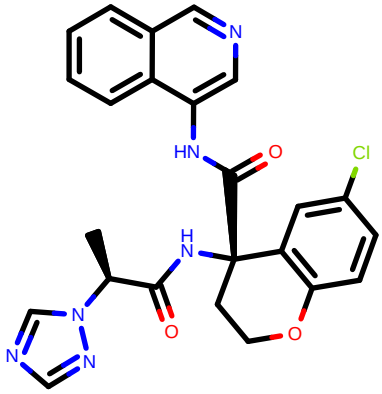
CID:	EN300-7003350_3_1
SMILES:	CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1484
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.25

EN300-1600517_2_2



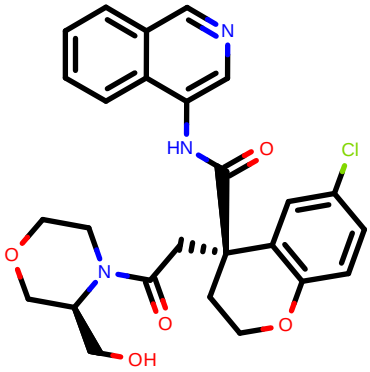
CID:	EN300-1600517_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F
RUN:	RUN1134
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.27

EN300-30397_1_1



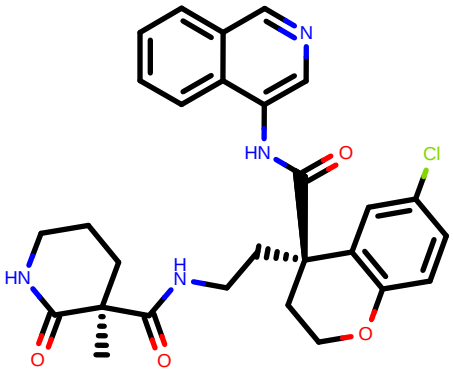
CID:	EN300-30397_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN3817
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.25

EN300-154201_1_1



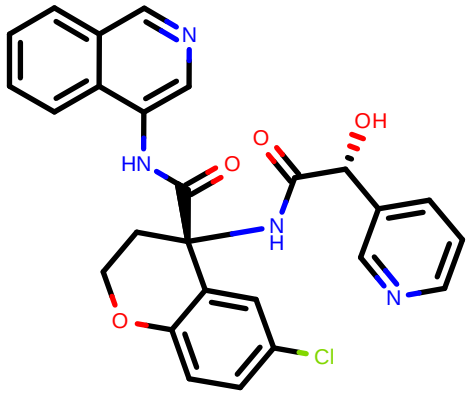
CID:	EN300-154201_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CO
RUN:	RUN9778
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.28

EN300-178876_3_2



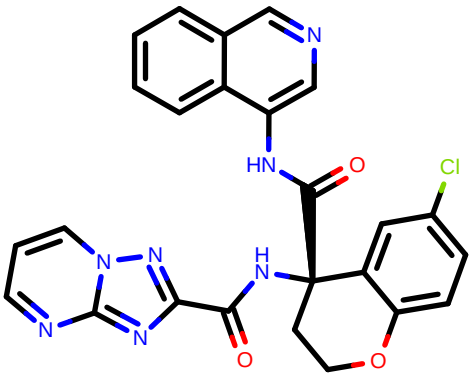
CID:	EN300-178876_3_2
SMILES:	C[C@]1(CCCNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2820
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.48

EN300-134855_1_1



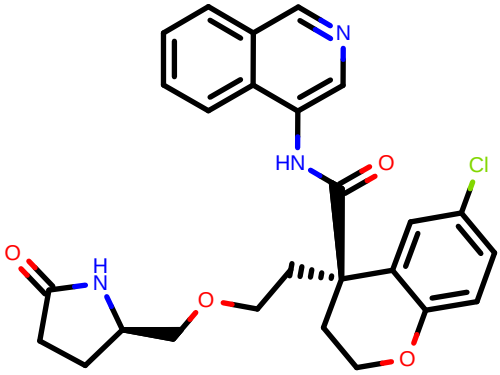
CID:	EN300-134855_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5cccnc5)O
RUN:	RUN7750
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.30

EN300-83529_1_1



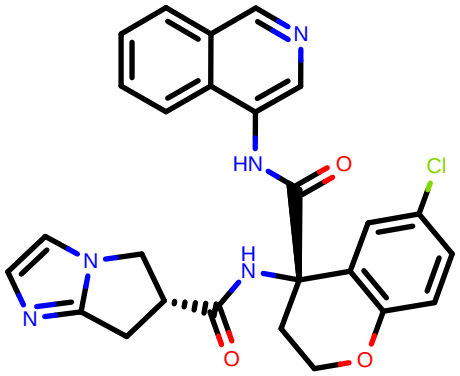
CID:	EN300-83529_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nc6ncccn6n5
RUN:	RUN8818
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.24

EN300-195756_3_2



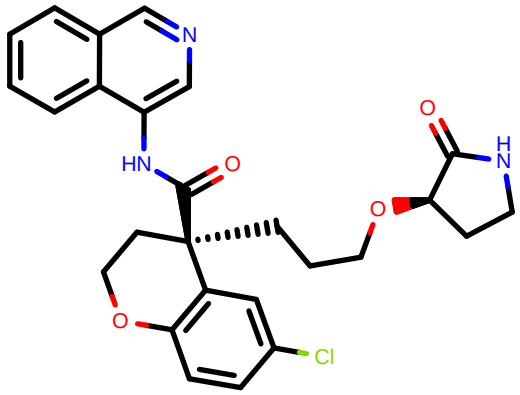
CID:	EN300-195756_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCC(=O)N5
RUN:	RUN1084
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.24

EN300-7385329_1_1



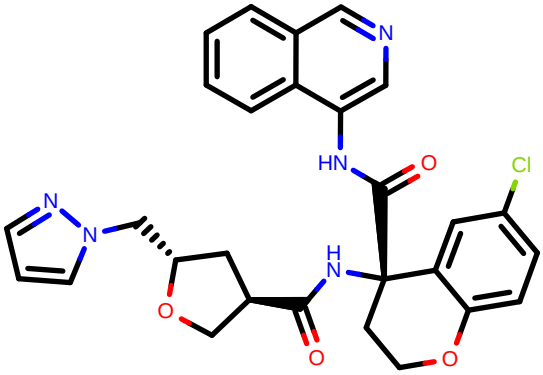
CID:	EN300-7385329_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5Cc6nccn6C5
RUN:	RUN8118
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.29

EN300-6736413_4_1



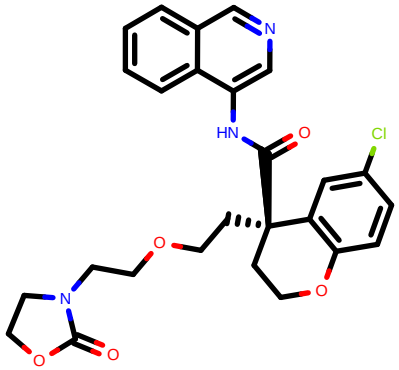
CID:	EN300-6736413_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@@H]5CCNC5=O
RUN:	RUN975
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.35

EN300-6494859_1_3



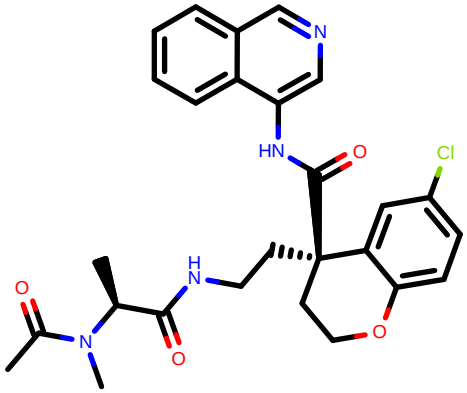
CID:	EN300-6494859_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@H](OC5)Cn6cccn6
RUN:	RUN8182
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.33

EN300-370967_3_1



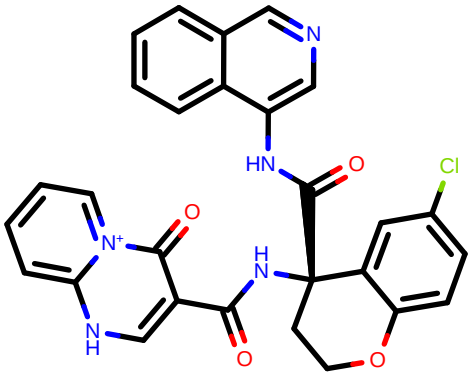
CID:	EN300-370967_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOC5=O
RUN:	RUN1907
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.29

EN300-863933_3_1



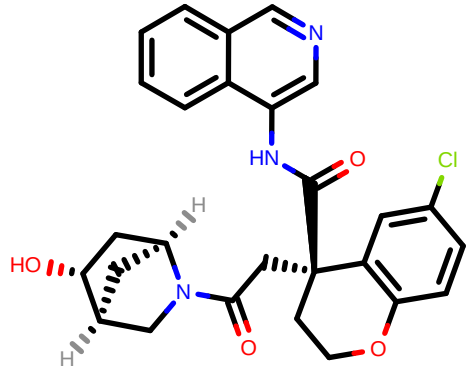
CID:	EN300-863933_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C)C(=O)C
RUN:	RUN2001
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.32

EN300-35781_1_1



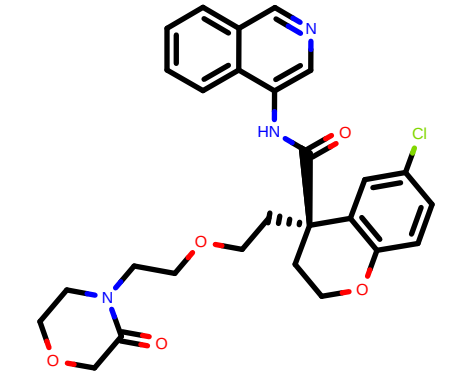
CID:	EN300-35781_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6ccccn6c5=O
RUN:	RUN8966
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.33

EN300-307084_1_2



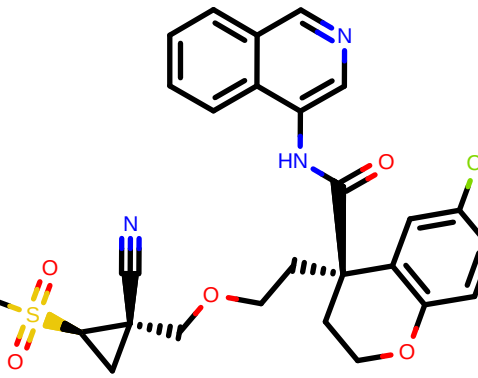
CID:	EN300-307084_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6CC5C[C@H]6O
RUN:	RUN4231
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.27

EN300-219330_3_1



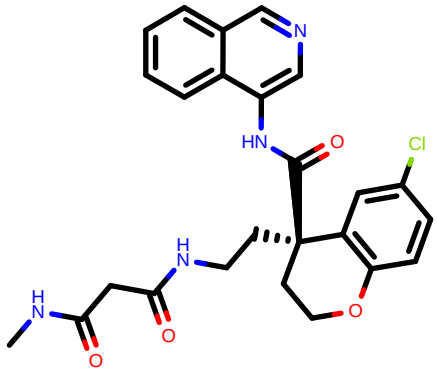
CID:	EN300-219330_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOCC5=O
RUN:	RUN536
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.27

EN300-633533_3_1



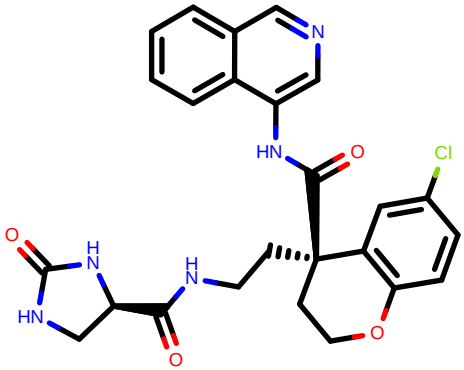
CID:	EN300-633533_3_1
SMILES:	CS(=O)(=O)[C@@H]1C[C@]1(COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN781
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.37

EN300-128463_3_1



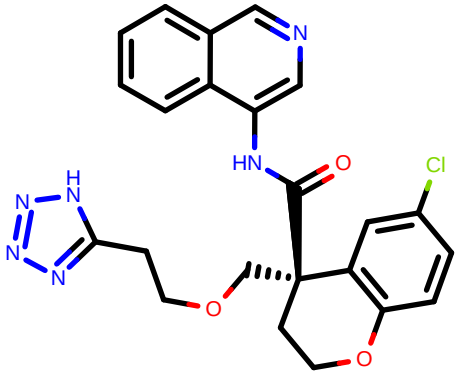
CID:	EN300-128463_3_1
SMILES:	CNC(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1090
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.31

EN300-222145_3_1



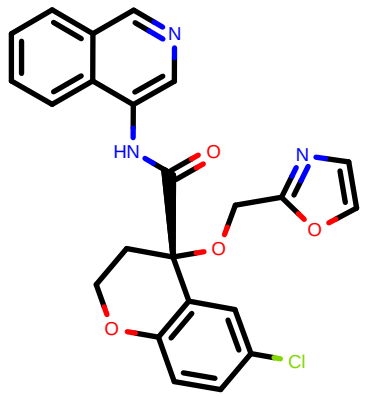
CID:	EN300-222145_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CNC(=O)N5
RUN:	RUN10612
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.26

EN300-183231_2_1



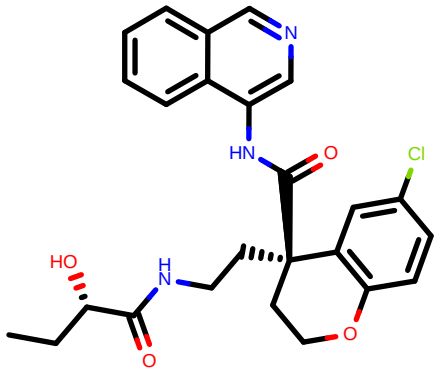
CID:	EN300-183231_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCc5[nH]nnn5
RUN:	RUN1518
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.33

EN300-317555_1_1



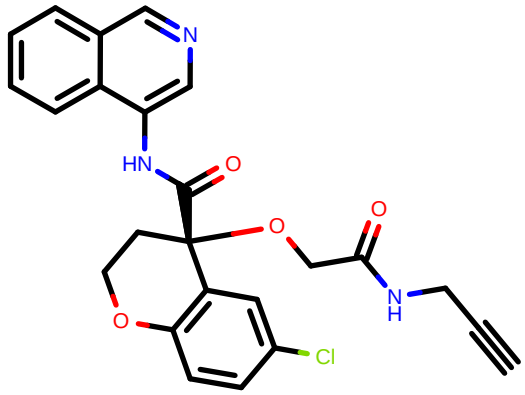
CID:	EN300-317555_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5
RUN:	RUN397
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.19

EN300-181492_3_1



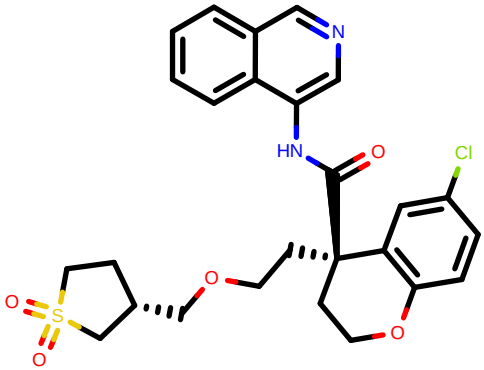
CID:	EN300-181492_3_1
SMILES:	C=C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5782
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.29

EN300-1659582_1_1



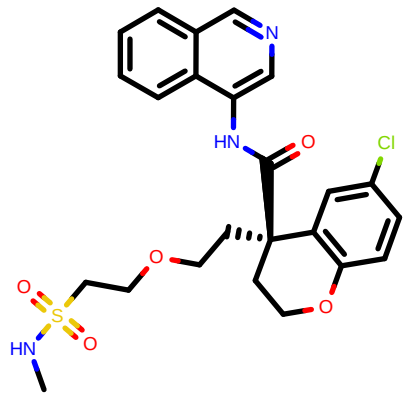
CID:	EN300-1659582_1_1
SMILES:	C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN461
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.23

EN300-1448603_3_2



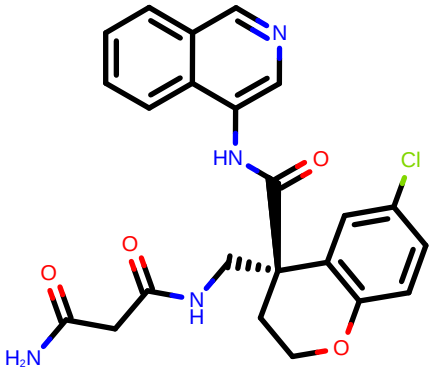
CID:	EN300-1448603_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCS(=O)(=O)C5
RUN:	RUN1244
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.30

EN300-6482967_3_1



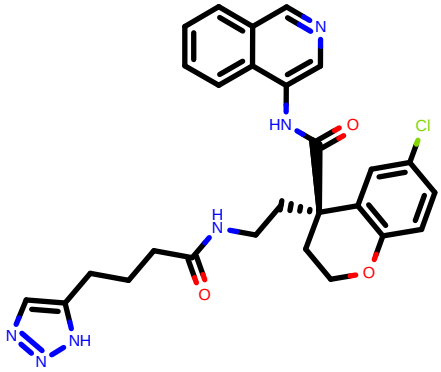
CID:	EN300-6482967_3_1
SMILES:	CNS(=O)(=O)CCOCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN329
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.35

EN300-82179_2_1



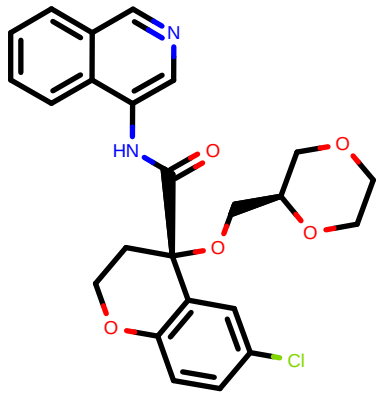
CID:	EN300-82179_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CC(=O)N
RUN:	RUN2402
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.25

EN300-156995_3_1



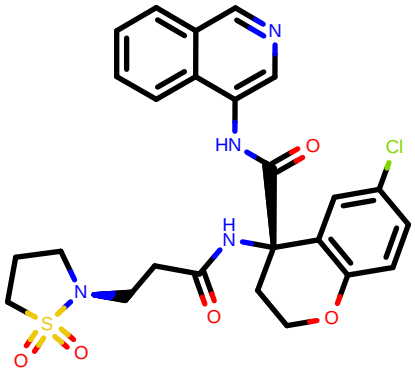
CID:	EN300-156995_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCc5c[nH]nn5
RUN:	RUN9644
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.39

EN300-139167_1_2



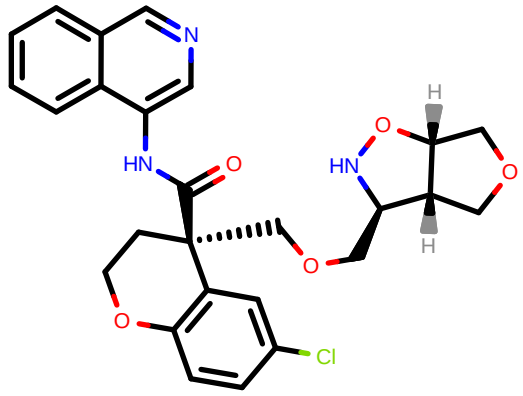
CID:	EN300-139167_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5COCCO5
RUN:	RUN2681
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.25

EN300-44873_1_1



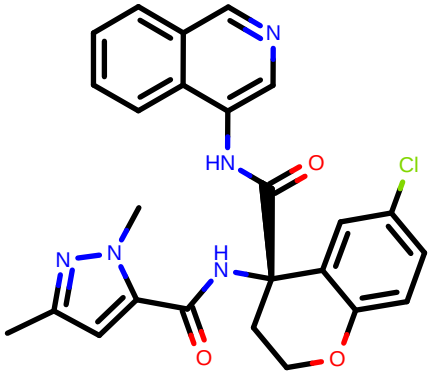
CID:	EN300-44873_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCN5CCCS5(=O)=O
RUN:	RUN506
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.40

EN300-7436306_2_1



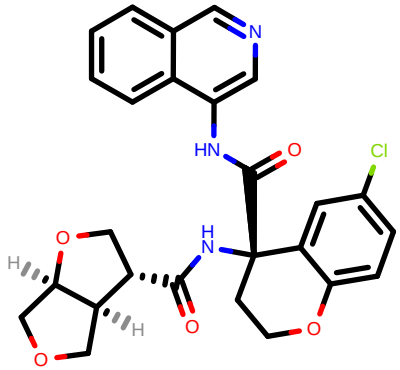
CID:	EN300-7436306_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5=NO[C@H]6[C@@H]5COC6
RUN:	RUN2101
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.30

EN300-51244_1_1



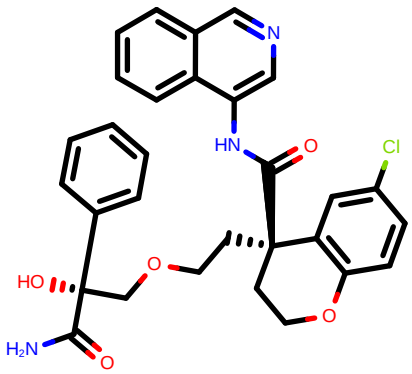
CID:	EN300-51244_1_1
SMILES:	Cc1cc(n(n1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4637
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.23

EN300-6482296_1_4



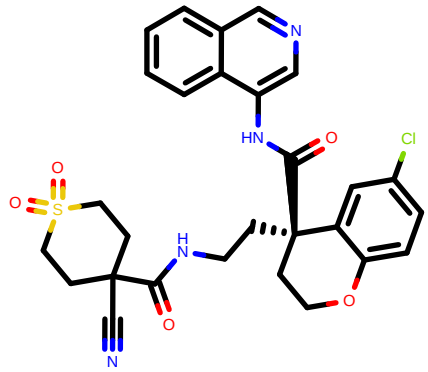
CID:	EN300-6482296_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CO[C@H]6[C@@H]5COC6
RUN:	RUN3857
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.32

EN300-248526_3_1



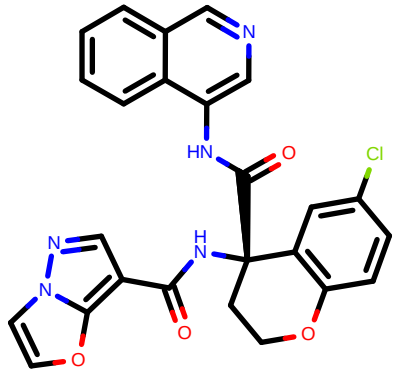
CID:	EN300-248526_3_1
SMILES:	c1ccc(cc1)[C@@](COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(C(=O)N)O
RUN:	RUN703
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.38

EN300-73967_3_1



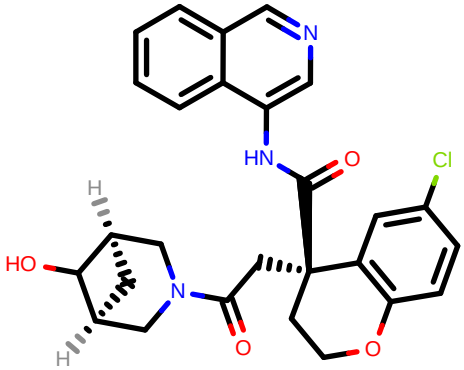
CID:	EN300-73967_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCS(=O)(=O)CC5)C#N
RUN:	RUN2812
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.37

EN300-303519_1_1



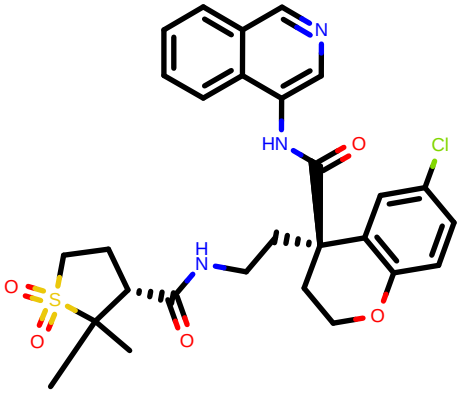
CID:	EN300-303519_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5OCC6
RUN:	RUN7434
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.23

EN300-90206_1_1



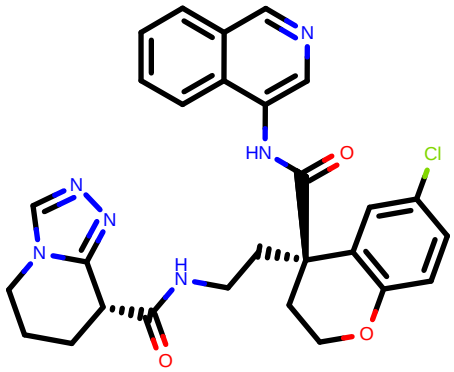
CID:	EN300-90206_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6CC(C5)C6O
RUN:	RUN6433
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.31

EN300-2007564_3_2



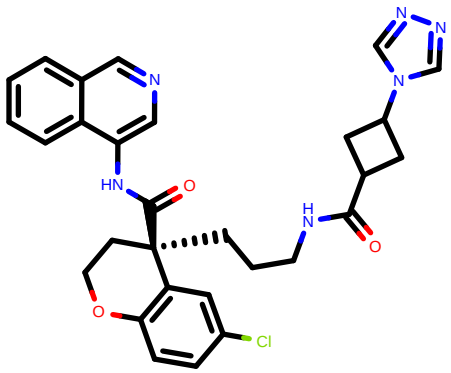
CID:	EN300-2007564_3_2
SMILES:	CC1([C@H](CCS1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN10434
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.33

EN300-748981_3_1



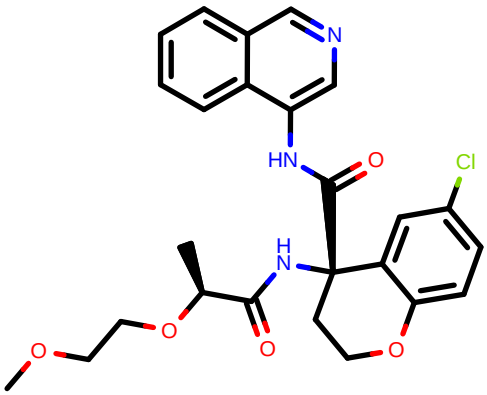
CID:	EN300-748981_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCn6c5nnc6
RUN:	RUN8488
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.35

EN300-7463161_4_1



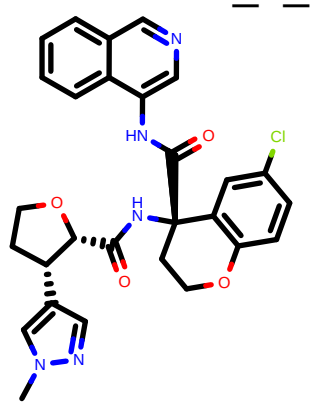
CID:	EN300-7463161_4_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)CCCNC(=O)[C@H]5C[C@H](C5)n6cnnc6)cc1
RUN:	RUN10699
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.35

EN300-77359_1_1



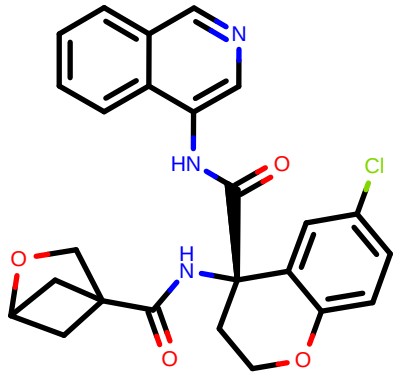
CID:	EN300-77359_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OCCOC
RUN:	RUN2490
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.27

EN300-305454_1_1



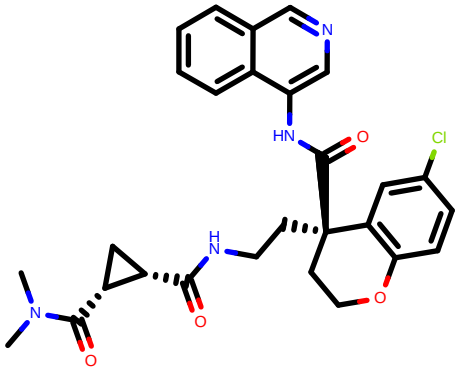
CID:	EN300-305454_1_1
SMILES:	Cn1cc(cn1)[C@@H]2CCO[C@@H]2C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7346
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.36

EN300-1604607_1_1



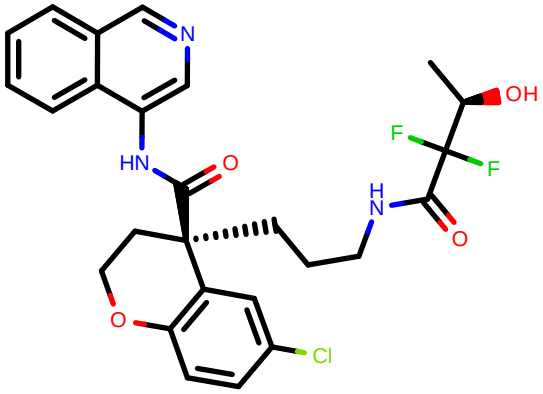
CID:	EN300-1604607_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C56CC(C5)OC6
RUN:	RUN3398
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.28

EN300-253462_3_1



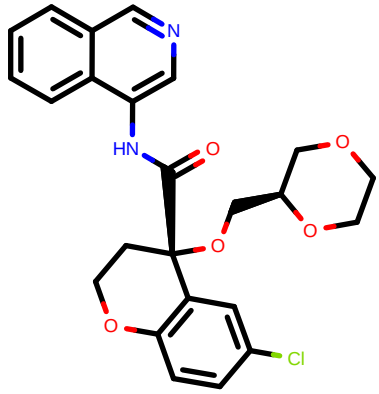
CID:	EN300-253462_3_1
SMILES:	CN(C)C(=O)[C@@H]1C[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4791
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.34

EN300-185398_4_2



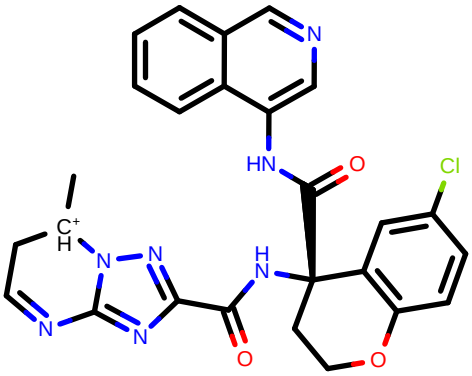
CID:	EN300-185398_4_2
SMILES:	C[C@H](C(C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F)O
RUN:	RUN11151
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.32

EN300-139167_1_2



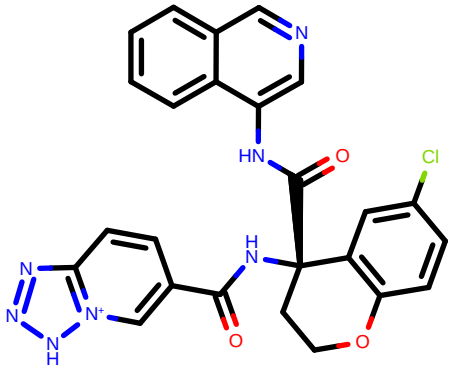
CID:	EN300-139167_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5COCCO5
RUN:	RUN2675
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.29

EN300-00903_1_1



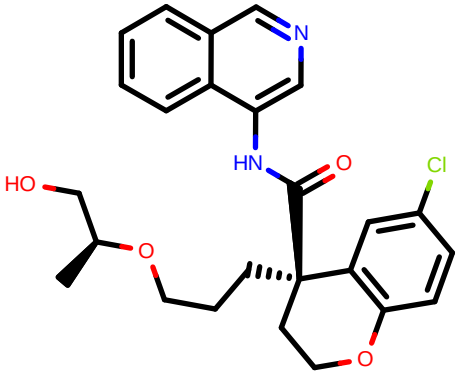
CID:	EN300-00903_1_1
SMILES:	Cc1ccnc2n1nc(n2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8897
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.30

EN300-102853_1_1



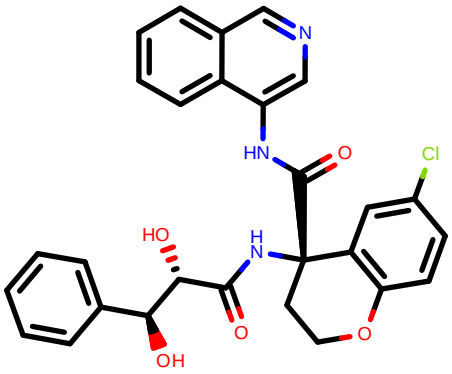
CID:	EN300-102853_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6nnnn6c5
RUN:	RUN6327
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.21

EN300-175186_4_1



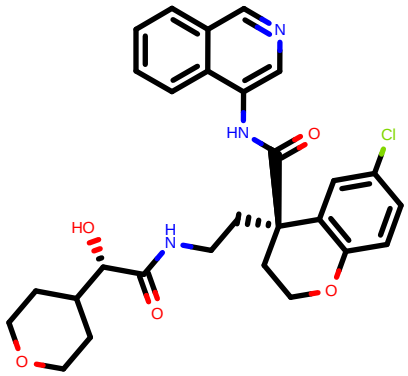
CID:	EN300-175186_4_1
SMILES:	C[C@@H](CO)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN911
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.35

EN300-2923949_1_1



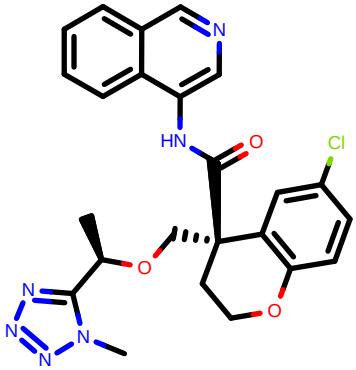
CID:	EN300-2923949_1_1
SMILES:	c1ccc(cc1)[C@@H]([C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O
RUN:	RUN7462
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.27

EN300-6792206_3_1



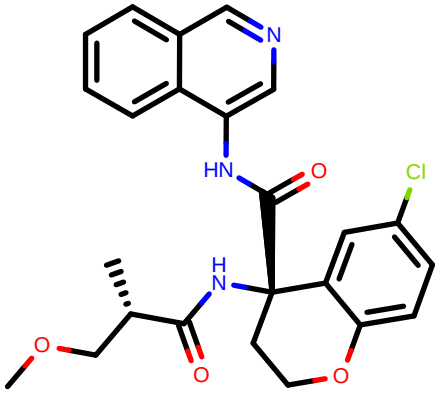
CID:	EN300-6792206_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5CCOCC5)O
RUN:	RUN5642
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.38

EN300-173006_2_2



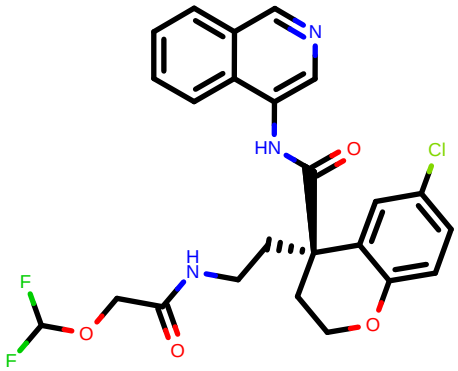
CID:	EN300-173006_2_2
SMILES:	C[C@H](c1nnnn1C)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1502
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.33

EN300-69162_1_1



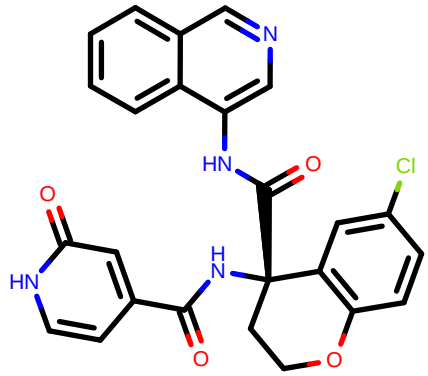
CID:	EN300-69162_1_1
SMILES:	C[C@@H](COC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3454
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.25

EN300-179091_3_1



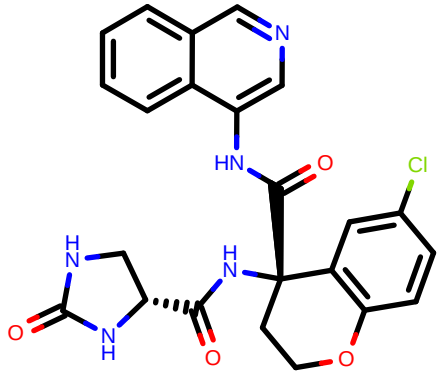
CID:	EN300-179091_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COC(F)F
RUN:	RUN3432
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.24

EN300-97661_1_1



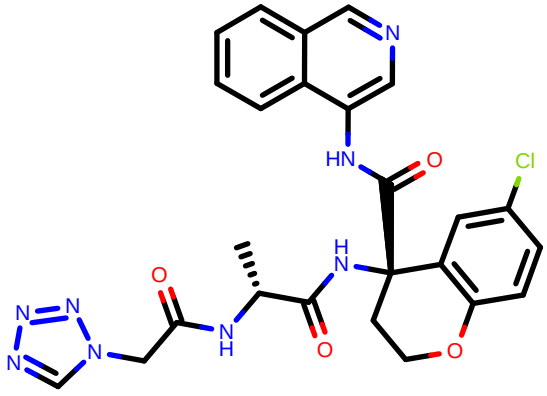
CID:	EN300-97661_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc[nH]c(=O)c5
RUN:	RUN4917
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.27

EN300-222145_1_1



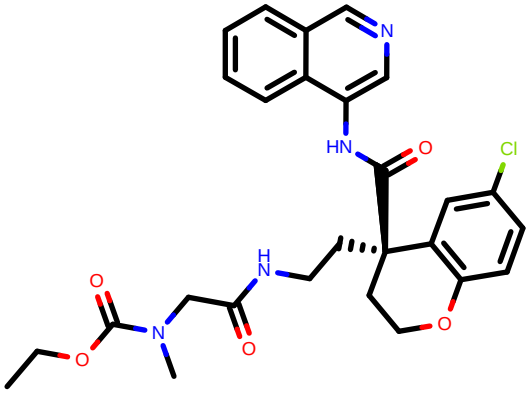
CID:	EN300-222145_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)N5
RUN:	RUN1557
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.21

EN300-649743_1_1



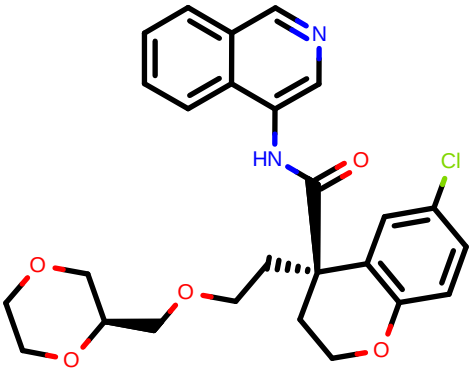
CID:	EN300-649743_1_1
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)Cn5cnnn5
RUN:	RUN5448
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.35

EN300-39101_3_1



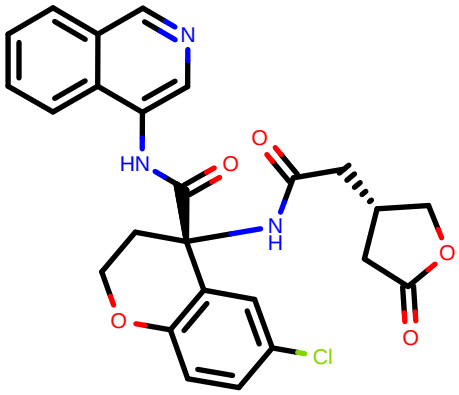
CID:	EN300-39101_3_1
SMILES:	CCOC(=O)N(C)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4535
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.35

EN300-139167_3_1



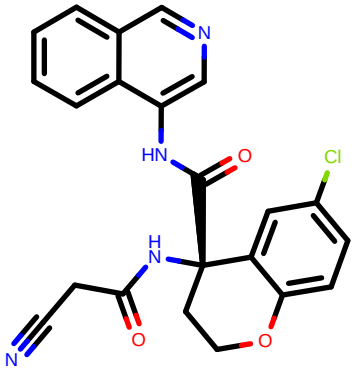
CID:	EN300-139167_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCCO5
RUN:	RUN640
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.27

EN300-109535_1_2



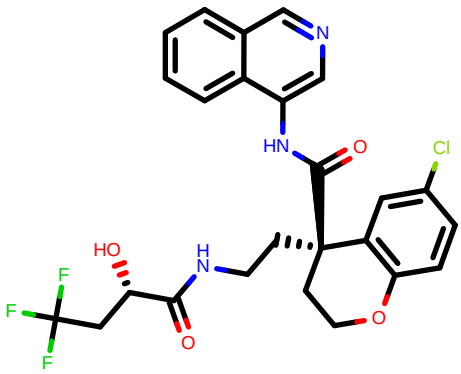
CID:	EN300-109535_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)OC5
RUN:	RUN869
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.29

EN300-19926_1_1



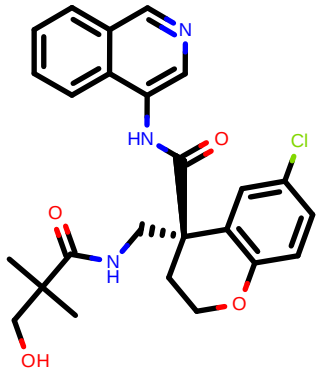
CID:	EN300-19926_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC#N
RUN:	RUN2156
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.17

EN300-1932013_3_2



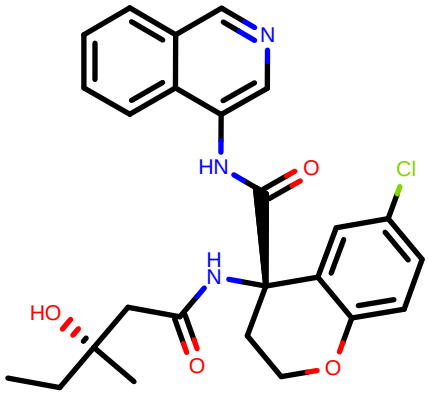
CID:	EN300-1932013_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](CC(F)(F)F)O
RUN:	RUN6190
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.34

EN300-65050_2_1



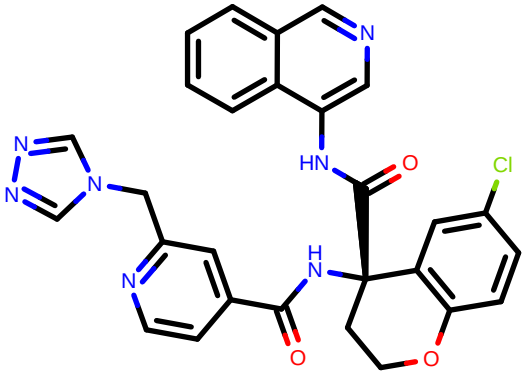
CID:	EN300-65050_2_1
SMILES:	CC(C)(CO)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3059
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.29

EN300-181938_1_2



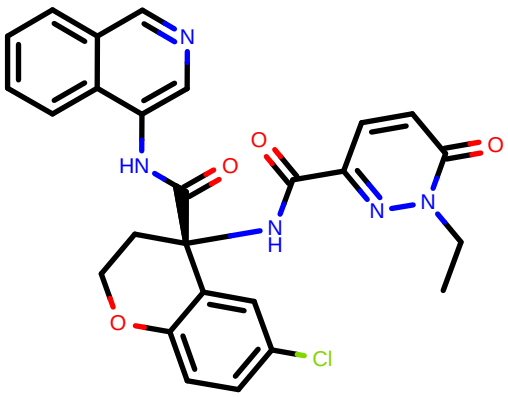
CID:	EN300-181938_1_2
SMILES:	C[C@](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C=C)O
RUN:	RUN4485
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.26

EN300-5309123_1_1



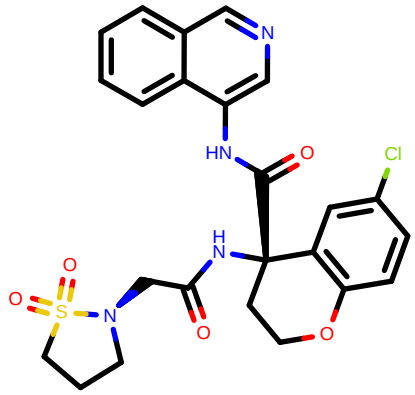
CID:	EN300-5309123_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)Cn6cnnc6
RUN:	RUN7982
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.33

EN300-74314_1_1



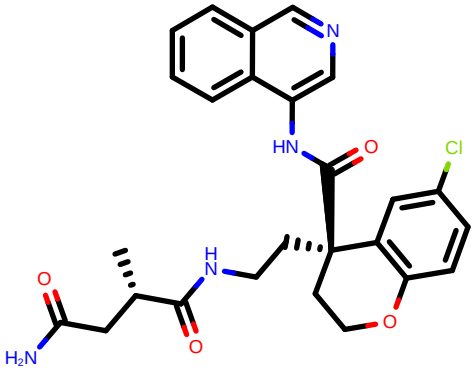
CID:	EN300-74314_1_1
SMILES:	CCn1c(=O)ccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4813
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.24

EN300-43206_1_1



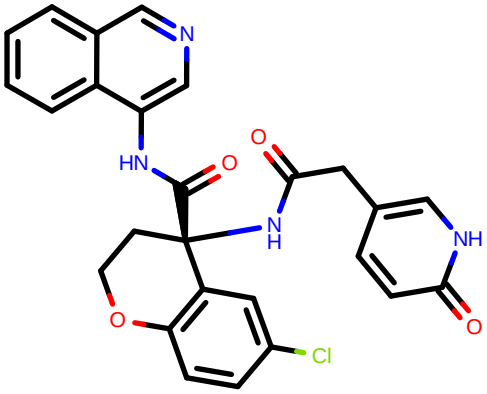
CID:	EN300-43206_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCS5(=O)=O
RUN:	RUN1636
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.31

EN300-202757_3_1



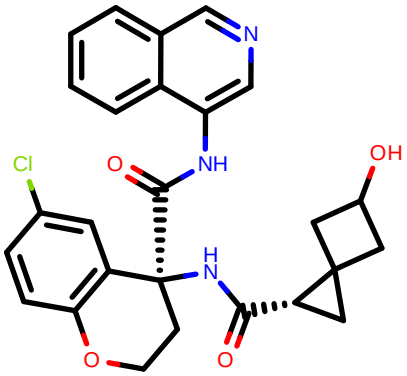
CID:	EN300-202757_3_1
SMILES:	C[C@@H](CC(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1442
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.36

EN300-189672_1_1



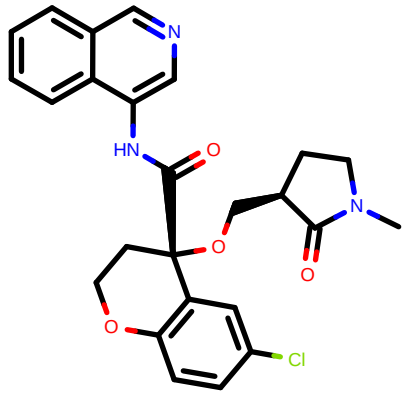
CID:	EN300-189672_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccc(=O)[nH]c5
RUN:	RUN7774
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.22

EN300-1717166_1_2



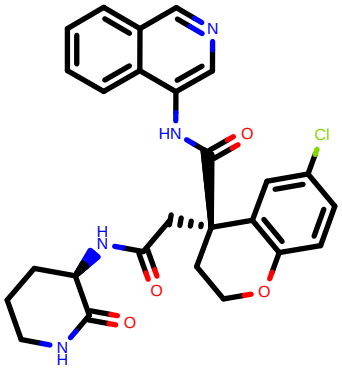
CID:	EN300-1717166_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC56CC(C6)O
RUN:	RUN861
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.25

EN300-260816_1_1



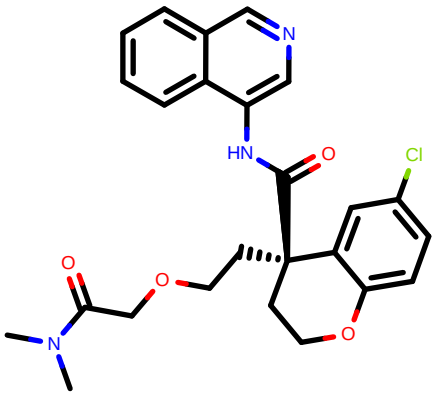
CID:	EN300-260816_1_1
SMILES:	CN1CC[C@@H](C1=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2646
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.30

EN300-60035_1_1



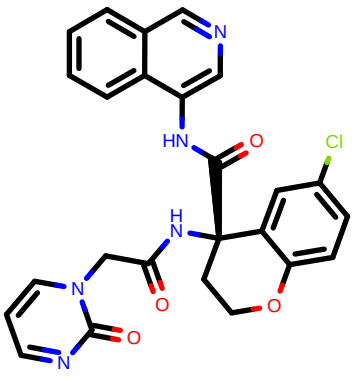
CID:	EN300-60035_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCNC5=O
RUN:	RUN11222
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.25

EN300-216063_3_1



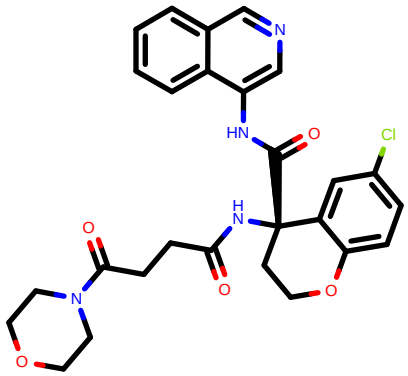
CID:	EN300-216063_3_1
SMILES:	CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1460
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.26

EN300-35789_1_1



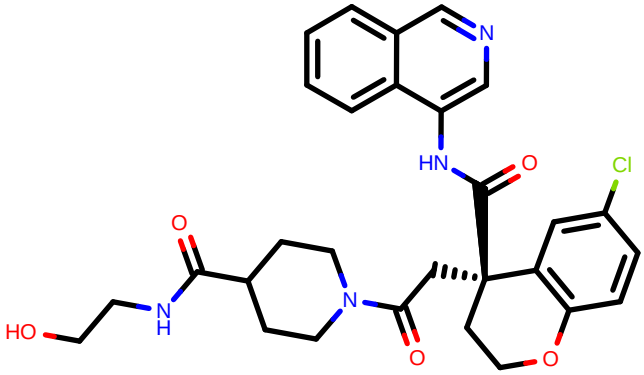
CID:	EN300-35789_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cccnc5=O
RUN:	RUN3877
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.30

EN300-05277_1_1



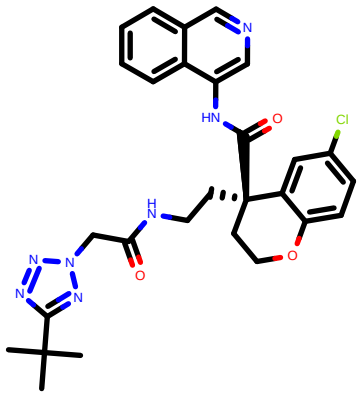
CID:	EN300-05277_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCC(=O)N5CCOCC5
RUN:	RUN5896
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.24

EN300-344753_1_1



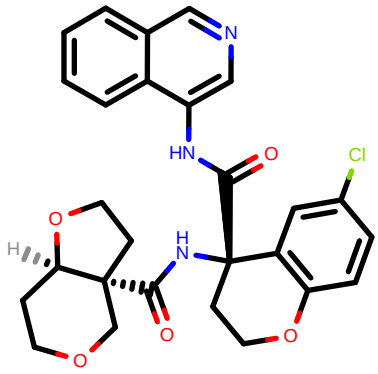
CID:	EN300-344753_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)C(=O)NCCO
RUN:	RUN8000
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.41

EN300-1703143_3_1



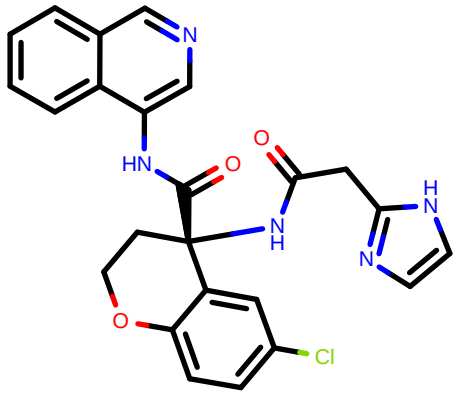
CID:	EN300-1703143_3_1
SMILES:	CC(C)(C)c1nnn(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11192
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.36

EN300-341337_1_1



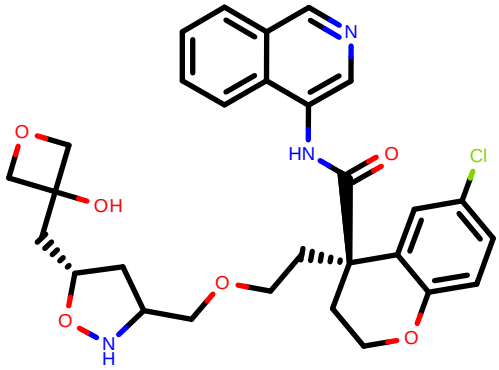
CID:	EN300-341337_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCO[C@@H]5CCOC6
RUN:	RUN4997
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.30

EN300-220527_1_1



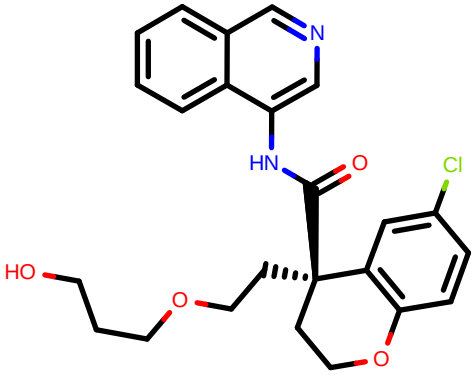
CID:	EN300-220527_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]ccn5
RUN:	RUN6759
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.22

EN300-7457160_3_1



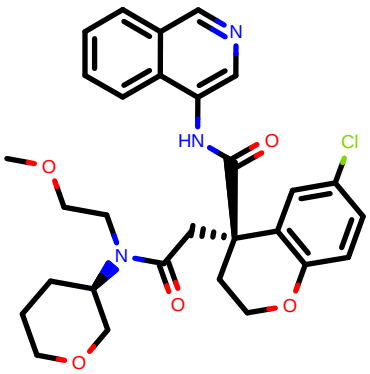
CID:	EN300-7457160_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NO[C@@H](C5)CC6(COC6)O
RUN:	RUN2426
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.31

EN300-221518_3_1



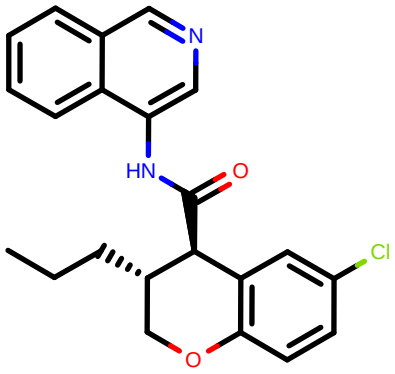
CID:	EN300-221518_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCO
RUN:	RUN1404
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.21

JAG-UCB-706446eb-5_1



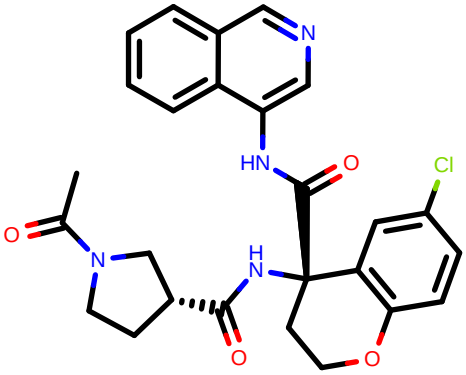
CID:	JAG-UCB-706446eb-5_1
SMILES:	COCCN([C@@H]1CCCOC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN264
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.31

EDJ-MED-e4b030d8-6_1



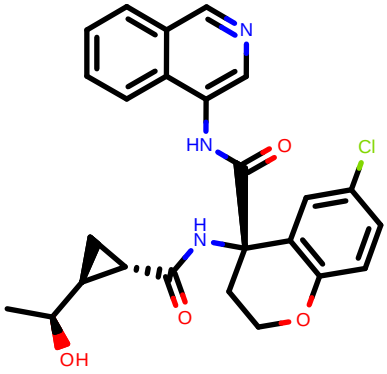
CID:	EDJ-MED-e4b030d8-6_1
SMILES:	CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN7
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.10

EN300-100180_1_2



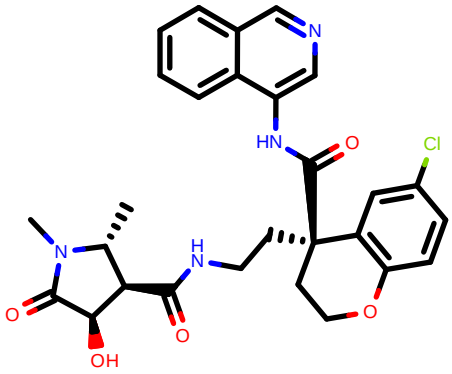
CID:	EN300-100180_1_2
SMILES:	CC(=O)N1CC[C@H](C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7670
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.36

EN300-6729572_1_3



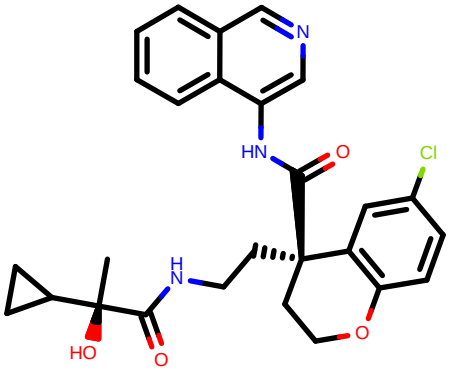
CID:	EN300-6729572_1_3
SMILES:	C[C@@H]([C@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2662
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.20

EN300-378828_3_1



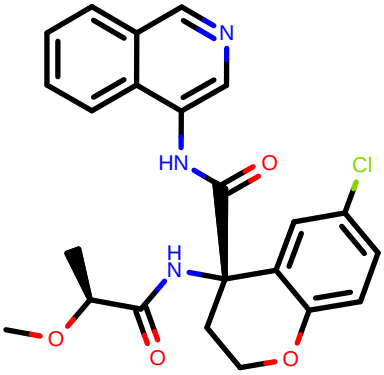
CID:	EN300-378828_3_1
SMILES:	C[C@@H]1[C@H]([C@H](C(=O)N1C)O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10542
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.41

EN300-118760_3_1



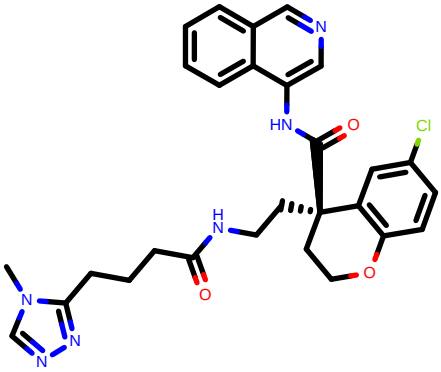
CID:	EN300-118760_3_1
SMILES:	C[C@@](C1CC1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1793
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.37

EN300-258477_1_1



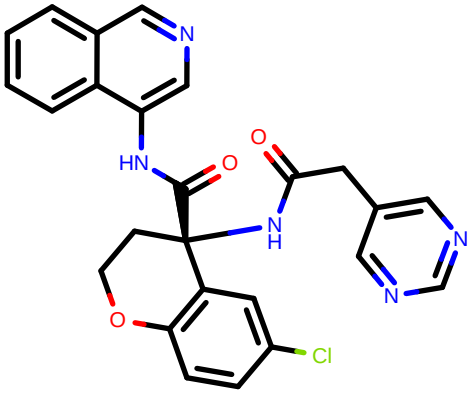
CID:	EN300-258477_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN774
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.24

EN300-6356960_3_1



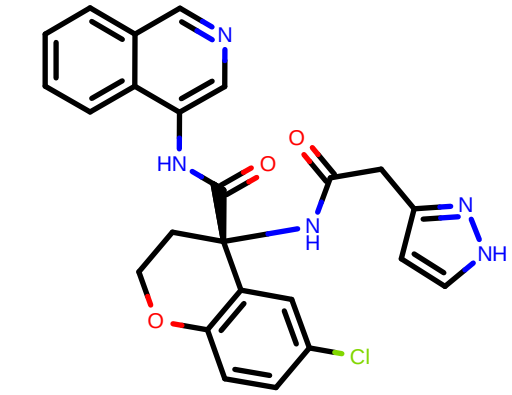
CID:	EN300-6356960_3_1
SMILES:	Cn1cnnc1CCCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6980
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.38

EN300-185751_1_1



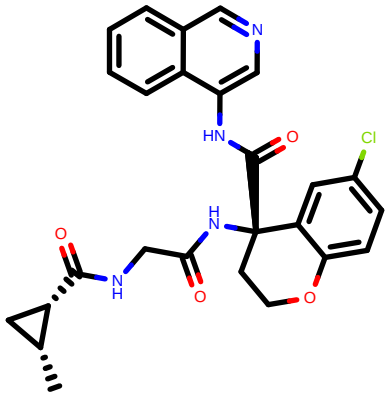
CID:	EN300-185751_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cncnc5
RUN:	RUN8054
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.28

VLA-UCB-34f3ed0c-4_1



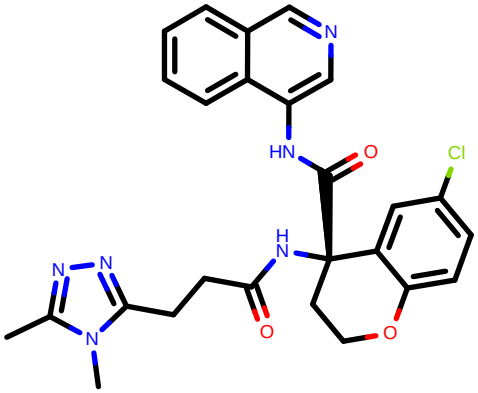
CID:	VLA-UCB-34f3ed0c-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cc[nH]n5
RUN:	RUN266
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.21

EN300-30768_1_1



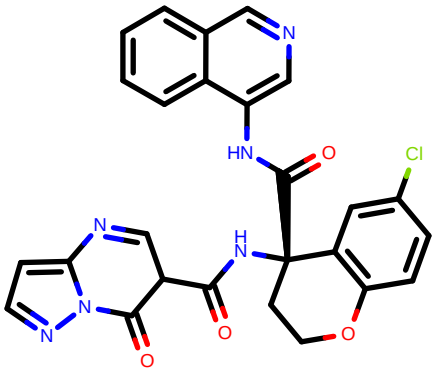
CID:	EN300-30768_1_1
SMILES:	C[C@@H]1C[C@@H]1C(=O)NCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3542
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.34

EN300-1721328_1_1



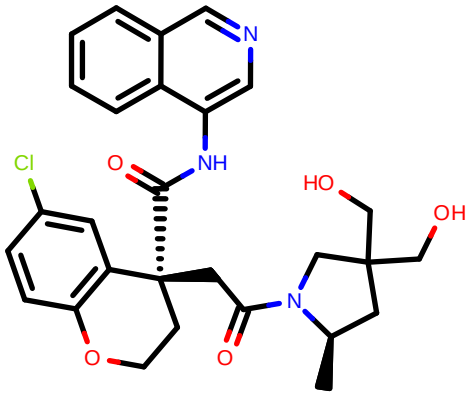
CID:	EN300-1721328_1_1
SMILES:	Cc1nnc(n1C)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6822
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.29

EN300-220228_1_1



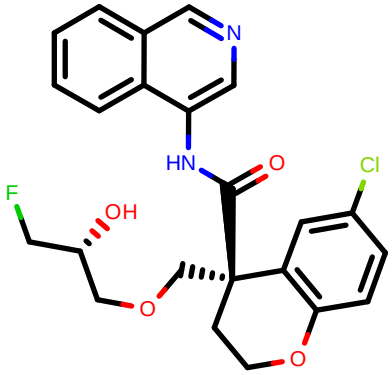
CID:	EN300-220228_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6ccnn6c5O
RUN:	RUN8242
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.28

EN300-6495717_1_1



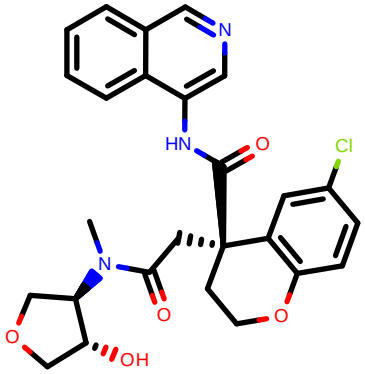
CID:	EN300-6495717_1_1
SMILES:	C[C@@H]1CC(CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(CO)CO
RUN:	RUN4055
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.40

EN300-1968342_2_2



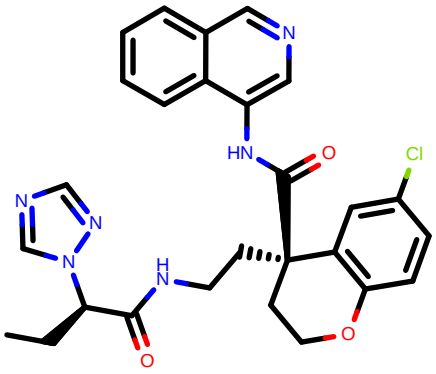
CID:	EN300-1968342_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O
RUN:	RUN514
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.34

EN300-371682_1_1



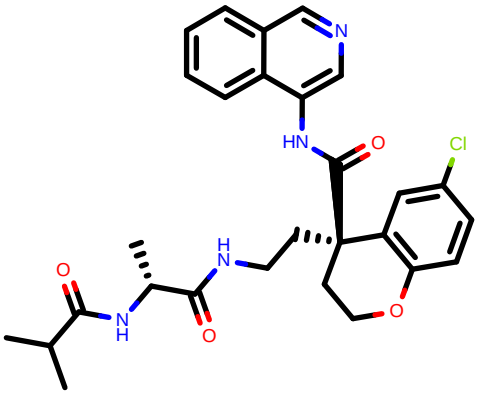
CID:	EN300-371682_1_1
SMILES:	CN([C@@H]1COC[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10065
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.27

EN300-651307_3_2



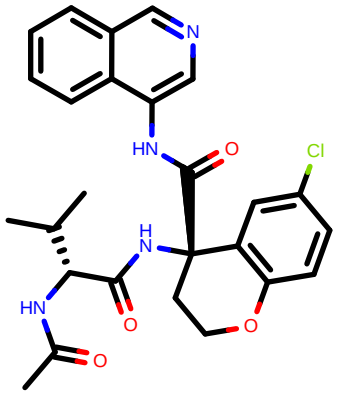
CID:	EN300-651307_3_2
SMILES:	CC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN3612
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.38

EN300-31184_3_2



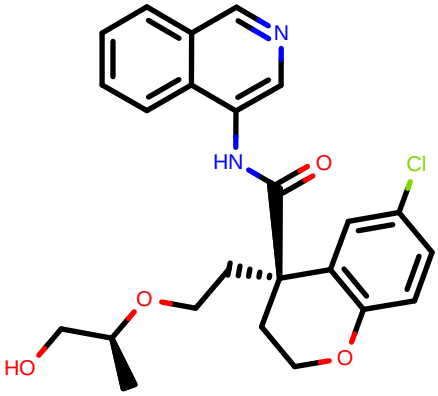
CID:	EN300-31184_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C(C)C
RUN:	RUN8970
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.34

EN300-16582_1_2



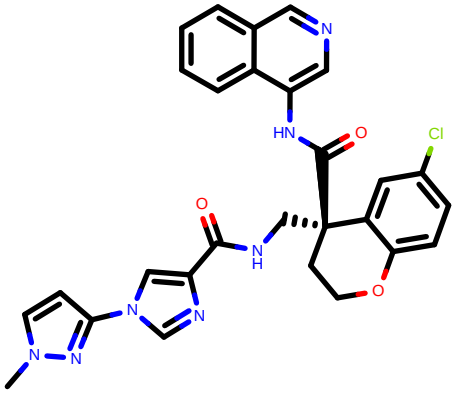
CID:	EN300-16582_1_2
SMILES:	CC(C)[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN3570
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.28

EN300-175186_3_1



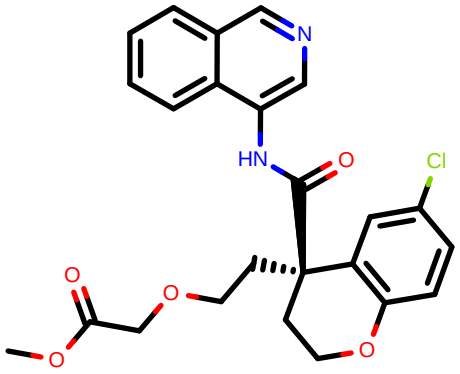
CID:	EN300-175186_3_1
SMILES:	C[C@@H](CO)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1172
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.27

EN300-1726340_2_1



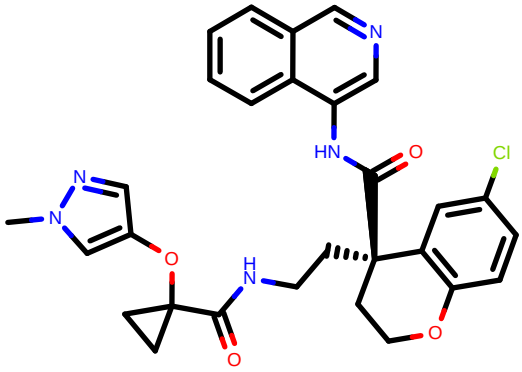
CID:	EN300-1726340_2_1
SMILES:	Cn1ccc(n1)n2cc(nc2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8803
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.33

EN300-19700_3_1



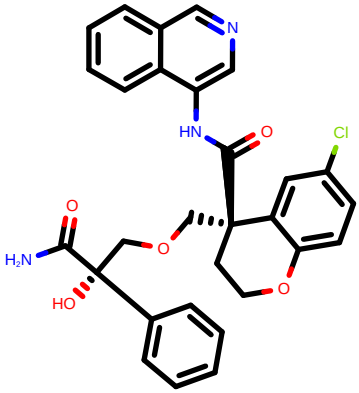
CID:	EN300-19700_3_1
SMILES:	COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1571
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.22

EN300-7352812_3_1



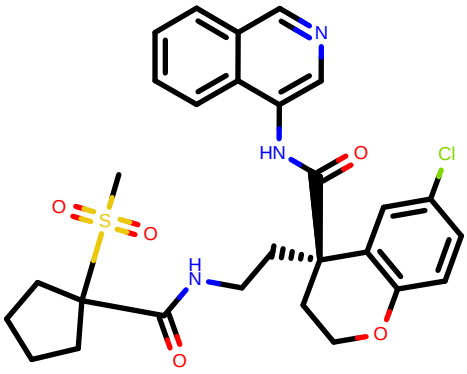
CID:	EN300-7352812_3_1
SMILES:	Cn1cc(cn1)OC2(CC2)C(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3088
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.33

EN300-248526_2_2



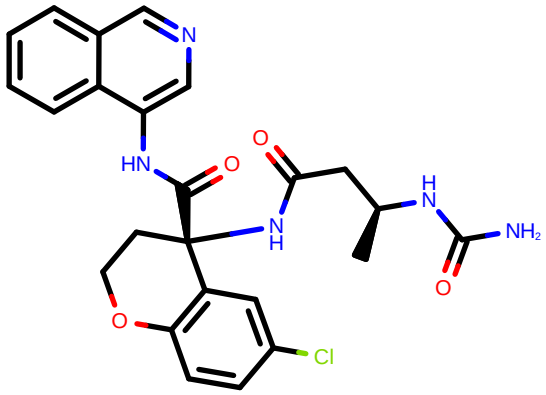
CID:	EN300-248526_2_2
SMILES:	c1ccc(cc1)[C@](COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(C(=O)N)O
RUN:	RUN1909
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.37

EN300-60831_3_1



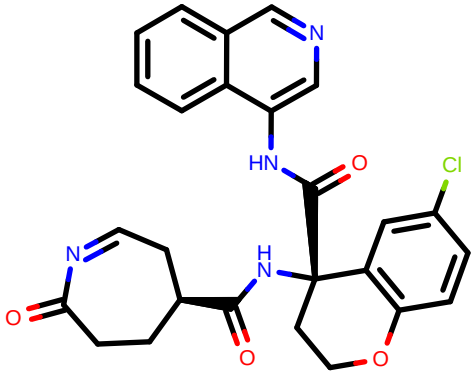
CID:	EN300-60831_3_1
SMILES:	CS(=O)(=O)C1(CCCC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3348
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.49

EN300-268198_1_1



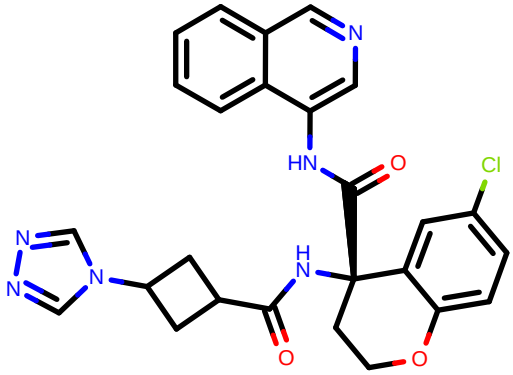
CID:	EN300-268198_1_1
SMILES:	C[C@@H](CC(=O)N[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN989
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.22

EN300-152337_1_2



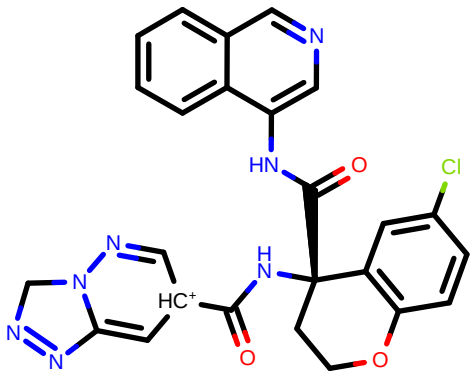
CID:	EN300-152337_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCC(=O)NCC5
RUN:	RUN4149
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.30

EN300-7463161_1_1



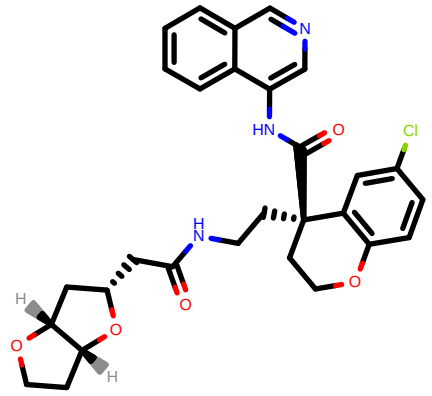
CID:	EN300-7463161_1_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@H]5C[C@H](C5)n6cnnc6)cc1
RUN:	RUN3030
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.29

EN300-7438185_1_1



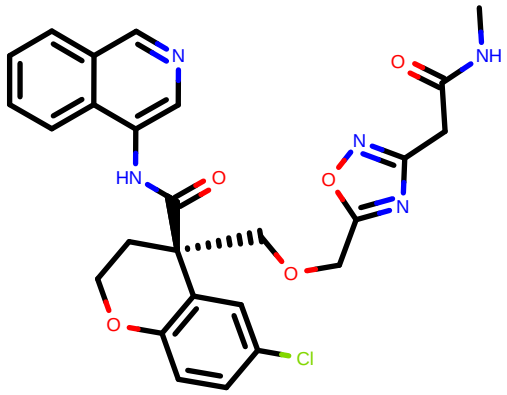
CID:	EN300-7438185_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6nncn6nc5
RUN:	RUN8810
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.25

EN300-7355519_3_6



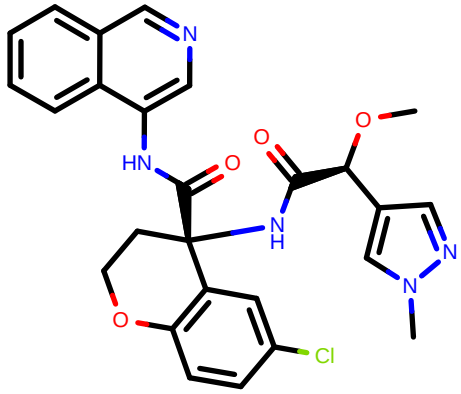
CID:	EN300-7355519_3_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5C[C@@H]6[C@H](O5)CCO6
RUN:	RUN11136
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.31

EN300-99983_2_1



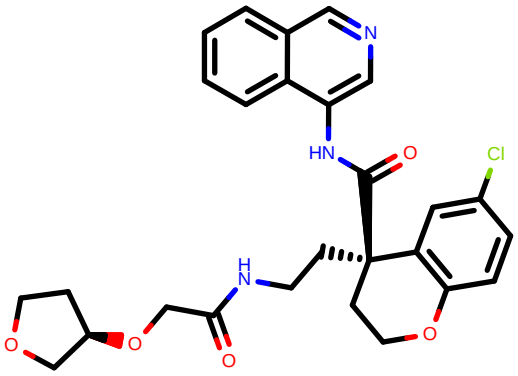
CID:	EN300-99983_2_1
SMILES:	CNC(=O)Cc1nc(on1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2428
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.33

EN300-198240_1_1



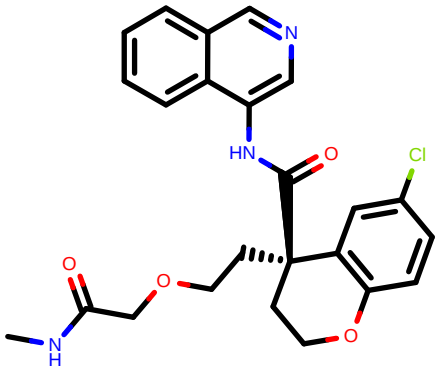
CID:	EN300-198240_1_1
SMILES:	Cn1cc(cn1)[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN7022
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.33

EN300-99391_3_1



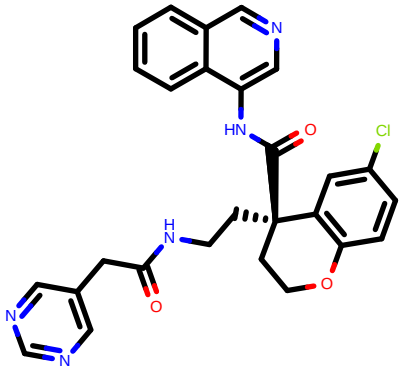
CID:	EN300-99391_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CO[C@@H]5CCOC5
RUN:	RUN6613
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.32

EN300-2977549_3_1



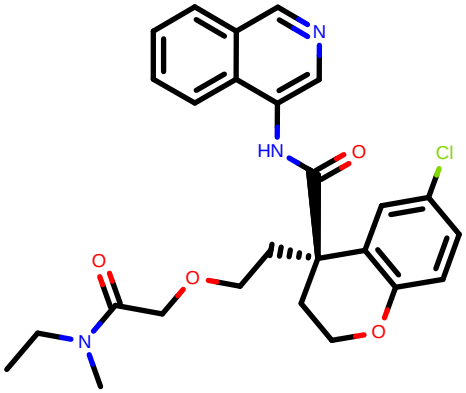
CID:	EN300-2977549_3_1
SMILES:	CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1739
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.26

EN300-185751_3_1



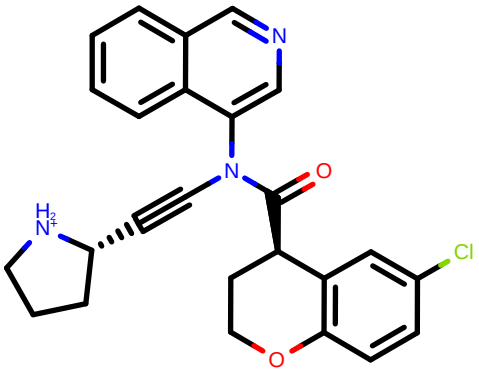
CID:	EN300-185751_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cncnc5
RUN:	RUN8316
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.32

EN300-1253122_3_1



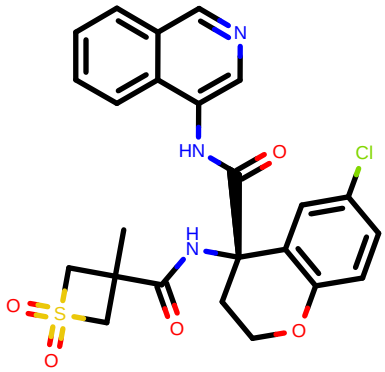
CID:	EN300-1253122_3_1
SMILES:	CCN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN576
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.28

DAR-DIA-5ff57136-12_1



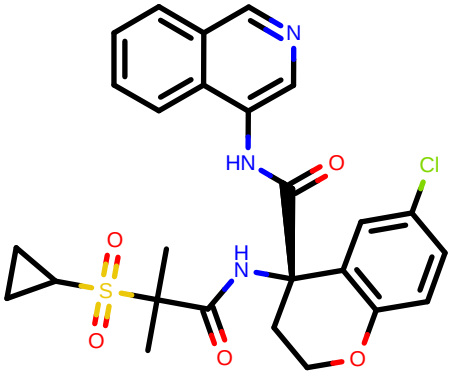
CID:	DAR-DIA-5ff57136-12_1
SMILES:	c1ccc2c(c1)cncc2N(C#C[C@@H]3CCCN3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN173
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.21

EN300-1718364_1_1



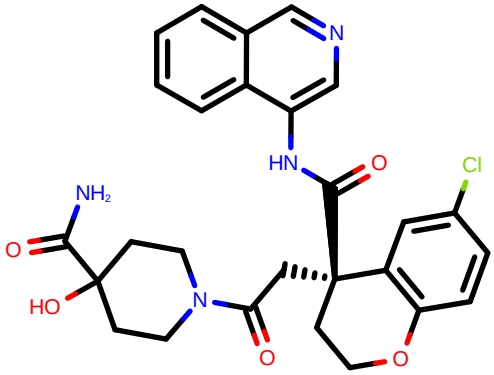
CID:	EN300-1718364_1_1
SMILES:	CC1(CS(=O)(=O)C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2954
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.26

EN300-193399_1_1



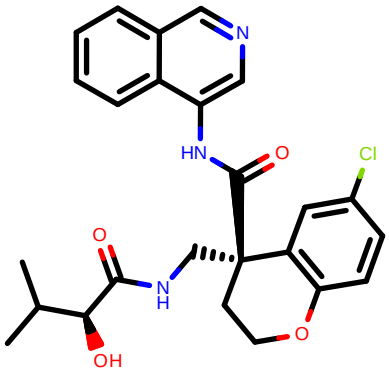
CID:	EN300-193399_1_1
SMILES:	CC(C)(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C5CC5
RUN:	RUN3114
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.47

EN300-203306_1_1



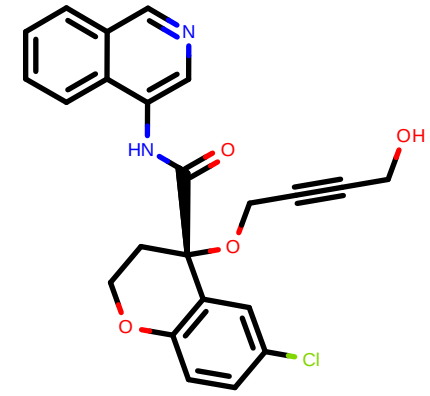
CID:	EN300-203306_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)(C(=O)N)O
RUN:	RUN1290
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.37

EN300-199359_2_1



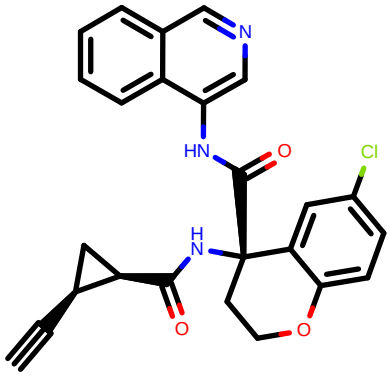
CID:	EN300-199359_2_1
SMILES:	CC(C)[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5258
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.30

EN300-83766_1_1



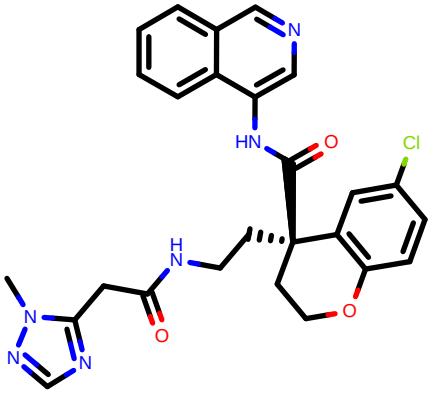
CID:	EN300-83766_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC#CCO
RUN:	RUN293
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.19

EN300-254137_1_1



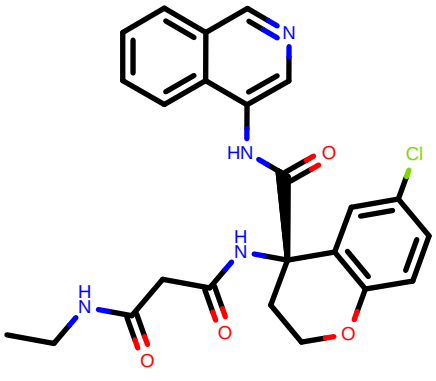
CID:	EN300-254137_1_1
SMILES:	C#C[C@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4757
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.20

EN300-209316_3_1



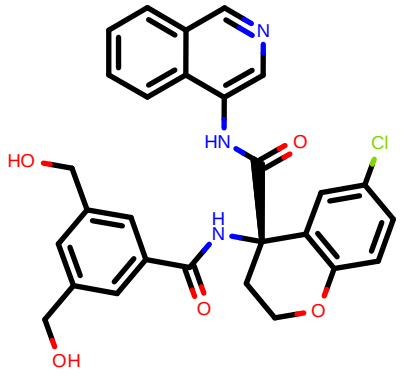
CID:	EN300-209316_3_1
SMILES:	Cn1c(ncn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10738
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.29

EN300-129455_1_1



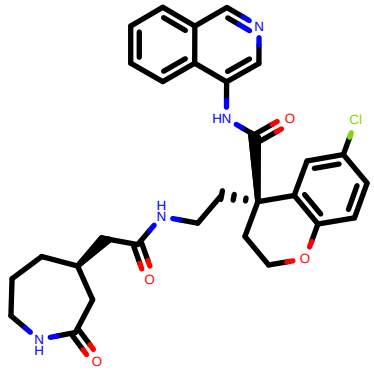
CID:	EN300-129455_1_1
SMILES:	CCNC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4821
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.29

EN300-211158_1_1



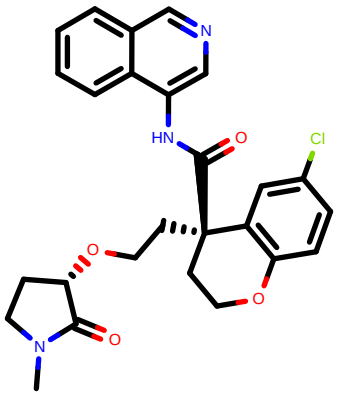
CID:	EN300-211158_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cc(c5)CO)CO
RUN:	RUN5436
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.29

EN300-195590_3_1



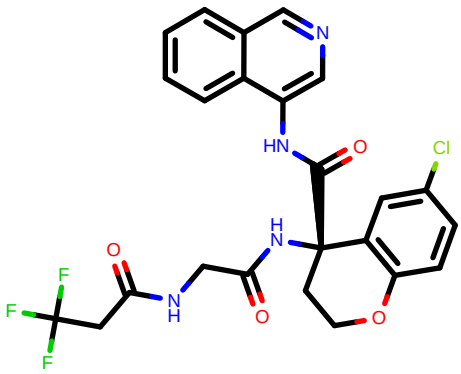
CID:	EN300-195590_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CCCNC(=O)C5
RUN:	RUN9270
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.32

EN300-98648_3_1



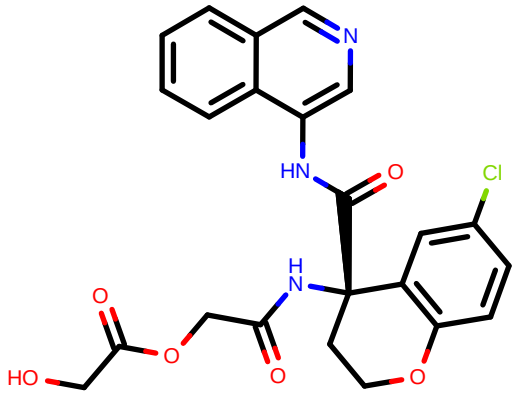
CID:	EN300-98648_3_1
SMILES:	CN1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2123
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.24

EN300-43939_1_1



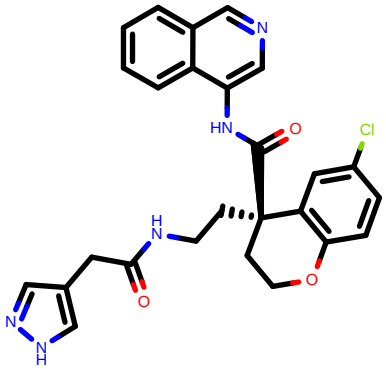
CID:	EN300-43939_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)CC(F)(F)F
RUN:	RUN6020
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.24

EN300-7459916_1_1



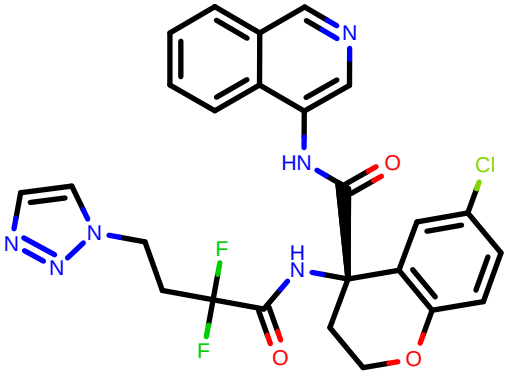
CID:	EN300-7459916_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COC(=O)CO
RUN:	RUN1660
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.31

EN300-1589101_3_1



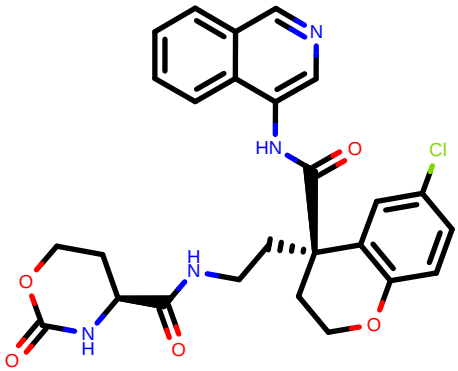
CID:	EN300-1589101_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5c[nH]nc5
RUN:	RUN8580
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.27

EN300-6474220_1_1



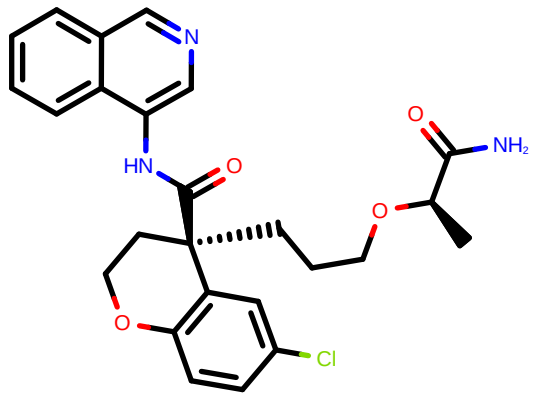
CID:	EN300-6474220_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CCn5ccnn5)(F)F
RUN:	RUN1461
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.32

EN300-249804_3_1



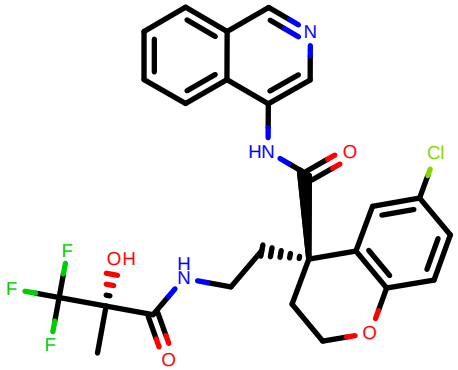
CID:	EN300-249804_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCOC(=O)N5
RUN:	RUN9191
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.25

EN300-17381_4_2



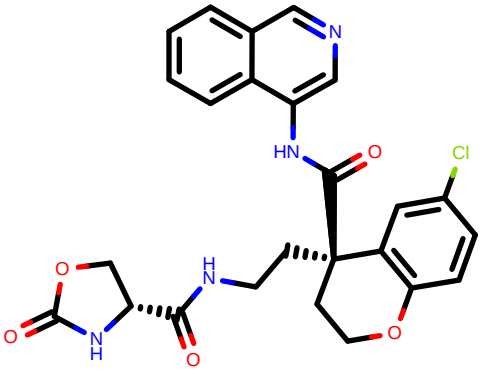
CID:	EN300-17381_4_2
SMILES:	C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN396
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.27

EN300-159633_3_2



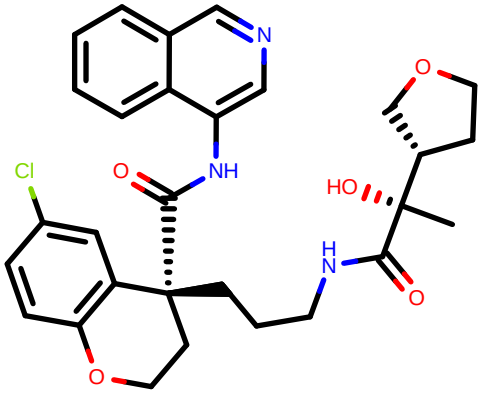
CID:	EN300-159633_3_2
SMILES:	C[C@](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN2864
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.30

EN300-305996_3_1



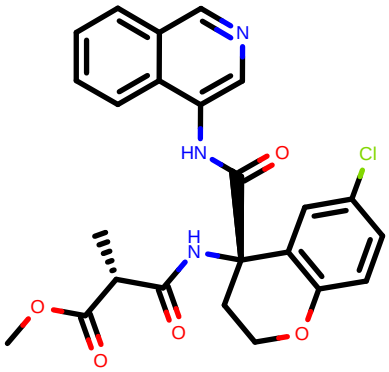
CID:	EN300-305996_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5COC(=O)N5
RUN:	RUN11040
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.24

EN300-217494_4_4



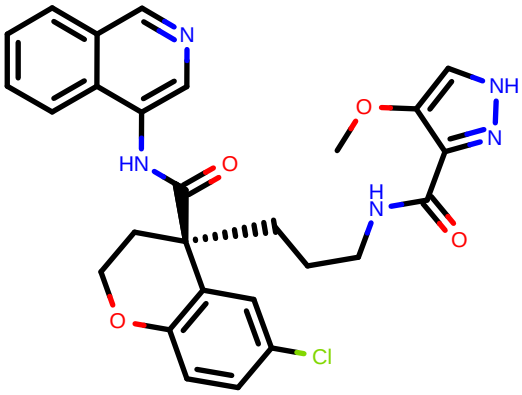
CID:	EN300-217494_4_4
SMILES:	C[C@]([C@H]1CCOC1)(C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10433
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.32

EN300-1239522_1_2



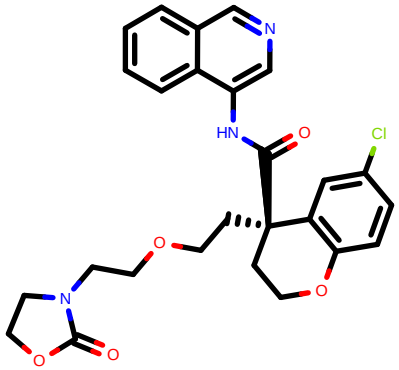
CID:	EN300-1239522_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN4873
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.24

EN300-7439284_4_1



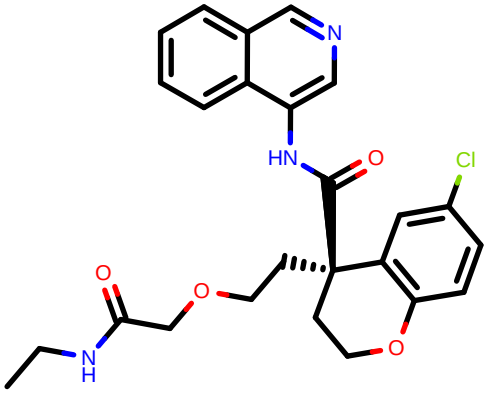
CID:	EN300-7439284_4_1
SMILES:	COc1cn[nH]c1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9337
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.35

EN300-370967_3_1



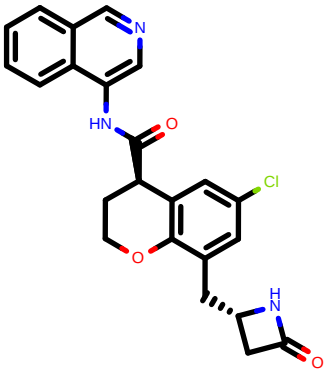
CID:	EN300-370967_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCN5CCOC5=O
RUN:	RUN1899
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.33

EN300-7003350_3_1



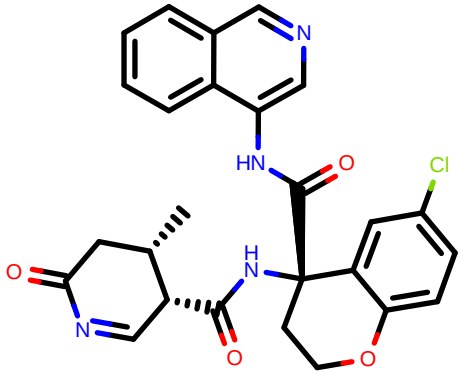
CID:	EN300-7003350_3_1
SMILES:	CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1500
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.24

DAR-DIA-6a508060-5_3



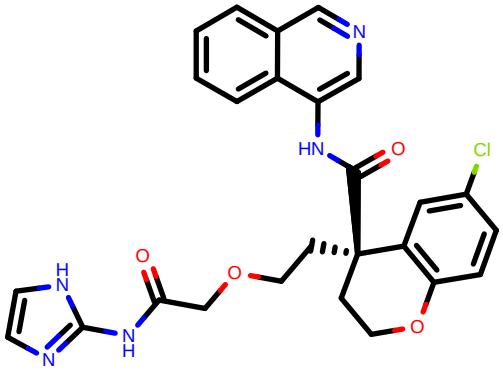
CID:	DAR-DIA-6a508060-5_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC(=O)N5)Cl
RUN:	RUN218
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.18

EN300-95698_1_4



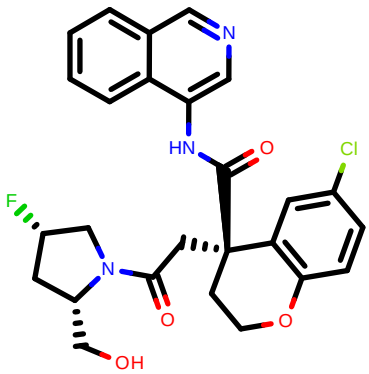
CID:	EN300-95698_1_4
SMILES:	C[C@H]1CC(=O)NC[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5065
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.27

EN300-331993_3_1



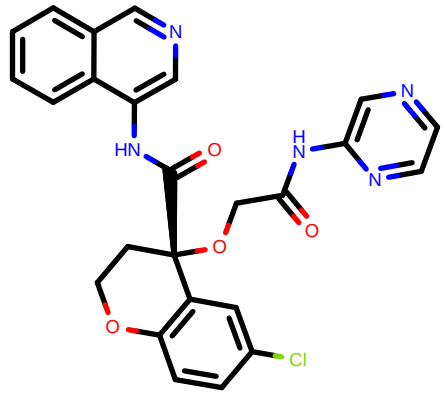
CID:	EN300-331993_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)Nc5[nH]ccn5
RUN:	RUN2107
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.27

EN300-244659_1_1



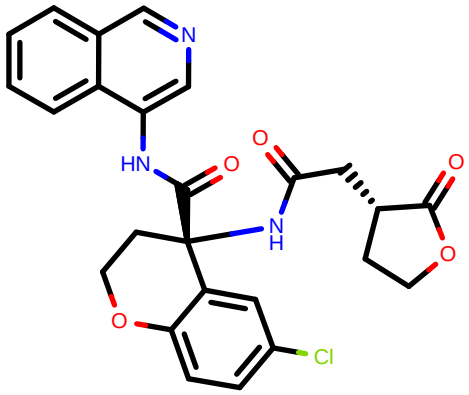
CID:	EN300-244659_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C[C@H]5CO)F
RUN:	RUN8744
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.29

EN300-105267_1_1



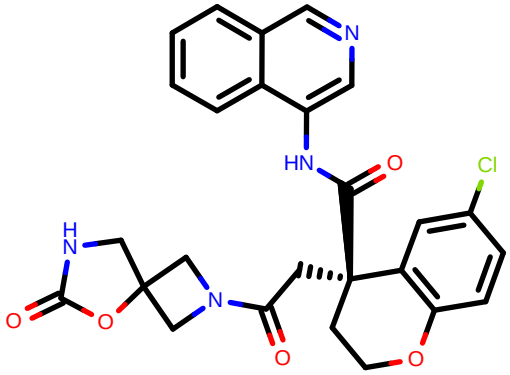
CID:	EN300-105267_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)Nc5cnccn5
RUN:	RUN676
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.25

EN300-1072972_1_2



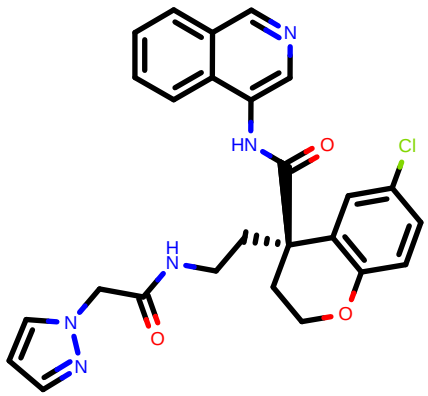
CID:	EN300-1072972_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCOC5=O
RUN:	RUN6072
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.24

EN300-6494361_1_1



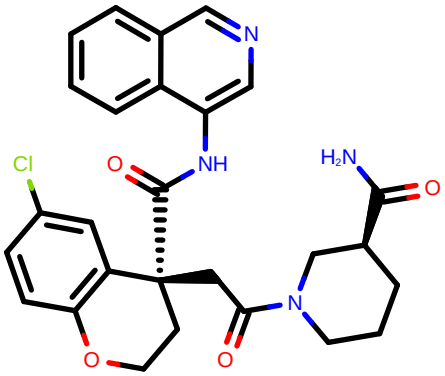
CID:	EN300-6494361_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CNC(=O)O6
RUN:	RUN9167
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.30

EN300-23942_3_1



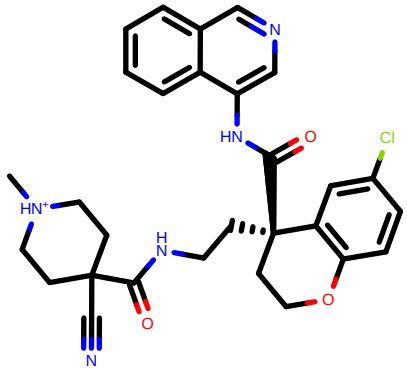
CID:	EN300-23942_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cccn5
RUN:	RUN9039
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.27

EN300-18610_1_1



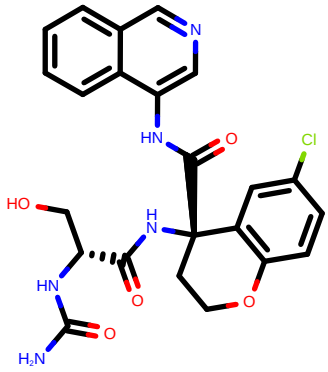
CID:	EN300-18610_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H](C5)C(=O)N
RUN:	RUN2452
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.38

EN300-7473378_3_1



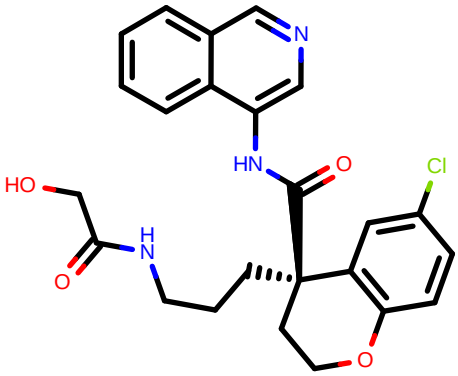
CID:	EN300-7473378_3_1
SMILES:	CN1CCC(CC1)(C#N)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6114
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.41

EN300-10170_1_1



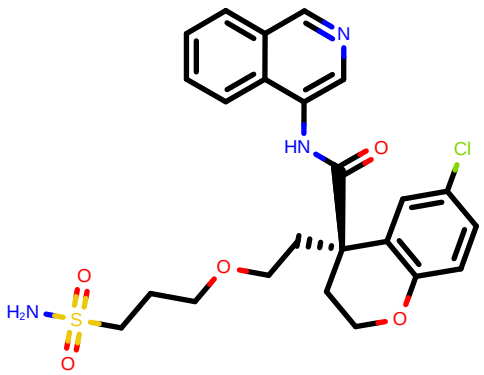
CID:	EN300-10170_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CO)NC(=O)N
RUN:	RUN5093
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.24

EN300-19242_4_1



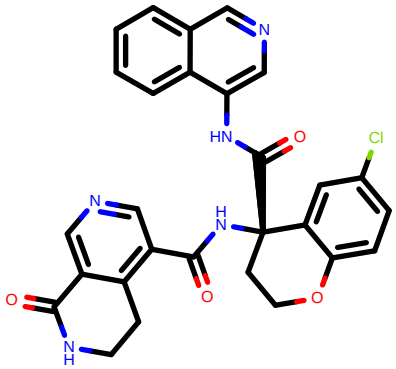
CID:	EN300-19242_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CO
RUN:	RUN9339
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.30

EN300-79588_3_1



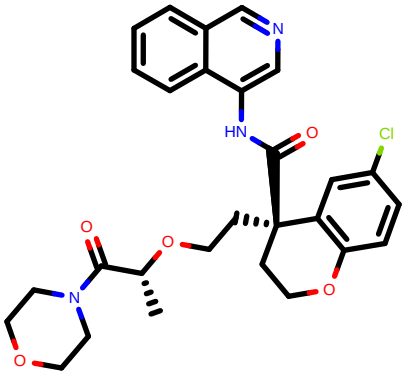
CID:	EN300-79588_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCS(=O)(=O)N
RUN:	RUN2243
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.30

EN300-314274_1_1



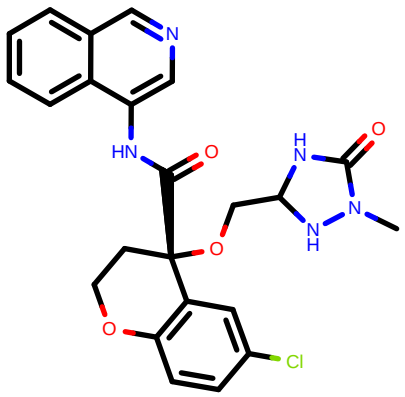
CID:	EN300-314274_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncc6c5CCNC6=O
RUN:	RUN8638
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.30

EN300-05754_3_2



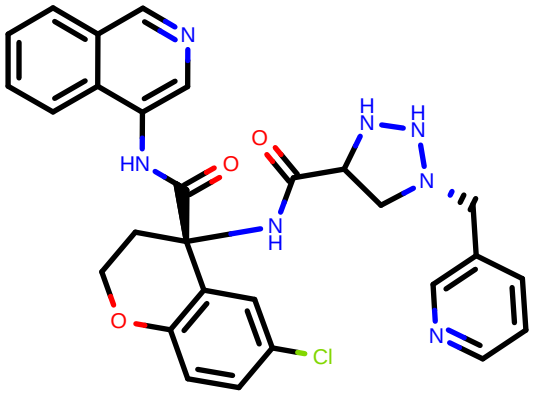
CID:	EN300-05754_3_2
SMILES:	C[C@H](C(=O)N1CCOCC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1803
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.27

EN300-124918_1_1



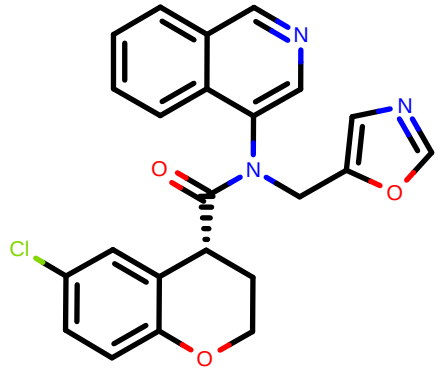
CID:	EN300-124918_1_1
SMILES:	Cn1c(=O)[nH]c(n1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN684
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.21

EN300-91314_1_1



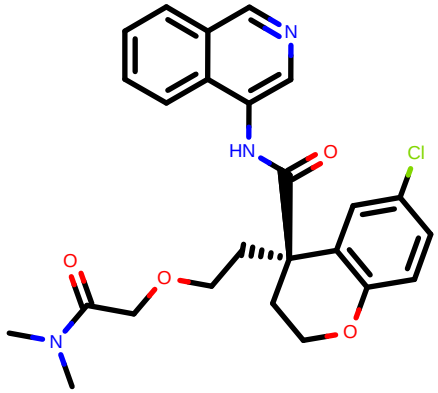
CID:	EN300-91314_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)Cc6cccnc6
RUN:	RUN7962
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.28

ALP-UNI-44c99a80-3_1



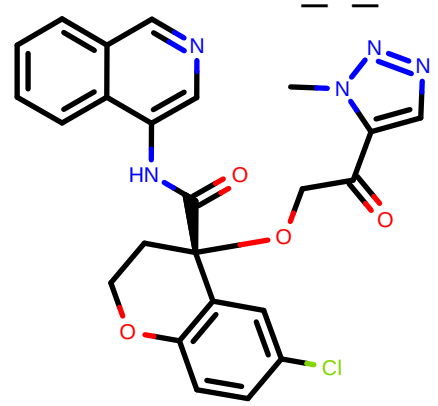
CID:	ALP-UNI-44c99a80-3_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN229
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.22

EN300-216063_3_1



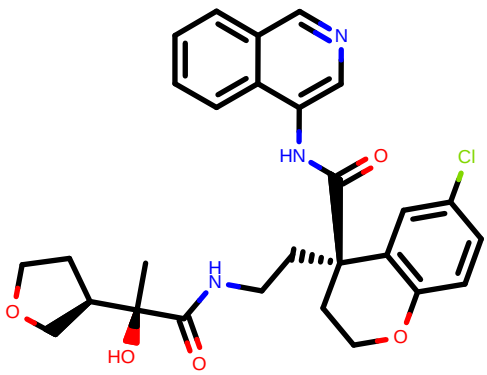
CID:	EN300-216063_3_1
SMILES:	CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1468
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.26

EN300-204936_1_1



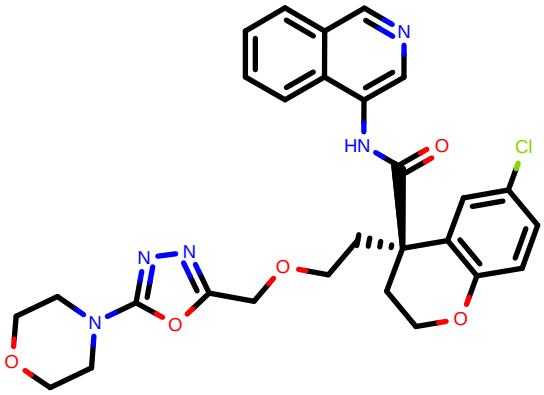
CID:	EN300-204936_1_1
SMILES:	Cn1c(cnn1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN944
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.24

EN300-217494_3_1



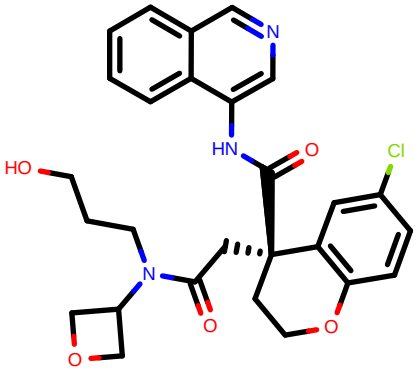
CID:	EN300-217494_3_1
SMILES:	C[C@@][[C@@H]1CCOC1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3648
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.27

EN300-6486576_3_1



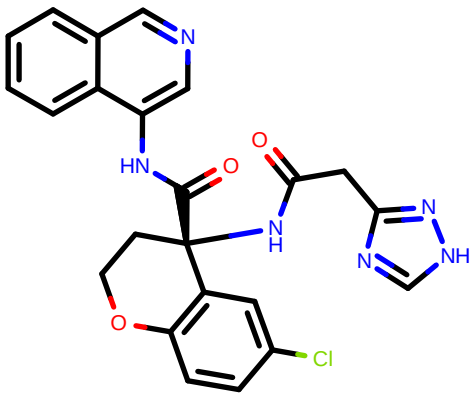
CID:	EN300-6486576_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nnc(o5)N6CCOCC6
RUN:	RUN2524
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.24

EN300-1725529_1_1



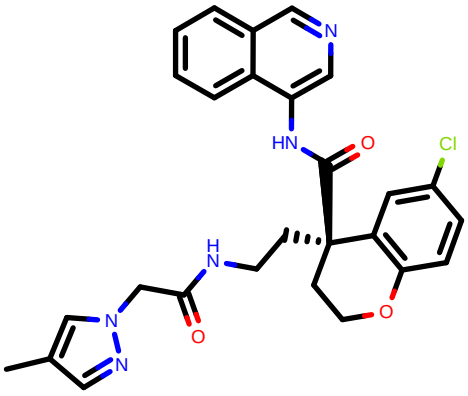
CID:	EN300-1725529_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCCO)C5COC5
RUN:	RUN9488
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.33

EN300-96159_1_1



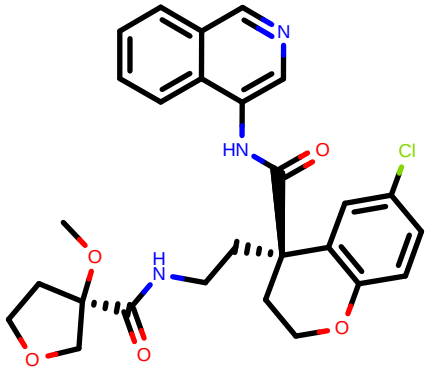
CID:	EN300-96159_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]cnn5
RUN:	RUN5500
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.22

EN300-51832_3_1



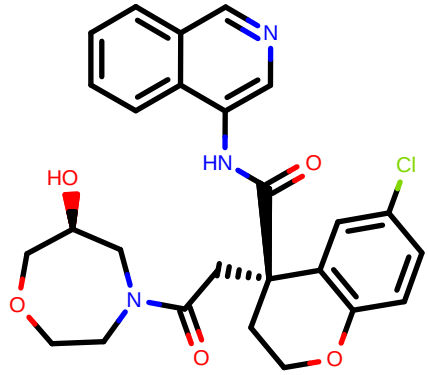
CID:	EN300-51832_3_1
SMILES:	Cc1cnn(c1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9894
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.30

EN300-174668_3_1



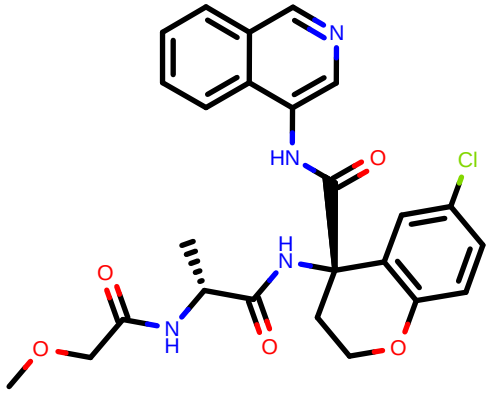
CID:	EN300-174668_3_1
SMILES:	CO[C@@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2748
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.44

EN300-233951_1_2



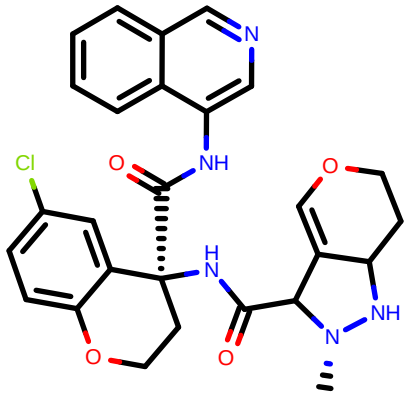
CID:	EN300-233951_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)O
RUN:	RUN1977
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.33

EN300-31183_1_2



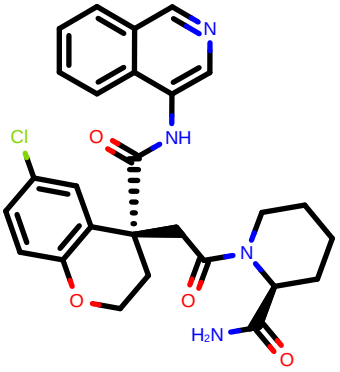
CID:	EN300-31183_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)COC
RUN:	RUN5516
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.36

EN300-6481960_1_1



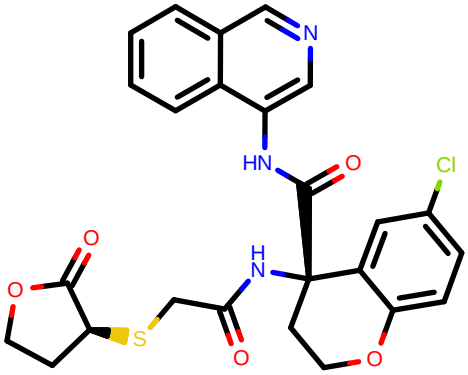
CID:	EN300-6481960_1_1
SMILES:	Cn1c(c2c(n1)CCOC2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8939
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.30

EN300-34542_1_2



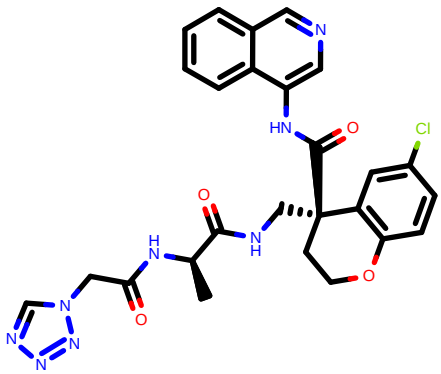
CID:	EN300-34542_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5C(=O)N
RUN:	RUN9264
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.43

EN300-113218_1_2



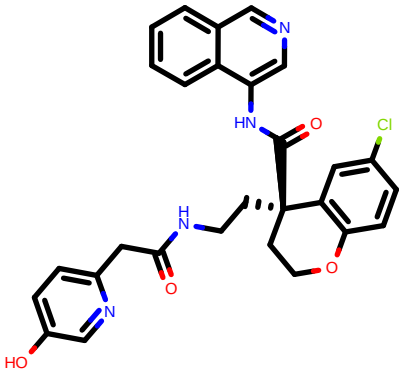
CID:	EN300-113218_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CS[C@H]5CCOC5=O
RUN:	RUN513
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.29

EN300-649743_2_1



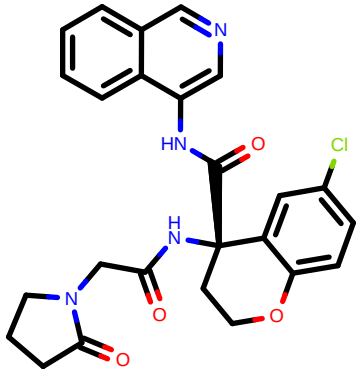
CID:	EN300-649743_2_1
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)Cn5cnnn5
RUN:	RUN1161
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.39

EN300-188341_3_1



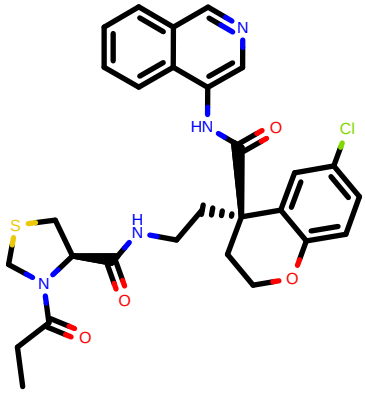
CID:	EN300-188341_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(cn5)O
RUN:	RUN9590
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.37

EN300-11934_1_1



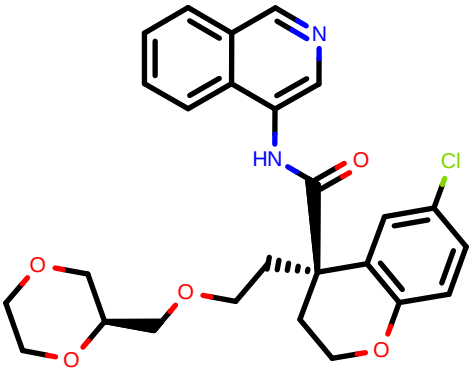
CID:	EN300-11934_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC5=O
RUN:	RUN1405
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.29

EN300-1697005_3_1



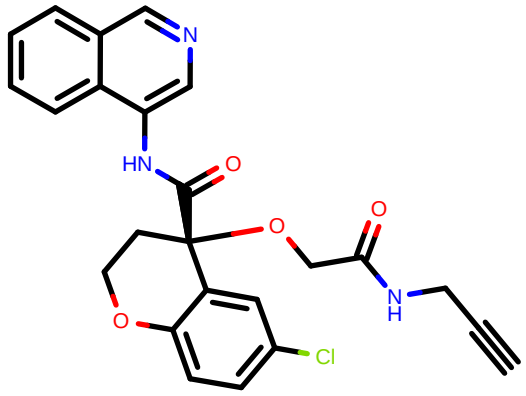
CID:	EN300-1697005_3_1
SMILES:	CCC(=O)N1CSC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4603
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.34

EN300-139167_3_1



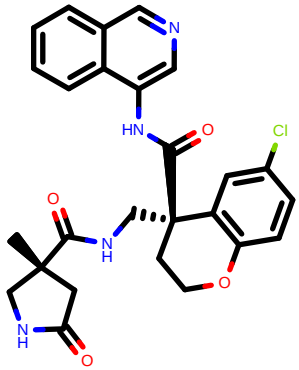
CID:	EN300-139167_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5COCCO5
RUN:	RUN656
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.34

EN300-1659582_1_1



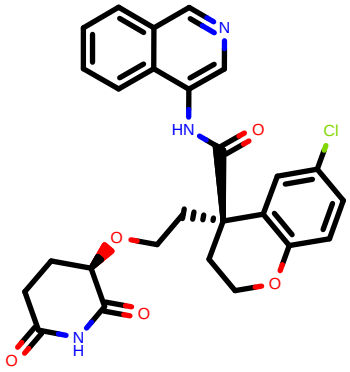
CID:	EN300-1659582_1_1
SMILES:	C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN453
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.27

EN300-132157_2_2



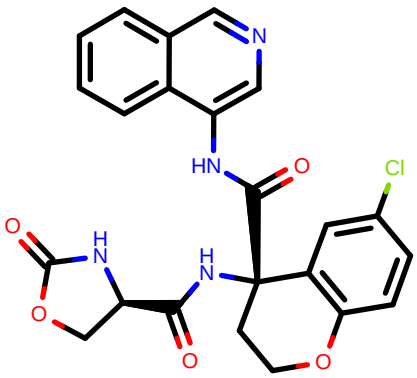
CID:	EN300-132157_2_2
SMILES:	C[C@]1(CC(=O)NC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3938
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.28

EN300-120920_3_1



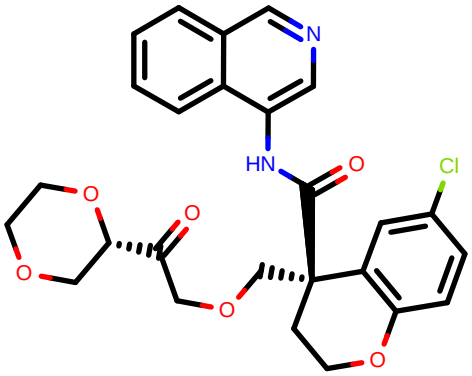
CID:	EN300-120920_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H]5CCC(=O)NC5=O
RUN:	RUN2440
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.25

EN300-201346_1_2



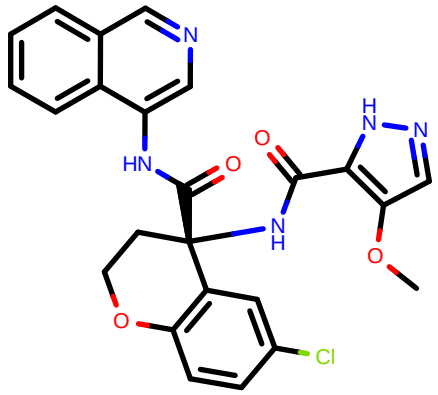
CID:	EN300-201346_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5COC(=O)N5
RUN:	RUN2084
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.22

EN300-6238494_2_1



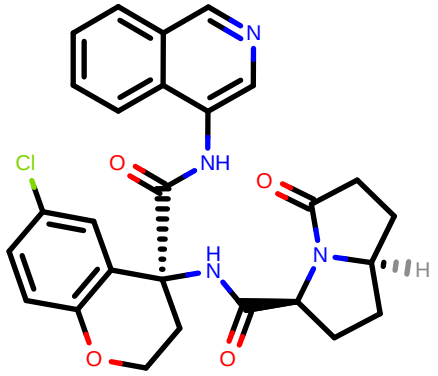
CID:	EN300-6238494_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)[C@@H]5COCCO5
RUN:	RUN759
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.27

EN300-7439284_1_1



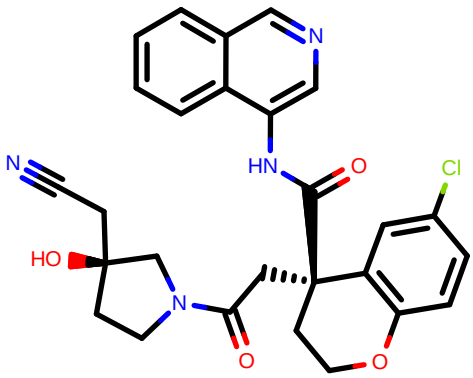
CID:	EN300-7439284_1_1
SMILES:	COc1cn[nH]c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7282
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.27

EN300-6479181_1_3



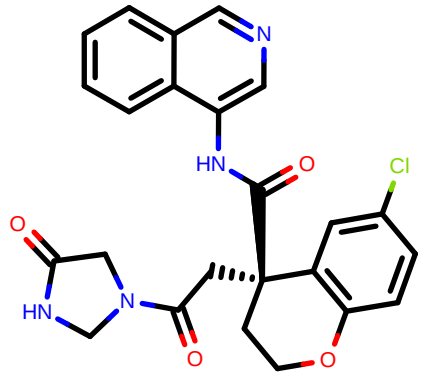
CID:	EN300-6479181_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC[C@H]6N5C(=O)CC6
RUN:	RUN7970
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.27

EN300-257405_1_1



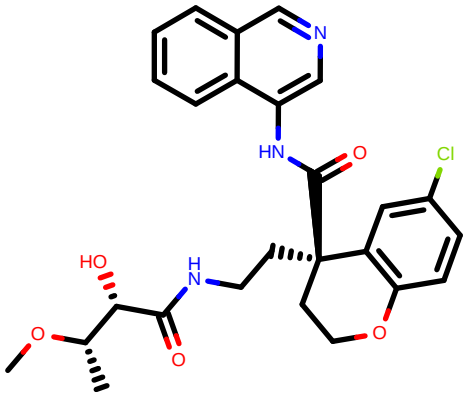
CID:	EN300-257405_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(CC#N)O
RUN:	RUN2270
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.30

EN300-154156_1_1



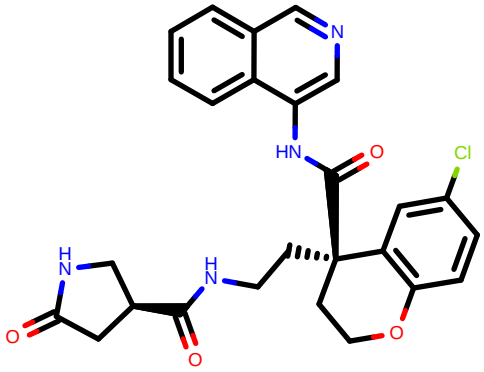
CID:	EN300-154156_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NC5
RUN:	RUN5518
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.25

EN300-220194_3_1



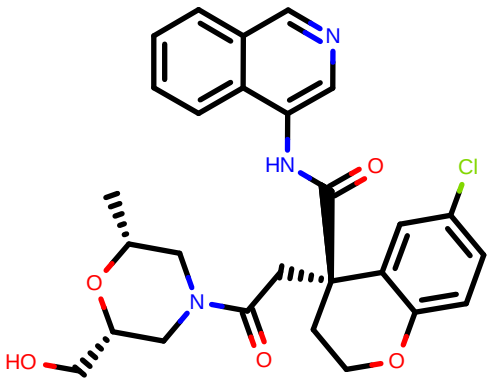
CID:	EN300-220194_3_1
SMILES:	C[C@@H]([C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN3024
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.30

EN300-59487_3_2



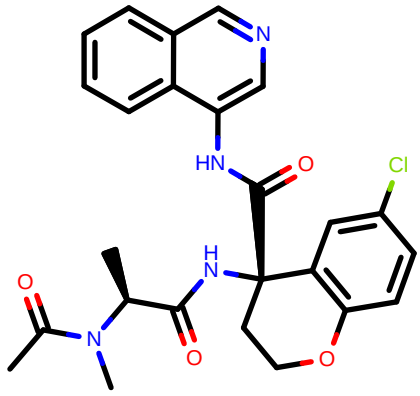
CID:	EN300-59487_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)NC5
RUN:	RUN3124
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.28

EN300-157776_1_1



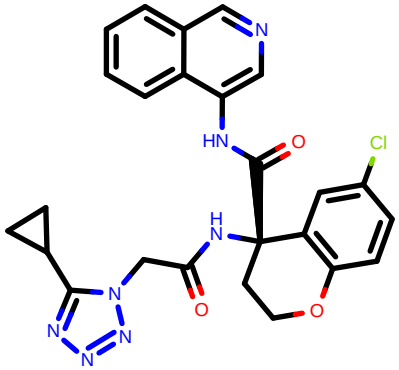
CID:	EN300-157776_1_1
SMILES:	C[C@@H]1CN(C[C@@H](O1)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4715
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.30

EN300-863933_1_1



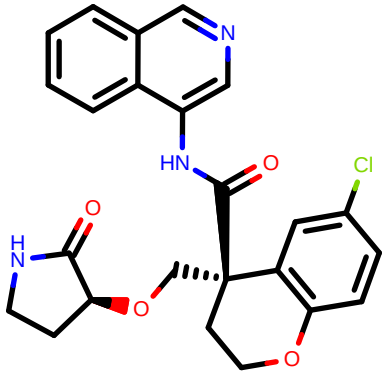
CID:	EN300-863933_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)N(C)C(=O)C
RUN:	RUN4169
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.33

EN300-872798_1_1



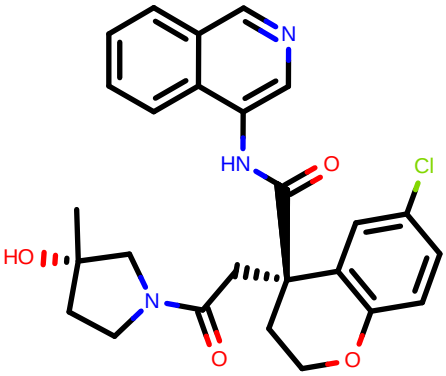
CID:	EN300-872798_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(nnn5)C6CC6
RUN:	RUN3430
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.31

EN300-6736413_2_2



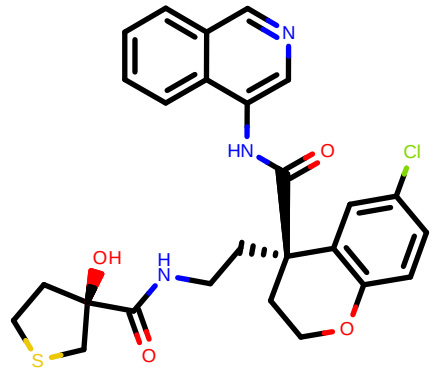
CID:	EN300-6736413_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O
RUN:	RUN1174
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.26

EN300-99161_1_1



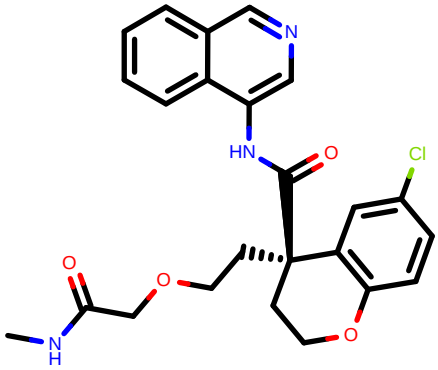
CID:	EN300-99161_1_1
SMILES:	C[C@@]1(CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN8116
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.28

EN300-122656_3_2



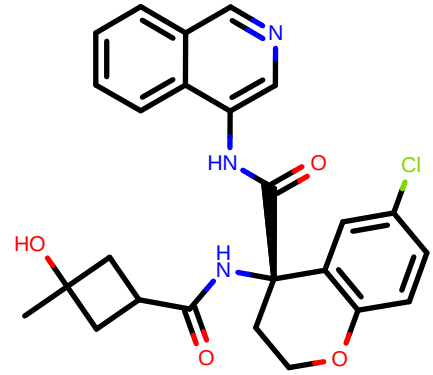
CID:	EN300-122656_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCSC5)O
RUN:	RUN7204
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.42

EN300-2977549_3_1



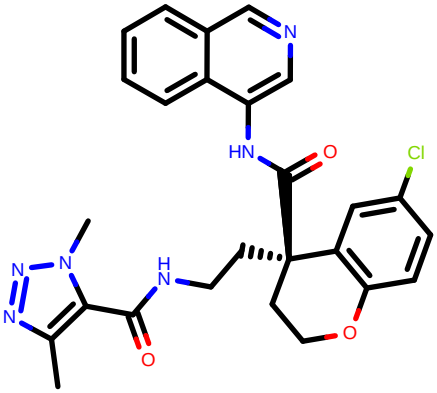
CID:	EN300-2977549_3_1
SMILES:	CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1755
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.27

EN300-7183657_1_1



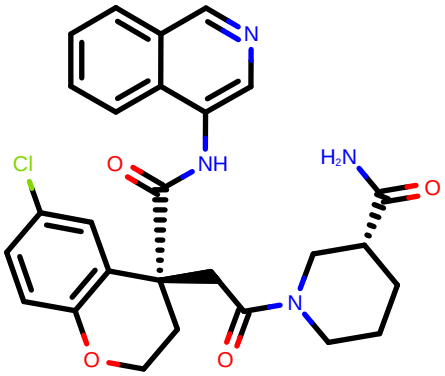
CID:	EN300-7183657_1_1
SMILES:	C[C@]1(C[C@@H](C1)C(=O)N[C@@]2(c3c(ccc(c3)Cl)OCC2)C(=O)Nc4c5c(cnc4)cccc5)O
RUN:	RUN3482
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.24

EN300-649738_3_1



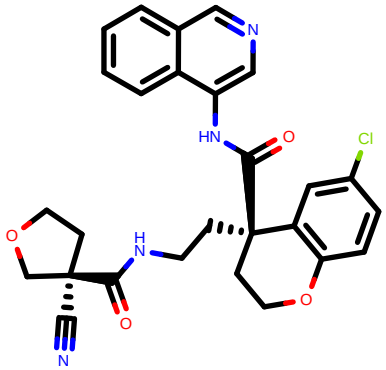
CID:	EN300-649738_3_1
SMILES:	Cc1c(n(nn1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10966
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.30

EN300-18610_1_2



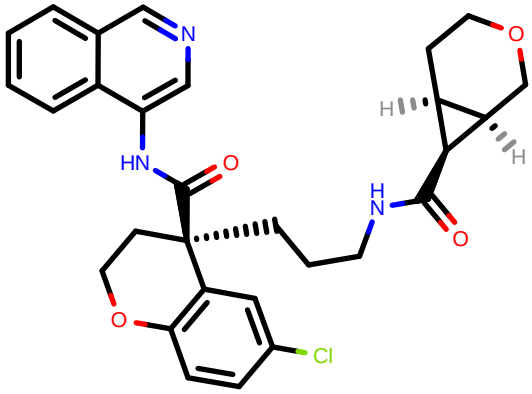
CID:	EN300-18610_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H](C5)C(=O)N
RUN:	RUN6257
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.27

EN300-261210_3_1



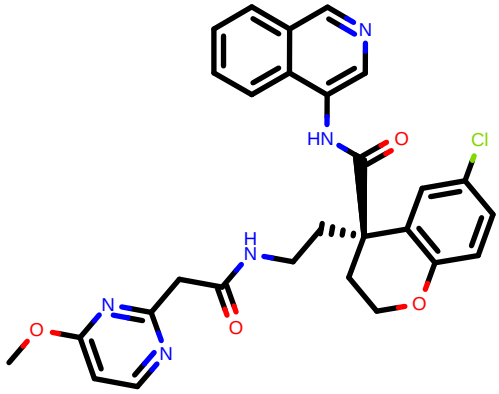
CID:	EN300-261210_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOC5)C#N
RUN:	RUN3176
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.35

EN300-1644723_4_6



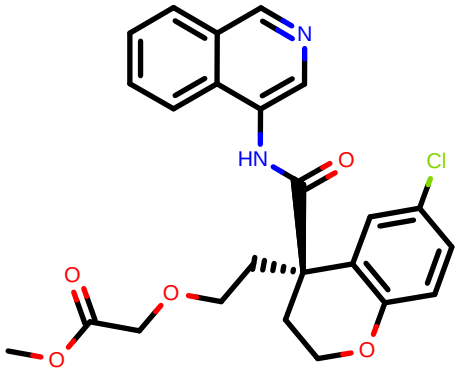
CID:	EN300-1644723_4_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5[C@@H]6[C@H]5COCC6
RUN:	RUN10169
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.32

EN300-6480588_3_1



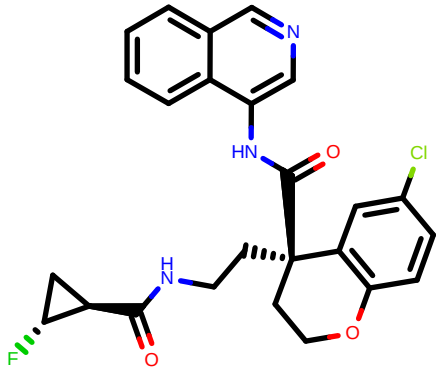
CID:	EN300-6480588_3_1
SMILES:	COc1ccnc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11030
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.31

EN300-19700_3_1



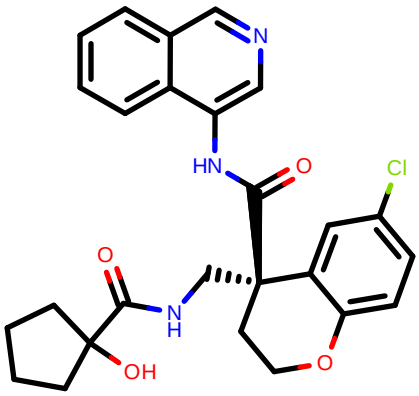
CID:	EN300-19700_3_1
SMILES:	COC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1579
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.22

EN300-4698402_3_1



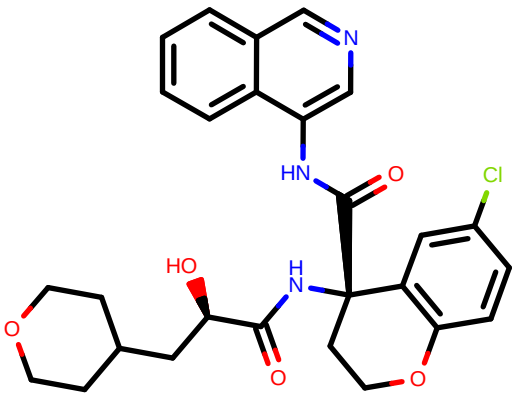
CID:	EN300-4698402_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@H]5F
RUN:	RUN11114
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.24

EN300-25960_2_1



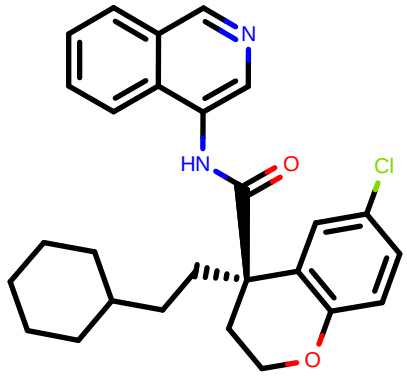
CID:	EN300-25960_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCCC5)O
RUN:	RUN4306
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.49

EN300-1452069_1_1



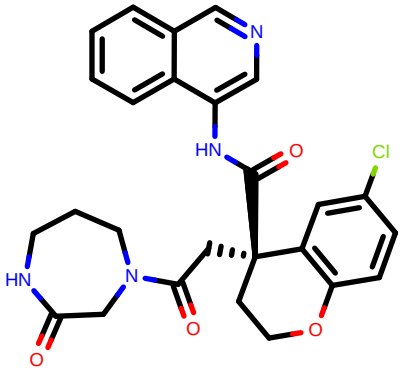
CID:	EN300-1452069_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CC5CCOCC5)O
RUN:	RUN2212
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.26

DAR-DIA-6a508060-9_1



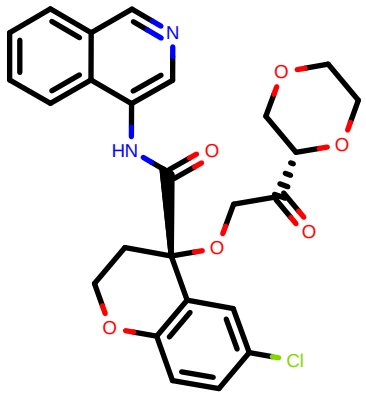
CID:	DAR-DIA-6a508060-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN142
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.31

EN300-366468_1_1



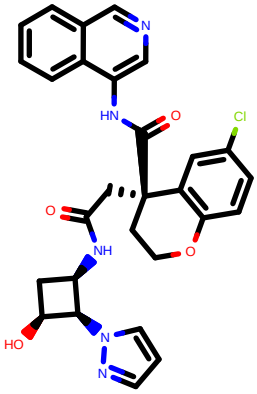
CID:	EN300-366468_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCNC(=O)C5
RUN:	RUN4587
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.26

EN300-6238494_1_1



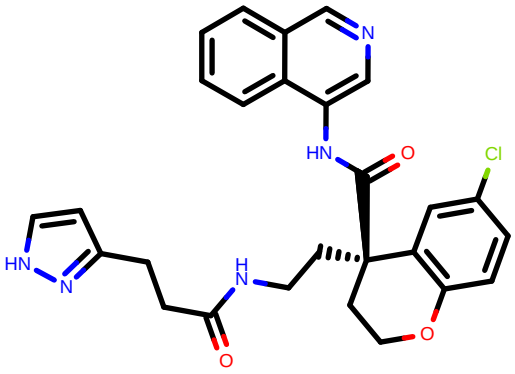
CID:	EN300-6238494_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@@H]5COCCO5
RUN:	RUN301
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.31

EN300-260696_1_1



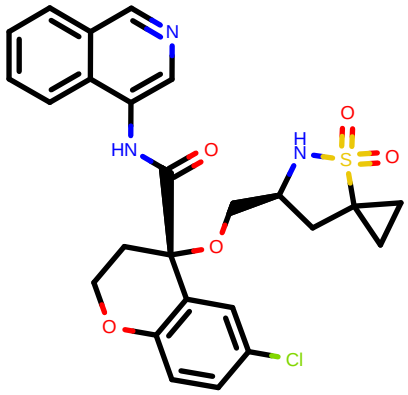
CID:	EN300-260696_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]([C@@H]5n6cccn6)O
RUN:	RUN9138
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.35

EN300-1664603_3_1



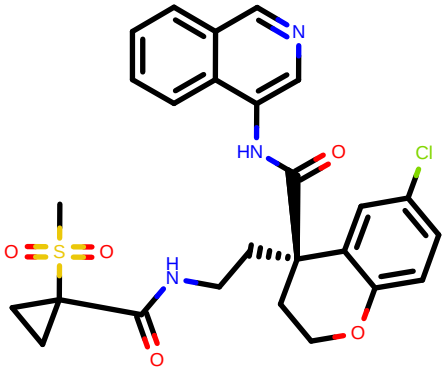
CID:	EN300-1664603_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5ccn[nH]5
RUN:	RUN4107
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.28

EN300-6504697_1_1



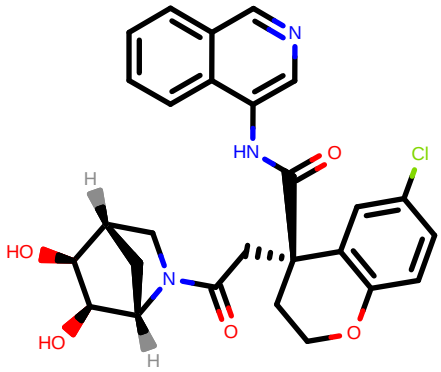
CID:	EN300-6504697_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CC6(CC6)S(=O)(=O)N5
RUN:	RUN2706
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.30

EN300-191495_3_1



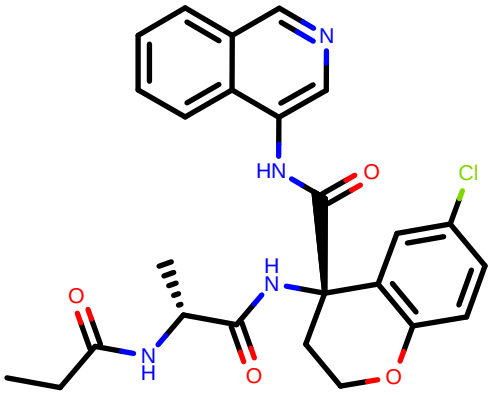
CID:	EN300-191495_3_1
SMILES:	CS(=O)(=O)C1(CC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3028
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.45

EN300-1722072_1_1



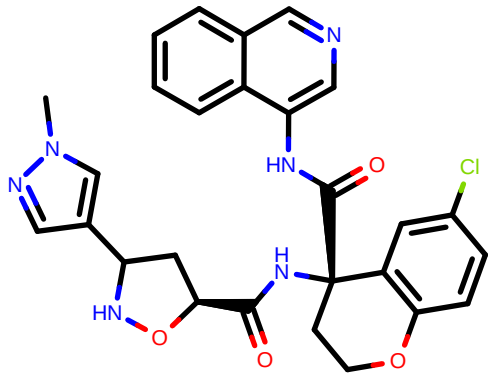
CID:	EN300-1722072_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@H]5[C@H]([C@H]6O)O
RUN:	RUN3032
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.29

EN300-31148_1_2



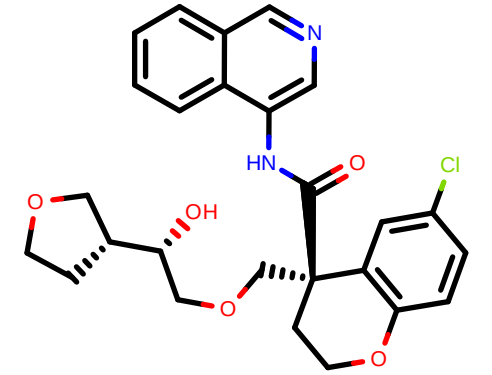
CID:	EN300-31148_1_2
SMILES:	CCC(=O)N[C@H](C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4521
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.28

EN300-92605_1_1



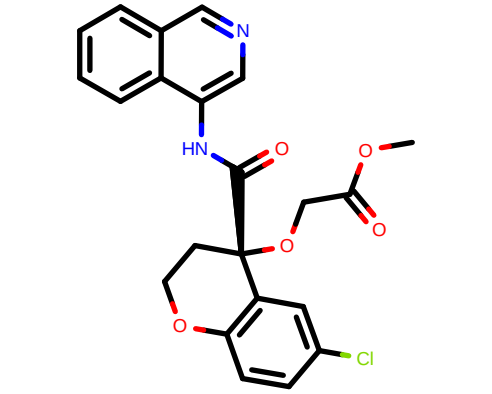
CID:	EN300-92605_1_1
SMILES:	Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8582
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.29

EN300-1911992_2_2



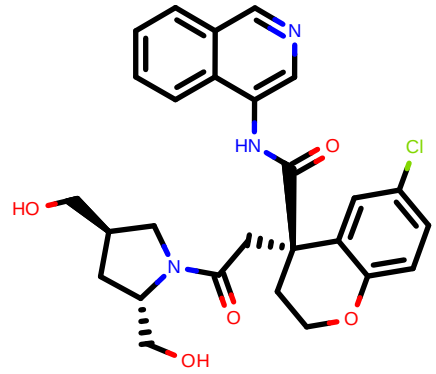
CID:	EN300-1911992_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]([C@@H]5CCOC5)O
RUN:	RUN1853
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.37

EN300-19700_1_1



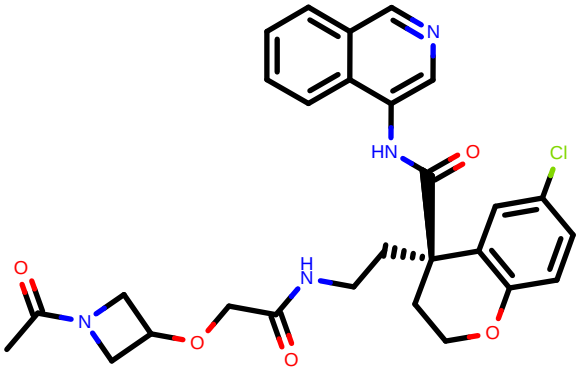
CID:	EN300-19700_1_1
SMILES:	COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN389
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.19

EN300-1212400_1_3



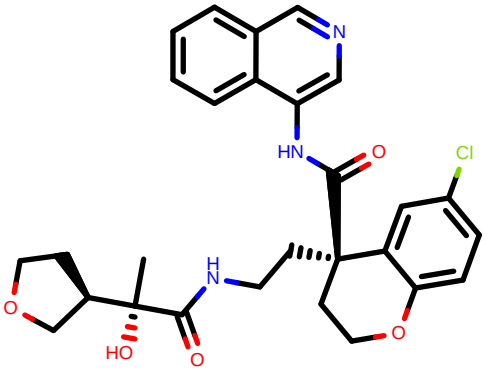
CID:	EN300-1212400_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@H]5CO)CO
RUN:	RUN10286
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.39

EN300-259004_3_1



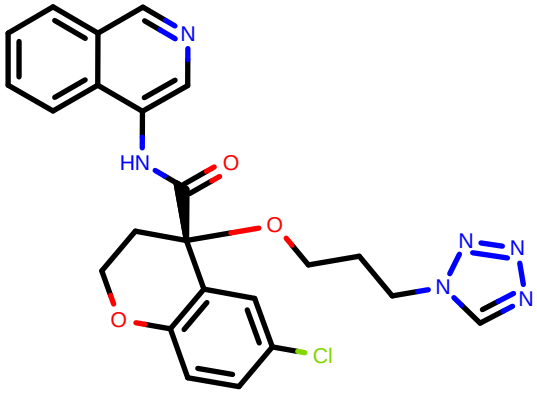
CID:	EN300-259004_3_1
SMILES:	CC(=O)N1CC(C1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11170
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.42

EN300-217494_3_2



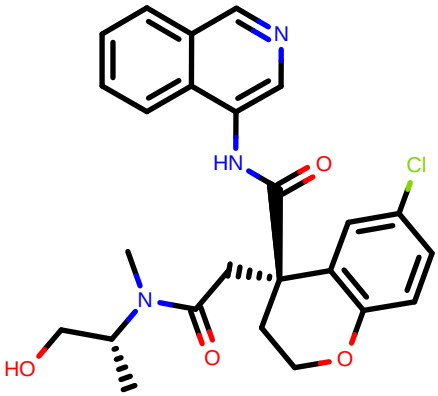
CID:	EN300-217494_3_2
SMILES:	C[C@]([C@@H]1CCOC1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6401
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.57

EN300-1696962_1_1



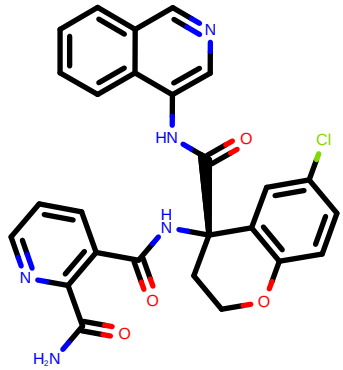
CID:	EN300-1696962_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCn5cnnn5
RUN:	RUN2610
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.24

EN300-117414_1_2



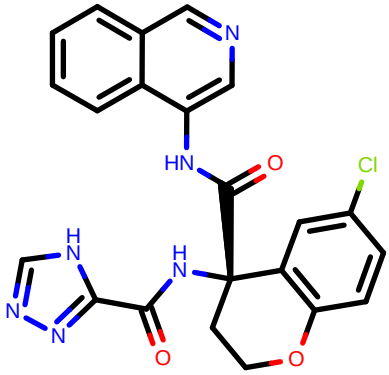
CID:	EN300-117414_1_2
SMILES:	C[C@H](CO)N(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8991
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.28

EN300-135530_1_1



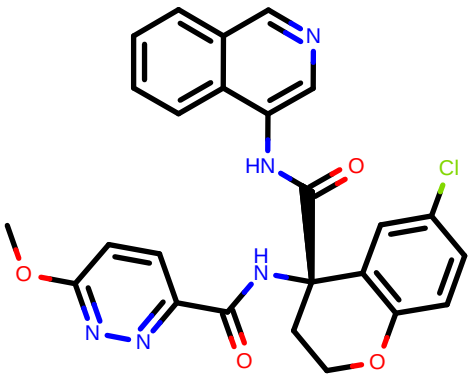
CID:	EN300-135530_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccnc5C(=O)N
RUN:	RUN7650
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.24

EN300-100741_1_1



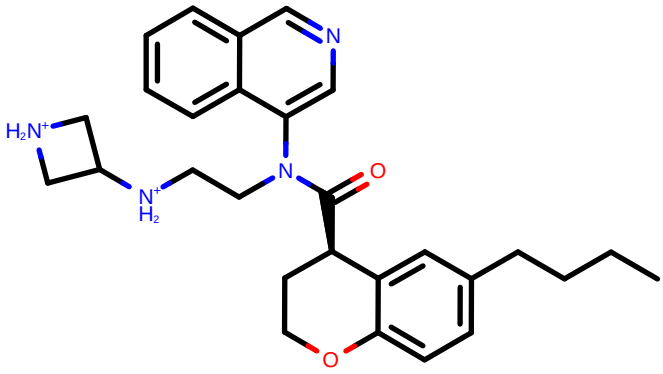
CID:	EN300-100741_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]cnn5
RUN:	RUN2994
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.17

EN300-82553_1_1



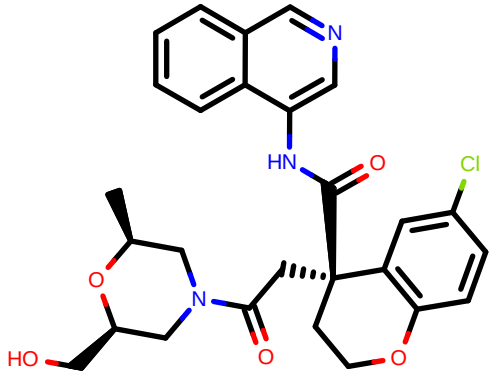
CID:	EN300-82553_1_1
SMILES:	COc1ccc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8750
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.22

MAK-UNK-83e0a0b4-4_1



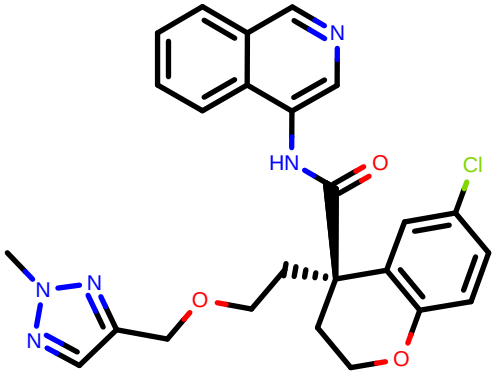
CID:	MAK-UNK-83e0a0b4-4_1
SMILES:	CCCCc1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCNC3CNC3)c4cncc5c4cccc5
RUN:	RUN238
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.47

EN300-157776_1_4



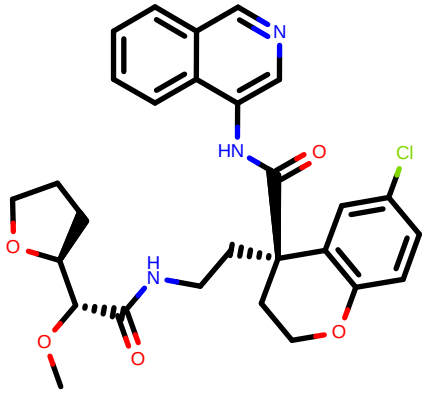
CID:	EN300-157776_1_4
SMILES:	C[C@H]1CN(C[C@H](O1)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8264
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.37

EN300-219020_3_1



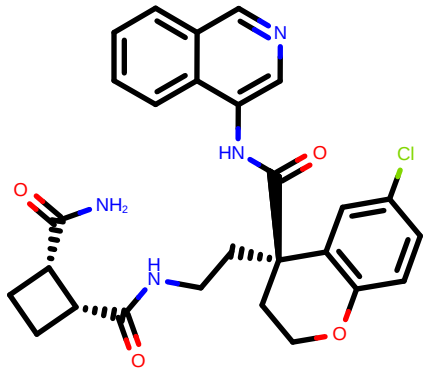
CID:	EN300-219020_3_1
SMILES:	Cn1ncc(n1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1635
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.27

EN300-6277108_3_2



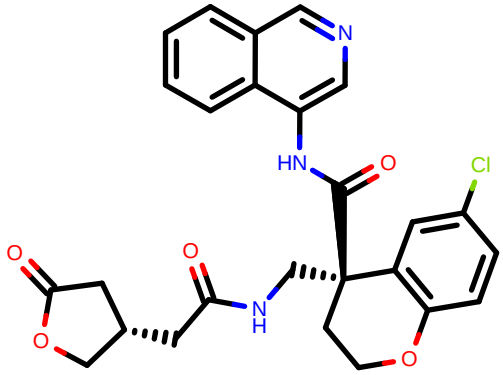
CID:	EN300-6277108_3_2
SMILES:	CO[C@H]([C@@H]1CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3755
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.38

EN300-217107_3_1



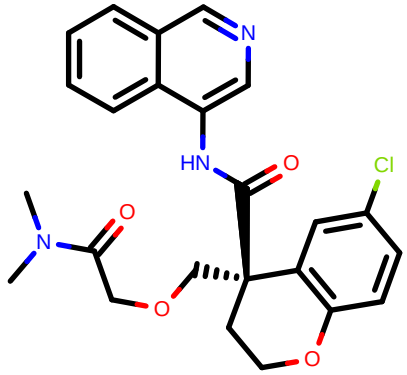
CID:	EN300-217107_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@@H]5C(=O)N
RUN:	RUN4539
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.31

EN300-109535_2_2



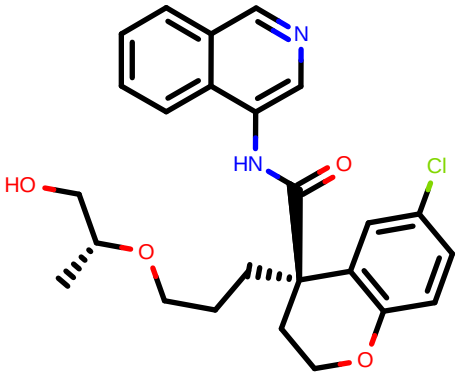
CID:	EN300-109535_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@H]5CC(=O)OC5
RUN:	RUN3479
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.29

EN300-216063_2_1



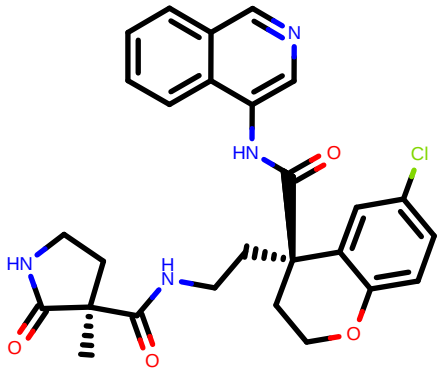
CID:	EN300-216063_2_1
SMILES:	CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1190
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.22

EN300-175186_4_2



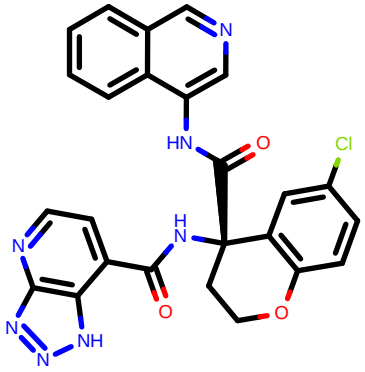
CID:	EN300-175186_4_2
SMILES:	C[C@H](CO)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN460
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.31

EN300-207959_3_2



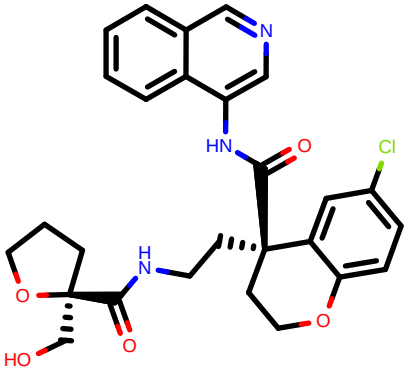
CID:	EN300-207959_3_2
SMILES:	C[C@]1(CCNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1729
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.35

EN300-188377_1_1



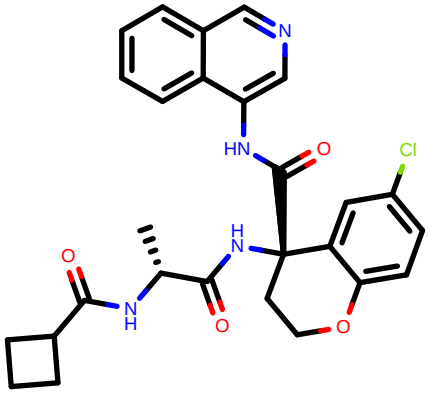
CID:	EN300-188377_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc6c5[nH]nn6
RUN:	RUN7758
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.23

EN300-1425677_3_1



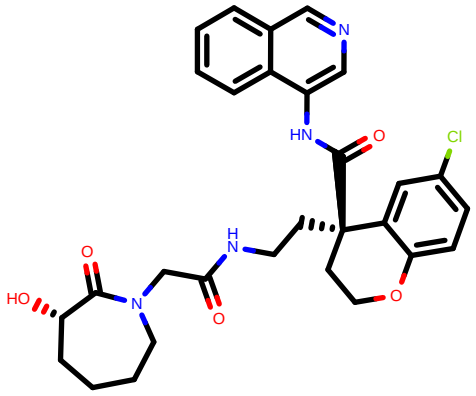
CID:	EN300-1425677_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCO5)CO
RUN:	RUN1817
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.33

EN300-66082_1_2



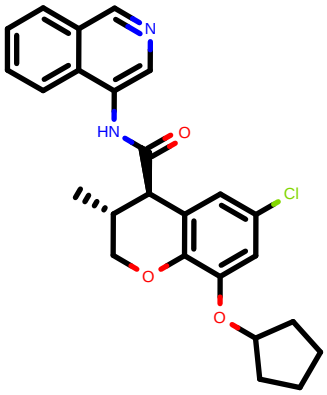
CID:	EN300-66082_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCC5
RUN:	RUN5888
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.28

EN300-259849_3_1



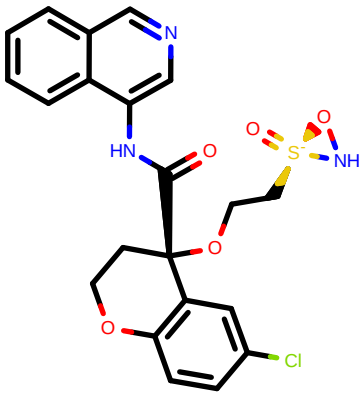
CID:	EN300-259849_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCC[C@@H](C5=O)O
RUN:	RUN5854
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.35

DAR-DIA-0d514e7d-4_1



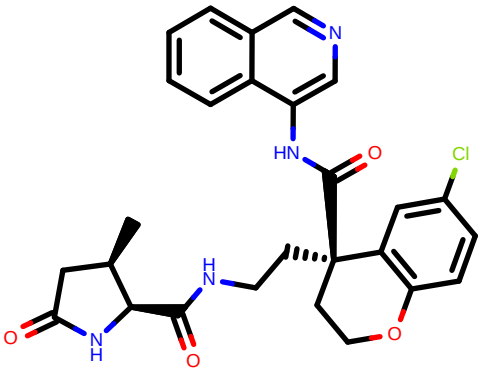
CID:	DAR-DIA-0d514e7d-4_1
SMILES:	C[C@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN93
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.21

EN300-270710_1_1



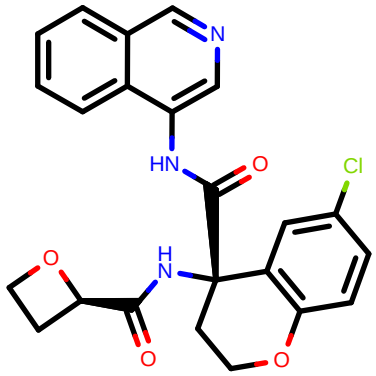
CID:	EN300-270710_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)N
RUN:	RUN2580
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.21

EN300-155362_3_1



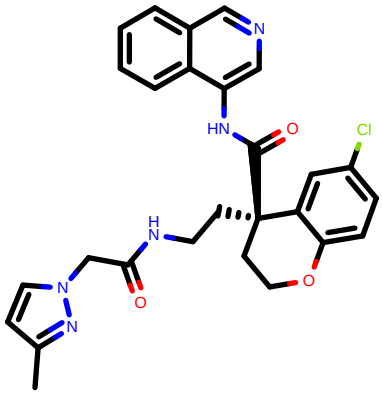
CID:	EN300-155362_3_1
SMILES:	C[C@@H]1CC(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4547
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.27

EN300-85760_1_2



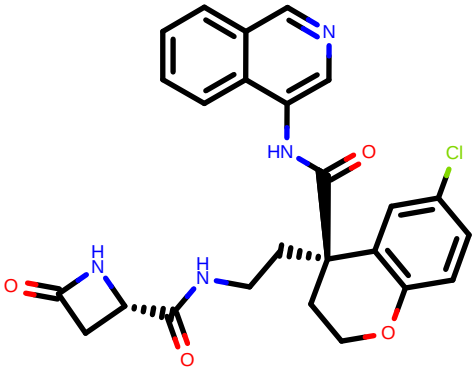
CID:	EN300-85760_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCO5
RUN:	RUN909
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.19

EN300-226964_3_1



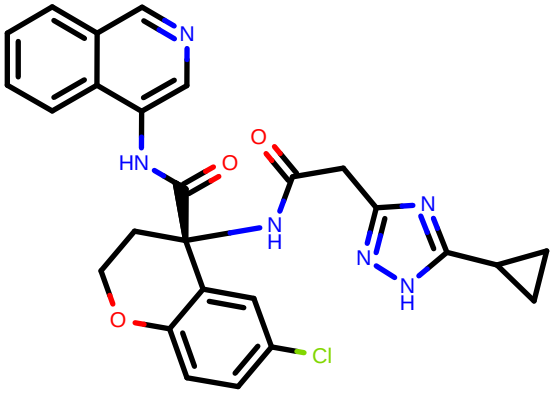
CID:	EN300-226964_3_1
SMILES:	Cc1ccn(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9808
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.37

EN300-101505_3_1



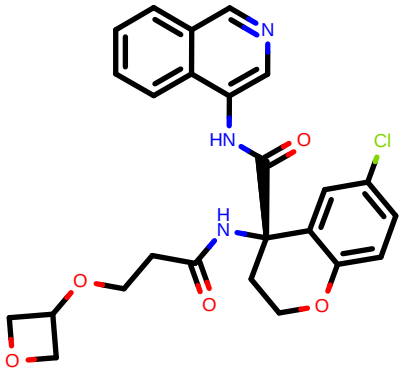
CID:	EN300-101505_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)N5
RUN:	RUN10954
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.28

EN300-657211_1_1



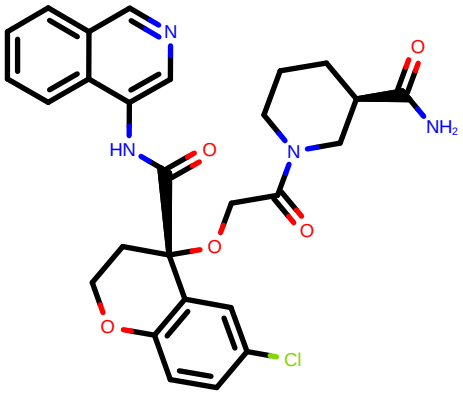
CID:	EN300-657211_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]c(nn5)C6CC6
RUN:	RUN6870
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.30

EN300-321703_1_1



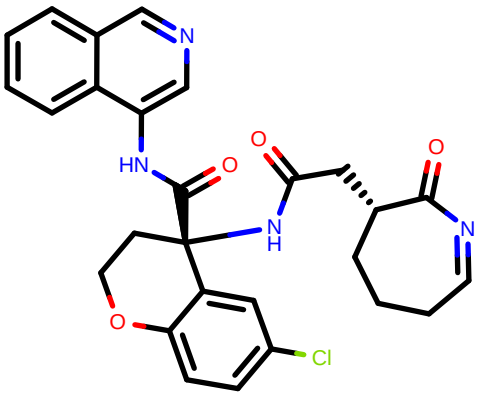
CID:	EN300-321703_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCOC5COC5
RUN:	RUN3789
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.21

EN300-22880_1_2



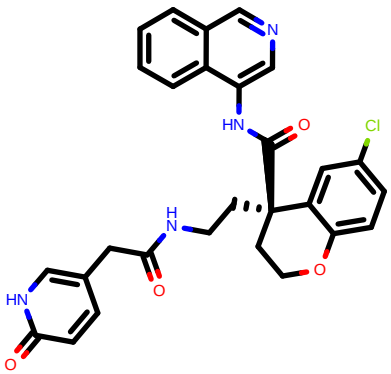
CID:	EN300-22880_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N5CCC[C@H](C5)C(=O)N
RUN:	RUN880
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.37

EN300-198633_1_2



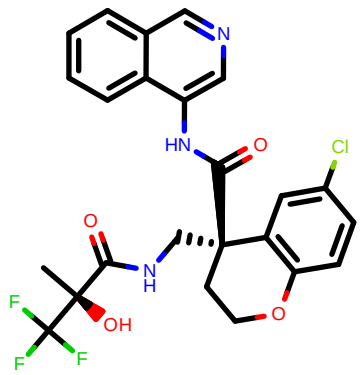
CID:	EN300-198633_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCCNC5=O
RUN:	RUN593
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.30

EN300-189672_3_1



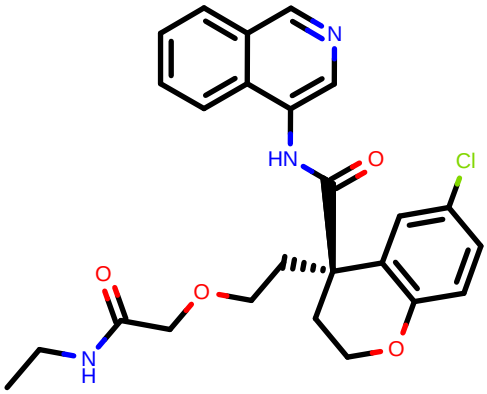
CID:	EN300-189672_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(=O)[nH]c5
RUN:	RUN8979
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.33

EN300-159633_2_2



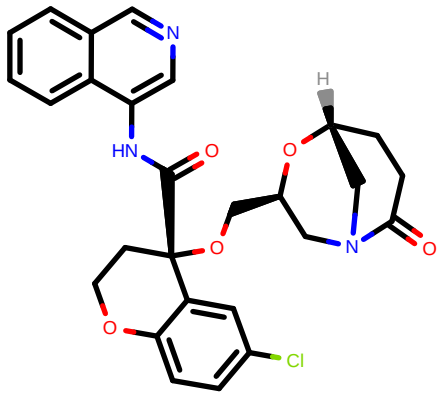
CID:	EN300-159633_2_2
SMILES:	C[C@](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN5477
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.32

EN300-7003350_3_1



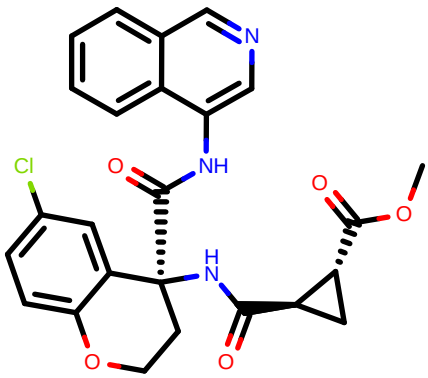
CID:	EN300-7003350_3_1
SMILES:	CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1492
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.24

EN300-2008102_1_1



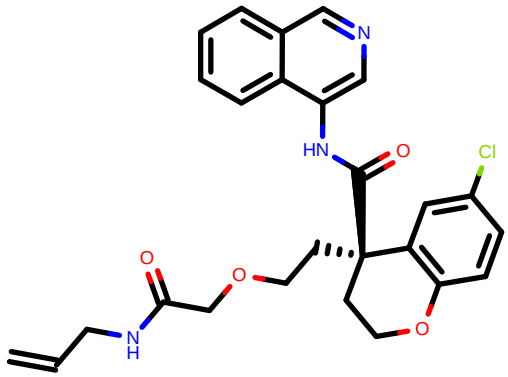
CID:	EN300-2008102_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CN6CC(O5)CCC6=O
RUN:	RUN2047
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.30

EN300-765003_1_1



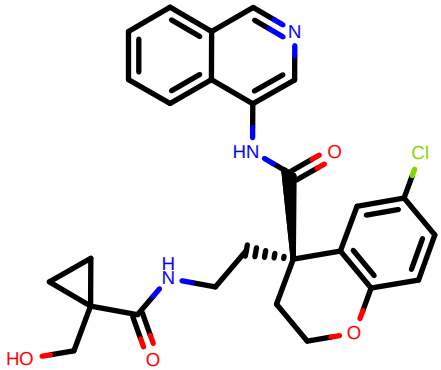
CID:	EN300-765003_1_1
SMILES:	COC(=O)[C@@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3698
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.24

EN300-17184_3_1



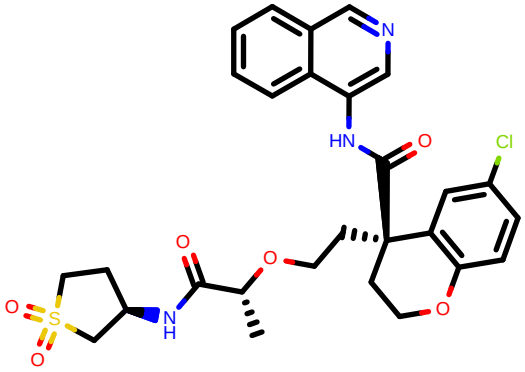
CID:	EN300-17184_3_1
SMILES:	C=CCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN560
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.30

EN300-146174_3_1



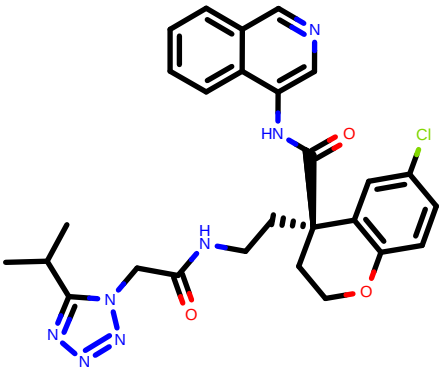
CID:	EN300-146174_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)CO
RUN:	RUN882
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.30

EN300-23318_3_2



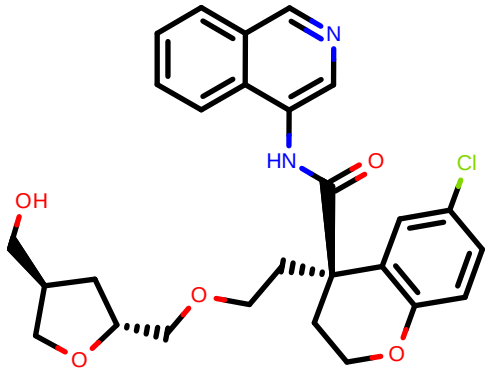
CID:	EN300-23318_3_2
SMILES:	C[C@H](C(=O)N[C@@H]1CCS(=O)(=O)C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2293
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.31

EN300-96933_3_1



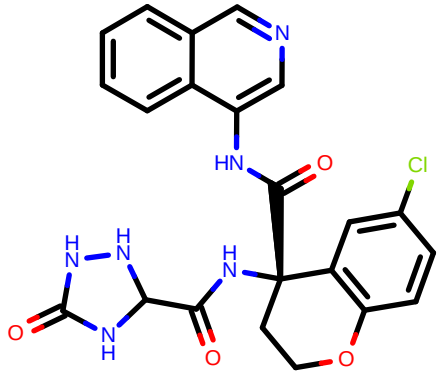
CID:	EN300-96933_3_1
SMILES:	CC(C)c1nnnn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7968
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.33

EN300-6494158_3_2



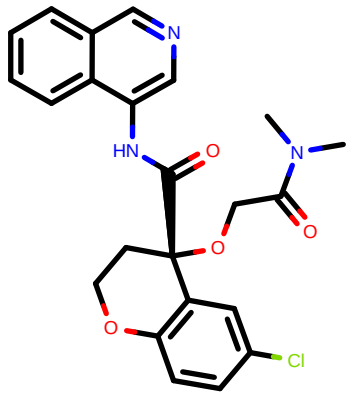
CID:	EN300-6494158_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C[C@@H](CO5)CO
RUN:	RUN1004
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.39

EN300-35843_1_1



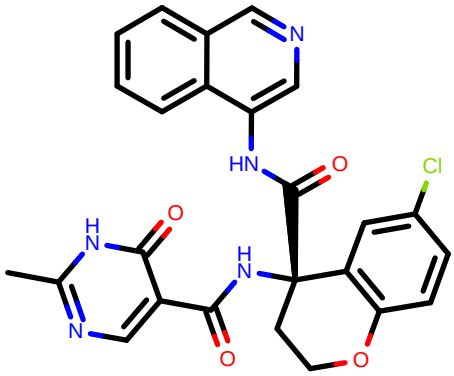
CID:	EN300-35843_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5[nH]c(=O)[nH]n5
RUN:	RUN4069
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.26

EN300-216063_1_1



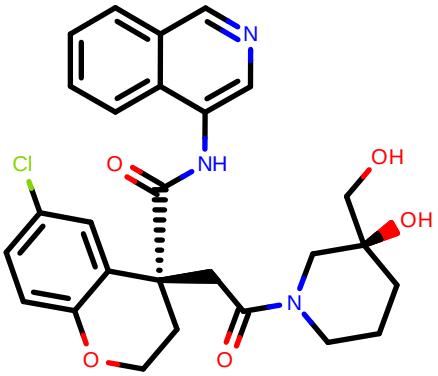
CID:	EN300-216063_1_1
SMILES:	CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN785
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.23

EN300-67267_1_1



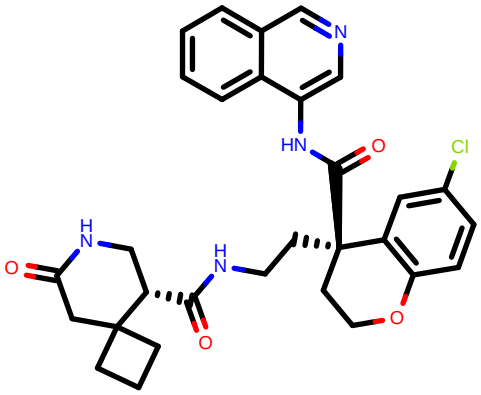
CID:	EN300-67267_1_1
SMILES:	Cc1[nH]c(=O)c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8738
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.29

EN300-251396_1_2



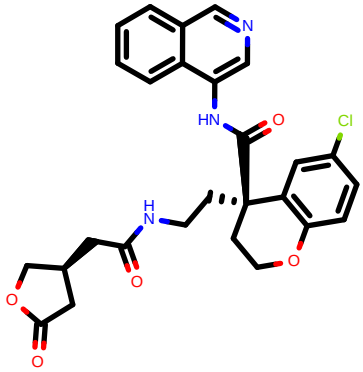
CID:	EN300-251396_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@](C5)(CO)O
RUN:	RUN835
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.50

EN300-1704404_3_2



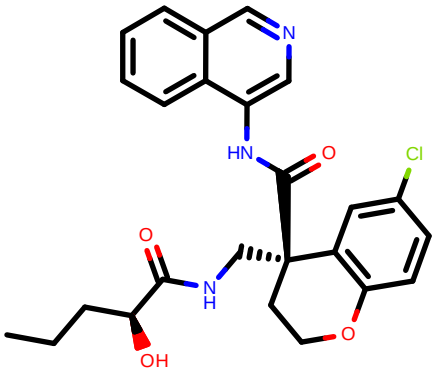
CID:	EN300-1704404_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CNC(=O)CC56CCC6
RUN:	RUN10686
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.40

EN300-109535_3_2



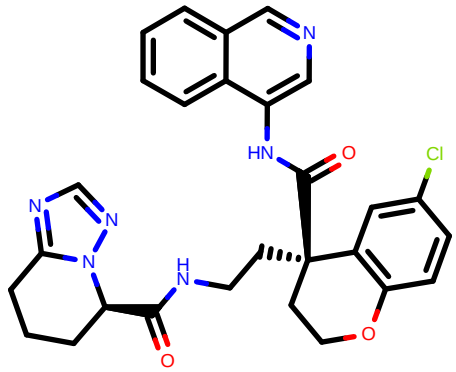
CID:	EN300-109535_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CC(=O)OC5
RUN:	RUN7624
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.31

EN300-300217_2_1



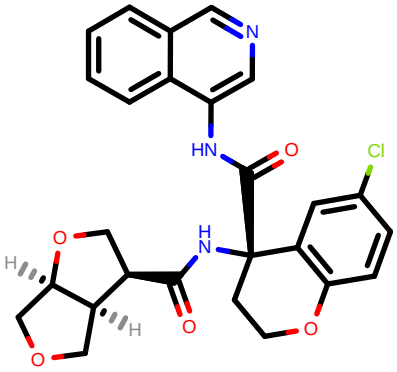
CID:	EN300-300217_2_1
SMILES:	C/C=C\[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2722
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.29

EN300-1273016_3_2



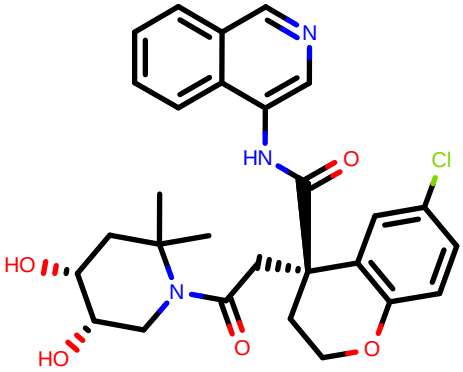
CID:	EN300-1273016_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCc6n5ncn6
RUN:	RUN9213
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.26

EN300-6482296_1_3



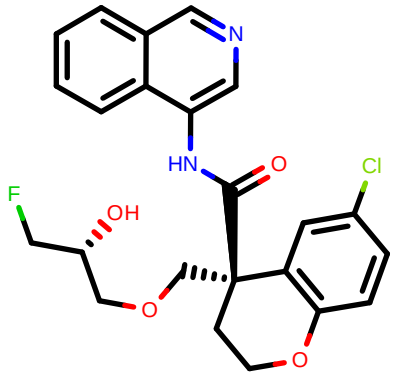
CID:	EN300-6482296_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CO[C@H]6[C@@H]5COC6
RUN:	RUN4989
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.39

EN300-7539819_1_1



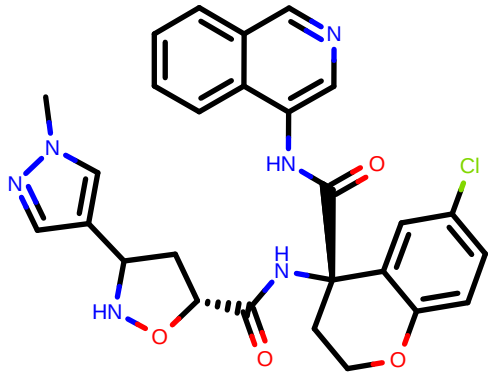
CID:	EN300-7539819_1_1
SMILES:	CC1(C[C@H]([C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O)C
RUN:	RUN11106
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.42

EN300-1968342_2_2



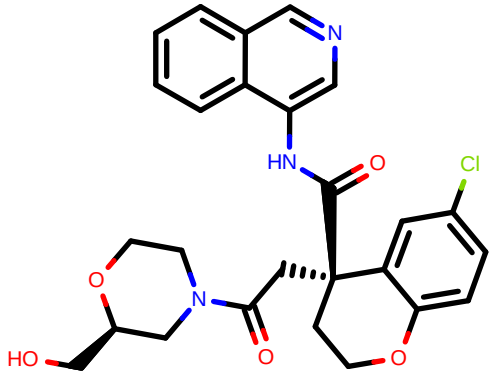
CID:	EN300-1968342_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CF)O
RUN:	RUN507
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.33

EN300-92605_1_2



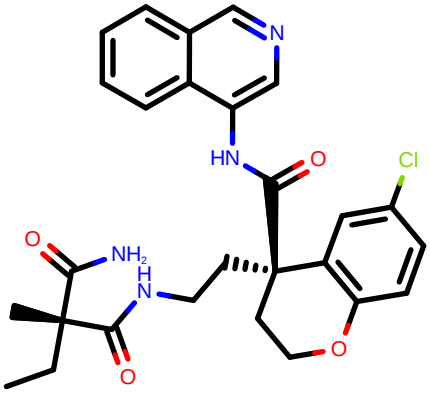
CID:	EN300-92605_1_2
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8490
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.27

EN300-175487_1_1



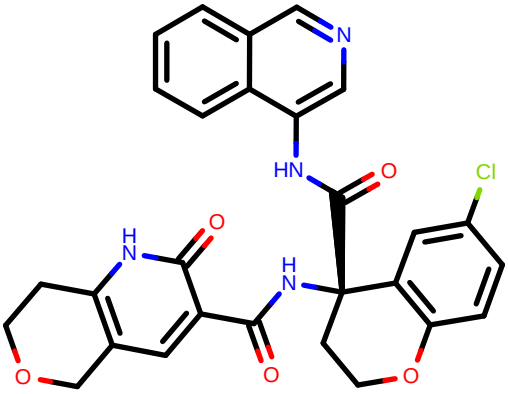
CID:	EN300-175487_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CO
RUN:	RUN2201
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.38

EN300-2908024_3_2



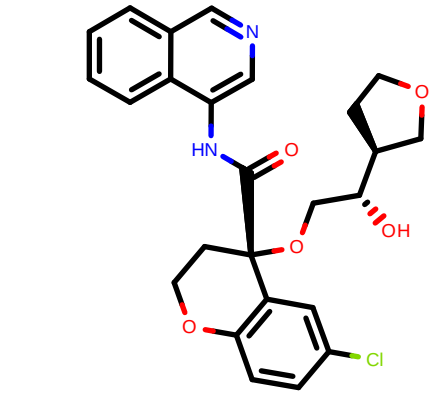
CID:	EN300-2908024_3_2
SMILES:	CC[C@](C)(C(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3863
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.31

EN300-383824_1_1



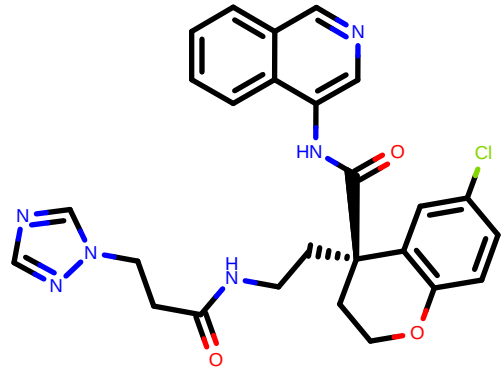
CID:	EN300-383824_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c([nH]c5=O)CCOC6
RUN:	RUN9059
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.38

EN300-1911992_1_4



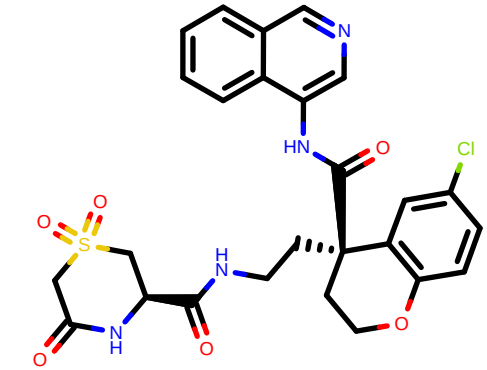
CID:	EN300-1911992_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]([C@H]5CCOC5)O
RUN:	RUN1703
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.33

EN300-26147_3_1



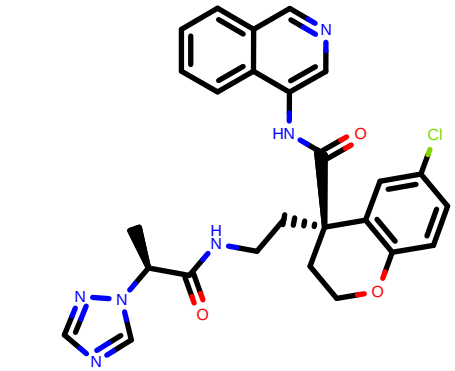
CID:	EN300-26147_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5cncn5
RUN:	RUN5223
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.31

EN300-702756_3_1



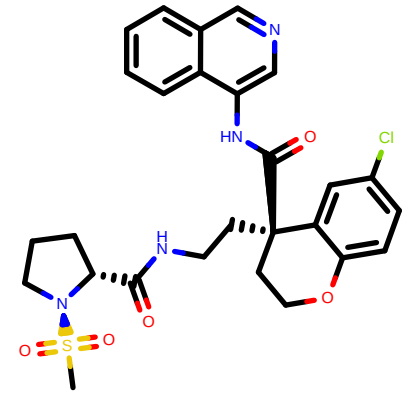
CID:	EN300-702756_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CS(=O)(=O)CC(=O)N5
RUN:	RUN9436
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.31

EN300-30397_3_1



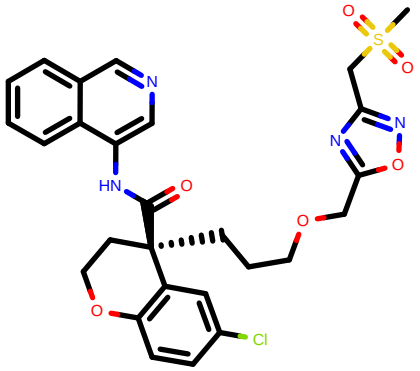
CID:	EN300-30397_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN5203
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.33

EN300-10402_3_1



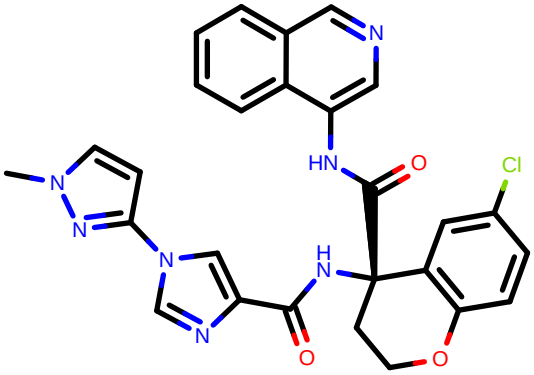
CID:	EN300-10402_3_1
SMILES:	CS(=O)(=O)N1CCC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5542
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.45

EN300-94900_4_1



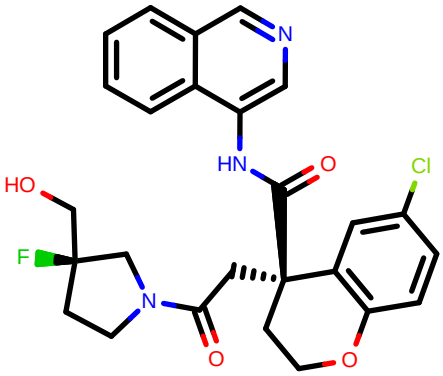
CID:	EN300-94900_4_1
SMILES:	CS(=O)(=O)Cc1nc(on1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2086
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.41

EN300-1726340_1_1



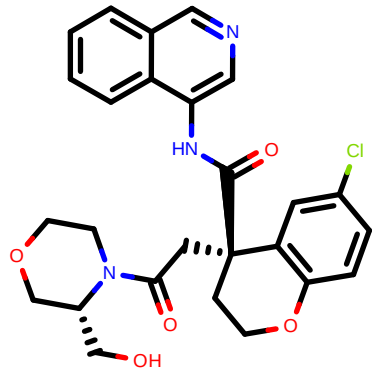
CID:	EN300-1726340_1_1
SMILES:	Cn1ccc(n1)n2cc(nc2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9020
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.22

EN300-203118_1_1



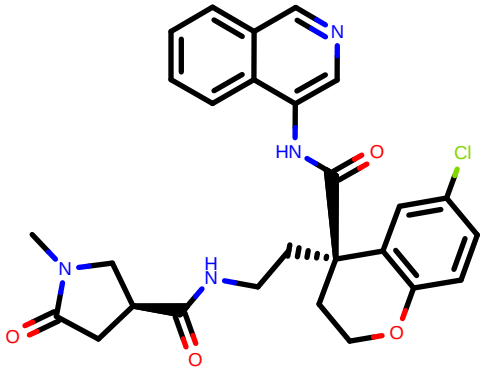
CID:	EN300-203118_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(CO)F
RUN:	RUN1737
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.31

EN300-173903_1_1



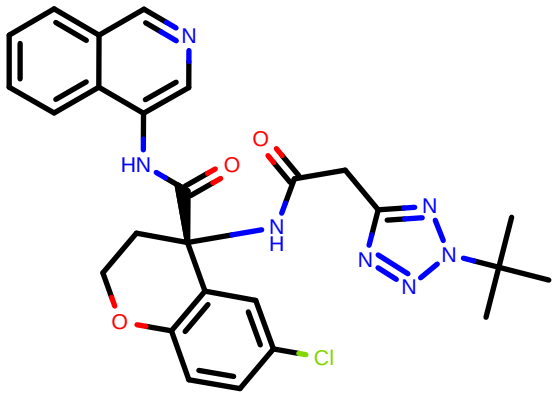
CID:	EN300-173903_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CO
RUN:	RUN1210
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.37

EN300-33601_3_2



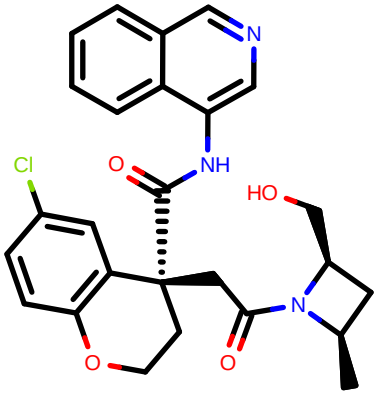
CID:	EN300-33601_3_2
SMILES:	CN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6625
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.34

EN300-297927_1_1



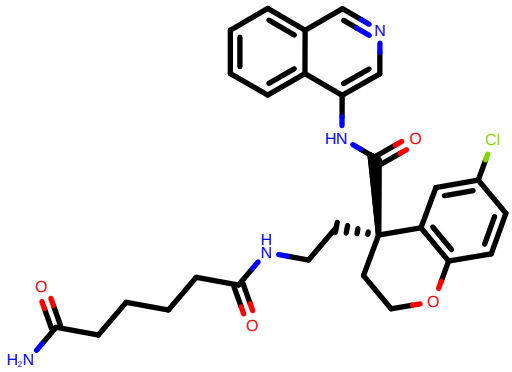
CID:	EN300-297927_1_1
SMILES:	CC(C)(C)n1nc(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7638
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.27

EN300-1709410_1_1



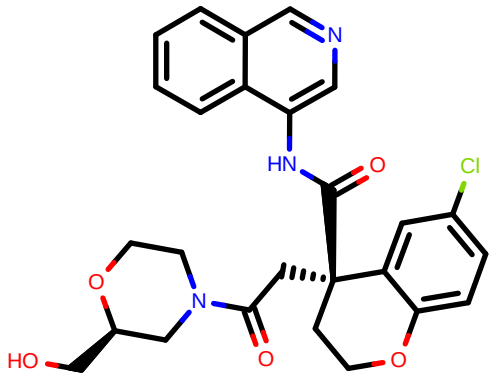
CID:	EN300-1709410_1_1
SMILES:	C[C@@H]1C[C@@H](N1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN8716
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.28

EN300-142412_3_1



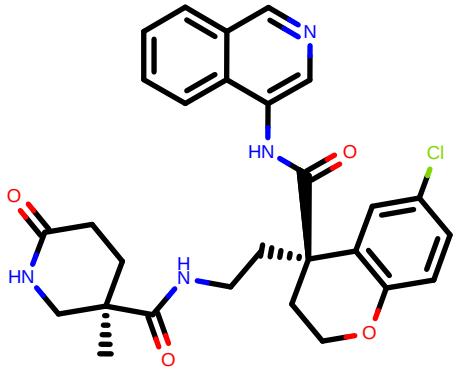
CID:	EN300-142412_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCCC(=O)N
RUN:	RUN10416
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.29

EN300-101373_1_1



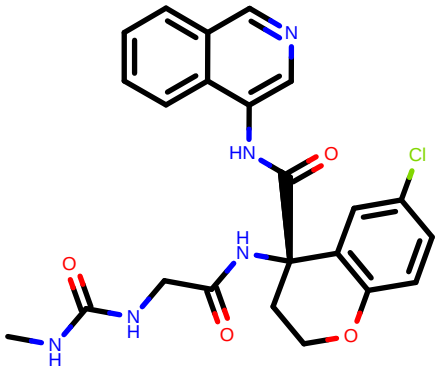
CID:	EN300-101373_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CO
RUN:	RUN2193
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.41

EN300-195924_3_2



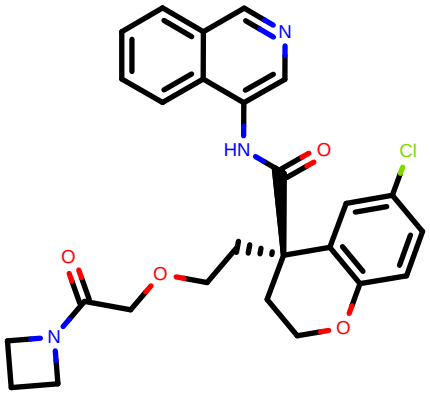
CID:	EN300-195924_3_2
SMILES:	C[C@]1(CCC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1530
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.36

EN300-36911_1_1



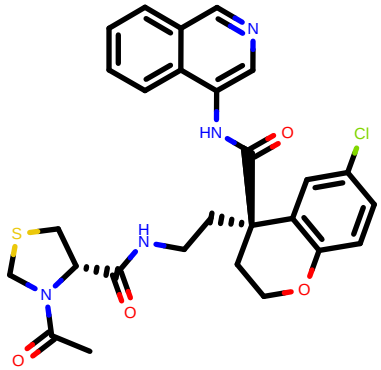
CID:	EN300-36911_1_1
SMILES:	CNC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2910
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.28

EN300-11195_3_1



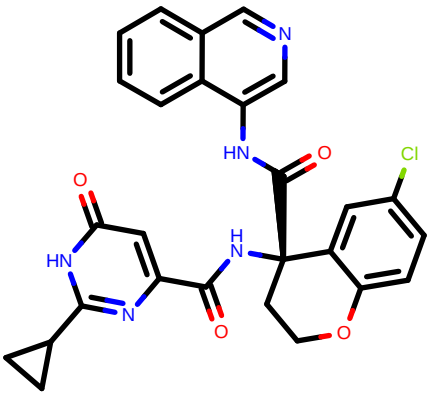
CID:	EN300-11195_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCC5
RUN:	RUN1356
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.27

EN300-56202_3_1



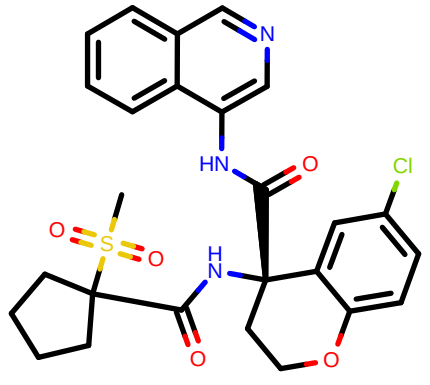
CID:	EN300-56202_3_1
SMILES:	CC(=O)N1CSC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4171
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.33

EN300-204239_1_1



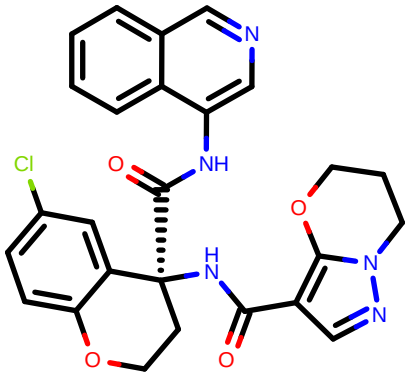
CID:	EN300-204239_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]c(n5)C6CC6
RUN:	RUN6551
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.27

EN300-60831_1_1



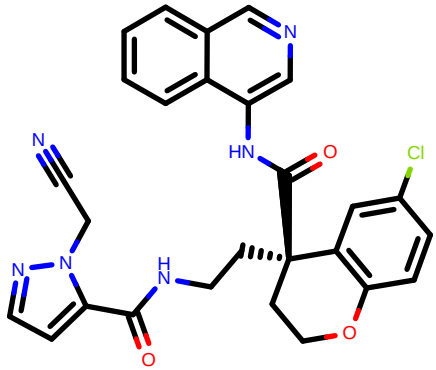
CID:	EN300-60831_1_1
SMILES:	CS(=O)(=O)C1(CCCC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6419
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.47

EN300-103722_1_1



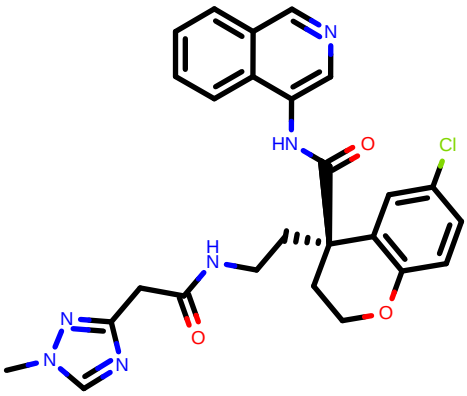
CID:	EN300-103722_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5OCCC6
RUN:	RUN8370
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.22

EN300-373791_3_1



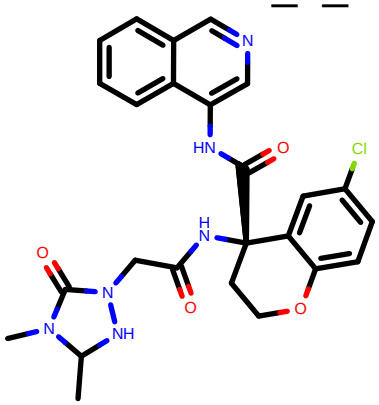
CID:	EN300-373791_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccnn5CC#N
RUN:	RUN9560
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.24

EN300-7493922_3_1



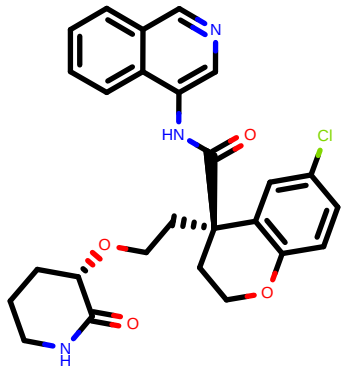
CID:	EN300-7493922_3_1
SMILES:	Cn1cnc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9802
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.36

EN300-269525_1_1



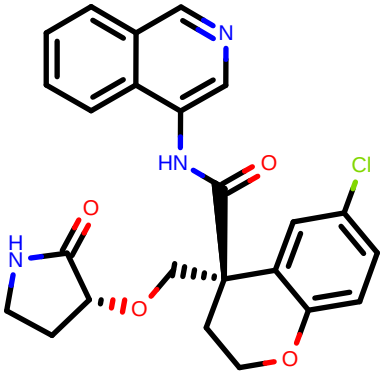
CID:	EN300-269525_1_1
SMILES:	Cc1nn(c(=O)n1C)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6695
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.35

EN300-107267_3_2



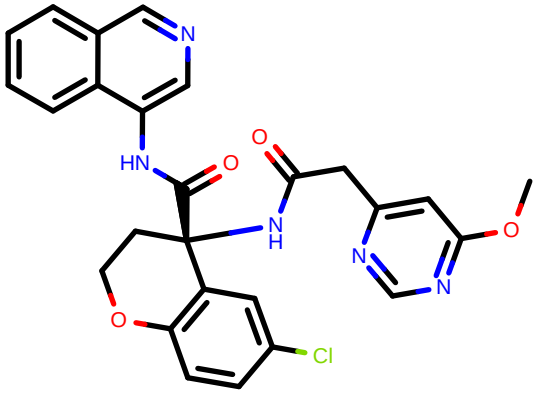
CID:	EN300-107267_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@H]5CCCNC5=O
RUN:	RUN2384
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.28

EN300-6736413_2_1



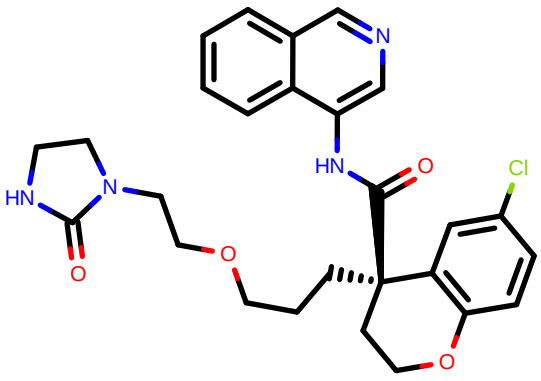
CID:	EN300-6736413_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCNC5=O
RUN:	RUN2021
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.23

EN300-7444950_1_1



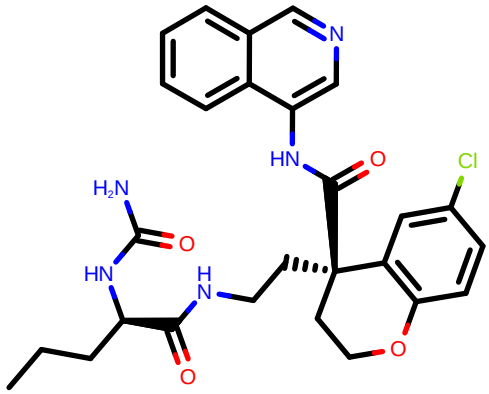
CID:	EN300-7444950_1_1
SMILES:	COc1cc(ncn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4905
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.26

EN300-214800_4_1



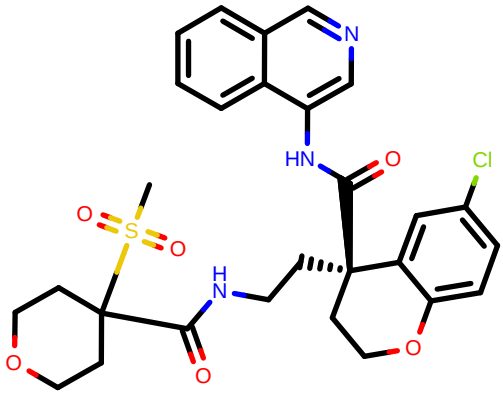
CID:	EN300-214800_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCN5CCNC5=O
RUN:	RUN2150
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.33

EN300-102901_3_1



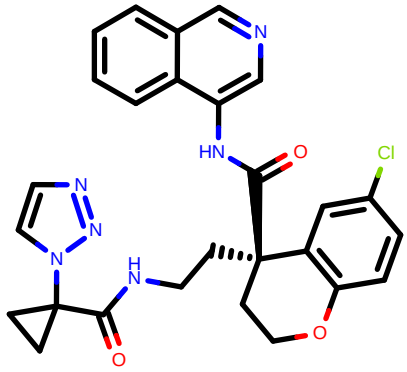
CID:	EN300-102901_3_1
SMILES:	CCC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN9150
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.31

EN300-220536_3_1



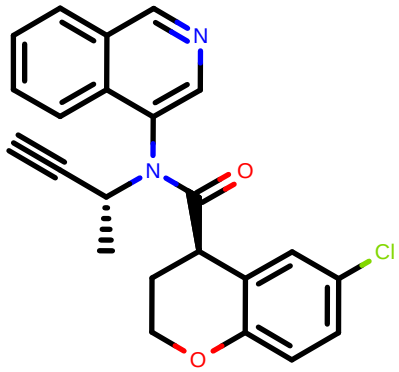
CID:	EN300-220536_3_1
SMILES:	CS(=O)(=O)C1(CCOCC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10658
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.40

EN300-658559_3_1



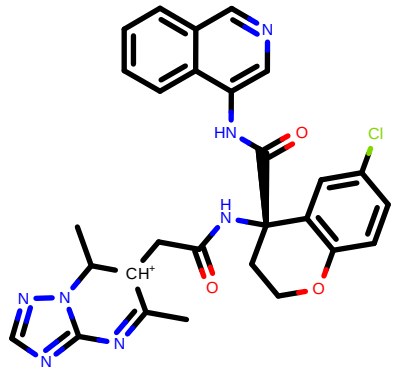
CID:	EN300-658559_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CC5)n6ccnn6
RUN:	RUN2209
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.32

DAR-DIA-5ff57136-16_2



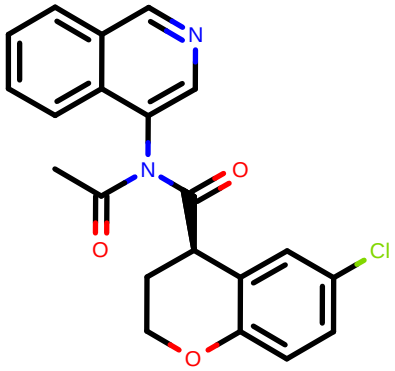
CID:	DAR-DIA-5ff57136-16_2
SMILES:	C[C@H](C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN192
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.13

EN300-13343_1_1



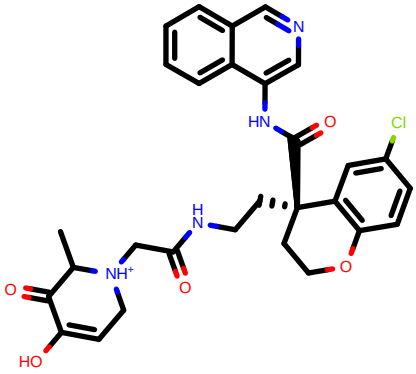
CID:	EN300-13343_1_1
SMILES:	Cc1c(c(n2c(n1)ncn2)C)CC(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8654
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.38

VLA-UCB-50c39ae8-1_1



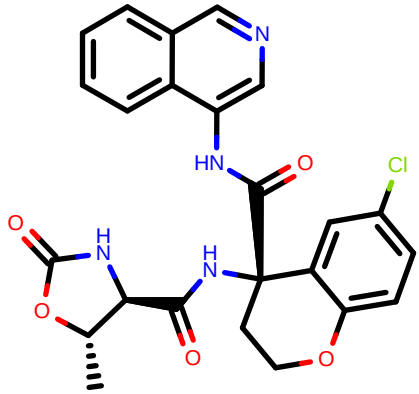
CID:	VLA-UCB-50c39ae8-1_1
SMILES:	CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN94
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.16

EN300-6498076_3_1



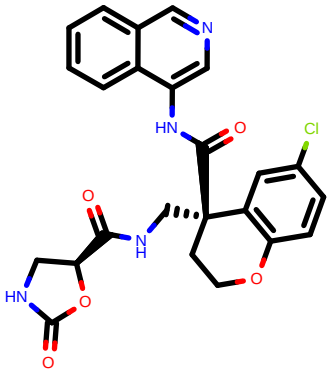
CID:	EN300-6498076_3_1
SMILES:	Cc1c(c(=O)ccn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6904
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.34

EN300-172640_1_2



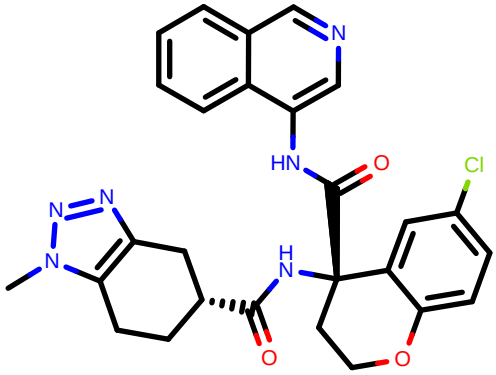
CID:	EN300-172640_1_2
SMILES:	C[C@H]1[C@@H](NC(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2814
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.28

EN300-244403_2_1



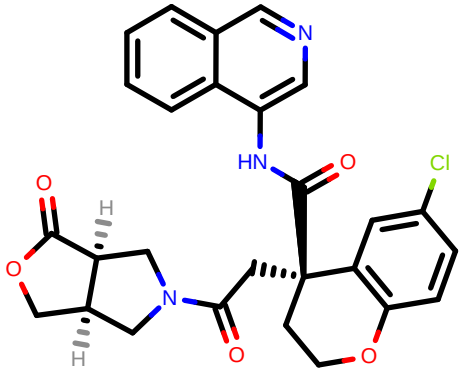
CID:	EN300-244403_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CNC(=O)O5
RUN:	RUN6835
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.23

EN300-185727_1_1



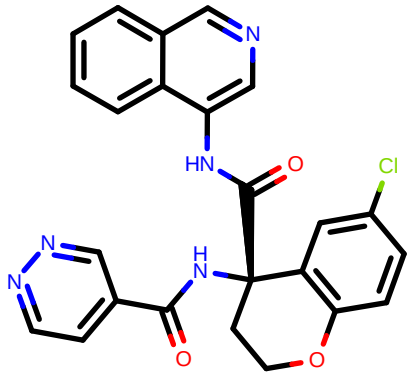
CID:	EN300-185727_1_1
SMILES:	Cn1c2c(nn1)C[C@@H](CC2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8494
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.32

EN300-316193_1_1



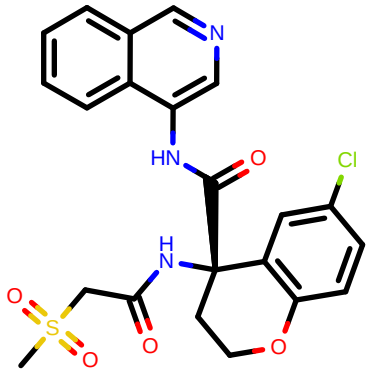
CID:	EN300-316193_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6COC(=O)[C@H]6C5
RUN:	RUN3312
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.26

EN300-75875_1_1



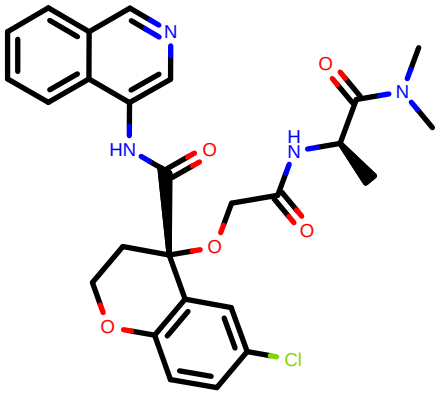
CID:	EN300-75875_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnnc5
RUN:	RUN3706
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.20

EN300-53677_1_1



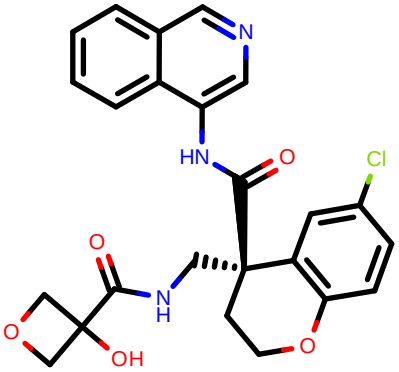
CID:	EN300-53677_1_1
SMILES:	CS(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2998
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.25

EN300-47657_1_2



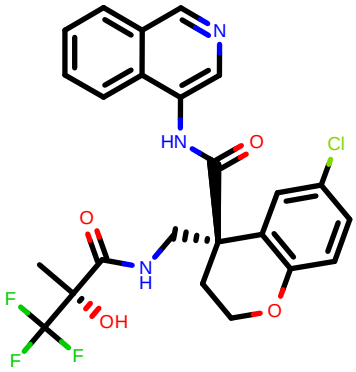
CID:	EN300-47657_1_2
SMILES:	C[C@H](C(=O)N(C)C)NC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1168
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.32

EN300-101443_2_1



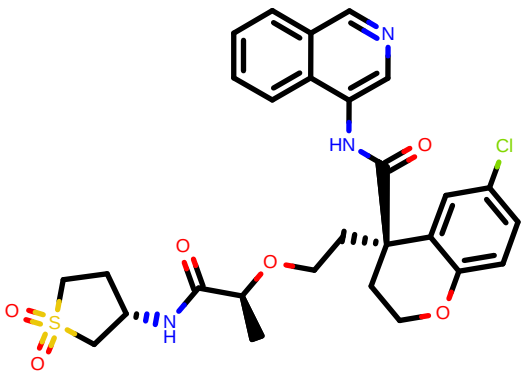
CID:	EN300-101443_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(COC5)O
RUN:	RUN5337
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.28

EN300-159633_2_1



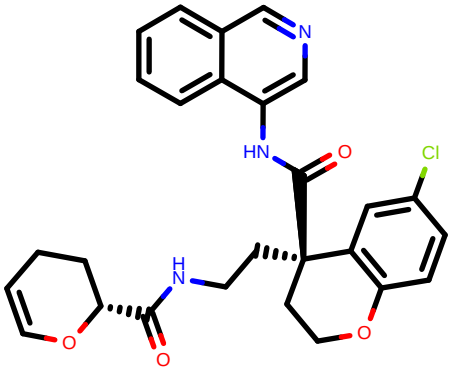
CID:	EN300-159633_2_1
SMILES:	C[C@@](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN5845
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.31

EN300-23318_3_3



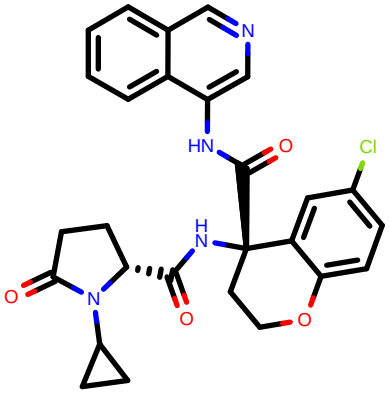
CID:	EN300-23318_3_3
SMILES:	C[C@@H](C(=O)N[C@H]1CCS(=O)(=O)C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1348
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.40

EN300-378044_3_2



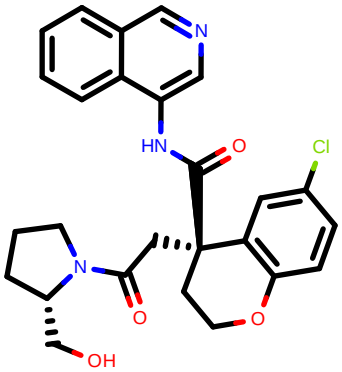
CID:	EN300-378044_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC=CCO5
RUN:	RUN3660
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.28

EN300-3044054_1_2



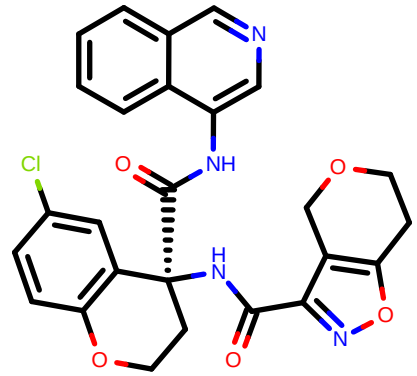
CID:	EN300-3044054_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCC(=O)N5C6CC6
RUN:	RUN5684
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.27

EN300-55109_1_2



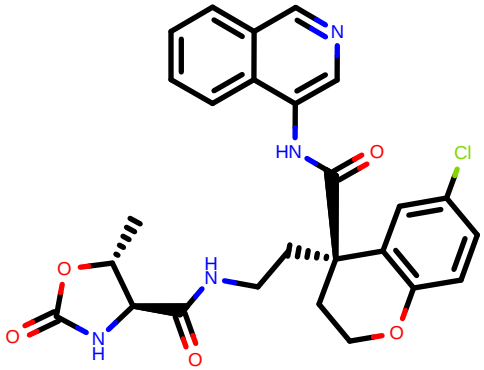
CID:	EN300-55109_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5CO
RUN:	RUN9308
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.29

EN300-88819_1_1



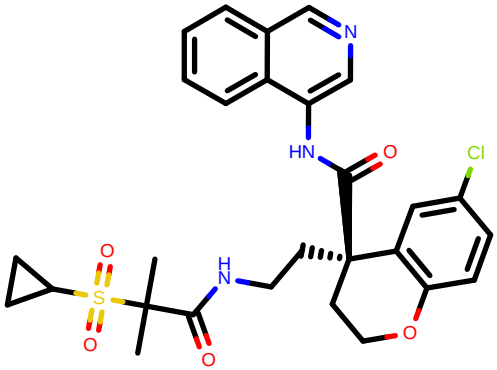
CID:	EN300-88819_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6c(on5)CCOC6
RUN:	RUN8246
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.24

EN300-172640_3_3



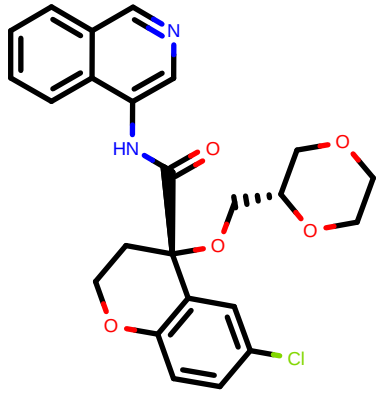
CID:	EN300-172640_3_3
SMILES:	C[C@@H]1[C@H](NC(=O)O1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10570
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.31

EN300-193399_3_1



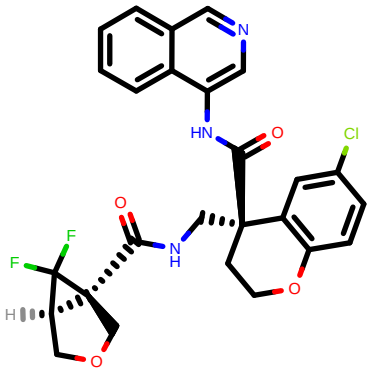
CID:	EN300-193399_3_1
SMILES:	CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C5CC5
RUN:	RUN5350
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.35

EN300-139167_1_1



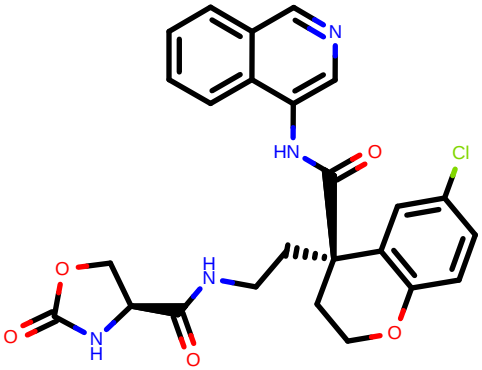
CID:	EN300-139167_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5COCCO5
RUN:	RUN2239
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.30

EN300-6738732_2_1



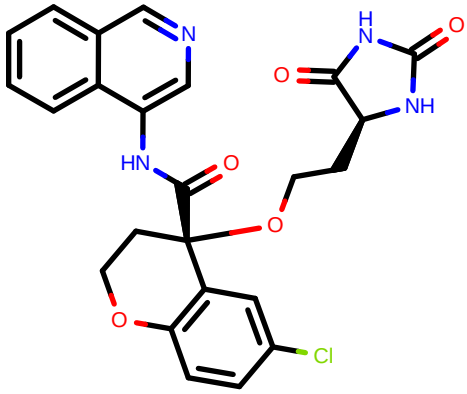
CID:	EN300-6738732_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]56COC[C@H]5C6(F)F
RUN:	RUN6436
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.28

EN300-201346_3_1



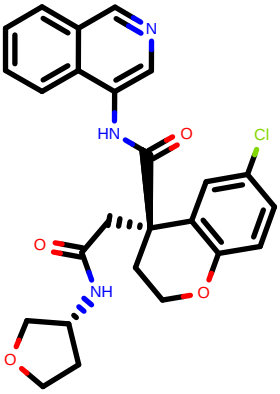
CID:	EN300-201346_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COC(=O)N5
RUN:	RUN8408
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.29

EN300-6498856_1_2



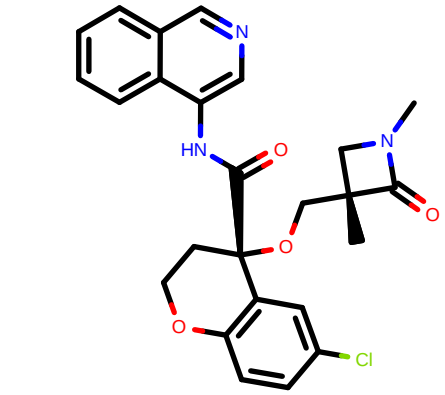
CID:	EN300-6498856_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[C@H]5C(=O)NC(=O)N5
RUN:	RUN2275
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.29

EN300-256939_1_1



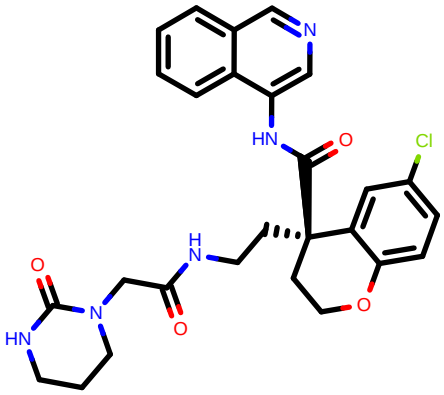
CID:	EN300-256939_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC5
RUN:	RUN10762
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.28

EN300-1273362_1_2



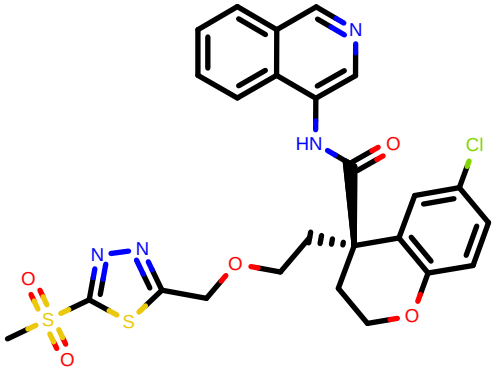
CID:	EN300-1273362_1_2
SMILES:	C[C@]1(CN(C1=O)C)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2183
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.27

EN300-36096_3_1



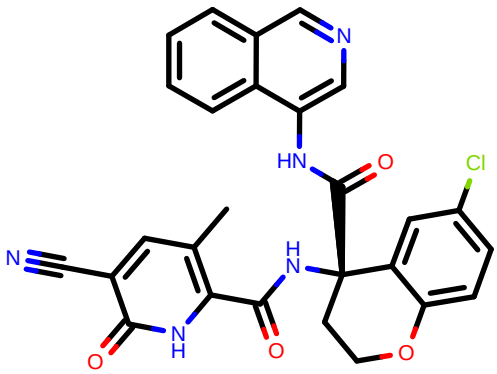
CID:	EN300-36096_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCNC5=O
RUN:	RUN6780
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.35

EN300-160080_3_1



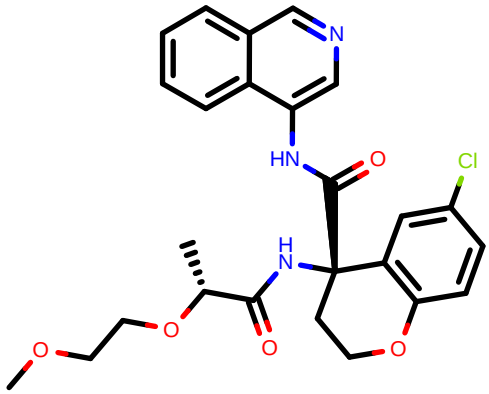
CID:	EN300-160080_3_1
SMILES:	CS(=O)(=O)c1nnc(s1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2496
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.32

EN300-358956_1_1



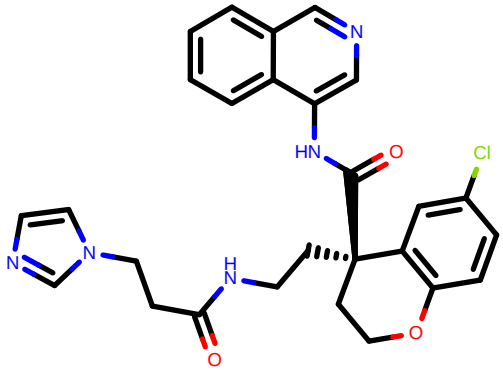
CID:	EN300-358956_1_1
SMILES:	Cc1cc(c(=O)[nH]c1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN8885
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.25

EN300-77359_1_2



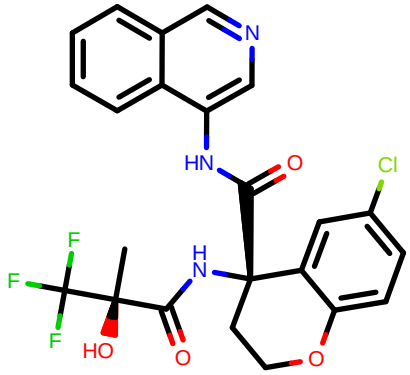
CID:	EN300-77359_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OCCOC
RUN:	RUN1333
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.29

EN300-75342_3_1



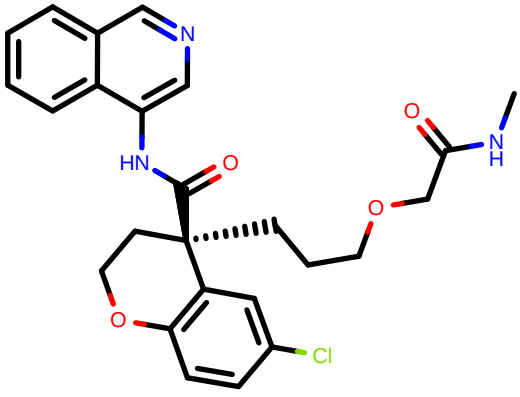
CID:	EN300-75342_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5ccnc5
RUN:	RUN8632
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.35

EN300-159633_1_2



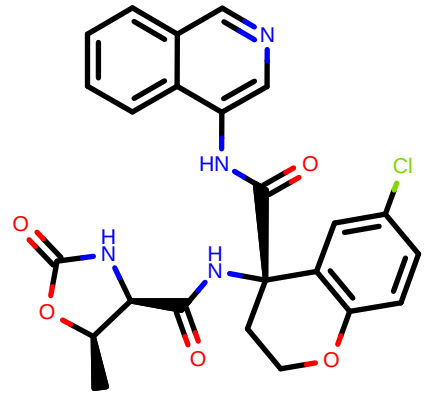
CID:	EN300-159633_1_2
SMILES:	C[C@](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN6036
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.28

EN300-2977549_4_1



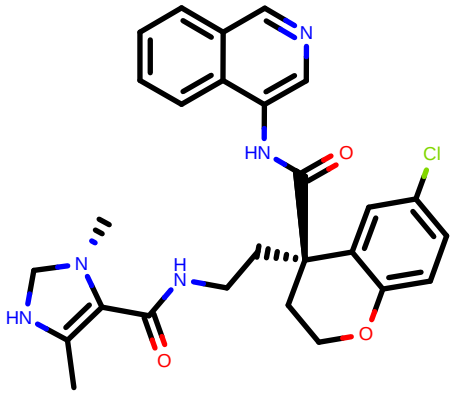
CID:	EN300-2977549_4_1
SMILES:	CNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN619
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.29

EN300-172640_1_1



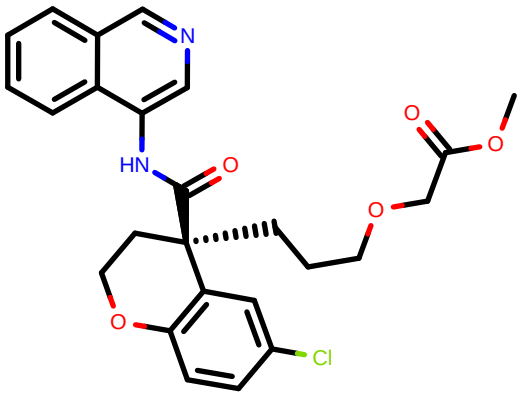
CID:	EN300-172640_1_1
SMILES:	C[C@@H]1[C@@H](NC(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4857
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.23

EN300-6498351_3_1



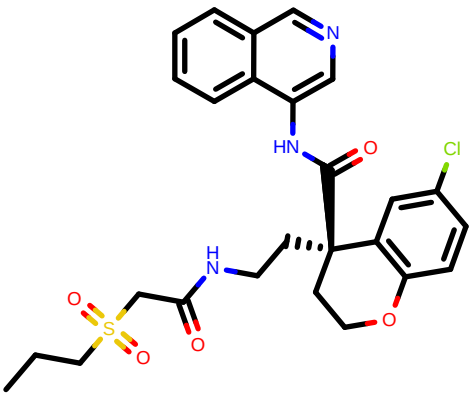
CID:	EN300-6498351_3_1
SMILES:	Cc1c(n(cn1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10133
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.25

EN300-19700_4_1



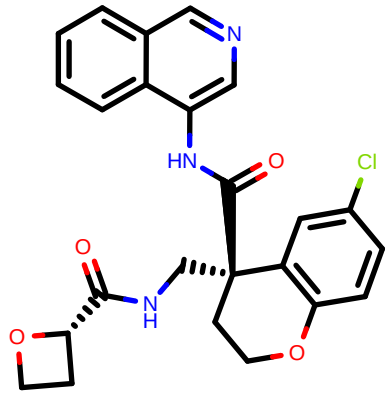
CID:	EN300-19700_4_1
SMILES:	COC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN428
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.27

EN300-52325_3_1



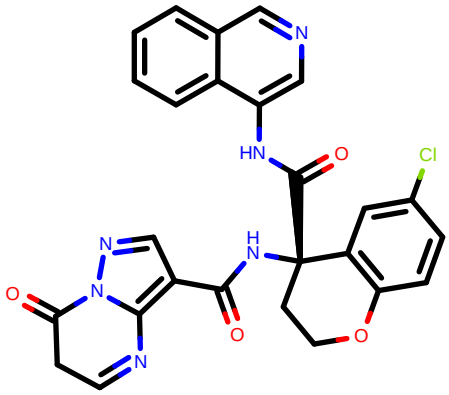
CID:	EN300-52325_3_1
SMILES:	CCCS(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4211
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.46

EN300-85760_2_1



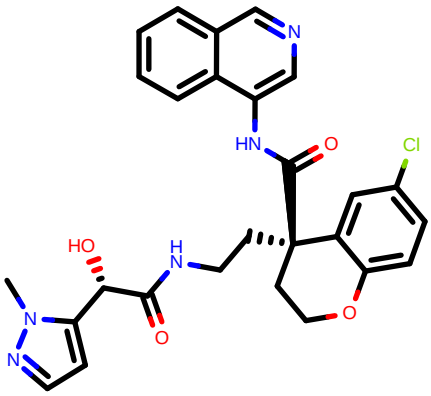
CID:	EN300-85760_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCO5
RUN:	RUN6432
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.23

EN300-203940_1_1



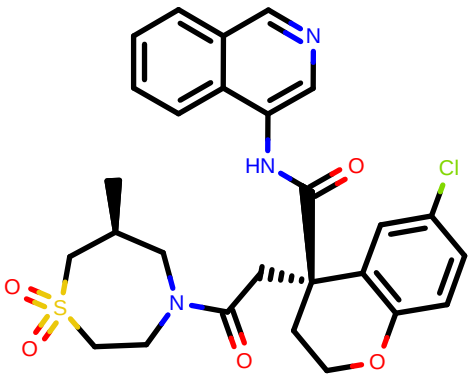
CID:	EN300-203940_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5[nH]ccc6=O
RUN:	RUN8558
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.24

EN300-6473273_3_1



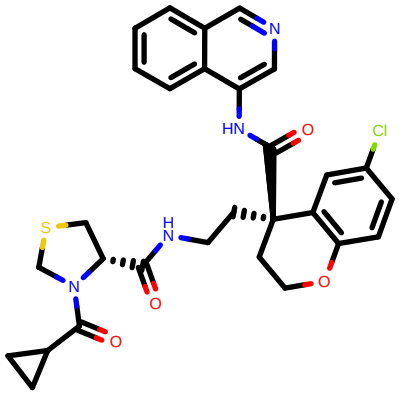
CID:	EN300-6473273_3_1
SMILES:	Cn1c(ccn1)[C@@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1689
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.33

EN300-180532_1_2



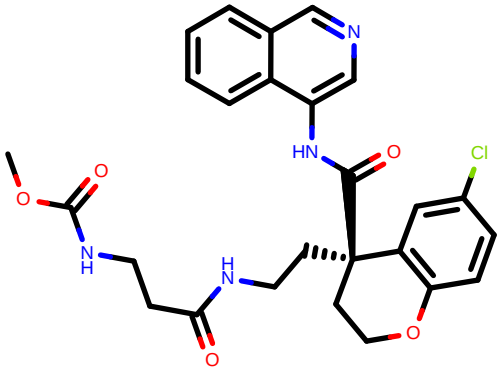
CID:	EN300-180532_1_2
SMILES:	C[C@H]1CN(CCS(=O)(=O)C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10422
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.35

EN300-18928_3_2



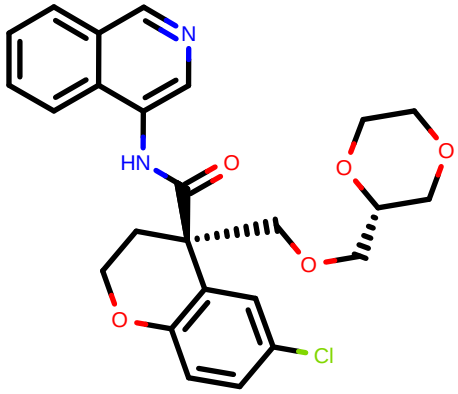
CID:	EN300-18928_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CSCN5C(=O)C6CC6
RUN:	RUN7376
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.33

EN300-71558_3_1



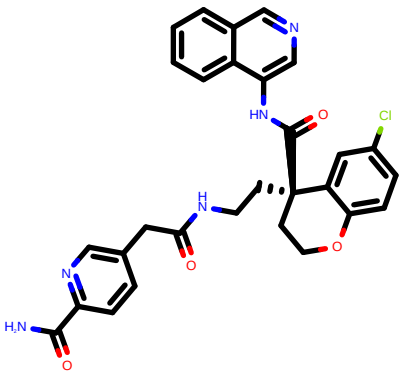
CID:	EN300-71558_3_1
SMILES:	COC(=O)NCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8874
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.30

EN300-139167_2_2



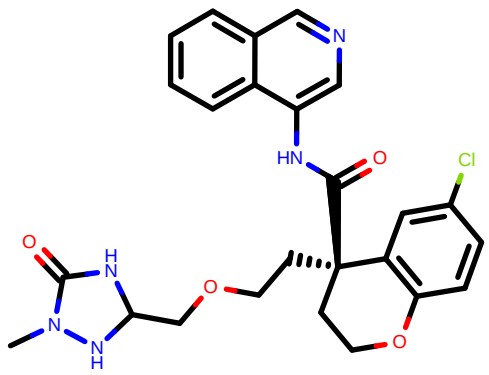
CID:	EN300-139167_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5COCCO5
RUN:	RUN2281
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.27

EN300-322332_3_1



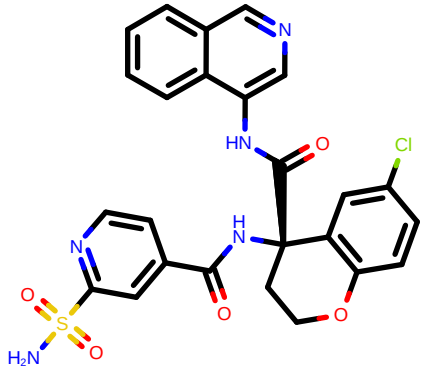
CID:	EN300-322332_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccc(nc5)C(=O)N
RUN:	RUN5830
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.38

EN300-124918_3_1



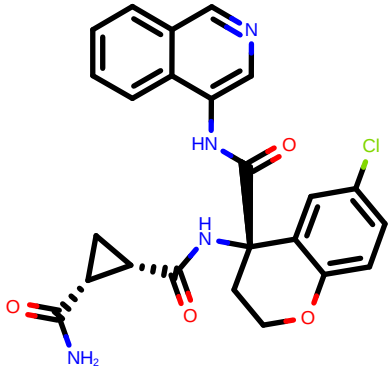
CID:	EN300-124918_3_1
SMILES:	Cn1c(=O)[nH]c(n1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1963
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.26

EN300-141628_1_1



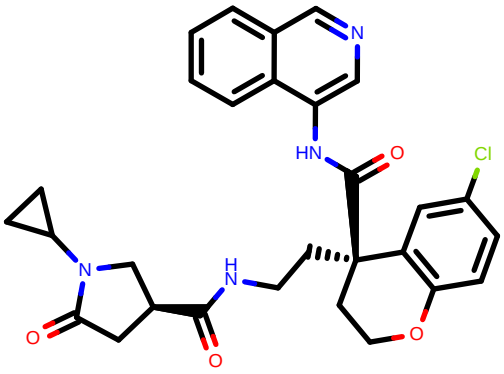
CID:	EN300-141628_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)S(=O)(=O)N
RUN:	RUN9089
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.43

EN300-331941_1_1



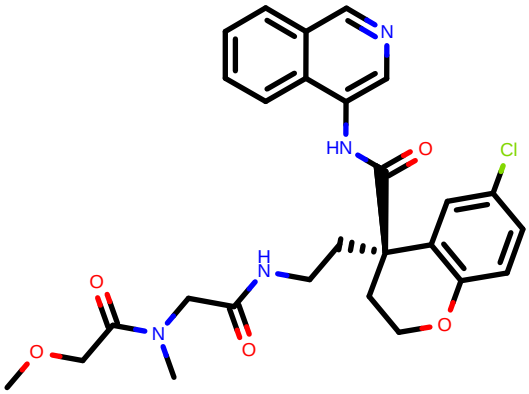
CID:	EN300-331941_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5C(=O)N
RUN:	RUN1580
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.25

EN300-12440_3_2



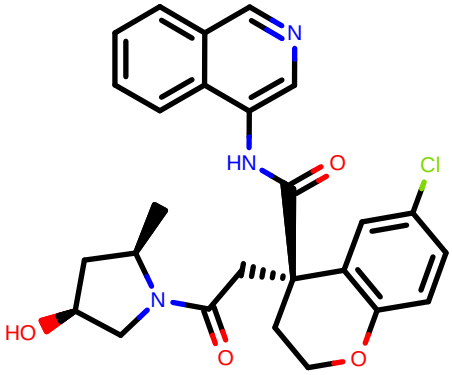
CID:	EN300-12440_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC(=O)N(C5)C6CC6
RUN:	RUN8492
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.40

EN300-35612_3_1



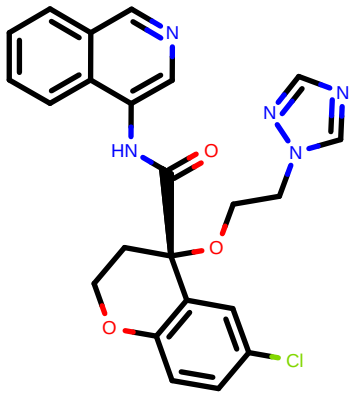
CID:	EN300-35612_3_1
SMILES:	CN(CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)COC
RUN:	RUN10598
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.33

EN300-173562_1_1



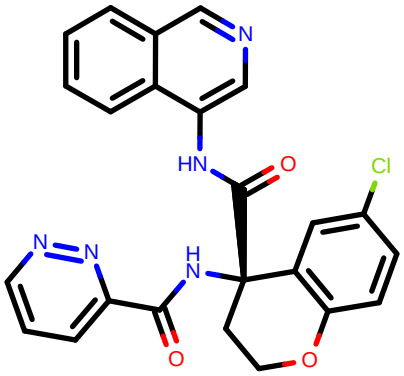
CID:	EN300-173562_1_1
SMILES:	C[C@@H]1C[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN9398
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.30

EN300-6255179_1_1



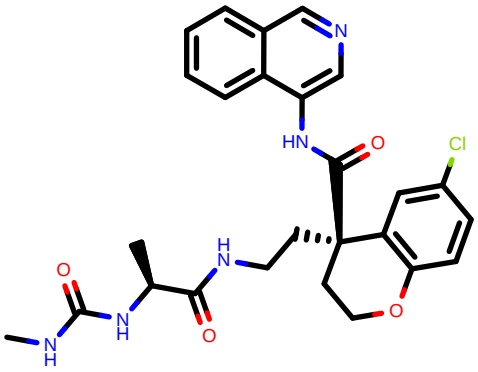
CID:	EN300-6255179_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cncn5
RUN:	RUN1088
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.21

EN300-79022_1_1



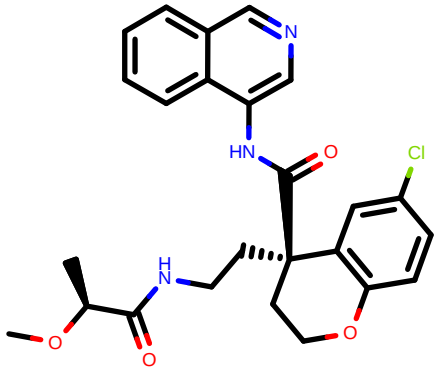
CID:	EN300-79022_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccnn5
RUN:	RUN5864
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.17

EN300-1258964_3_1



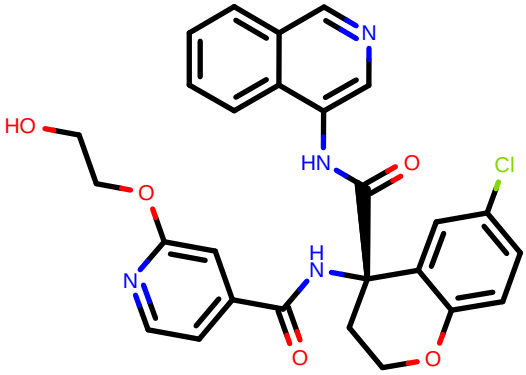
CID:	EN300-1258964_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)NC
RUN:	RUN5171
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.36

EN300-51257_3_1



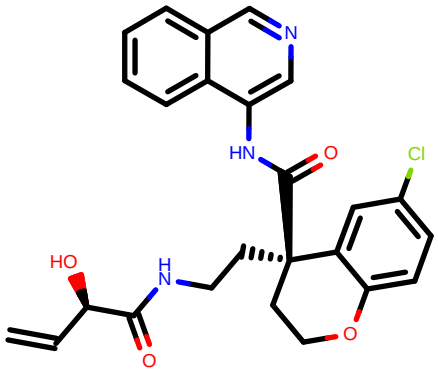
CID:	EN300-51257_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN3240
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.27

EN300-101796_1_1



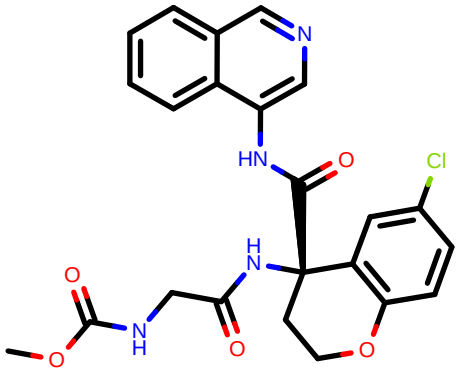
CID:	EN300-101796_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccnc(c5)OCCO
RUN:	RUN3586
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.44

EN300-181492_3_2



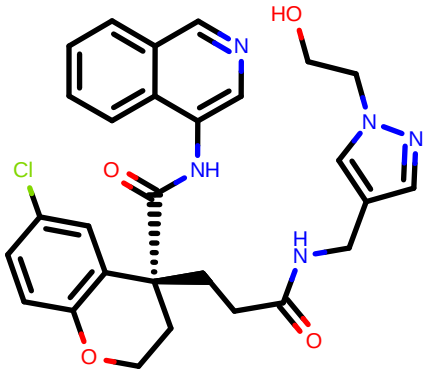
CID:	EN300-181492_3_2
SMILES:	C=C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1713
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.27

EN300-50009_1_1



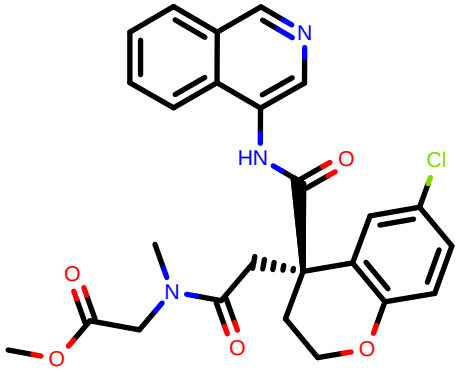
CID:	EN300-50009_1_1
SMILES:	COC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3386
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.21

EN300-1692858_2_1



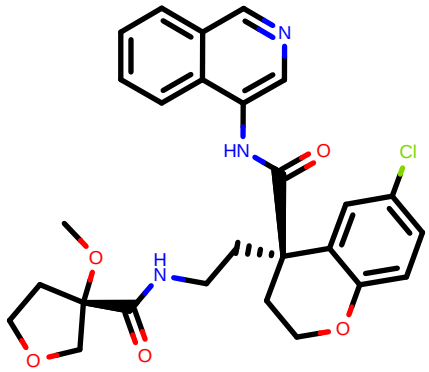
CID:	EN300-1692858_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cnn(c5)CCO
RUN:	RUN11131
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.32

EN300-13000_1_1



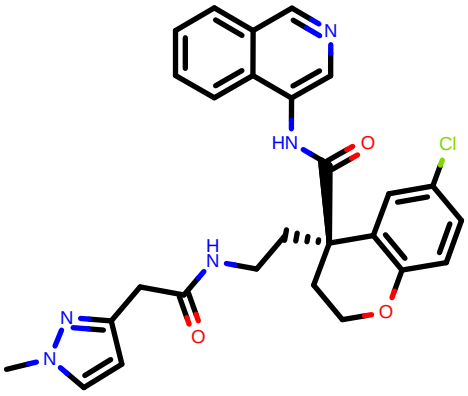
CID:	EN300-13000_1_1
SMILES:	CN(CC(=O)OC)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9926
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.25

EN300-174668_3_2



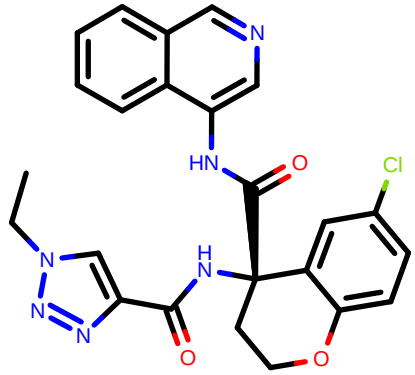
CID:	EN300-174668_3_2
SMILES:	CO[C@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5382
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.37

EN300-258702_3_1



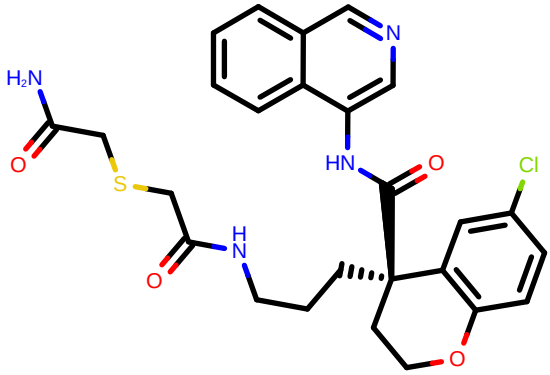
CID:	EN300-258702_3_1
SMILES:	Cn1ccc(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6210
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.29

EN300-262745_1_1



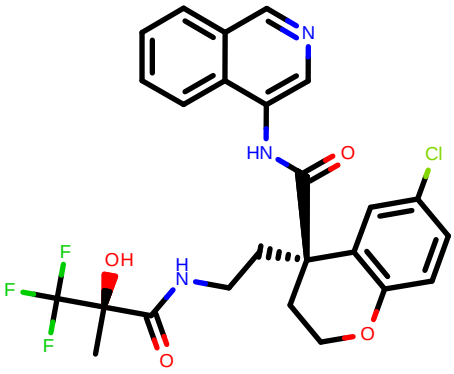
CID:	EN300-262745_1_1
SMILES:	CCn1cc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4597
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.20

EN300-33513_4_1



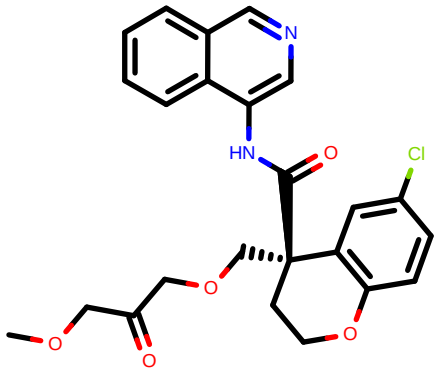
CID:	EN300-33513_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CSCC(=O)N
RUN:	RUN10997
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.34

EN300-159633_3_1



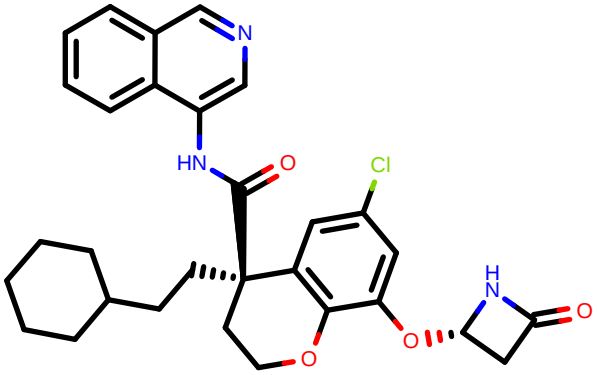
CID:	EN300-159633_3_1
SMILES:	C[C@@](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN8476
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.28

EN300-125140_2_1



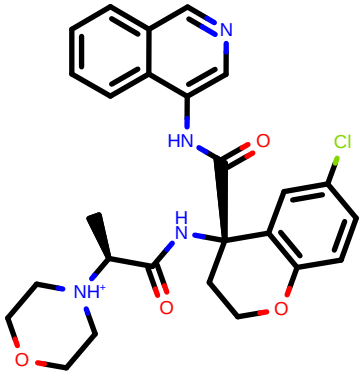
CID:	EN300-125140_2_1
SMILES:	COCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN918
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.25

VLA-UCB-50c39ae8-9_2



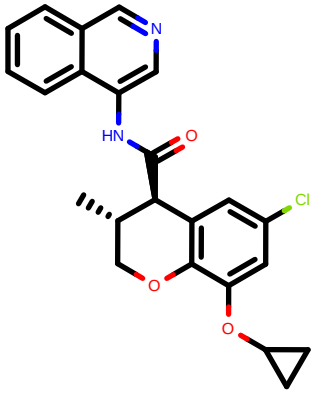
CID:	VLA-UCB-50c39ae8-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O[C@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN124
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.50

EN300-41473_1_1



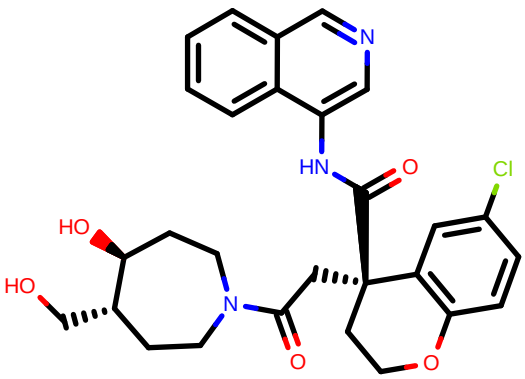
CID:	EN300-41473_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N5CCOCC5
RUN:	RUN4733
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-6_1



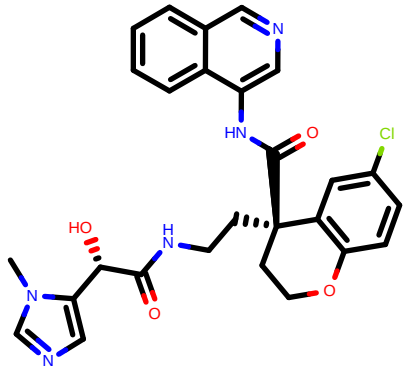
CID:	DAR-DIA-0d514e7d-6_1
SMILES:	C[C@H]1COc2c(cc(cc2OC3CC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN105
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.17

EN300-7353672_1_3



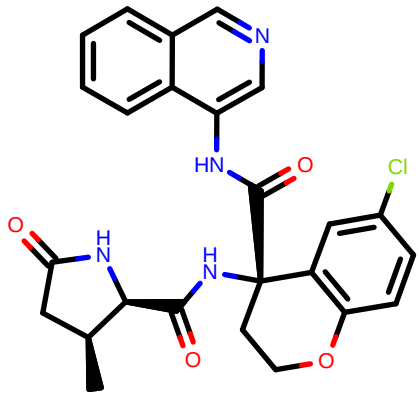
CID:	EN300-7353672_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H][C@H](C5)O)CO
RUN:	RUN1985
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.37

EN300-190283_3_1



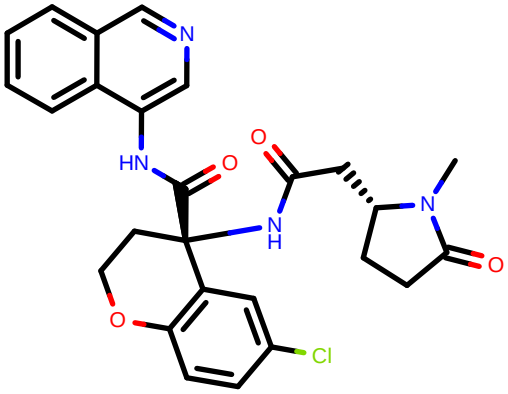
CID:	EN300-190283_3_1
SMILES:	Cn1cncc1[C@@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4835
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.41

EN300-155362_1_4



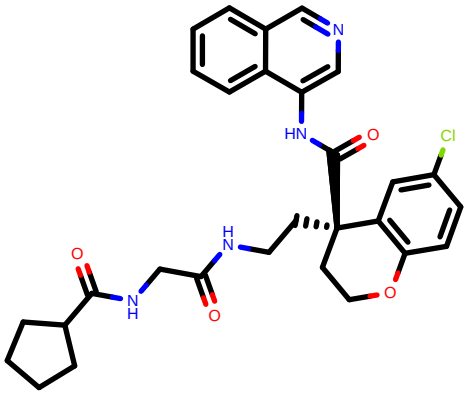
CID:	EN300-155362_1_4
SMILES:	C[C@H]1CC(=O)N[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4049
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.24

EN300-207765_1_2



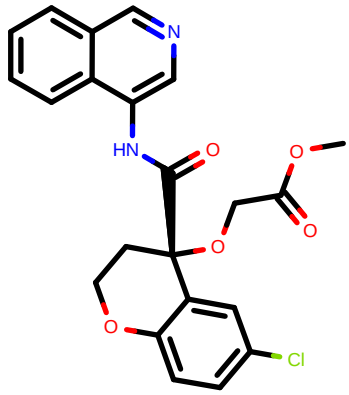
CID:	EN300-207765_1_2
SMILES:	CN1[C@H](CCC1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3422
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.28

EN300-36845_3_1



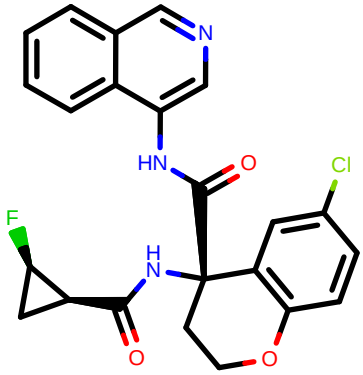
CID:	EN300-36845_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CCCC5
RUN:	RUN11238
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.32

EN300-19700_1_1



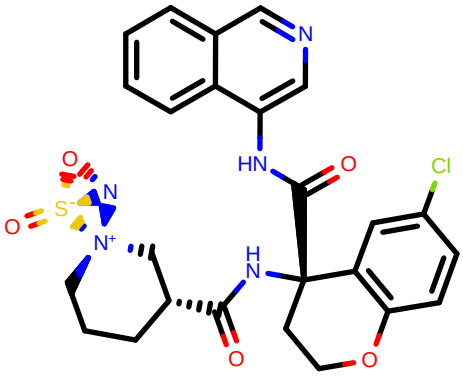
CID:	EN300-19700_1_1
SMILES:	COC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN373
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.21

EN300-97300_1_4



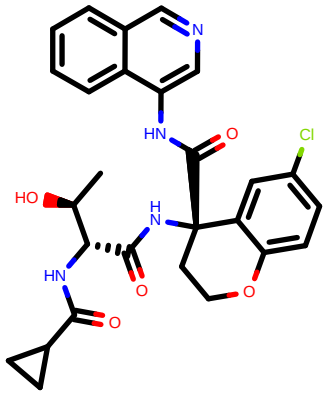
CID:	EN300-97300_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5F
RUN:	RUN2775
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.21

EN300-219496_1_1



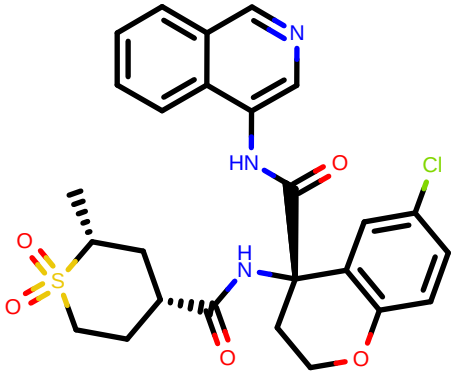
CID:	EN300-219496_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCN(C5)S(=O)(=O)N
RUN:	RUN7046
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.28

EN300-96362_1_3



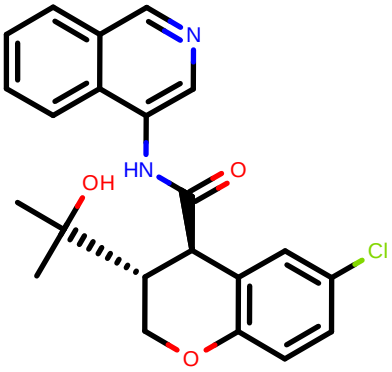
CID:	EN300-96362_1_3
SMILES:	C[C@@H]([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CC5)O
RUN:	RUN6866
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.35

EN300-6082676_1_1



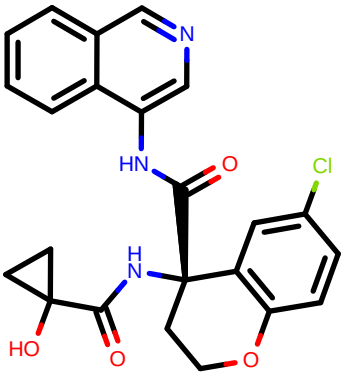
CID:	EN300-6082676_1_1
SMILES:	C[C@@H]1C[C@@H](CCS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6938
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.29

BEN-BAS-5c03e89e-1_2



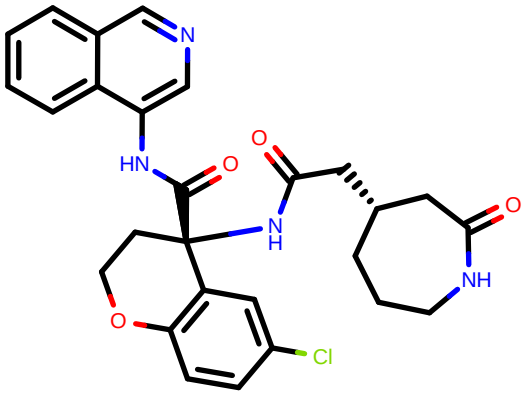
CID:	BEN-BAS-5c03e89e-1_2
SMILES:	CC(C)([C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN14
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.11

EN300-25702_1_1



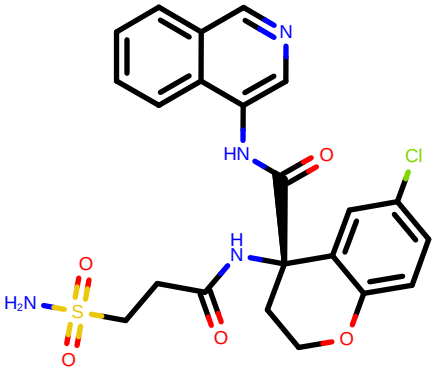
CID:	EN300-25702_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)O
RUN:	RUN2644
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.24

EN300-195590_1_2



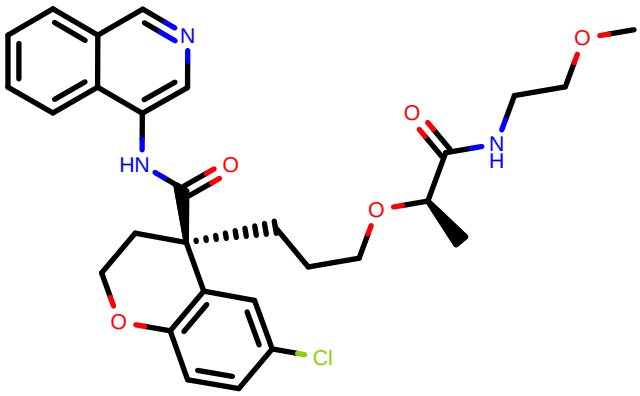
CID:	EN300-195590_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCNC(=O)C5
RUN:	RUN743
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.26

EN300-31553_1_1



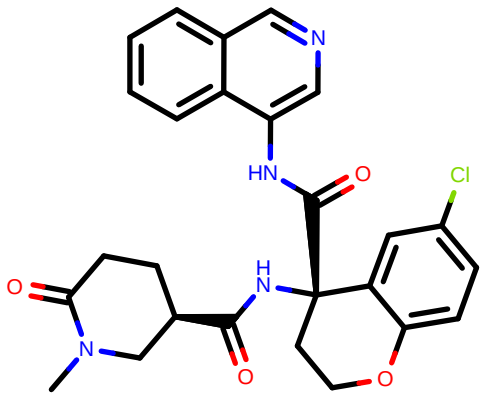
CID:	EN300-31553_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCS(=O)(=O)N
RUN:	RUN2914
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.24

EN300-23317_4_2



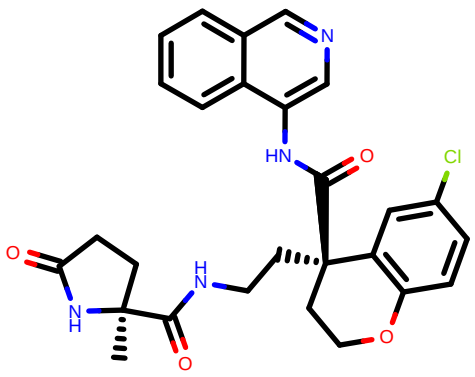
CID:	EN300-23317_4_2
SMILES:	C[C@H](C(=O)NCCOC)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1551
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.38

EN300-52983_1_1



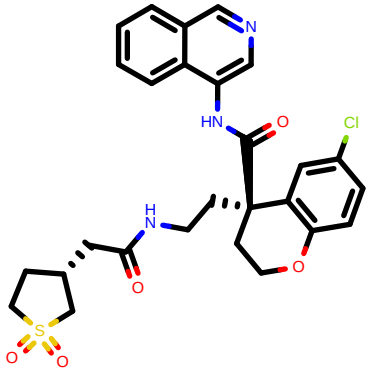
CID:	EN300-52983_1_1
SMILES:	CN1C[C@@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7894
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.32

EN300-370280_3_1



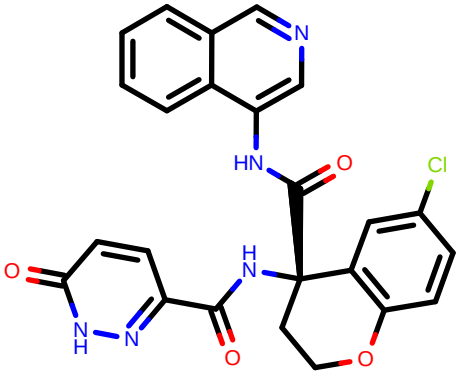
CID:	EN300-370280_3_1
SMILES:	C[C@]1(CCC(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1857
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.27

EN300-14006_3_2



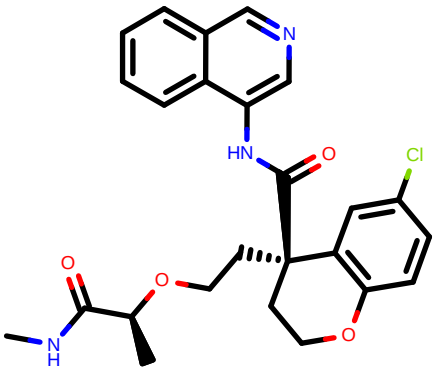
CID:	EN300-14006_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCS(=O)(=O)C5
RUN:	RUN10770
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.40

EN300-04614_1_1



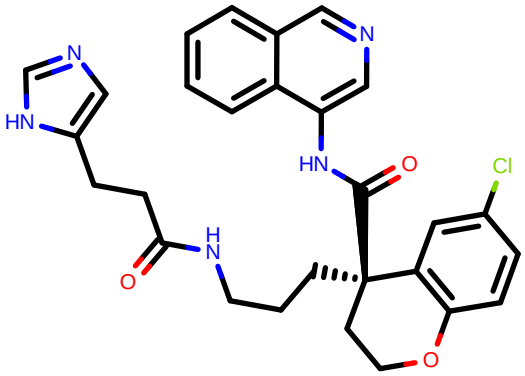
CID:	EN300-04614_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(=O)[nH]n5
RUN:	RUN5668
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.22

EN300-211482_3_1



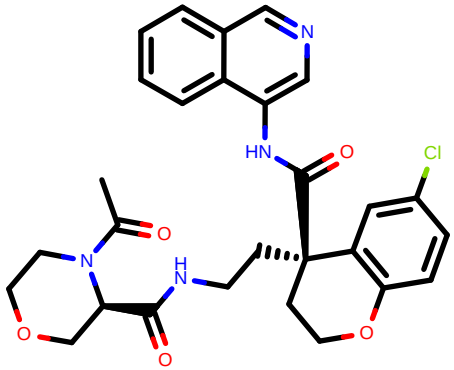
CID:	EN300-211482_3_1
SMILES:	C[C@@H](C(=O)NC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1931
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.33

EN300-145616_4_1



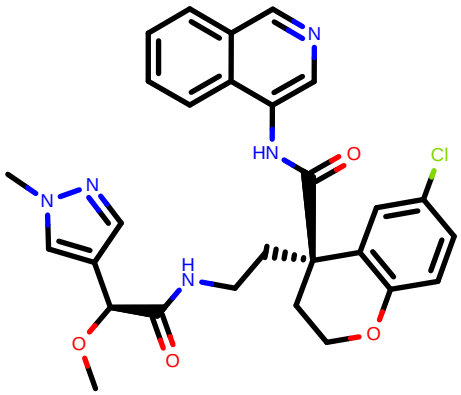
CID:	EN300-145616_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCc5cnc[nH]5
RUN:	RUN10199
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.38

EN300-116313_3_1



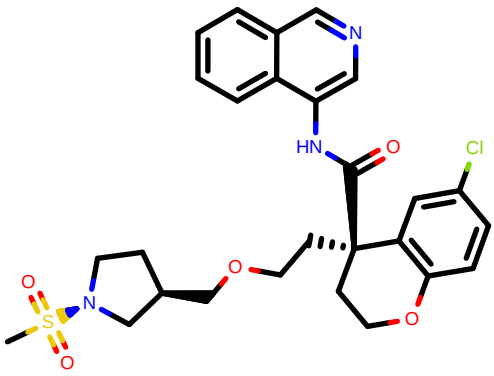
CID:	EN300-116313_3_1
SMILES:	CC(=O)N1CCOC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2522
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.39

EN300-198240_3_1



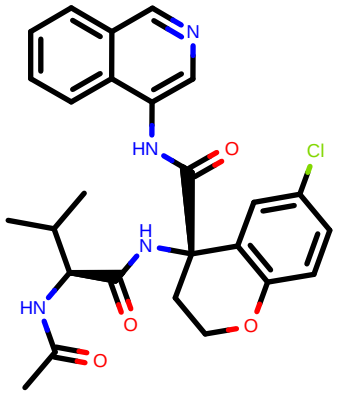
CID:	EN300-198240_3_1
SMILES:	Cn1cc(cn1)[C@@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN4935
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.39

EN300-261986_3_2



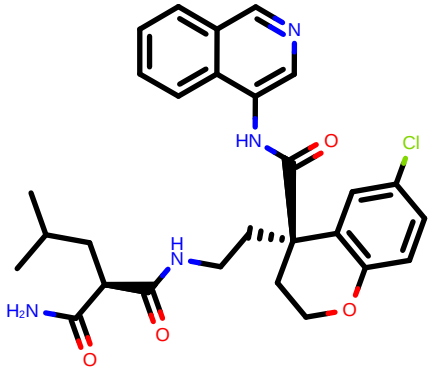
CID:	EN300-261986_3_2
SMILES:	CS(=O)(=O)N1CC[C@H](C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2377
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.32

EN300-297451_1_1



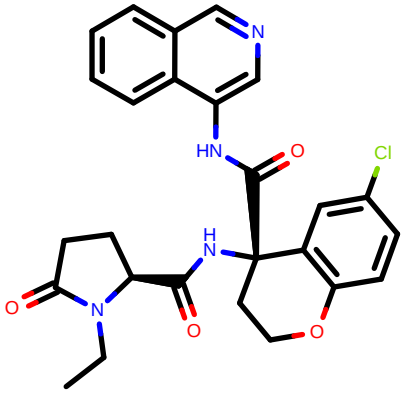
CID:	EN300-297451_1_1
SMILES:	CC(C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN5676
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.25

EN300-250126_3_2



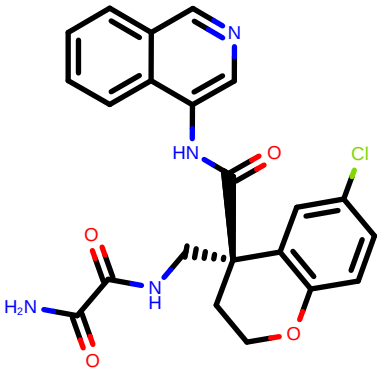
CID:	EN300-250126_3_2
SMILES:	CC(C)C[C@H](C(=O)N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10095
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.30

EN300-718785_1_1



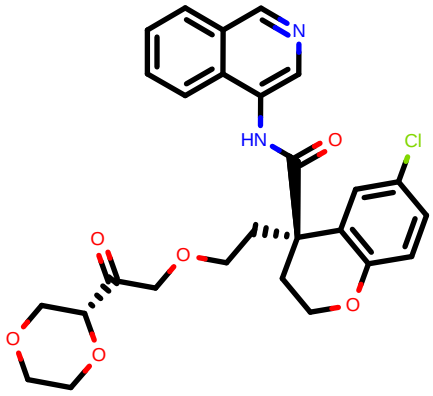
CID:	EN300-718785_1_1
SMILES:	CCN1[C@@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5960
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.27

EN300-113507_2_1



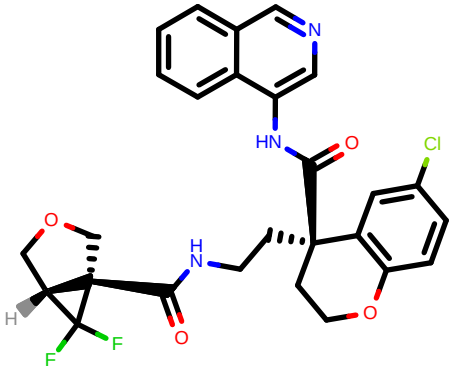
CID:	EN300-113507_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C(=O)N
RUN:	RUN5297
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.21

EN300-6238494_3_2



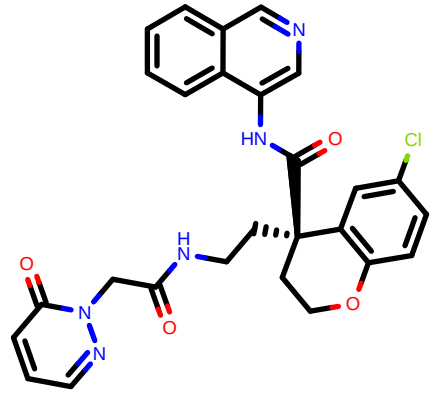
CID:	EN300-6238494_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@H]5COCCO5
RUN:	RUN1076
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.32

EN300-6738732_3_1



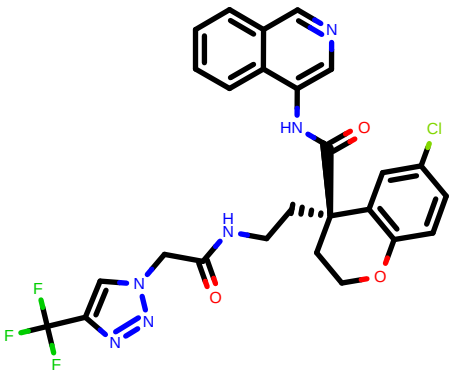
CID:	EN300-6738732_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56COC[C@H]5C6(F)F
RUN:	RUN9024
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.28

EN300-237561_3_1



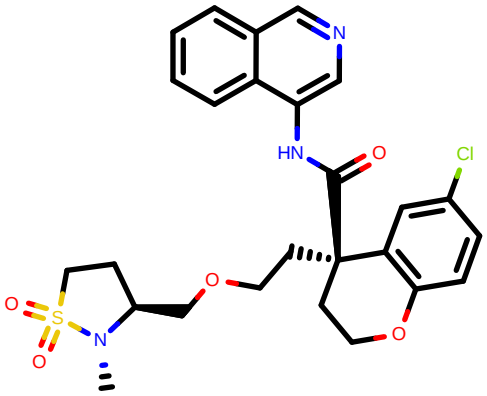
CID:	EN300-237561_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5c(=O)cccn5
RUN:	RUN10934
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.37

EN300-2910941_3_1



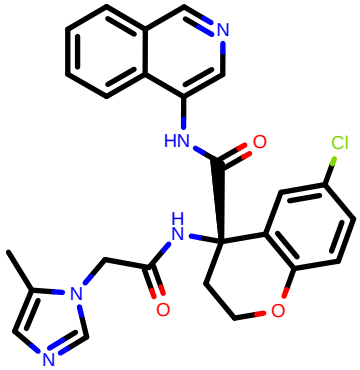
CID:	EN300-2910941_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(nn5)C(F)(F)F
RUN:	RUN10518
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.28

EN300-393148_3_1



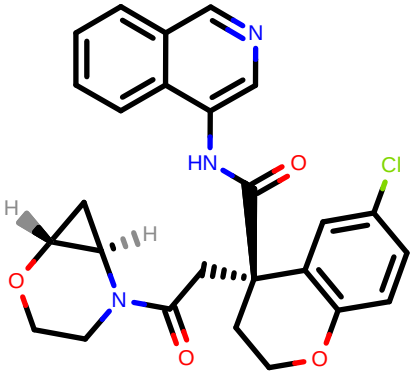
CID:	EN300-393148_3_1
SMILES:	CN1[C@@H](CCS1(=O)=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN385
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.41

EN300-315453_1_1



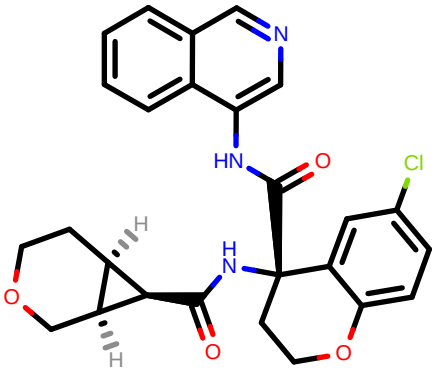
CID:	EN300-315453_1_1
SMILES:	Cc1cncn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7414
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.22

EN300-91609_1_4



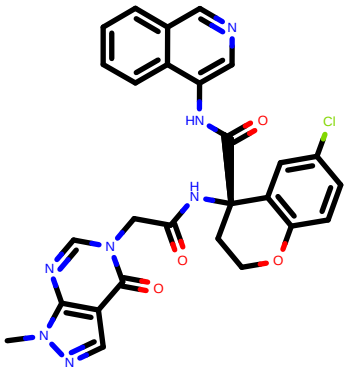
CID:	EN300-91609_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H]6[C@H]5C6
RUN:	RUN5526
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.27

EN300-1644723_1_3



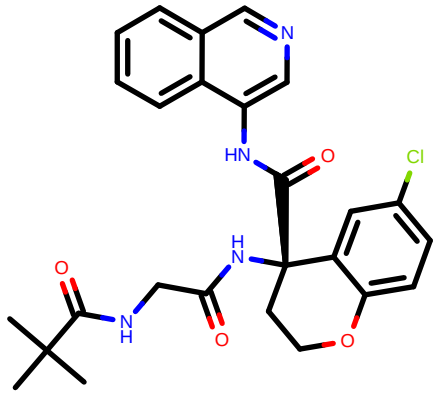
CID:	EN300-1644723_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@H]6[C@@H]5COCC6
RUN:	RUN6615
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.23

EN300-25865_1_1



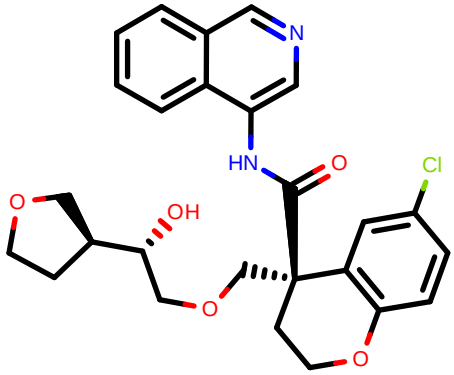
CID:	EN300-25865_1_1
SMILES:	Cn1c2c(cn1)c(=O)n(cn2)CC(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN6902
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.36

EN300-12247_1_1



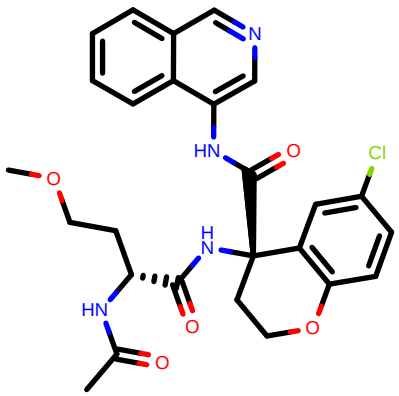
CID:	EN300-12247_1_1
SMILES:	CC(C)(C)C(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5165
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.27

EN300-1911992_2_4



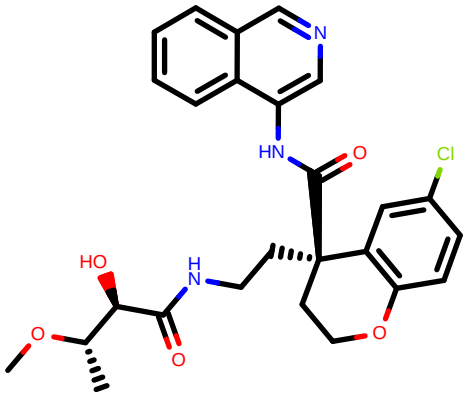
CID:	EN300-1911992_2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]([C@H]5CCOC5)O
RUN:	RUN1973
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.28

EN300-62074_1_2



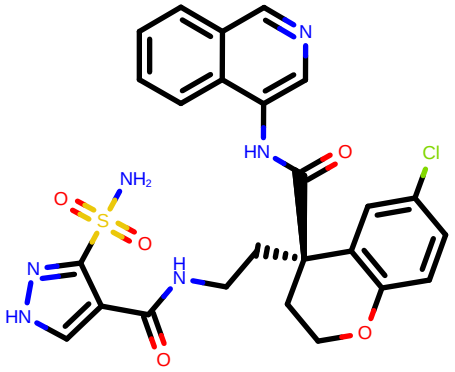
CID:	EN300-62074_1_2
SMILES:	CC(=O)N[C@H](CCOC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3154
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.28

EN300-220194_3_3



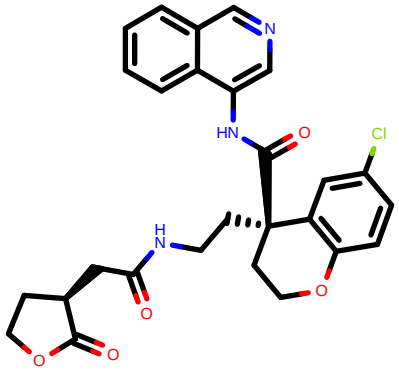
CID:	EN300-220194_3_3
SMILES:	C[C@@H]([C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN1721
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.35

EN300-144606_3_1



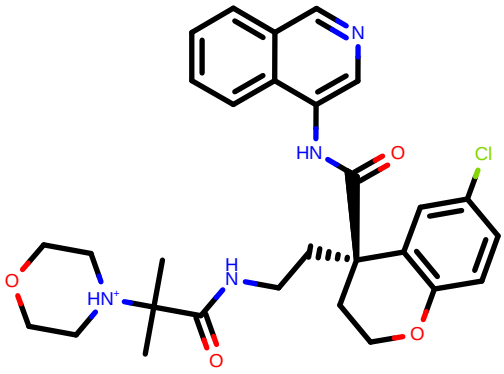
CID:	EN300-144606_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cn[nH]c5S(=O)(=O)N
RUN:	RUN11268
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.31

EN300-1072972_3_1



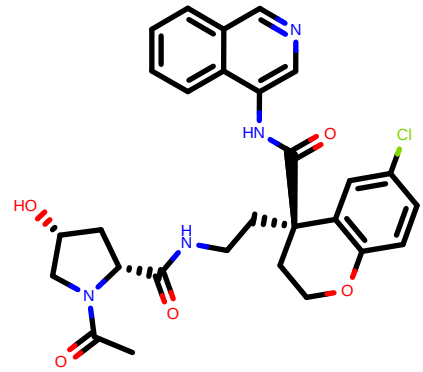
CID:	EN300-1072972_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CCOC5=O
RUN:	RUN8668
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.37

EN300-64247_3_1



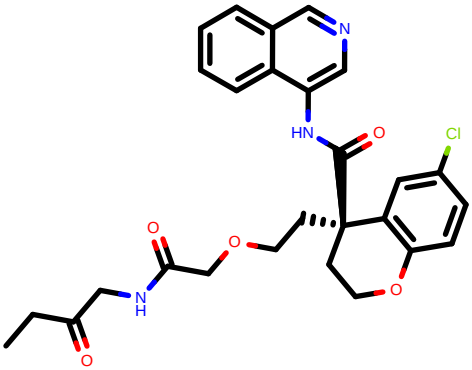
CID:	EN300-64247_3_1
SMILES:	CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N5CCOCC5
RUN:	RUN630
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.40

EN300-158260_3_1



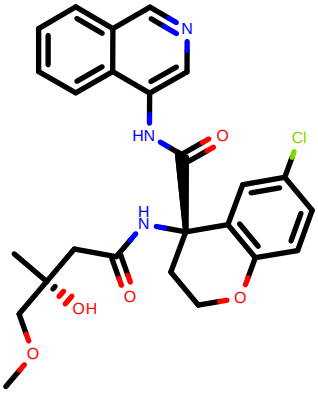
CID:	EN300-158260_3_1
SMILES:	CC(=O)N1C[C@@H](C[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10194
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.36

EN300-132624_3_1



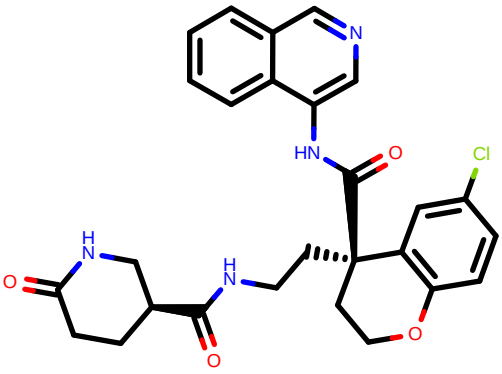
CID:	EN300-132624_3_1
SMILES:	CCC(=O)CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN948
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.36

EN300-1296824_1_1



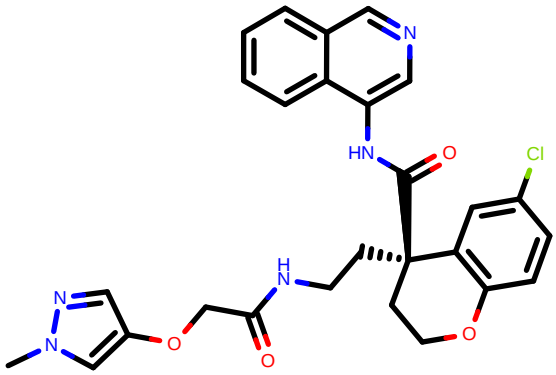
CID:	EN300-1296824_1_1
SMILES:	C[C@@](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(COC)O
RUN:	RUN957
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.33

EN300-42819_3_2



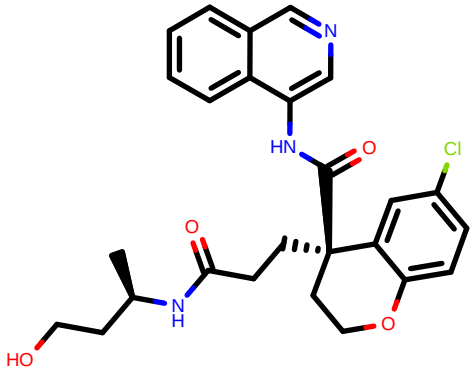
CID:	EN300-42819_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCC(=O)NC5
RUN:	RUN7360
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.31

EN300-201553_3_1



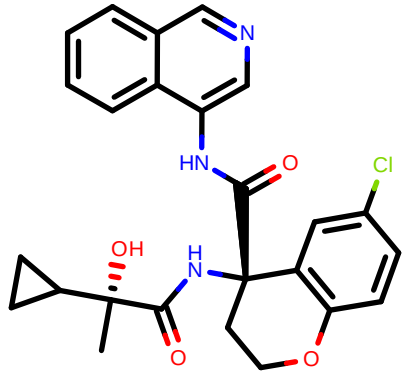
CID:	EN300-201553_3_1
SMILES:	Cn1cc(cn1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9744
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.31

EN300-117685_2_1



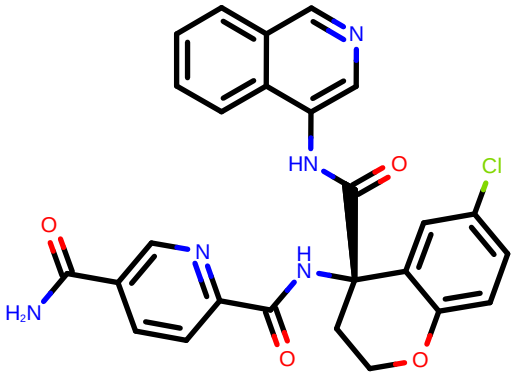
CID:	EN300-117685_2_1
SMILES:	C[C@H](CCO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1970
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.27

EN300-118760_1_1



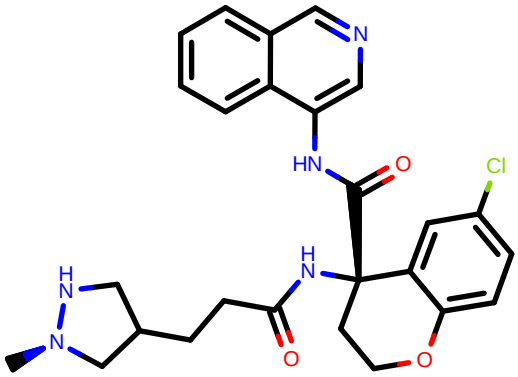
CID:	EN300-118760_1_1
SMILES:	C[C@@](C1CC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4417
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.27

EN300-58880_1_1



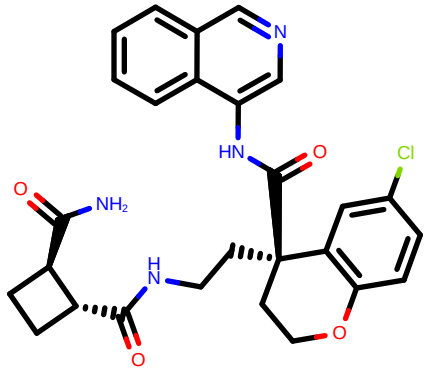
CID:	EN300-58880_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cn5)C(=O)N
RUN:	RUN8822
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.23

EN300-51411_1_1



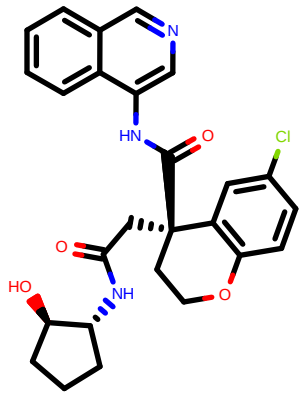
CID:	EN300-51411_1_1
SMILES:	Cn1cc(cn1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3082
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.26

EN300-217107_3_3



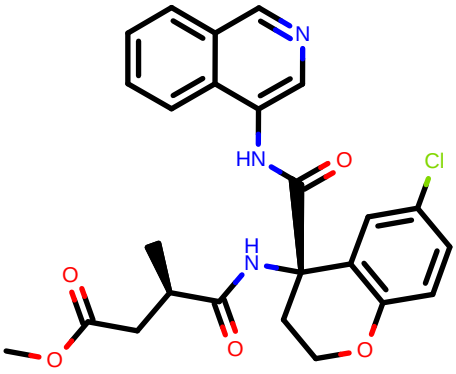
CID:	EN300-217107_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@H]5C(=O)N
RUN:	RUN503
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.30

EN300-60314_1_1



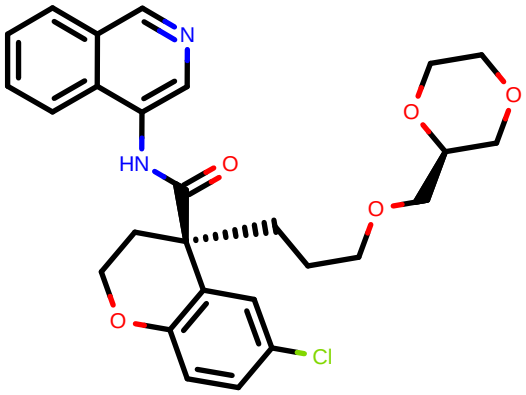
CID:	EN300-60314_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCC[C@H]5O
RUN:	RUN8704
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.21

EN300-106540_1_2



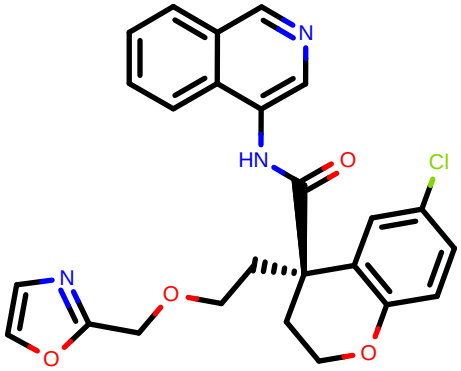
CID:	EN300-106540_1_2
SMILES:	C[C@H](CC(=O)OC)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2938
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.25

EN300-139167_4_1



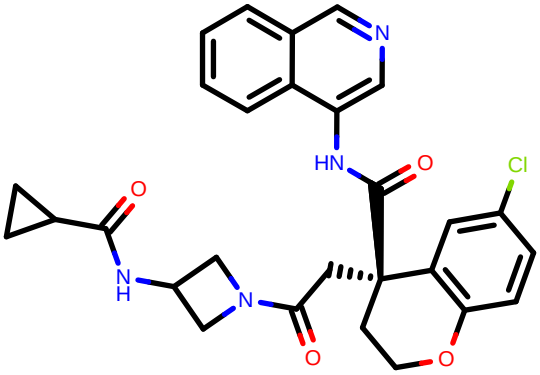
CID:	EN300-139167_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5COCCO5
RUN:	RUN508
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.47

EN300-317555_3_1



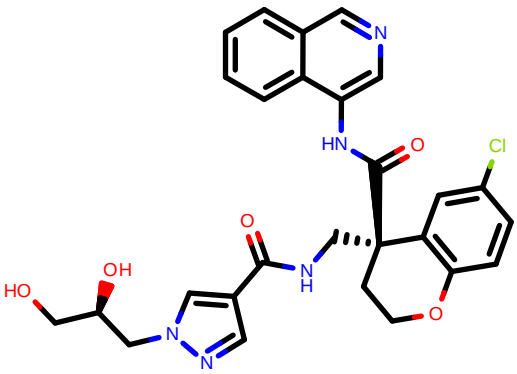
CID:	EN300-317555_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NCCO5
RUN:	RUN797
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.23

EN300-142432_1_1



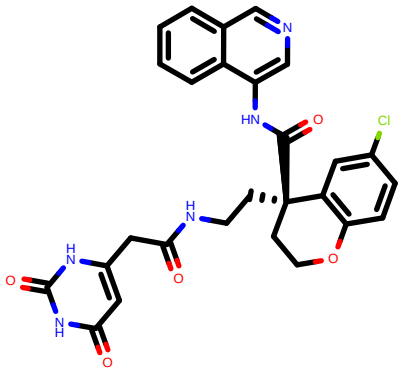
CID:	EN300-142432_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)NC(=O)C6CC6
RUN:	RUN11230
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.31

EN300-246178_2_1



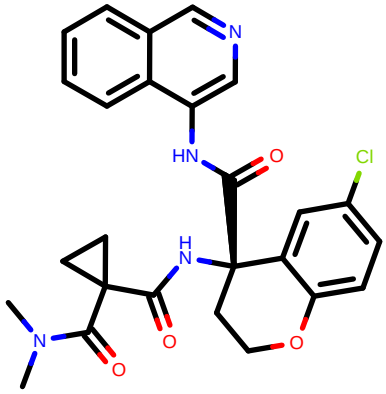
CID:	EN300-246178_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnn(c5)C[C@@H](CO)O
RUN:	RUN6931
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.49

EN300-11441_3_1



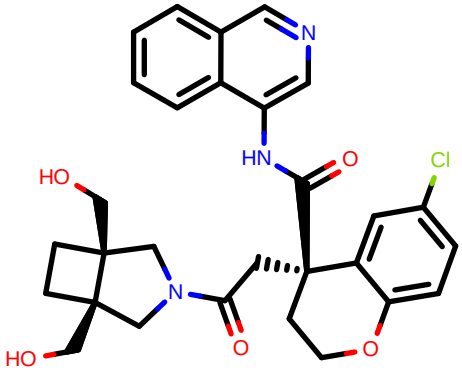
CID:	EN300-11441_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5cc(=O)[nH]c(=O)[nH]5
RUN:	RUN10246
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.34

EN300-180875_1_1



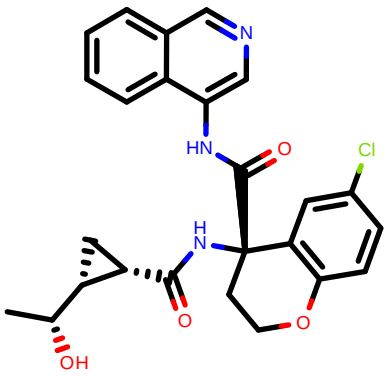
CID:	EN300-180875_1_1
SMILES:	CN(C)C(=O)C1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6946
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.28

EN300-1272865_1_1



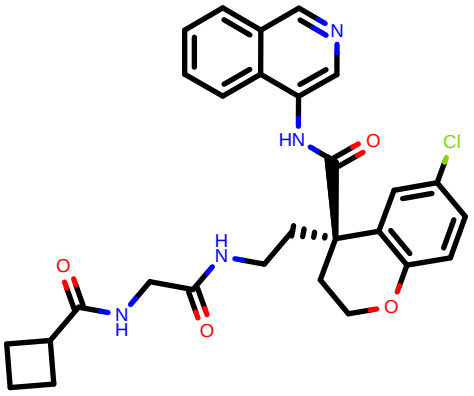
CID:	EN300-1272865_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@]6(CC[C@]6(C5)CO)CO
RUN:	RUN1905
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.31

EN300-6729572_1_2



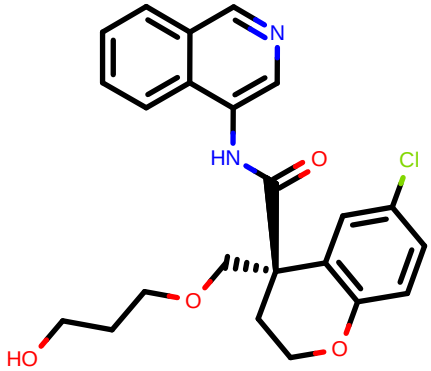
CID:	EN300-6729572_1_2
SMILES:	C[C@H]([C@@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1804
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.32

EN300-62448_3_1



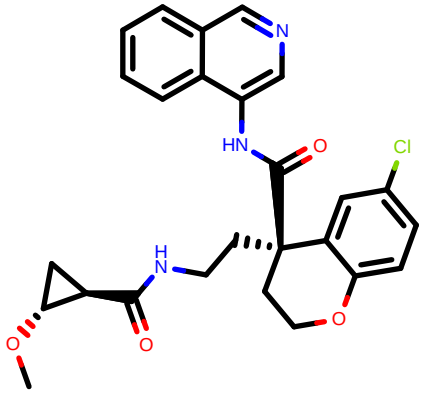
CID:	EN300-62448_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)C5CCC5
RUN:	RUN10400
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.30

EN300-221518_2_1



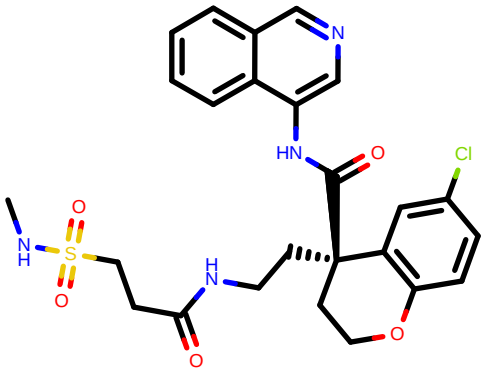
CID:	EN300-221518_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCO
RUN:	RUN823
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.21

EN300-650518_3_1



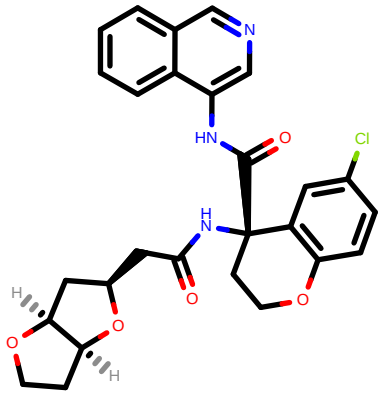
CID:	EN300-650518_3_1
SMILES:	CO[C@@H]1C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10412
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.27

EN300-123205_3_1



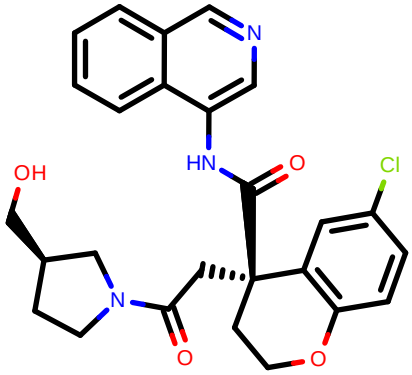
CID:	EN300-123205_3_1
SMILES:	CNS(=O)(=O)CCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7388
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.32

EN300-7355519_1_3



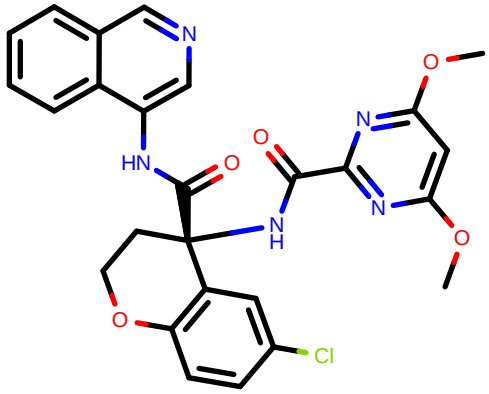
CID:	EN300-7355519_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5C[C@@H]6[C@@H](O5)CCO6
RUN:	RUN7382
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.30

EN300-144970_1_1



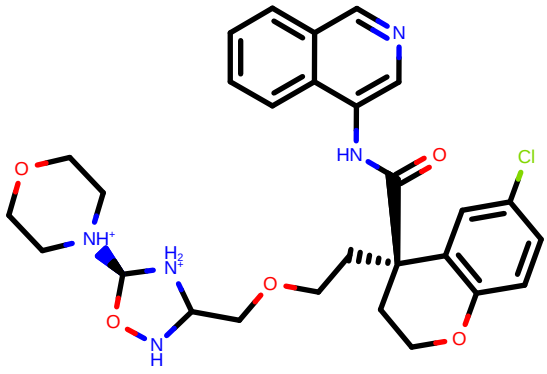
CID:	EN300-144970_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO
RUN:	RUN2630
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.25

EN300-393341_1_1



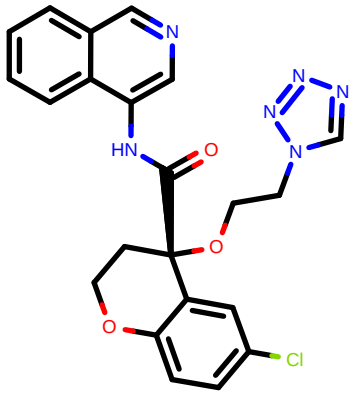
CID:	EN300-393341_1_1
SMILES:	COc1cc(nc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN6235
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.25

EN300-1608590_3_1



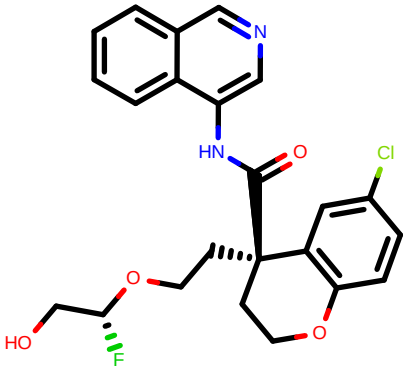
CID:	EN300-1608590_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5nc(on5)N6CCOCC6
RUN:	RUN2551
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.37

EN300-364679_1_1



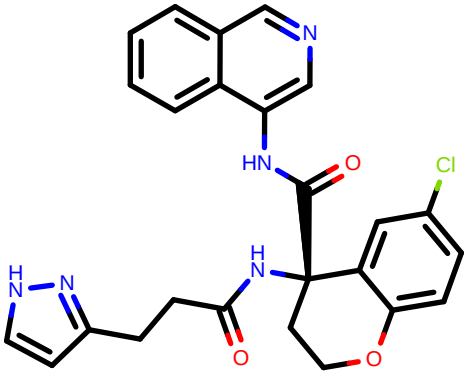
CID:	EN300-364679_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cnnn5
RUN:	RUN1408
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.22

EN300-861925_3_1



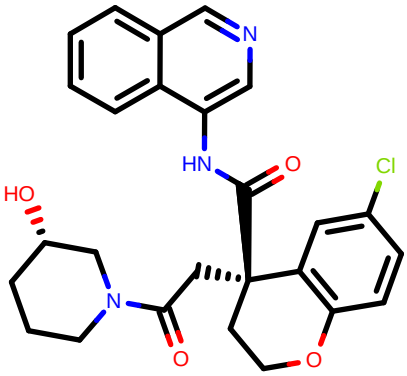
CID:	EN300-861925_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO[C@@H](CO)F
RUN:	RUN1068
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.30

EN300-1664603_1_1



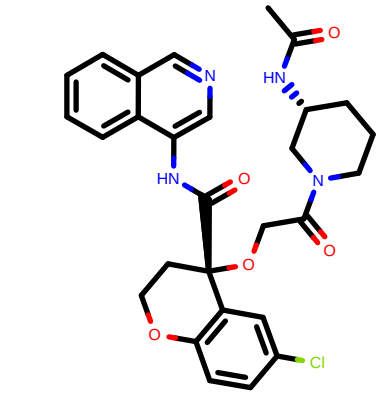
CID:	EN300-1664603_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCc5ccn[nH]5
RUN:	RUN5616
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.23

EN300-20284_1_1



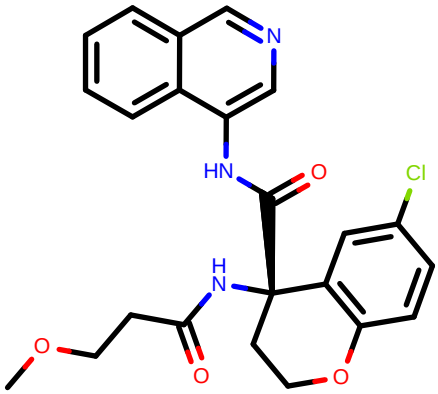
CID:	EN300-20284_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H](C5)O
RUN:	RUN2778
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.26

EN300-48886_1_1



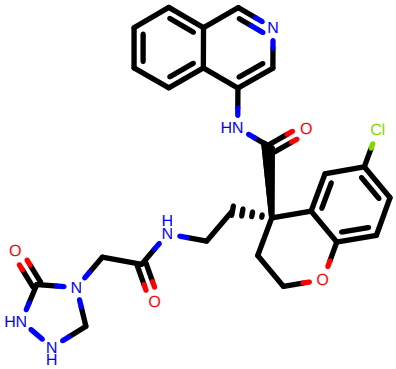
CID:	EN300-48886_1_1
SMILES:	CC(=O)N[C@@H]1CCCN(C1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1991
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.30

EN300-64536_1_1



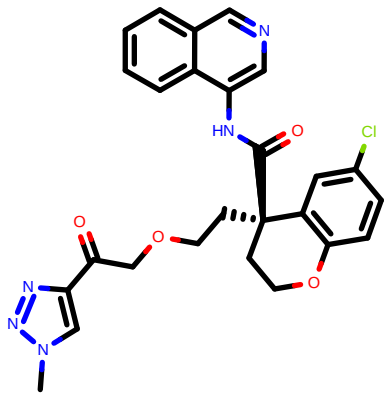
CID:	EN300-64536_1_1
SMILES:	COCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2538
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.22

EN300-120820_3_1



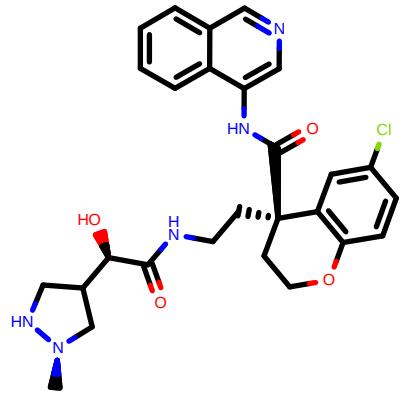
CID:	EN300-120820_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cn[nH]c5=O
RUN:	RUN914
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.26

EN300-263153_3_1



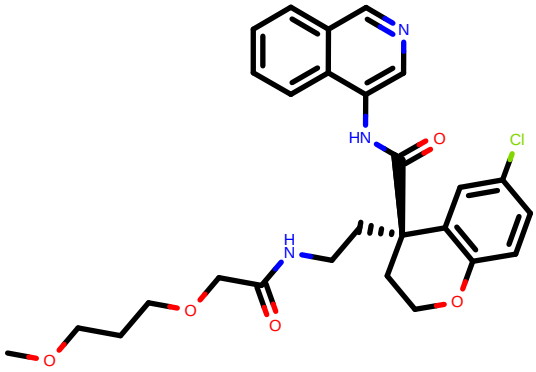
CID:	EN300-263153_3_1
SMILES:	Cn1cc(nn1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN719
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.30

EN300-198540_3_2



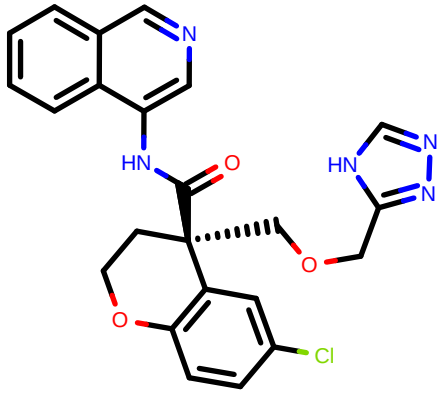
CID:	EN300-198540_3_2
SMILES:	Cn1cc(cn1)[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2487
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.45

EN300-125769_3_1



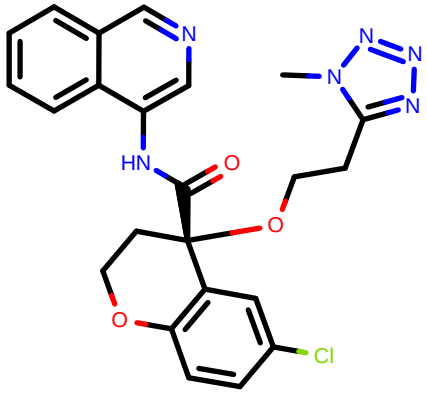
CID:	EN300-125769_3_1
SMILES:	COCCCOCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10206
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.27

EN300-306316_2_1



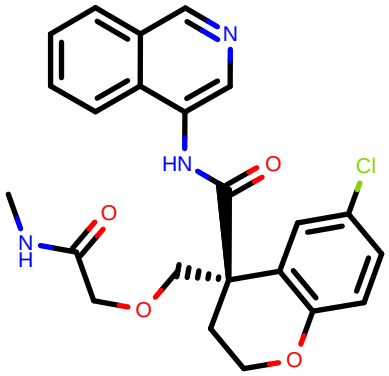
CID:	EN300-306316_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5[nH]cnn5
RUN:	RUN2141
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.23

EN300-365398_1_1



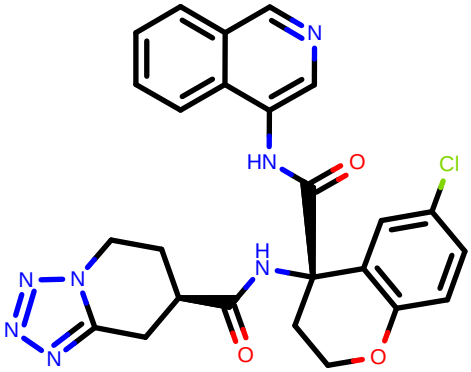
CID:	EN300-365398_1_1
SMILES:	Cn1c(nnn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2711
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.27

EN300-2977549_2_1



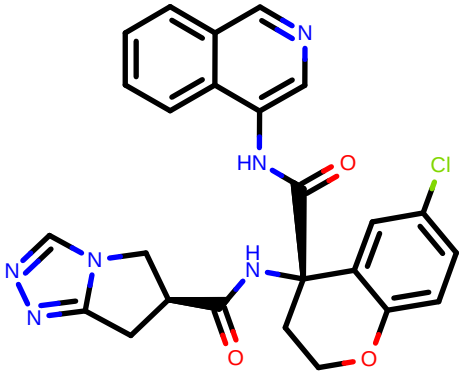
CID:	EN300-2977549_2_1
SMILES:	CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1078
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.17

EN300-1653482_1_1



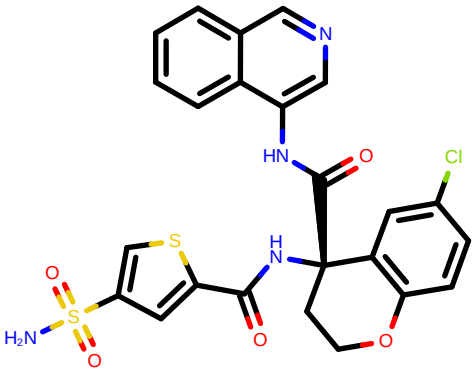
CID:	EN300-1653482_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCn6c(nnn6)C5
RUN:	RUN8266
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.28

EN300-6745453_1_2



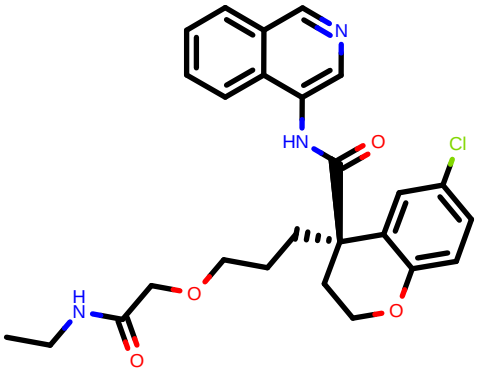
CID:	EN300-6745453_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5Cc6nncn6C5
RUN:	RUN6387
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.29

EN300-98099_1_1



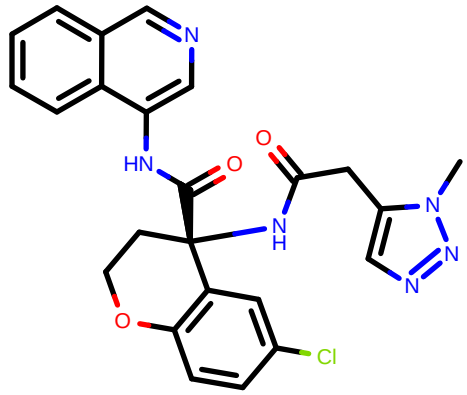
CID:	EN300-98099_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cs5)S(=O)(=O)N
RUN:	RUN9134
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.30

EN300-7003350_4_1



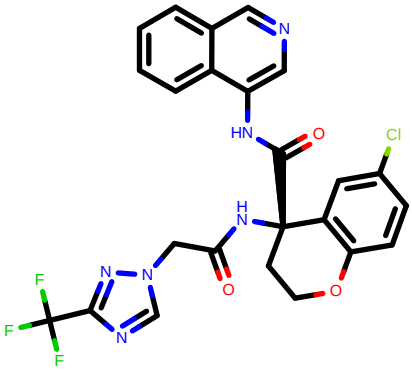
CID:	EN300-7003350_4_1
SMILES:	CCNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1047
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.27

EN300-6486855_1_1



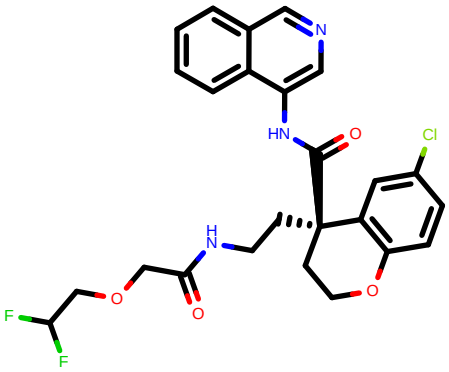
CID:	EN300-6486855_1_1
SMILES:	Cn1c(cnn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3622
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.27

EN300-7385389_1_1



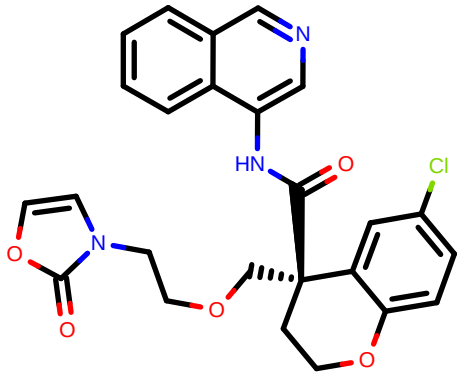
CID:	EN300-7385389_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cnc(n5)C(F)(F)F
RUN:	RUN6970
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.29

EN300-315792_3_1



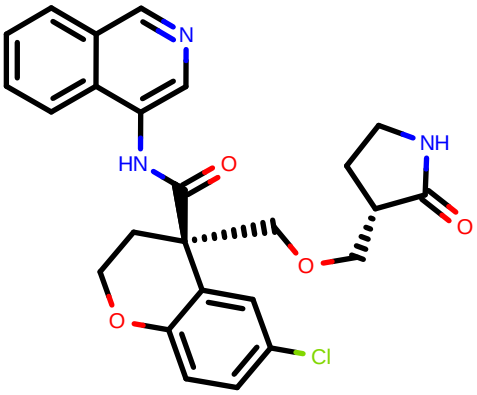
CID:	EN300-315792_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)COCC(F)F
RUN:	RUN3196
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.25

EN300-370967_2_1



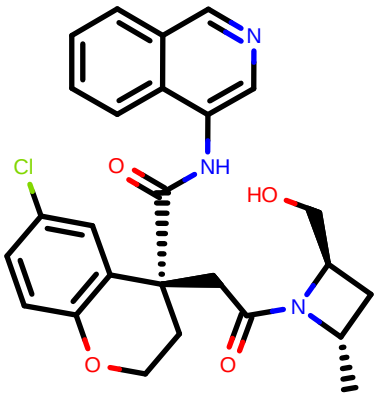
CID:	EN300-370967_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCN5CCOC5=O
RUN:	RUN815
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.32

EN300-246248_2_1



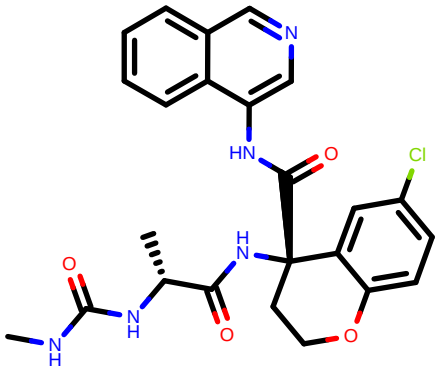
CID:	EN300-246248_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCNC5=O
RUN:	RUN323
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.26

EN300-1709410_1_2



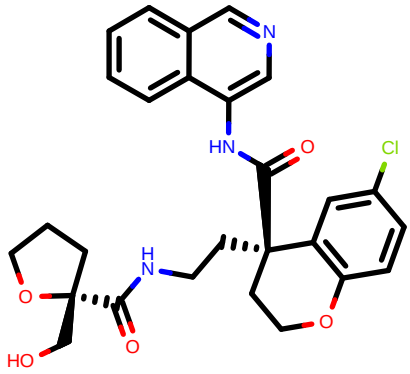
CID:	EN300-1709410_1_2
SMILES:	C[C@H]1C[C@@H](N1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN6784
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.31

EN300-2958082_1_1



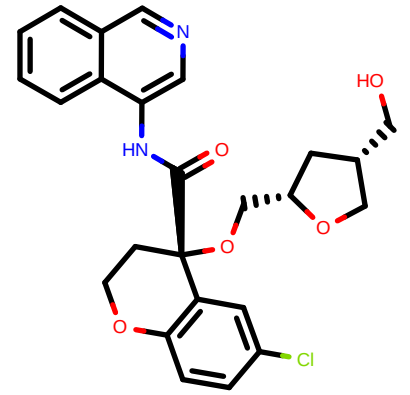
CID:	EN300-2958082_1_1
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)NC
RUN:	RUN4385
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.28

EN300-1425677_3_2



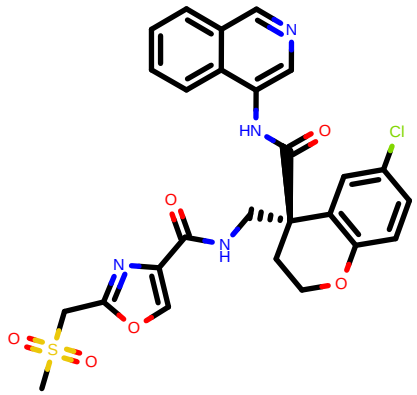
CID:	EN300-1425677_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCCO5)CO
RUN:	RUN1665
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.36

EN300-6494158_1_1



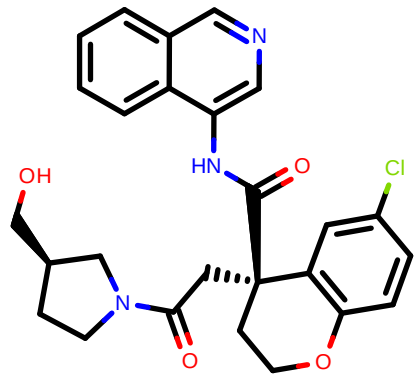
CID:	EN300-6494158_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[C@@H](CO5)CO
RUN:	RUN1360
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.35

EN300-263392_2_1



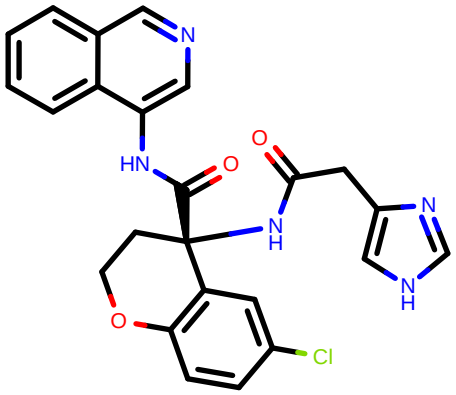
CID:	EN300-263392_2_1
SMILES:	CS(=O)(=O)Cc1nc(co1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6181
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.29

EN300-144970_1_1



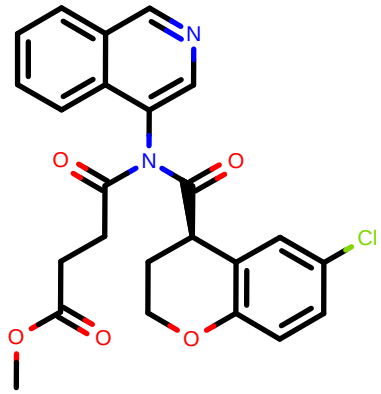
CID:	EN300-144970_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO
RUN:	RUN2624
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.34

EN300-342226_1_1



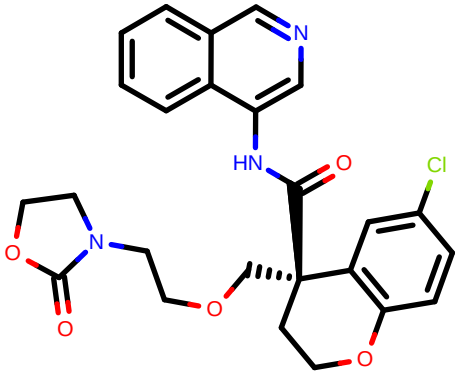
CID:	EN300-342226_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnc[nH]5
RUN:	RUN2336
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.29

DAR-DIA-5ff57136-9_1



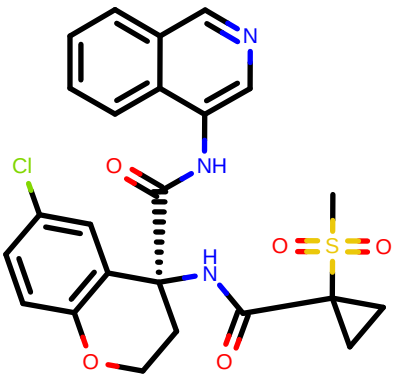
CID:	DAR-DIA-5ff57136-9_1
SMILES:	COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN256
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.33

EN300-370967_2_1



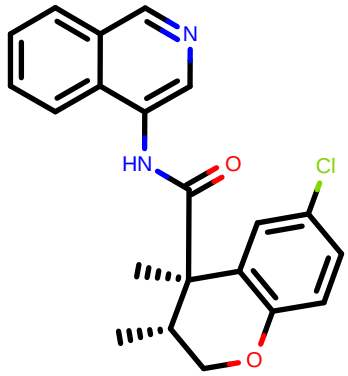
CID:	EN300-370967_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCN5CCOC5=O
RUN:	RUN807
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.31

EN300-191495_1_1



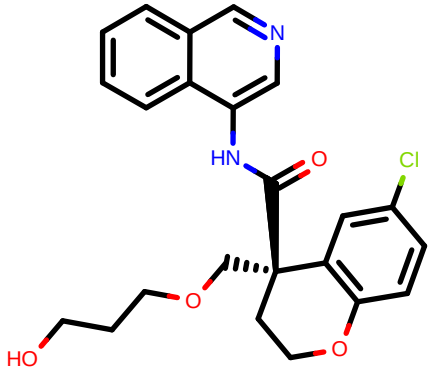
CID:	EN300-191495_1_1
SMILES:	CS(=O)(=O)C1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5736
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.32

DAR-DIA-0d514e7d-28_1



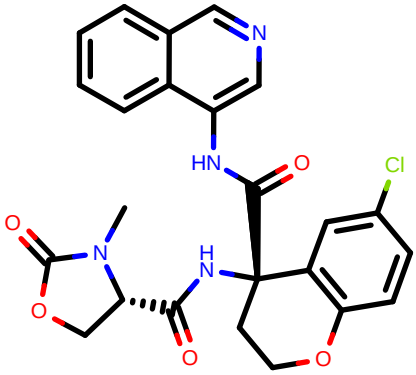
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	C[C@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN6
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.09

EN300-221518_2_1



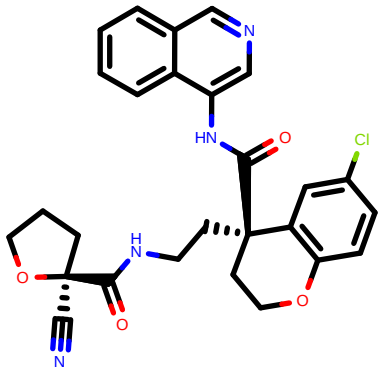
CID:	EN300-221518_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCCO
RUN:	RUN831
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.20

EN300-332838_1_1



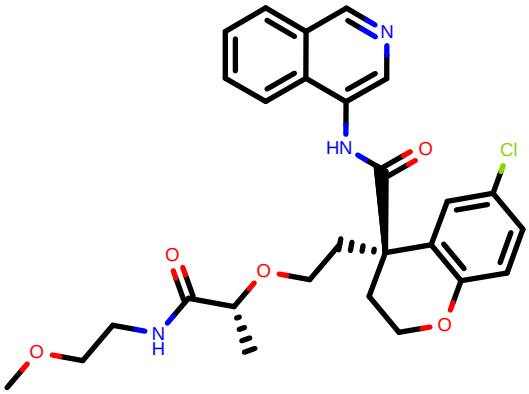
CID:	EN300-332838_1_1
SMILES:	CN1[C@@H](COC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7778
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.22

EN300-3710141_3_1



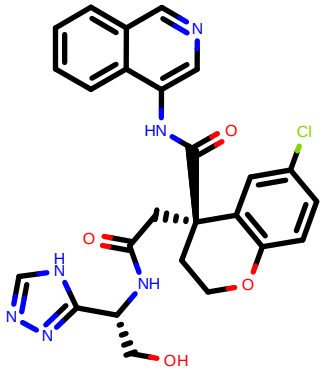
CID:	EN300-3710141_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCCO5)C#N
RUN:	RUN1002
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.30

EN300-23317_3_2



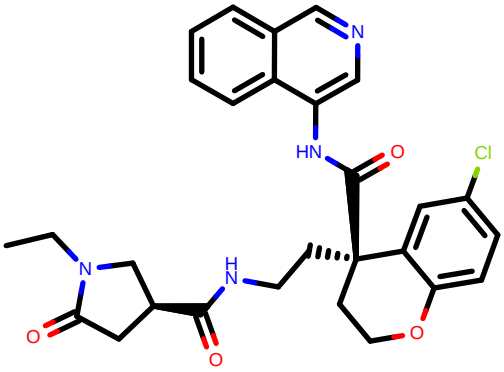
CID:	EN300-23317_3_2
SMILES:	C[C@H](C(=O)NCCOC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1795
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.34

EN300-1719401_1_1



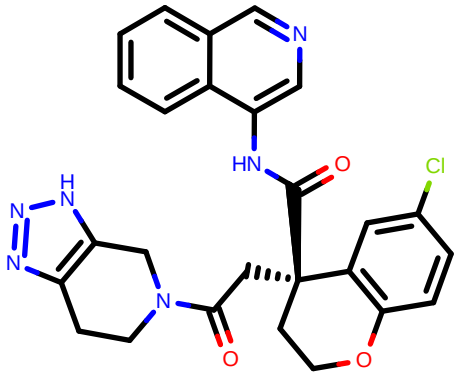
CID:	EN300-1719401_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](CO)c5[nH]cnn5
RUN:	RUN9756
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.31

EN300-33478_3_2



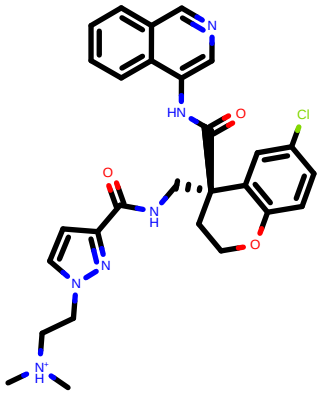
CID:	EN300-33478_3_2
SMILES:	CCN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7048
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.35

EN300-90293_1_1



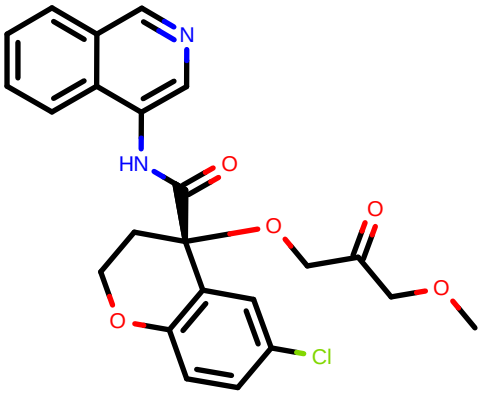
CID:	EN300-90293_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c([nH]nn6)C5
RUN:	RUN3955
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.29

EN300-255791_2_1



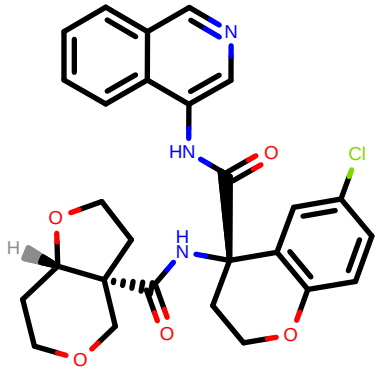
CID:	EN300-255791_2_1
SMILES:	CN(C)CCn1ccc(n1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6340
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.32

EN300-125140_1_1



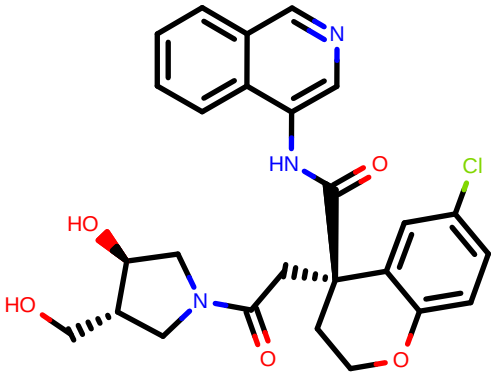
CID:	EN300-125140_1_1
SMILES:	COCC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN405
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.24

EN300-341337_1_3



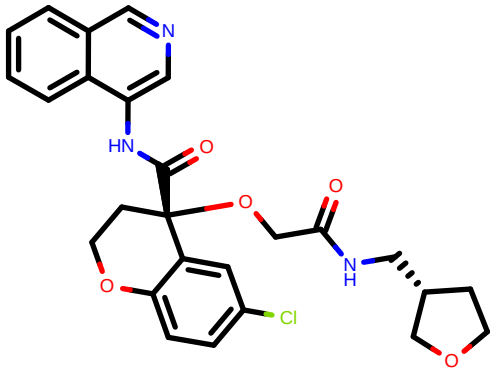
CID:	EN300-341337_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56CCO[C@H]5CCOC6
RUN:	RUN5916
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.28

EN300-248521_1_3



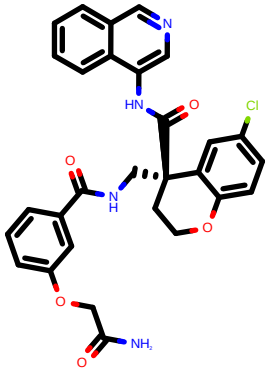
CID:	EN300-248521_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@H](C5)O)CO
RUN:	RUN2263
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.26

EN300-46832_1_1



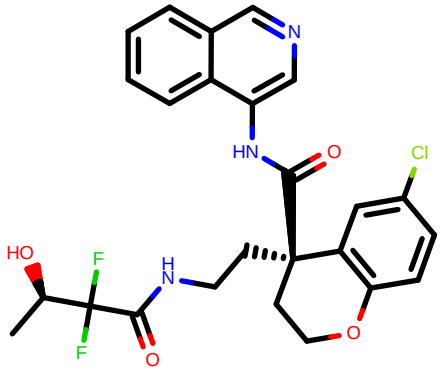
CID:	EN300-46832_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@@H]5CCOC5
RUN:	RUN1472
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.33

EN300-30687_2_1



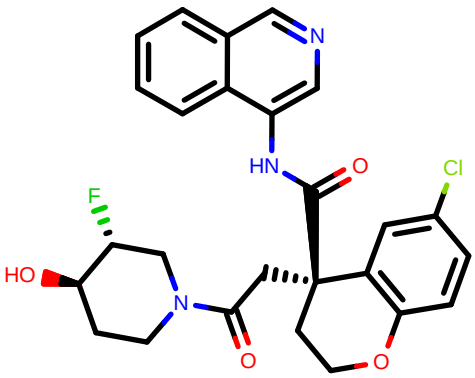
CID:	EN300-30687_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cccc(c5)OCC(=O)N
RUN:	RUN8315
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.34

EN300-185398_3_2



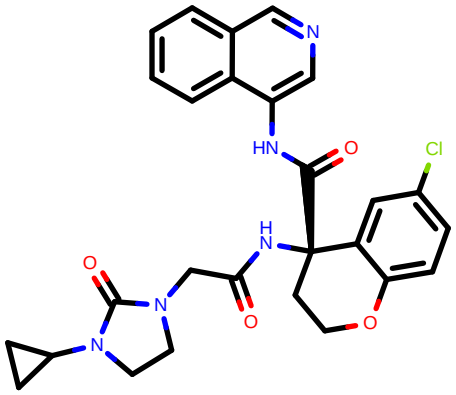
CID:	EN300-185398_3_2
SMILES:	C[C@H](C(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F)O
RUN:	RUN3751
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.28

EN300-741926_1_2



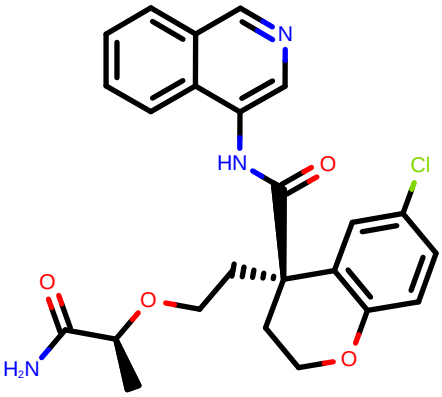
CID:	EN300-741926_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@@H](C5)F)O
RUN:	RUN2788
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.27

EN300-304771_1_1



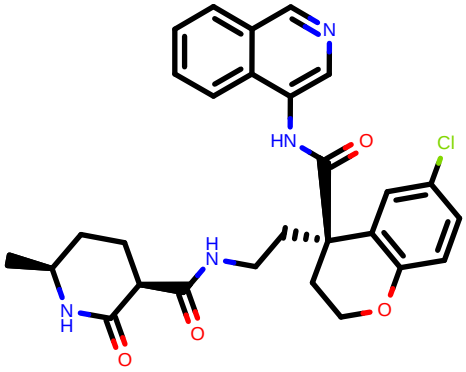
CID:	EN300-304771_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCN(C5=O)C6CC6
RUN:	RUN4013
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.33

EN300-17381_3_1



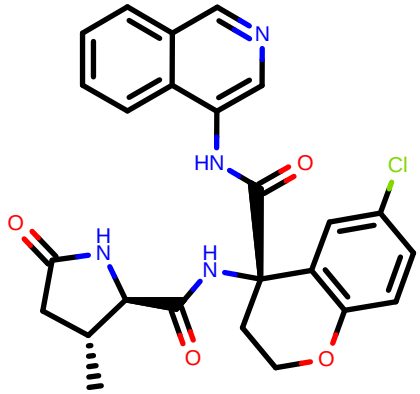
CID:	EN300-17381_3_1
SMILES:	C[C@@H](C(=O)N)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2027
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.28

EN300-6505003_3_4



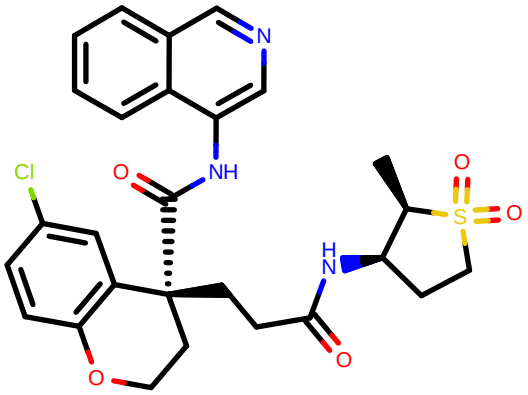
CID:	EN300-6505003_3_4
SMILES:	C[C@H]1CC[C@H](C(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7668
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.49

EN300-155362_1_3



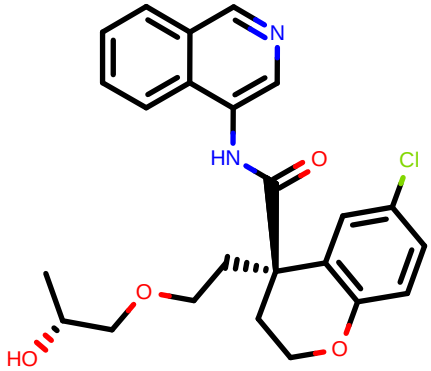
CID:	EN300-155362_1_3
SMILES:	C[C@@H]1CC(=O)N[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4337
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.24

EN300-321110_2_1



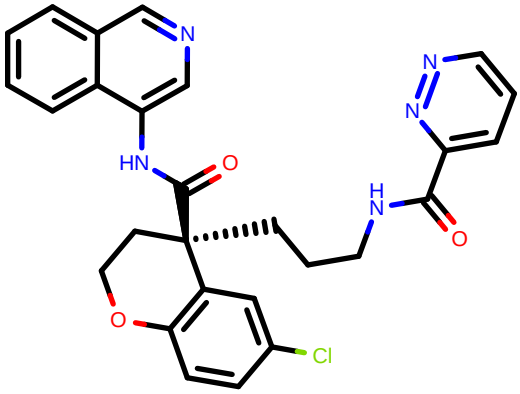
CID:	EN300-321110_2_1
SMILES:	C[C@@H]1[C@@H](CCS1(=O)=O)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6554
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.32

EN300-185378_3_2



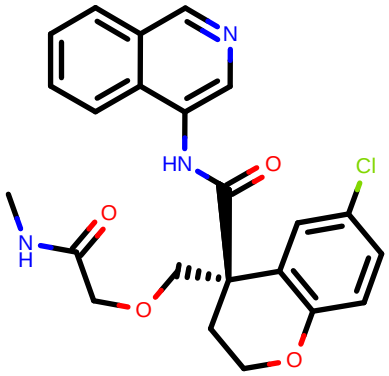
CID:	EN300-185378_3_2
SMILES:	C[C@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1643
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.25

EN300-79022_4_1



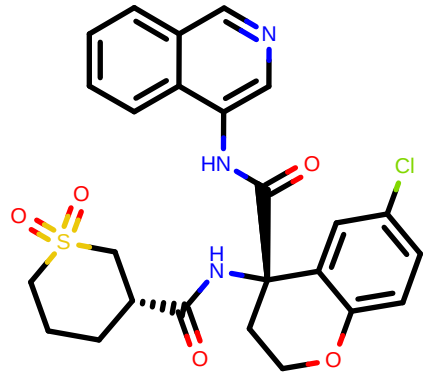
CID:	EN300-79022_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cccnn5
RUN:	RUN9799
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.27

EN300-2977549_2_1



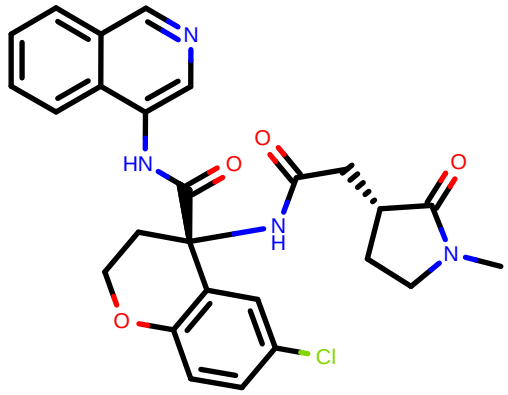
CID:	EN300-2977549_2_1
SMILES:	CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1062
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.21

EN300-77778_1_1



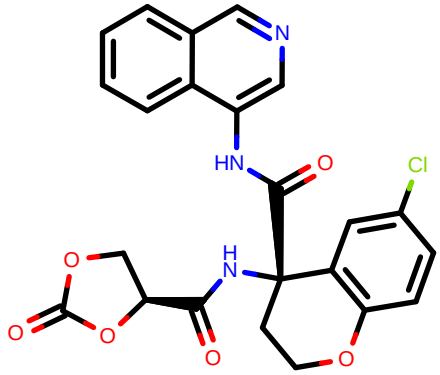
CID:	EN300-77778_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCCS(=O)(=O)C5
RUN:	RUN6096
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.28

EN300-378722_1_1



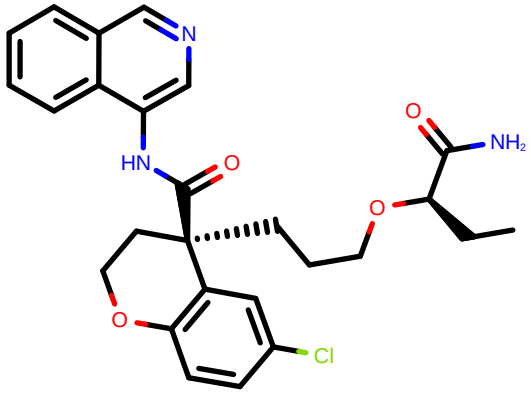
CID:	EN300-378722_1_1
SMILES:	CN1CC[C@@H](C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4377
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.30

EN300-5253939_1_1



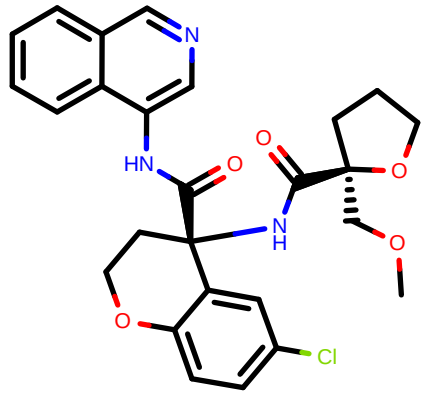
CID:	EN300-5253939_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COC(=O)O5
RUN:	RUN6056
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.19

EN300-65839_4_2



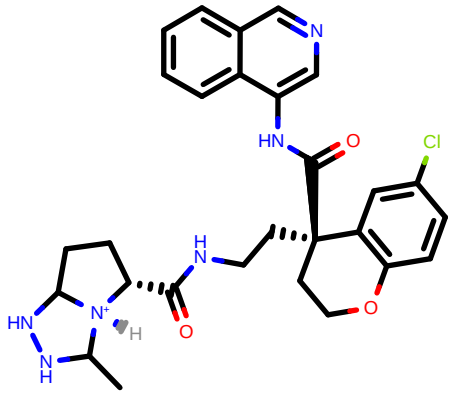
CID:	EN300-65839_4_2
SMILES:	CC[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN667
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.37

EN300-1301381_1_1



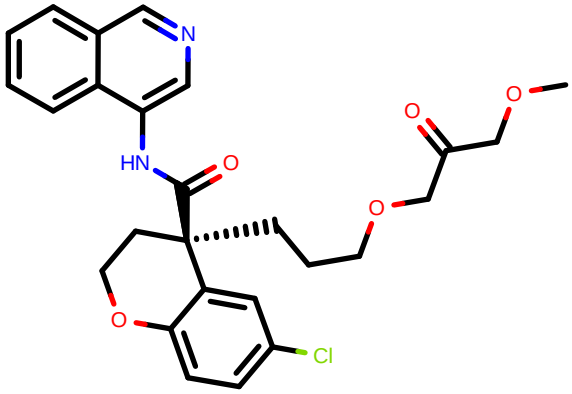
CID:	EN300-1301381_1_1
SMILES:	COC[C@@]1(CCCO1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4465
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.30

EN300-6489289_3_2



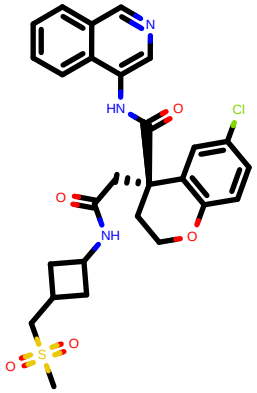
CID:	EN300-6489289_3_2
SMILES:	Cc1nnc2n1[C@H](CC2)C(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8904
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.35

EN300-125140_4_1



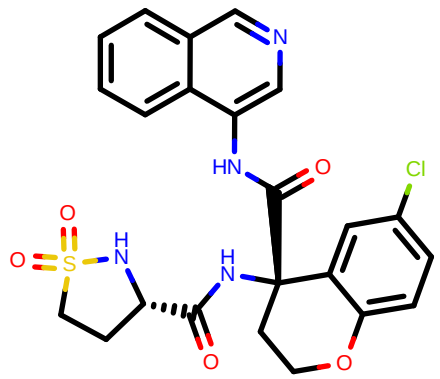
CID:	EN300-125140_4_1
SMILES:	COCC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN659
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.35

EN300-7429970_1_1



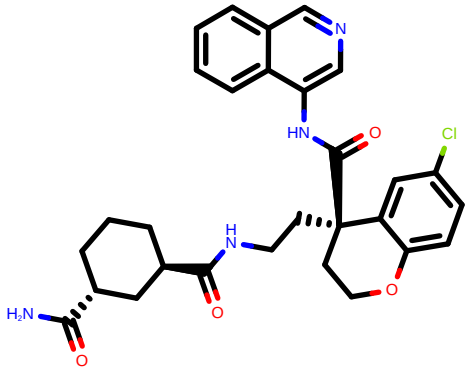
CID:	EN300-7429970_1_1
SMILES:	CS(=O)(=O)CC1CC(C1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8124
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.35

EN300-45049_1_1



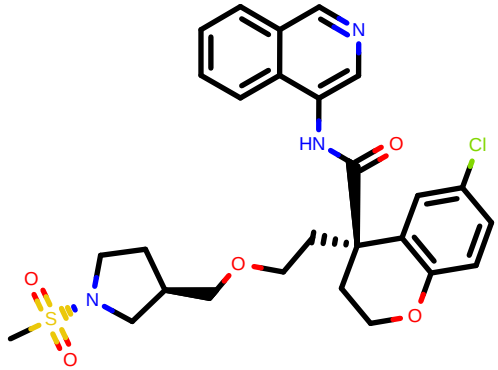
CID:	EN300-45049_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCS(=O)(=O)N5
RUN:	RUN4749
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.28

EN300-90142_3_3



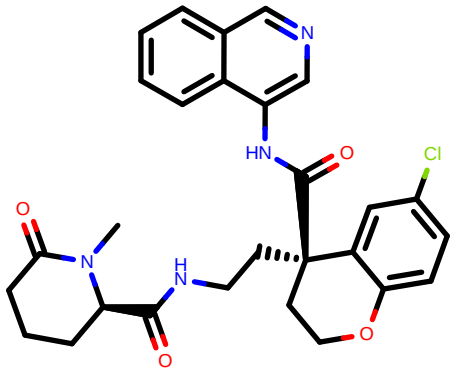
CID:	EN300-90142_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCC[C@H](C5)C(=O)N
RUN:	RUN3068
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.44

EN300-261986_3_2



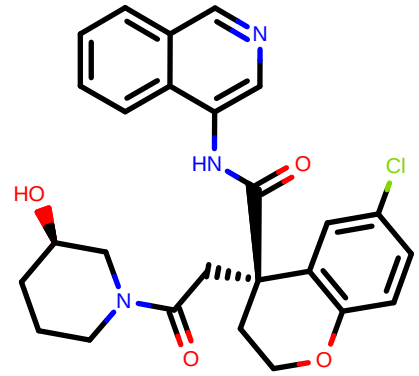
CID:	EN300-261986_3_2
SMILES:	CS(=O)(=O)N1CC[C@H](C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2370
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.46

EN300-325738_3_2



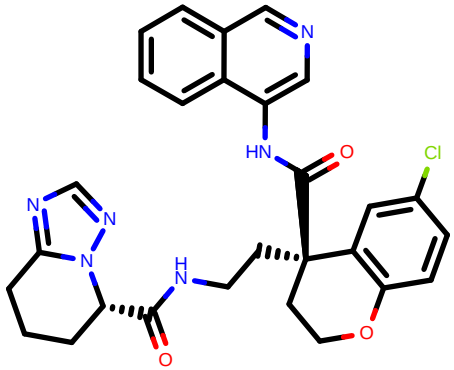
CID:	EN300-325738_3_2
SMILES:	CN1[C@H](CCCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2688
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.29

EN300-20284_1_2



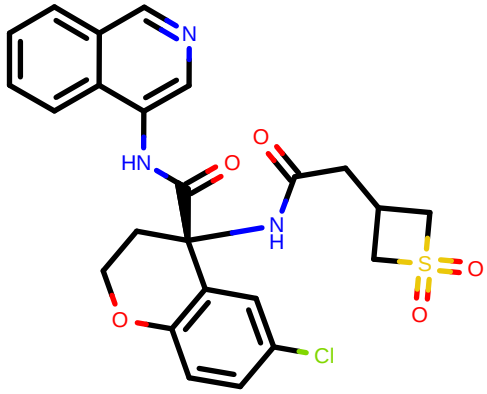
CID:	EN300-20284_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H](C5)O
RUN:	RUN3116
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.30

EN300-1273016_3_1



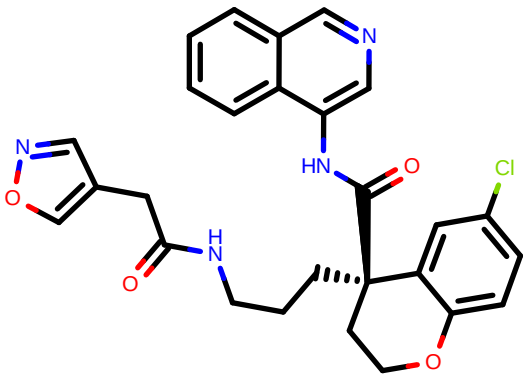
CID:	EN300-1273016_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCc6n5ncn6
RUN:	RUN10648
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.32

EN300-256583_1_1



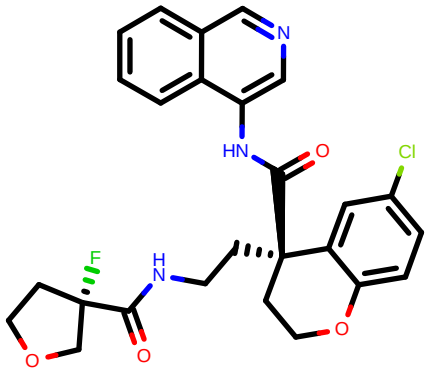
CID:	EN300-256583_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5CS(=O)(=O)C5
RUN:	RUN6104
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.24

EN300-315963_4_1



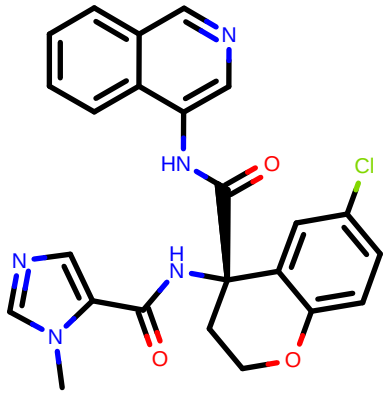
CID:	EN300-315963_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)Cc5cnoc5
RUN:	RUN8521
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.33

EN300-188356_3_1



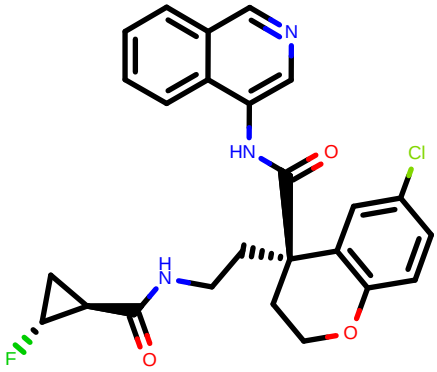
CID:	EN300-188356_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOC5)F
RUN:	RUN2097
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.28

EN300-88417_1_1



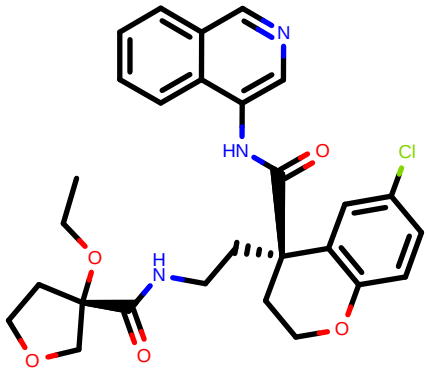
CID:	EN300-88417_1_1
SMILES:	Cn1cncc1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4033
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.25

EN300-97300_3_3



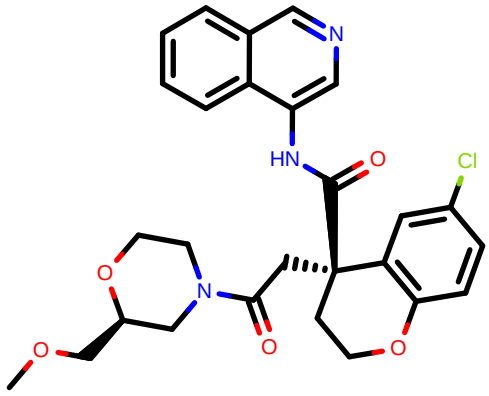
CID:	EN300-97300_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@H]5F
RUN:	RUN11112
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.25

EN300-259694_3_2



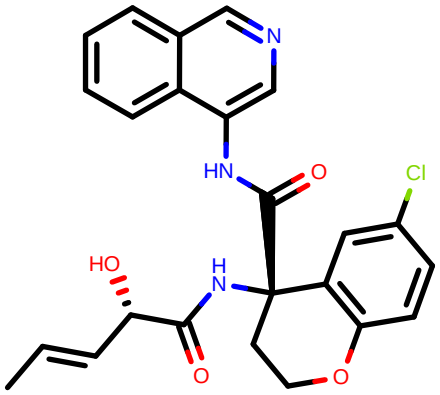
CID:	EN300-259694_3_2
SMILES:	CCO[C@]1(CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6166
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.54

EN300-6742996_1_1



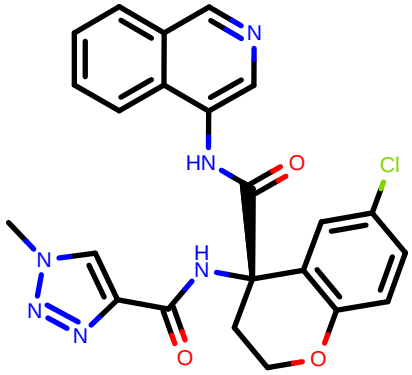
CID:	EN300-6742996_1_1
SMILES:	COC[C@@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9834
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.33

EN300-300217_1_2



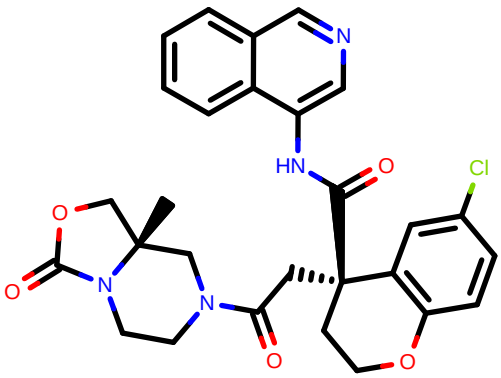
CID:	EN300-300217_1_2
SMILES:	C/C=C/[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3410
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.32

EN300-86357_1_1



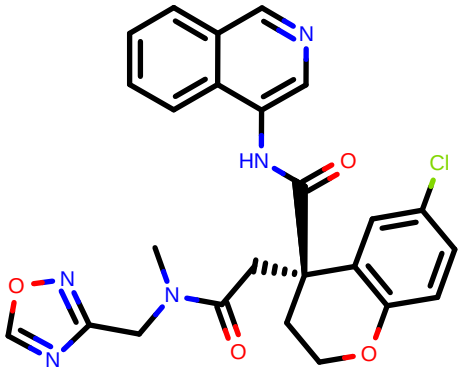
CID:	EN300-86357_1_1
SMILES:	Cn1cc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4209
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.19

EN300-395954_1_1



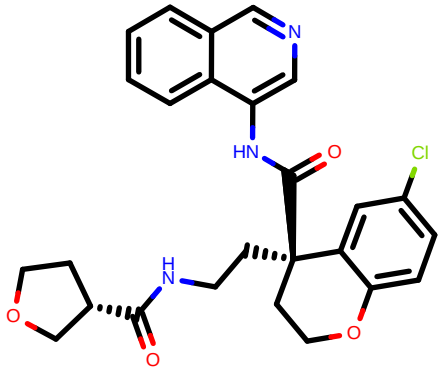
CID:	EN300-395954_1_1
SMILES:	C[C@@]12CN(CCN1C(=O)OC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3468
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.35

EN300-126412_1_1



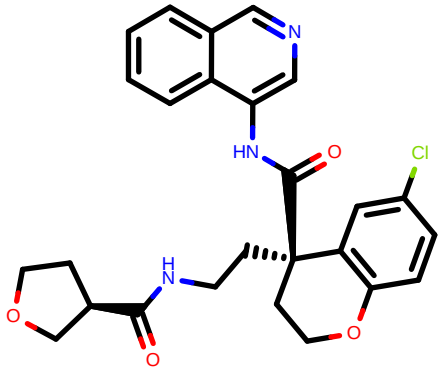
CID:	EN300-126412_1_1
SMILES:	CN(Cc1ncon1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3987
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.30

EN300-170463_3_1



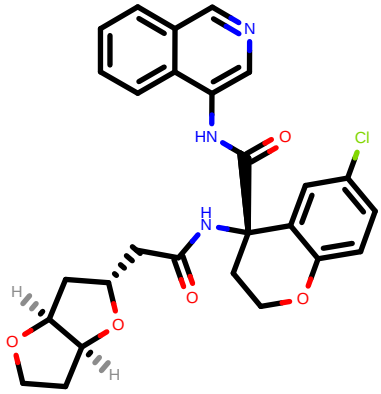
CID:	EN300-170463_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5
RUN:	RUN3971
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.32

EN300-53423_3_1



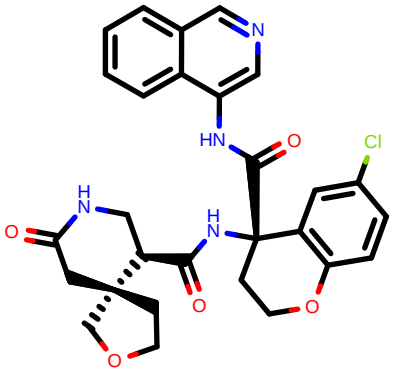
CID:	EN300-53423_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCOC5
RUN:	RUN8048
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.30

EN300-7355519_1_4



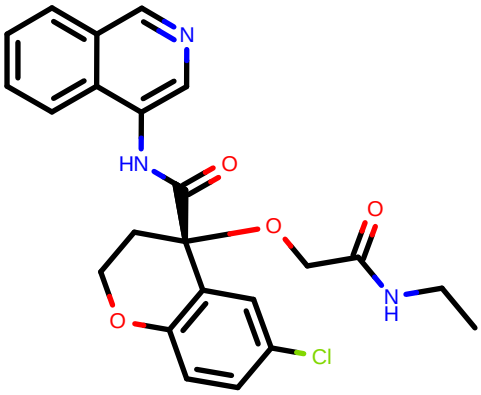
CID:	EN300-7355519_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5C[C@H]6[C@@H](O5)CCO6
RUN:	RUN7174
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.30

EN300-1707879_1_1



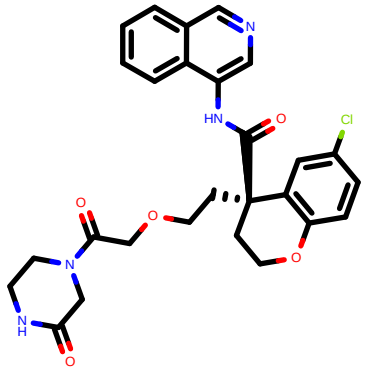
CID:	EN300-1707879_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CNC(=O)CC56CCOC6
RUN:	RUN5416
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.29

EN300-7003350_1_1



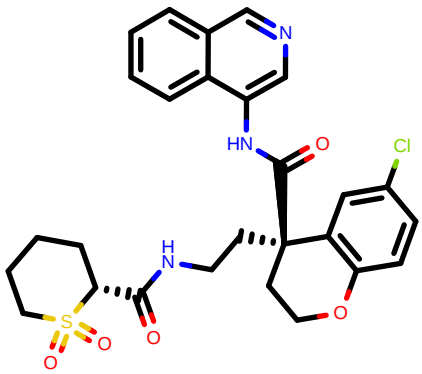
CID:	EN300-7003350_1_1
SMILES:	CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN738
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.19

EN300-22884_3_1



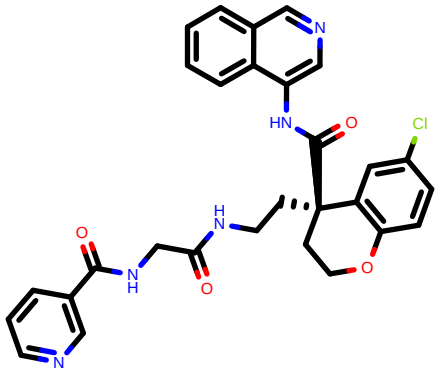
CID:	EN300-22884_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCNC(=O)C5
RUN:	RUN544
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.26

EN300-107435_3_2



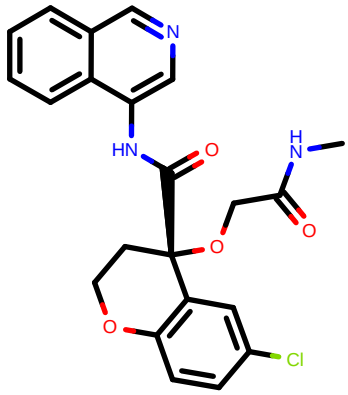
CID:	EN300-107435_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCCS5(=O)=O
RUN:	RUN6497
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.26

EN300-107990_3_1



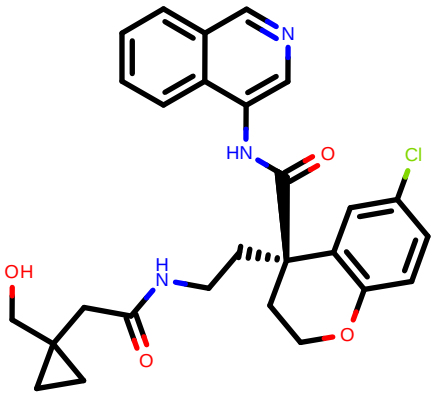
CID:	EN300-107990_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)c5cccnc5
RUN:	RUN11158
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.33

EN300-2977549_1_1



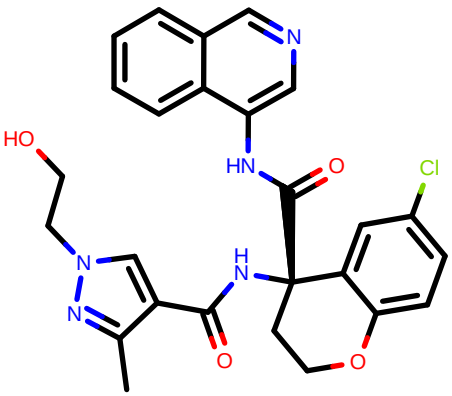
CID:	EN300-2977549_1_1
SMILES:	CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1064
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.21

EN300-107048_3_1



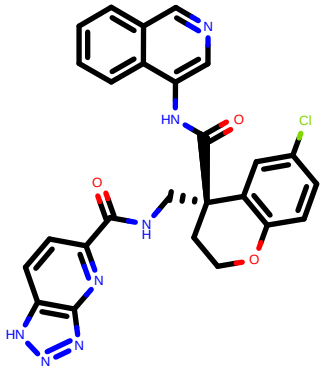
CID:	EN300-107048_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CC5)CO
RUN:	RUN1897
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.29

EN300-39476_1_1



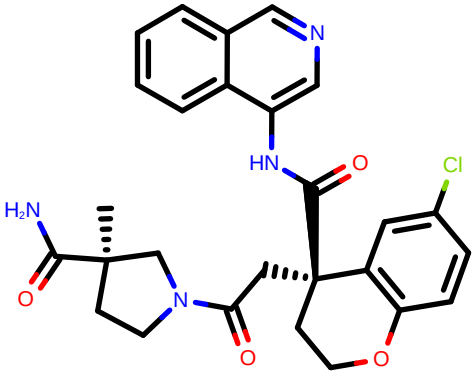
CID:	EN300-39476_1_1
SMILES:	Cc1c(cn(n1)CCO)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8876
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.40

EN300-133058_2_1



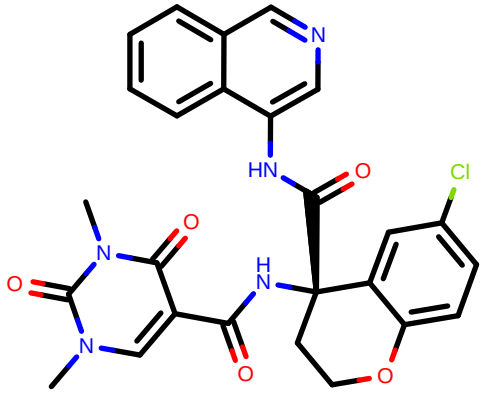
CID:	EN300-133058_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6c(n5)n[nH]n6
RUN:	RUN8423
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.29

EN300-194442_1_2



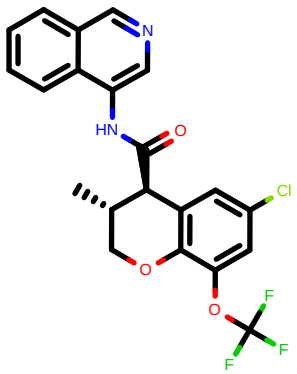
CID:	EN300-194442_1_2
SMILES:	C[C@]1(CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN3440
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.36

EN300-79497_1_1



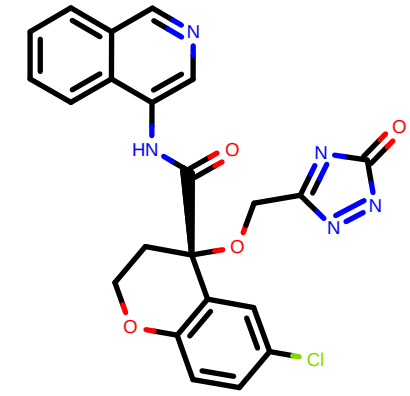
CID:	EN300-79497_1_1
SMILES:	Cn1cc(c(=O)n(c1=O)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7930
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.32

DAR-DIA-0d514e7d-18_1



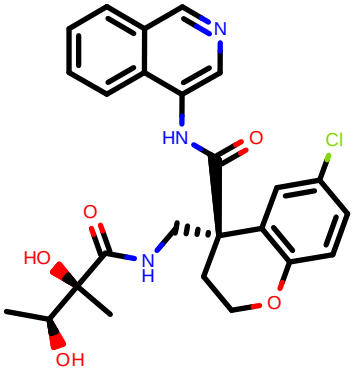
CID:	DAR-DIA-0d514e7d-18_1
SMILES:	C[C@H]1COc2c(cc(cc2OC(F)(F)F)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4
RUN:	RUN123
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.17

EN300-73772_1_1



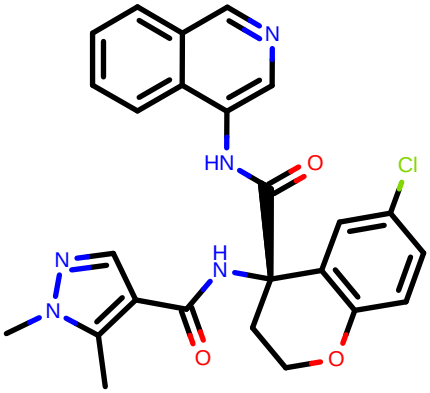
CID:	EN300-73772_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5[nH]c(=O)[nH]n5
RUN:	RUN1040
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.21

EN300-202922_2_1



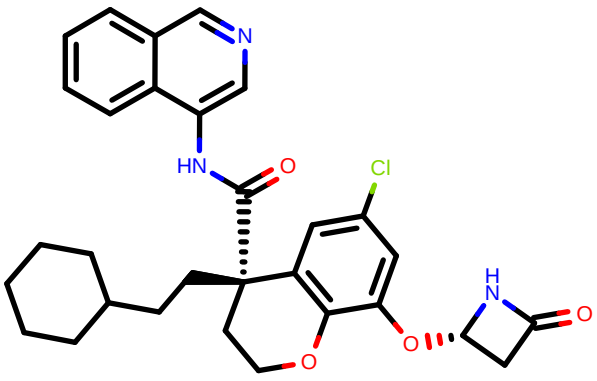
CID:	EN300-202922_2_1
SMILES:	C[C@@H]([C@@](C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN2782
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.33

EN300-25866_1_1



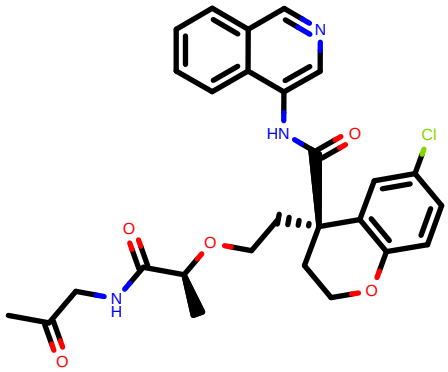
CID:	EN300-25866_1_1
SMILES:	Cc1c(cnn1C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6739
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.28

VLA-UCB-05e51b3f-12_2



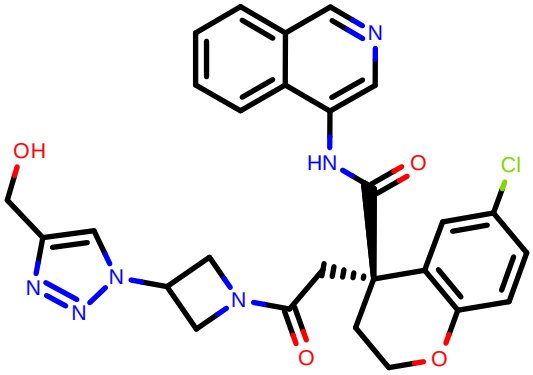
CID:	VLA-UCB-05e51b3f-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4O[C@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN247
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.41

EN300-131093_3_1



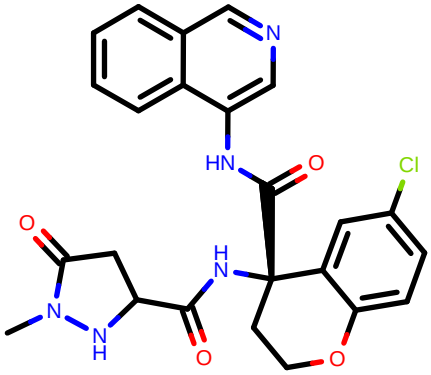
CID:	EN300-131093_3_1
SMILES:	C[C@@H](C(=O)NCC(=O)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN789
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.43

EN300-1664105_1_1



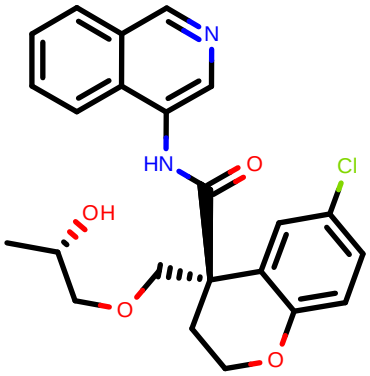
CID:	EN300-1664105_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)n6cc(nn6)CO
RUN:	RUN4475
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.27

EN300-150749_1_1



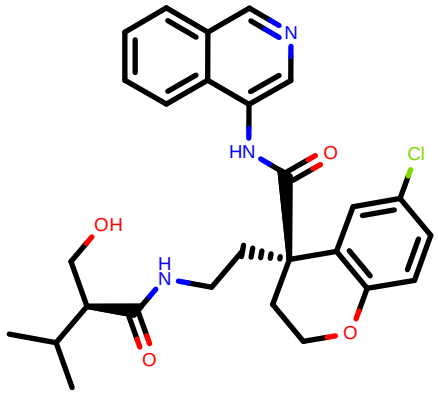
CID:	EN300-150749_1_1
SMILES:	Cn1c(=O)cc([nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3554
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.24

EN300-185378_2_1



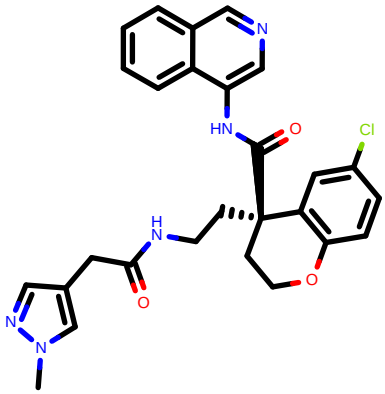
CID:	EN300-185378_2_1
SMILES:	C[C@@H](COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1054
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.25

EN300-153257_3_1



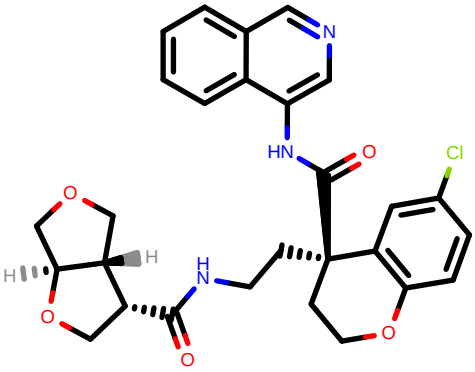
CID:	EN300-153257_3_1
SMILES:	CC(C)[C@@H](CO)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2473
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.35

EN300-63872_3_1



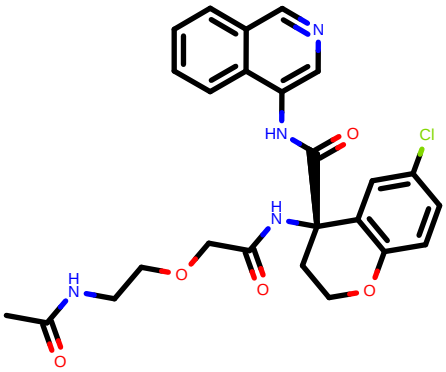
CID:	EN300-63872_3_1
SMILES:	Cn1cc(cn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1562
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.28

EN300-6482296_3_1



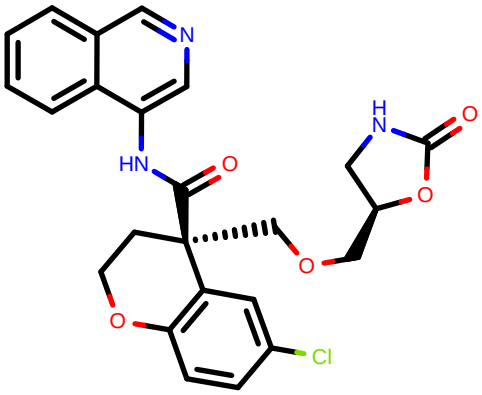
CID:	EN300-6482296_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CO[C@@H]6[C@@H]5COC6
RUN:	RUN7764
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.28

EN300-126555_1_1



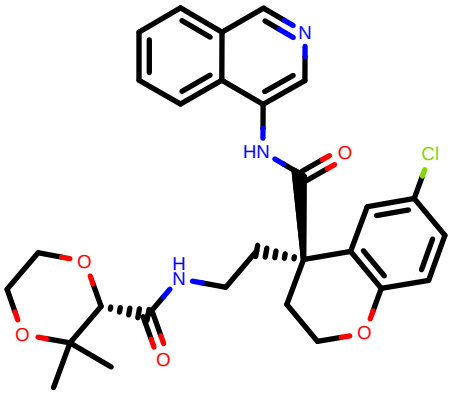
CID:	EN300-126555_1_1
SMILES:	CC(=O)NCCOCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2164
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.35

EN300-203293_2_2



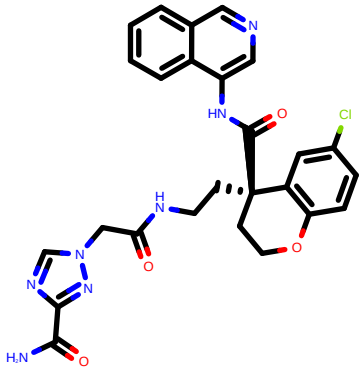
CID:	EN300-203293_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CNC(=O)O5
RUN:	RUN1637
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.28

EN300-1601684_3_2



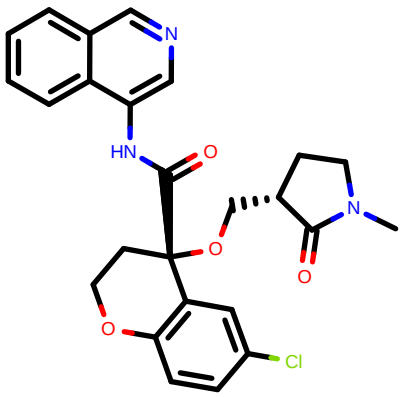
CID:	EN300-1601684_3_2
SMILES:	CC1([C@H](OCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN10506
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.28

EN300-262604_3_1



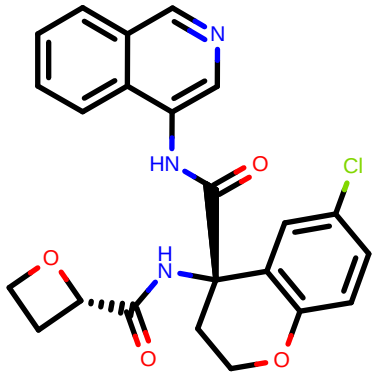
CID:	EN300-262604_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cnc(n5)C(=O)N
RUN:	RUN9356
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.33

EN300-260816_1_2



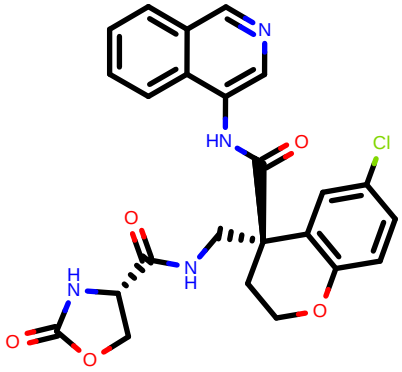
CID:	EN300-260816_1_2
SMILES:	CN1CC[C@H](C1=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2568
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.33

EN300-85760_1_1



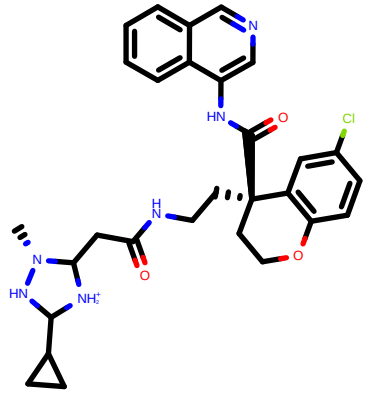
CID:	EN300-85760_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCO5
RUN:	RUN3346
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.22

EN300-126389_2_1



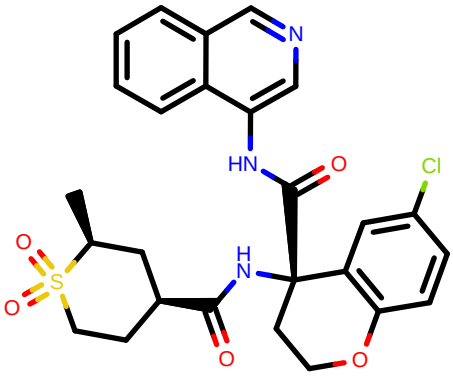
CID:	EN300-126389_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COC(=O)N5
RUN:	RUN4878
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.30

EN300-260418_3_1



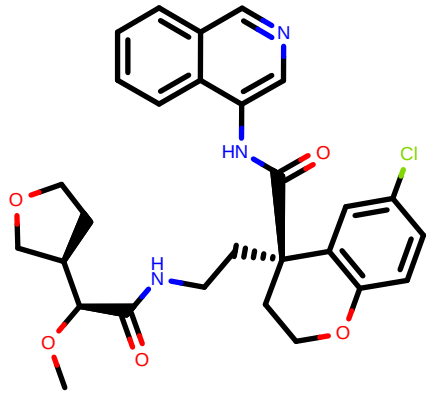
CID:	EN300-260418_3_1
SMILES:	Cn1c(nc(n1)C2CC2)CC(=O)NCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8468
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.42

EN300-6082676_1_4



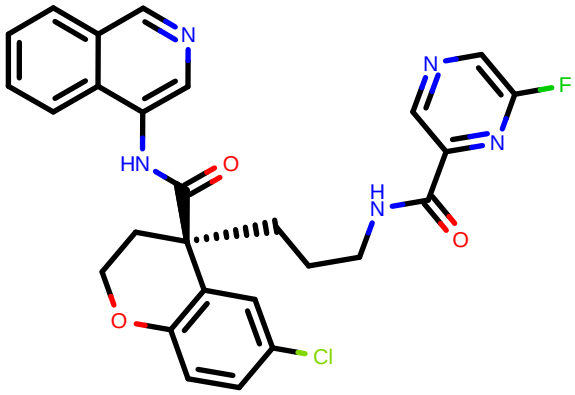
CID:	EN300-6082676_1_4
SMILES:	C[C@H]1C[C@H](CCS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6531
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.27

EN300-298552_3_1



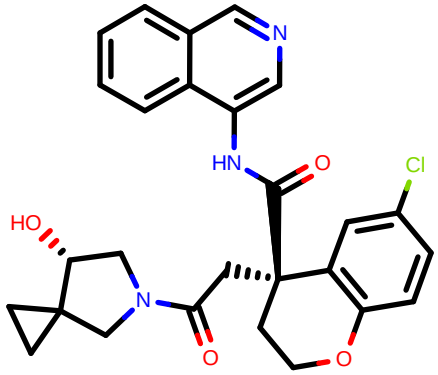
CID:	EN300-298552_3_1
SMILES:	CO[C@@H]([C@@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8871
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.35

EN300-373552_4_1



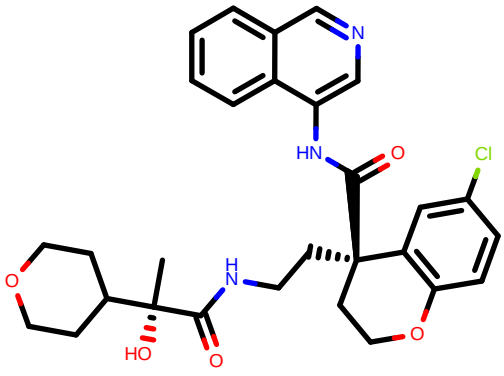
CID:	EN300-373552_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cncc(n5)F
RUN:	RUN10605
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.32

EN300-142333_1_2



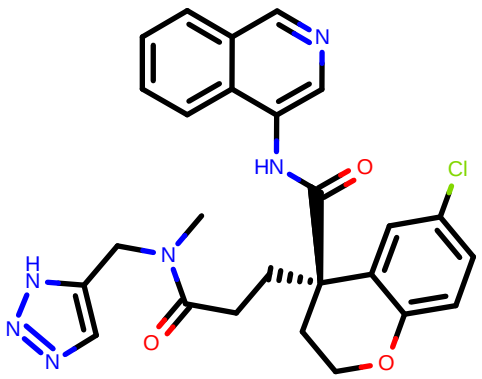
CID:	EN300-142333_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C6(C5)CC6)O
RUN:	RUN4191
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.29

EN300-217499_3_2



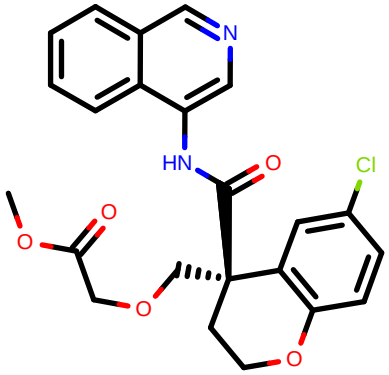
CID:	EN300-217499_3_2
SMILES:	C[C@](C1CCOCC1)(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN8328
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.41

EN300-1265071_2_1



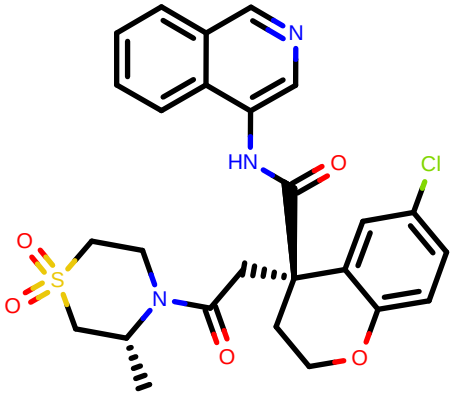
CID:	EN300-1265071_2_1
SMILES:	CN(Cc1c[nH]nn1)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6406
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.30

EN300-19700_2_1



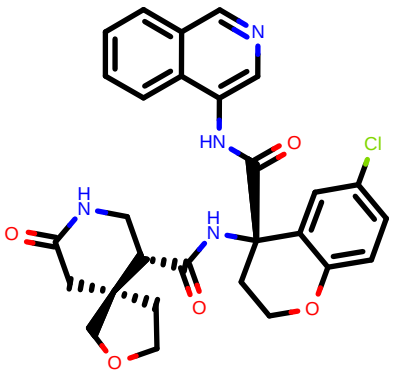
CID:	EN300-19700_2_1
SMILES:	COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1422
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.17

EN300-171215_1_1



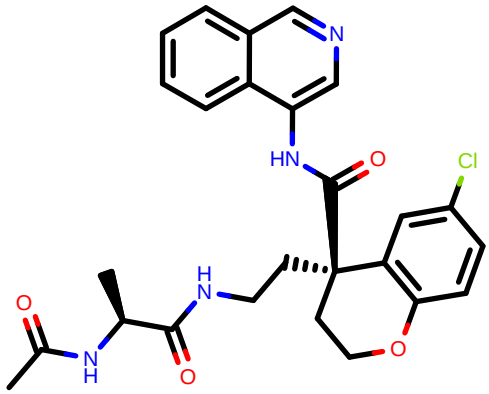
CID:	EN300-171215_1_1
SMILES:	C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10274
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.41

EN300-1707879_1_2



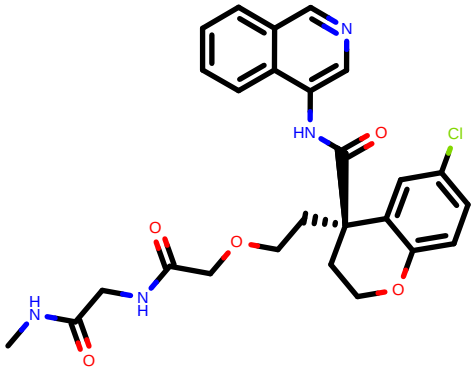
CID:	EN300-1707879_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)CC56CCOC6
RUN:	RUN8482
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.28

EN300-862647_3_1



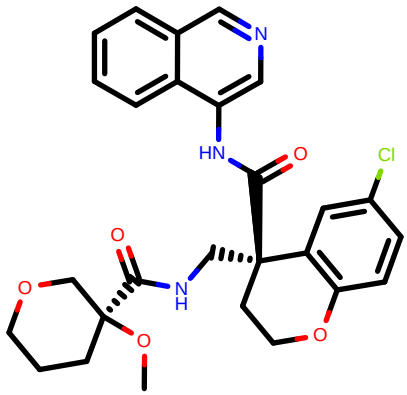
CID:	EN300-862647_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN2984
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.28

EN300-23223_3_1



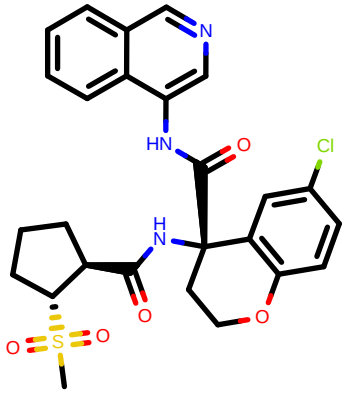
CID:	EN300-23223_3_1
SMILES:	CNC(=O)CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1148
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.27

EN300-1072199_2_2



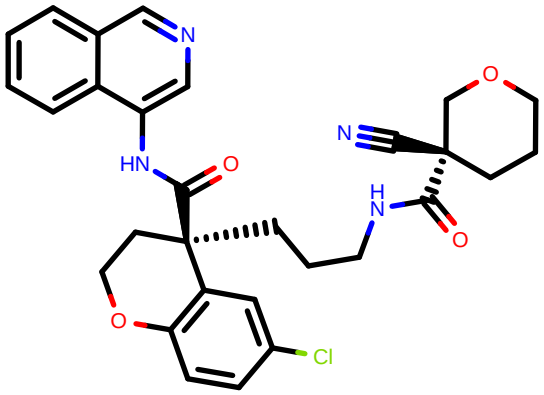
CID:	EN300-1072199_2_2
SMILES:	CO[C@]1(CCCOC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3023
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.38

EN300-1387145_1_3



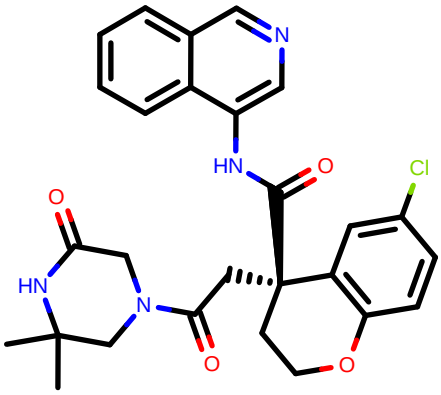
CID:	EN300-1387145_1_3
SMILES:	CS(=O)(=O)[C@@H]1CCC[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7162
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.62

EN300-301925_4_2



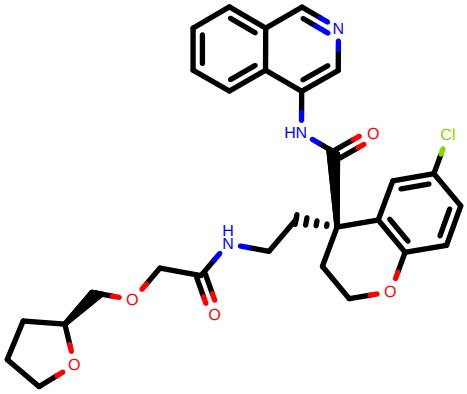
CID:	EN300-301925_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@]5(CCCOC5)C#N
RUN:	RUN10885
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.33

EN300-7493939_1_1



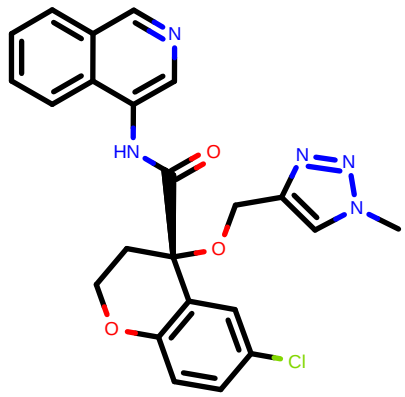
CID:	EN300-7493939_1_1
SMILES:	CC1(CN(CC(=O)N1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN9728
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.30

EN300-60033_3_1



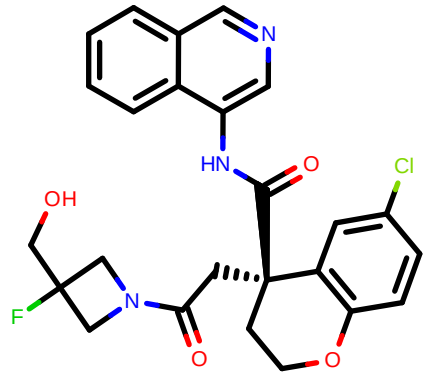
CID:	EN300-60033_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)OC[C@@H]5CCCO5
RUN:	RUN10478
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.45

EN300-120282_1_1



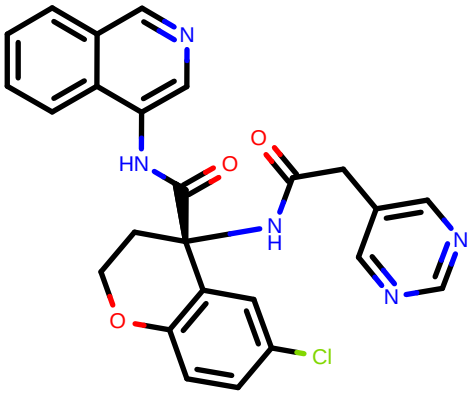
CID:	EN300-120282_1_1
SMILES:	Cn1cc(nn1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN485
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.19

EN300-204507_1_1



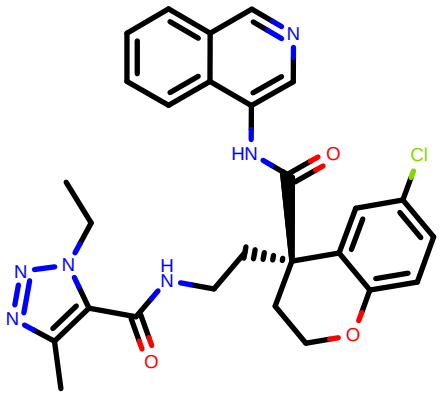
CID:	EN300-204507_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F
RUN:	RUN3899
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.31

EN300-185751_1_1



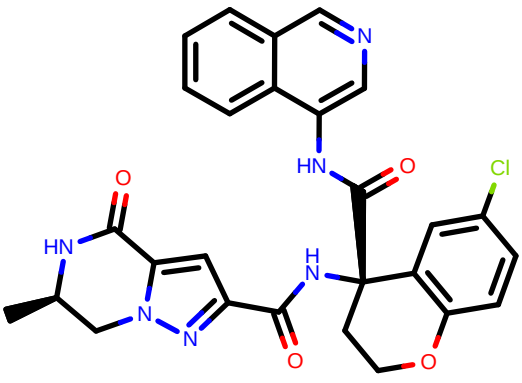
CID:	EN300-185751_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cncnc5
RUN:	RUN8050
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.28

EN300-217526_3_1



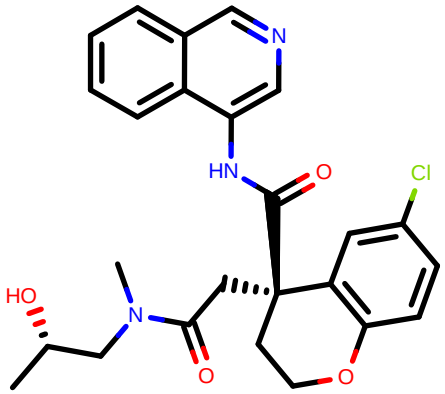
CID:	EN300-217526_3_1
SMILES:	CCn1c(c(nn1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10796
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.35

EN300-265285_1_1



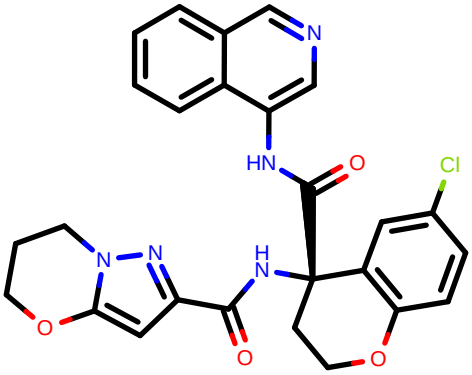
CID:	EN300-265285_1_1
SMILES:	C[C@@H]1Cn2c(cc(n2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)C(=O)N1
RUN:	RUN9065
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.35

EN300-210254_1_1



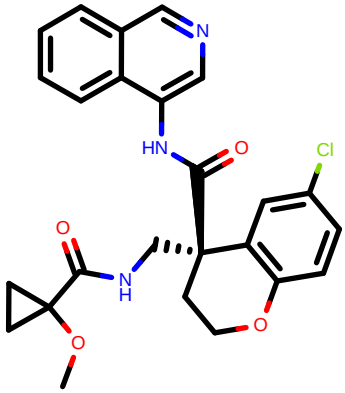
CID:	EN300-210254_1_1
SMILES:	C[C@@H](CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN6277
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.25

EN300-103720_1_1



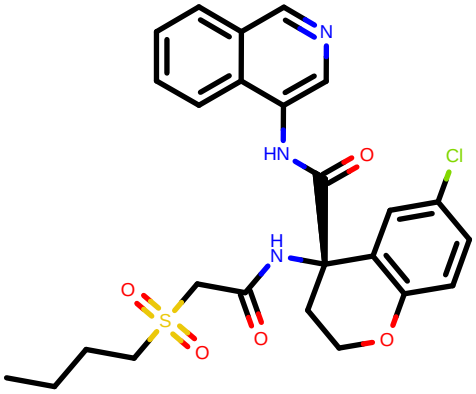
CID:	EN300-103720_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCCO6
RUN:	RUN8855
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.24

EN300-182124_2_1



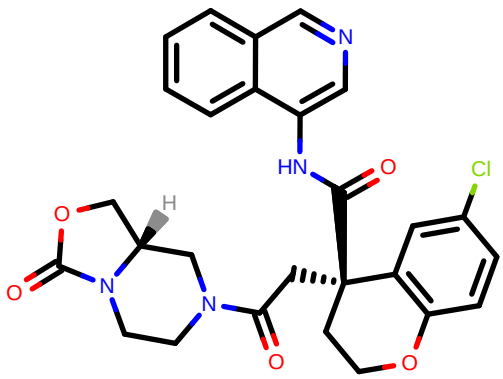
CID:	EN300-182124_2_1
SMILES:	COC1(CC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3471
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.26

EN300-686903_1_1



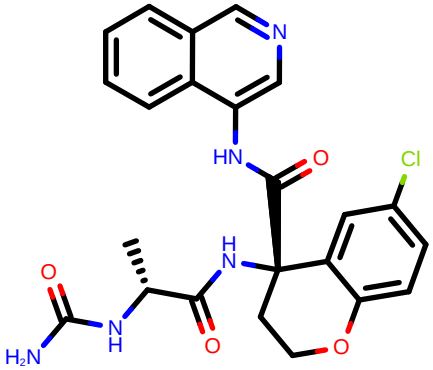
CID:	EN300-686903_1_1
SMILES:	CCCCS(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN712
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.40

EN300-109827_1_1



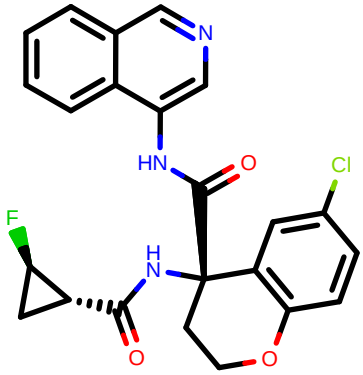
CID:	EN300-109827_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@H](C5)COC6=O
RUN:	RUN3420
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.31

EN300-00271_1_2



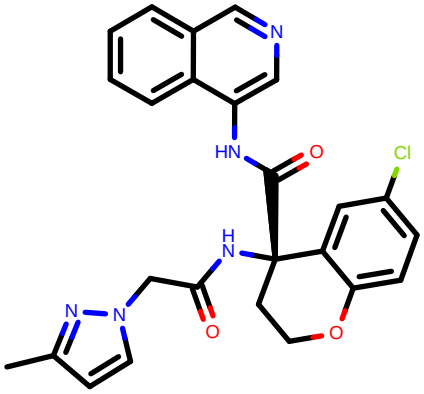
CID:	EN300-00271_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN3110
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.25

EN300-97300_1_3



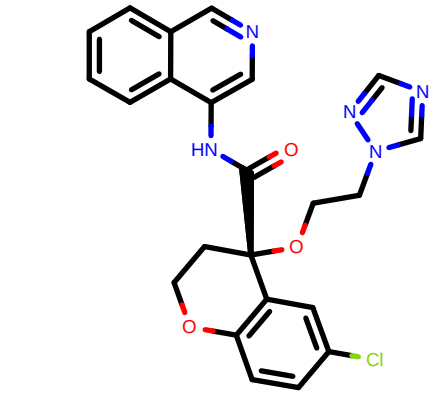
CID:	EN300-97300_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@H]5F
RUN:	RUN1884
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.18

EN300-226964_1_1



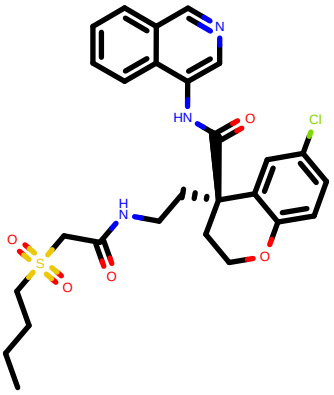
CID:	EN300-226964_1_1
SMILES:	Cc1ccn(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5344
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.26

EN300-6255179_1_1



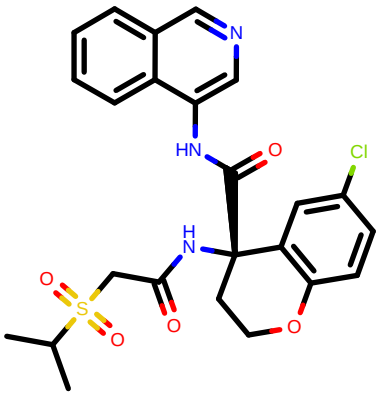
CID:	EN300-6255179_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cncn5
RUN:	RUN1096
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.24

EN300-686903_3_1



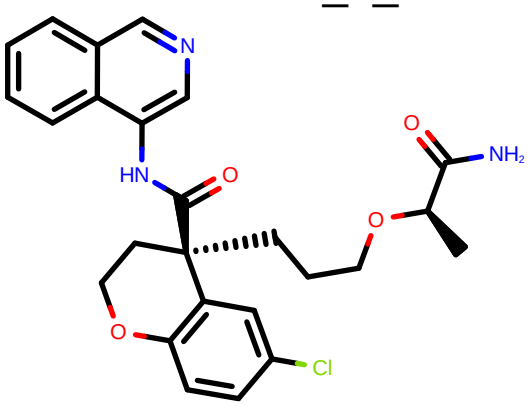
CID:	EN300-686903_3_1
SMILES:	CCCCS(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4063
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.62

EN300-51028_1_1



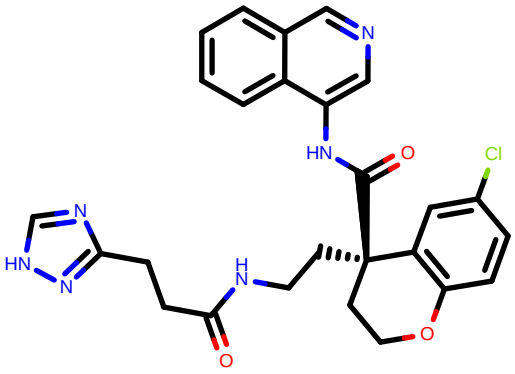
CID:	EN300-51028_1_1
SMILES:	CC(C)S(=O)(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN941
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.24

EN300-17381_4_2



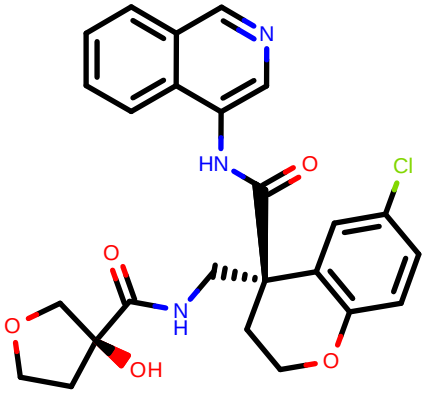
CID:	EN300-17381_4_2
SMILES:	C[C@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN388
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.28

EN300-101197_3_1



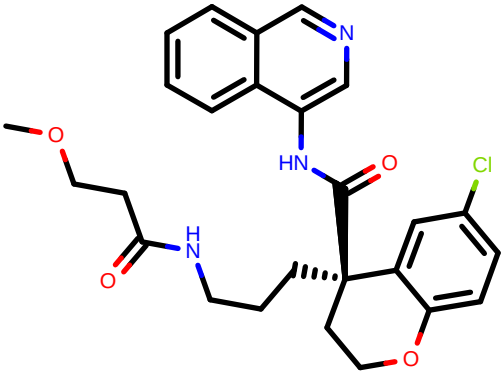
CID:	EN300-101197_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5[nH]cnn5
RUN:	RUN1178
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.33

EN300-148421_2_1



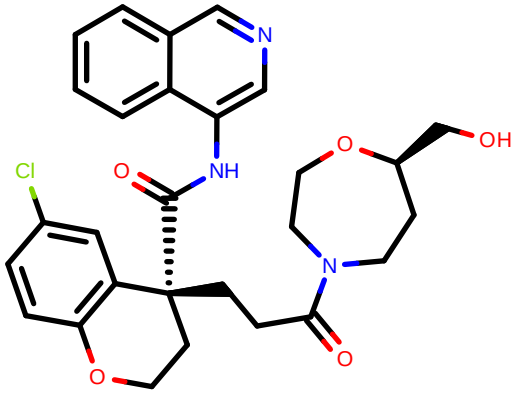
CID:	EN300-148421_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCOC5)O
RUN:	RUN5689
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.34

EN300-64536_4_1



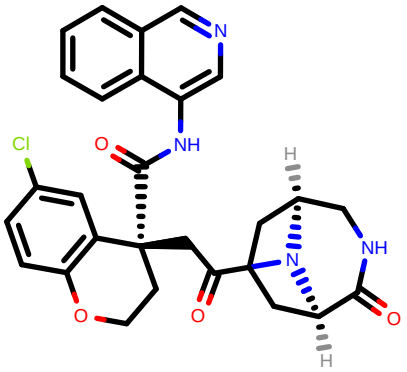
CID:	EN300-64536_4_1
SMILES:	COCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9899
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.34

EN300-2007620_2_1



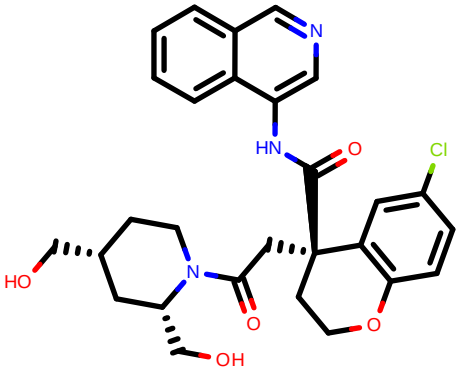
CID:	EN300-2007620_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](OCC5)CO
RUN:	RUN9291
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.32

EN300-6740329_1_1



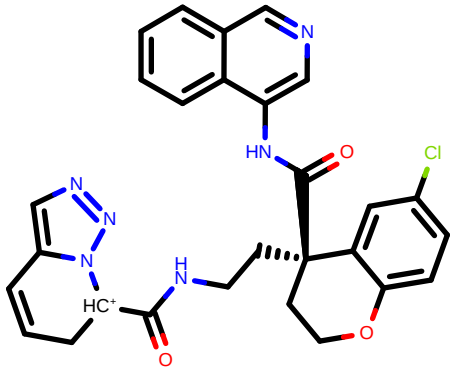
CID:	EN300-6740329_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C6CCCC5C(=O)NC6
RUN:	RUN9438
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.32

EN300-7470991_1_1



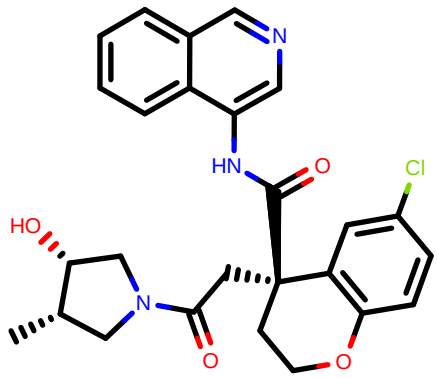
CID:	EN300-7470991_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C[C@H]5CO)CO
RUN:	RUN10456
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.41

EN300-2010167_3_1



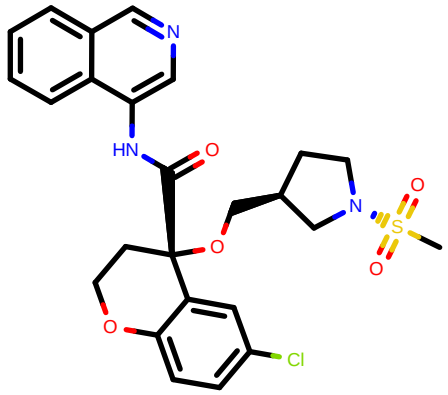
CID:	EN300-2010167_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cccc6n5nnc6
RUN:	RUN9766
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.26

EN300-124052_1_4



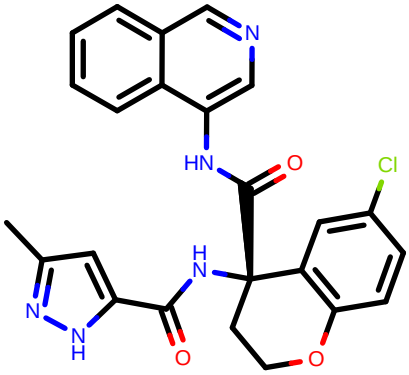
CID:	EN300-124052_1_4
SMILES:	C[C@H]1CN(C[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5558
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.33

EN300-261986_1_1



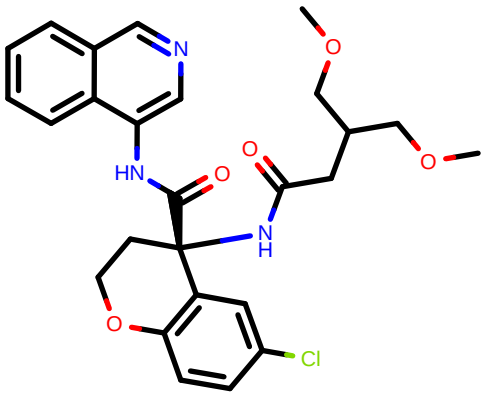
CID:	EN300-261986_1_1
SMILES:	CS(=O)(=O)N1CC[C@@H](C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN516
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.33

EN300-41425_1_1



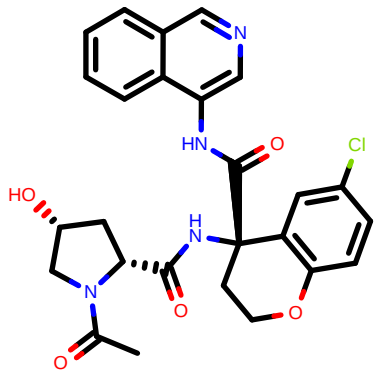
CID:	EN300-41425_1_1
SMILES:	Cc1cc(n[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4969
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.27

EN300-7102031_1_1



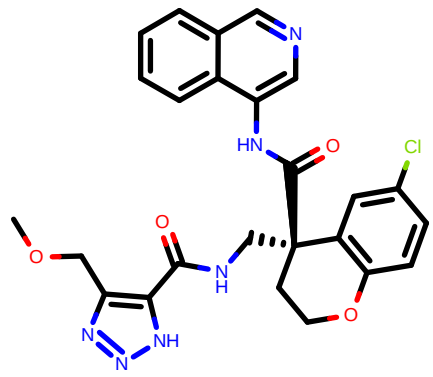
CID:	EN300-7102031_1_1
SMILES:	COCC(CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)COC
RUN:	RUN758
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.35

EN300-158260_1_1



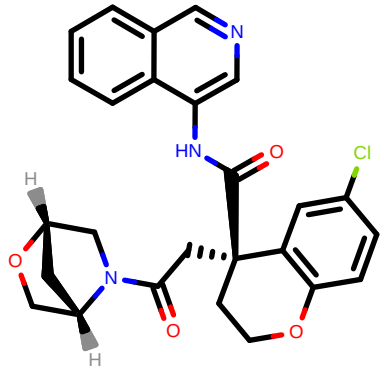
CID:	EN300-158260_1_1
SMILES:	CC(=O)N1C[C@@H](C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5552
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.32

EN300-785910_2_1



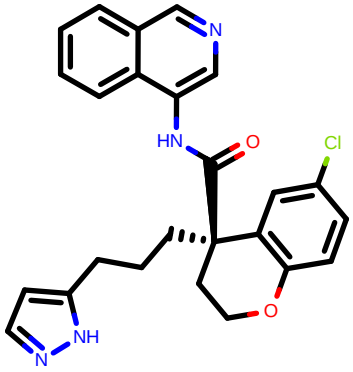
CID:	EN300-785910_2_1
SMILES:	COCc1c(nn[nH]1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2128
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.23

EN300-321790_1_1



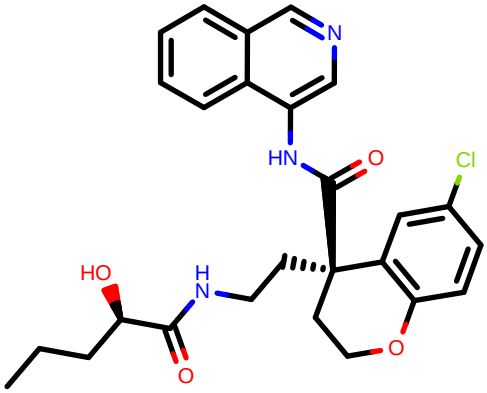
CID:	EN300-321790_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@H]5CO6
RUN:	RUN4875
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.26

VLA-UCB-34f3ed0c-10_1



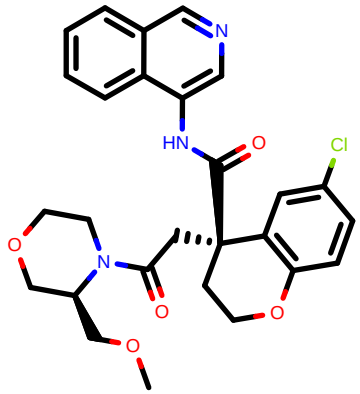
CID:	VLA-UCB-34f3ed0c-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5cc[nH]n5
RUN:	RUN125
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.27

EN300-300217_3_4



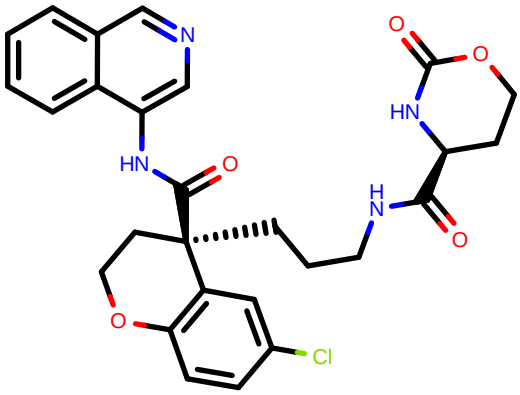
CID:	EN300-300217_3_4
SMILES:	C/C=C/[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4027
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.33

EN300-325729_1_2



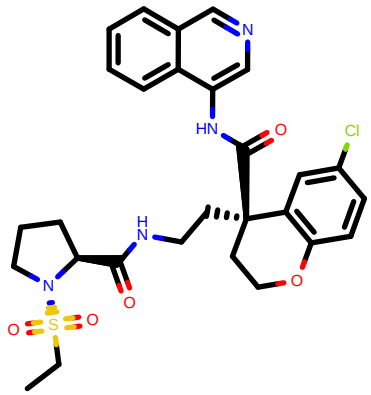
CID:	EN300-325729_1_2
SMILES:	COC[C@H]1COCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9870
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.30

EN300-249804_4_1



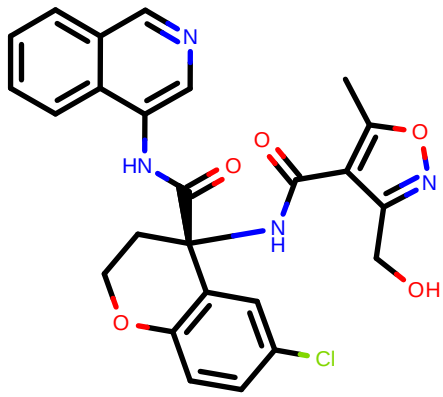
CID:	EN300-249804_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCOC(=O)N5
RUN:	RUN10759
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.44

EN300-16091_3_2



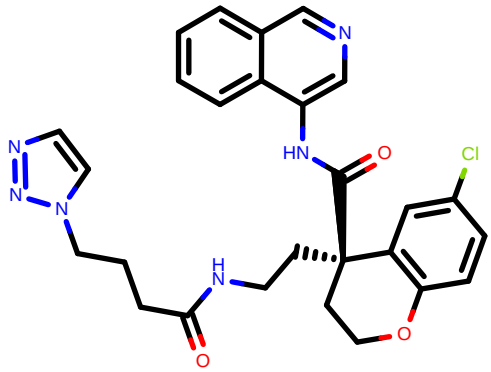
CID:	EN300-16091_3_2
SMILES:	CCS(=O)(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7320
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.49

EN300-215799_1_1



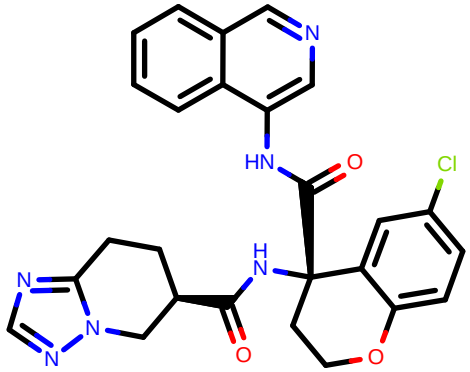
CID:	EN300-215799_1_1
SMILES:	Cc1c(c(no1)CO)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6024
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.25

EN300-124301_3_1



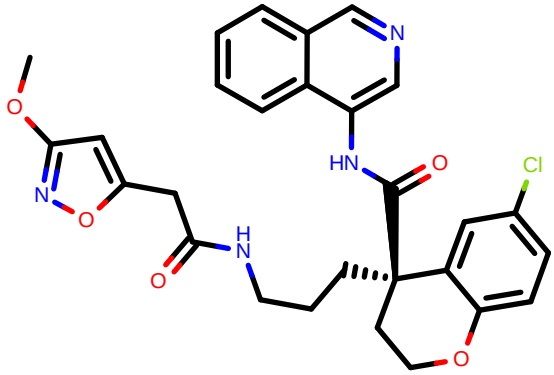
CID:	EN300-124301_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCn5ccnn5
RUN:	RUN5814
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.36

EN300-1662365_1_1



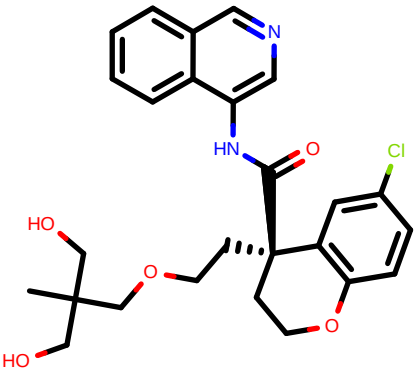
CID:	EN300-1662365_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCc6ncnn6C5
RUN:	RUN8294
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.25

EN300-127197_4_1



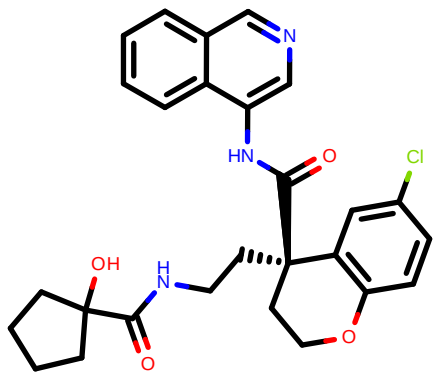
CID:	EN300-127197_4_1
SMILES:	COc1cc(on1)CC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11199
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.28

EN300-218116_3_1



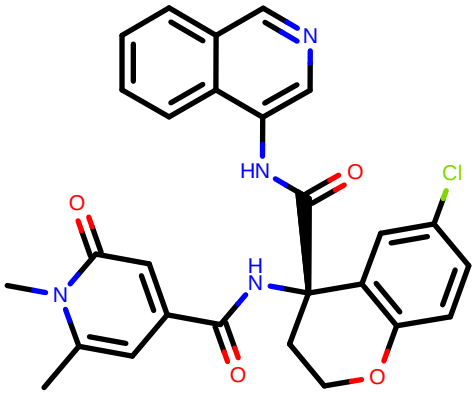
CID:	EN300-218116_3_1
SMILES:	CC(CO)(CO)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN289
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.36

EN300-25960_3_1



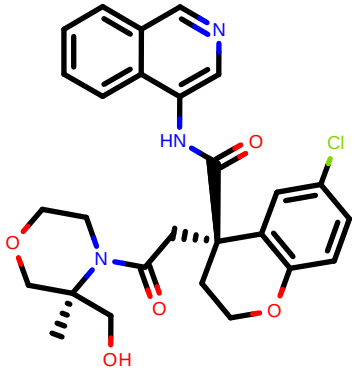
CID:	EN300-25960_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCC5)O
RUN:	RUN6505
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.33

EN300-4287199_1_1



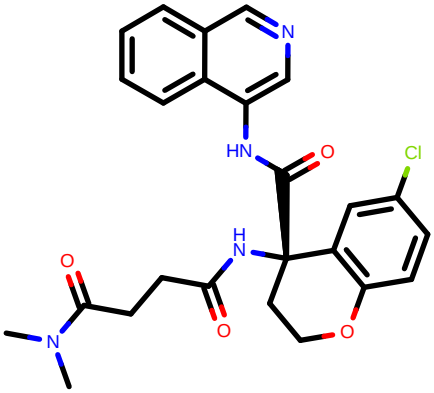
CID:	EN300-4287199_1_1
SMILES:	Cc1cc(cc(=O)n1C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5372
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.27

EN300-127629_1_1



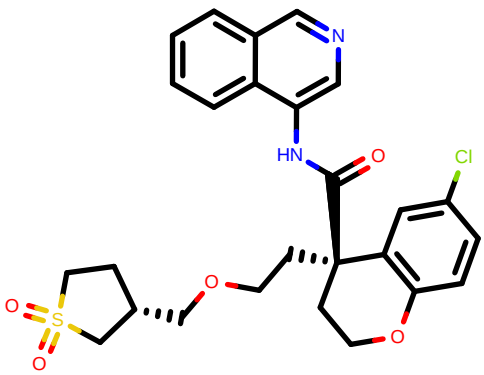
CID:	EN300-127629_1_1
SMILES:	C[C@@]1(COCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN6804
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.32

EN300-176877_1_1



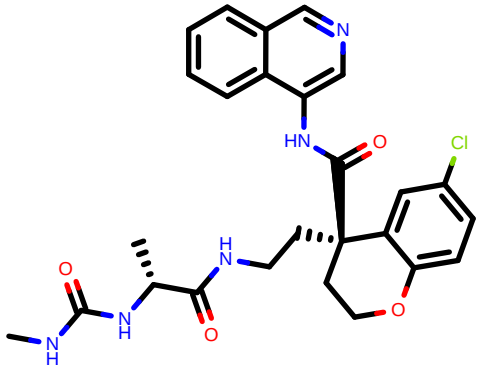
CID:	EN300-176877_1_1
SMILES:	CN(C)C(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3538
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.26

EN300-1448603_3_2



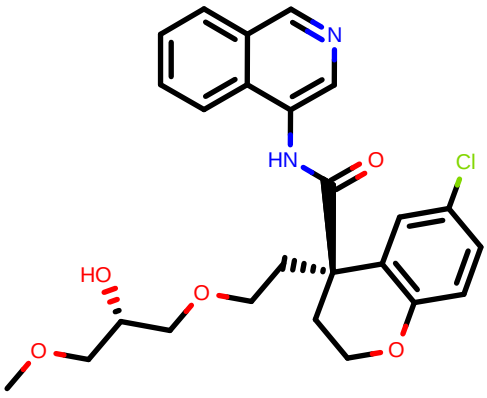
CID:	EN300-1448603_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CCS(=O)(=O)C5
RUN:	RUN1252
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.30

EN300-2958082_3_1



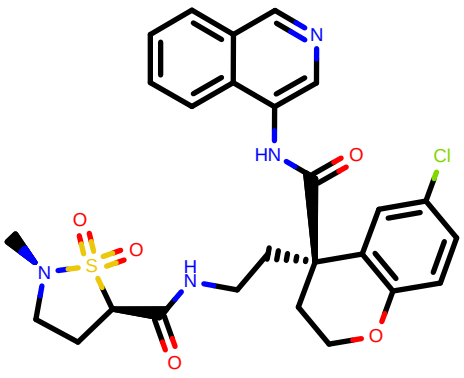
CID:	EN300-2958082_3_1
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)NC
RUN:	RUN1018
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.36

EN300-1915260_3_1



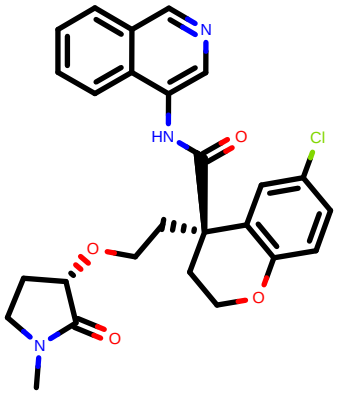
CID:	EN300-1915260_3_1
SMILES:	COC[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1540
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.38

EN300-255496_3_1



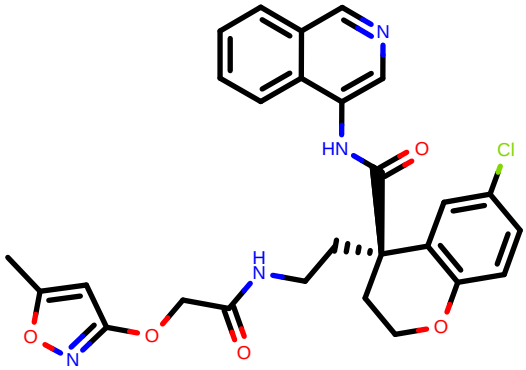
CID:	EN300-255496_3_1
SMILES:	CN1CC[C@@H](S1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8168
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.37

EN300-98648_3_1



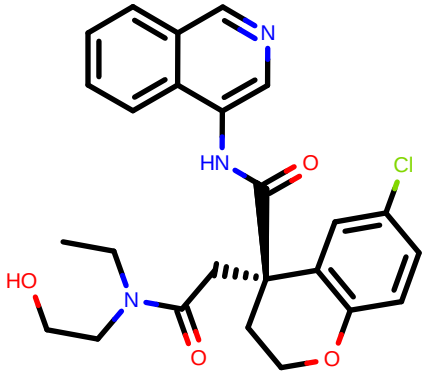
CID:	EN300-98648_3_1
SMILES:	CN1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2115
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.27

EN300-12929_3_1



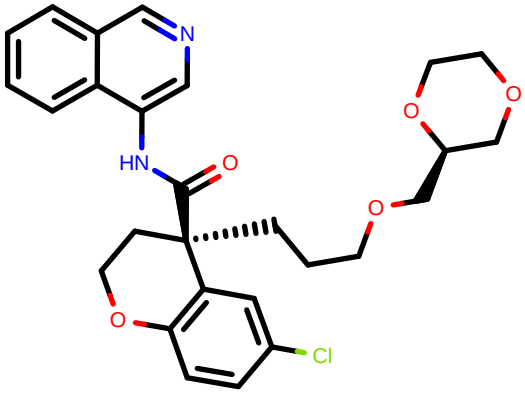
CID:	EN300-12929_3_1
SMILES:	Cc1cc(no1)OCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8136
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.26

EN300-74448_1_1



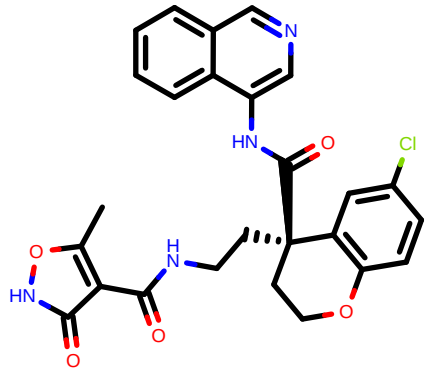
CID:	EN300-74448_1_1
SMILES:	CCN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7656
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.28

EN300-139167_4_1



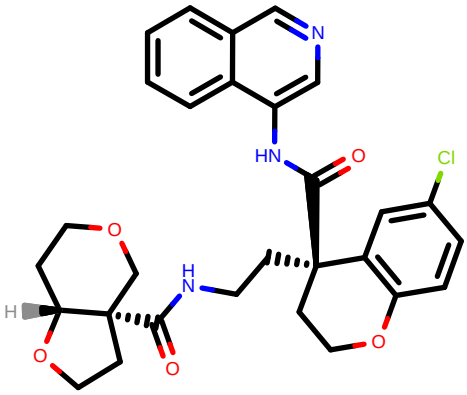
CID:	EN300-139167_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5COCCO5
RUN:	RUN523
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.37

EN300-110423_3_1



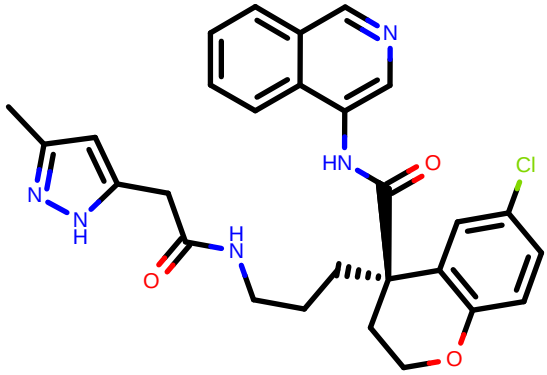
CID:	EN300-110423_3_1
SMILES:	Cc1c(c(=O)[nH]o1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10320
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.29

EN300-341337_3_2



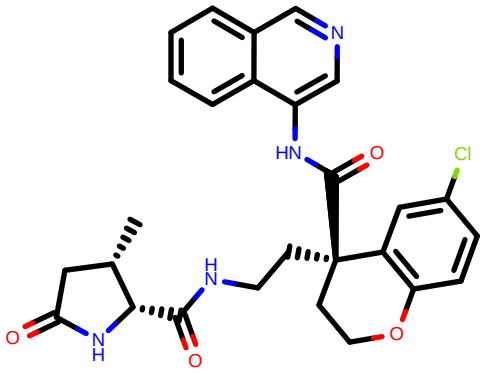
CID:	EN300-341337_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56CCO[C@@H]5CCOC6
RUN:	RUN3759
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.32

EN300-105110_4_1



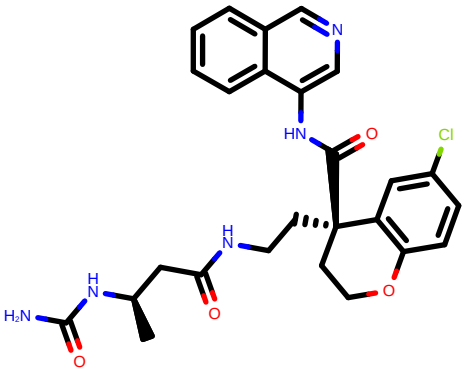
CID:	EN300-105110_4_1
SMILES:	Cc1cc(n[nH]1)CC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10479
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.34

EN300-155362_3_4



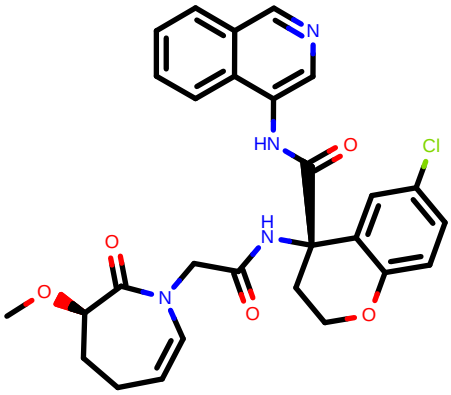
CID:	EN300-155362_3_4
SMILES:	C[C@H]1CC(=O)N[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9099
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.25

EN300-268198_3_2



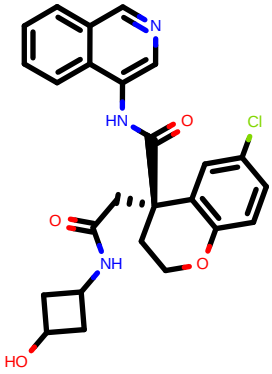
CID:	EN300-268198_3_2
SMILES:	C[C@H](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN2368
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.34

EN300-259847_1_1



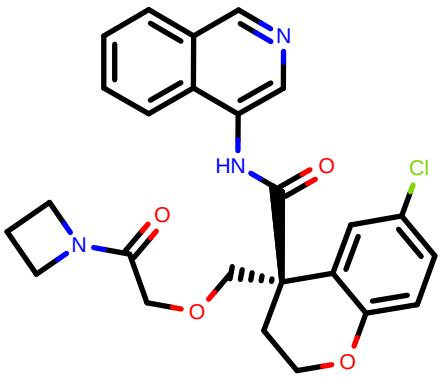
CID:	EN300-259847_1_1
SMILES:	CO[C@@H]1CCCCN(C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5924
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.38

EN300-100583_1_1



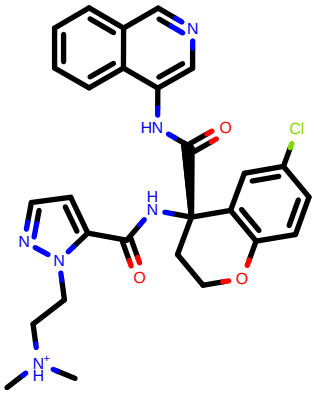
CID:	EN300-100583_1_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)CC(=O)N[C@H]5C[C@H](C5)O)cc1
RUN:	RUN10208
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.26

EN300-11195_2_1



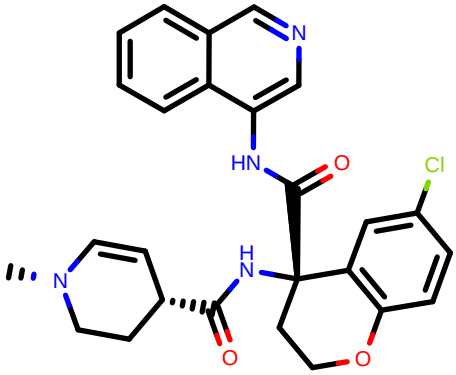
CID:	EN300-11195_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCC5
RUN:	RUN1142
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.27

EN300-256075_1_1



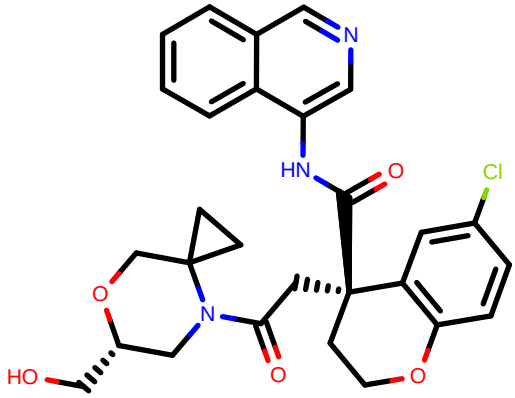
CID:	EN300-256075_1_1
SMILES:	CN(C)CCn1c(ccn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6355
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.33

EN300-51886_1_1



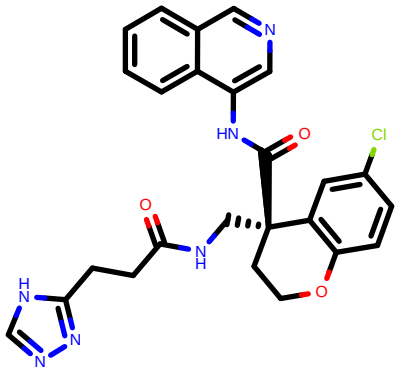
CID:	EN300-51886_1_1
SMILES:	CN1CCC(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7518
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.49

EN300-7493255_1_1



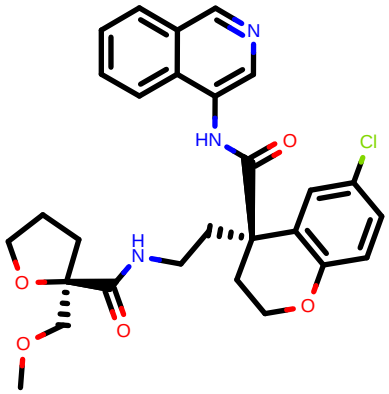
CID:	EN300-7493255_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](OCC56CC6)CO
RUN:	RUN9961
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.34

EN300-101197_2_1



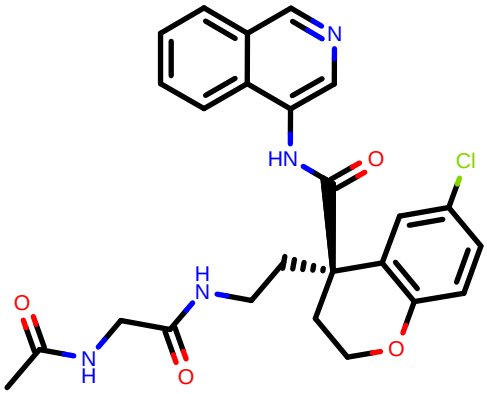
CID:	EN300-101197_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCc5[nH]cnn5
RUN:	RUN2762
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.28

EN300-1301381_3_2



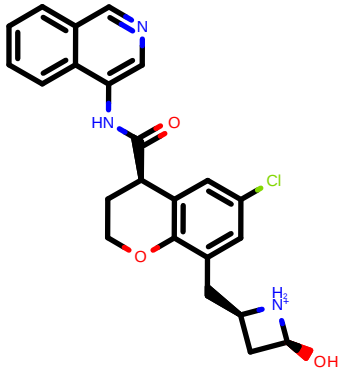
CID:	EN300-1301381_3_2
SMILES:	COC[C@]1(CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6705
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.35

EN300-18561_3_1



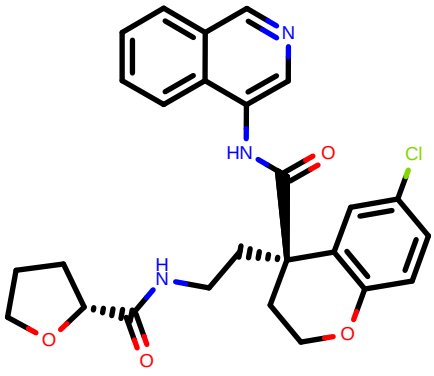
CID:	EN300-18561_3_1
SMILES:	CC(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3843
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.25

DAR-DIA-6a508060-5_1



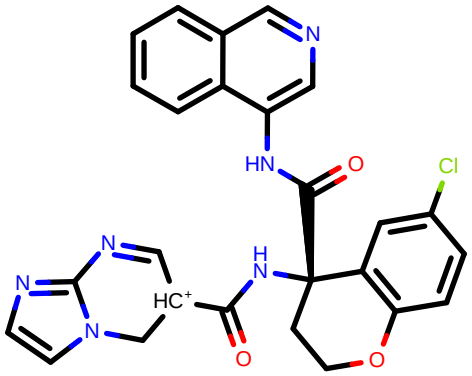
CID:	DAR-DIA-6a508060-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC(=O)N5)Cl
RUN:	RUN189
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.21

EN300-116234_3_1



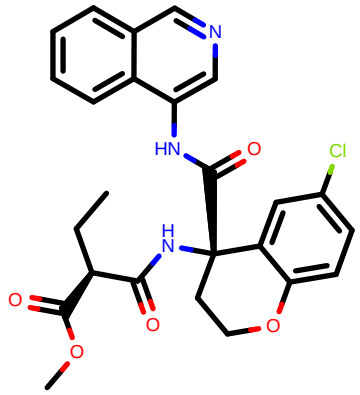
CID:	EN300-116234_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCO5
RUN:	RUN7592
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.28

EN300-147397_1_1



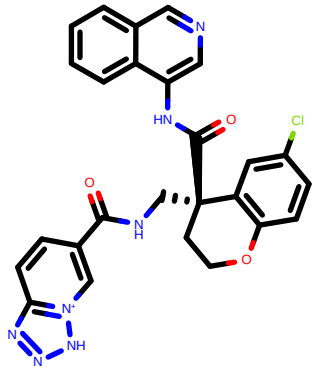
CID:	EN300-147397_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc6nccn6c5
RUN:	RUN8786
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.27

EN300-175425_1_1



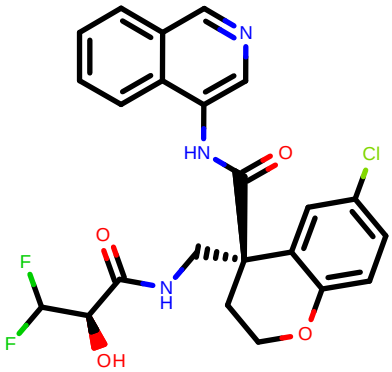
CID:	EN300-175425_1_1
SMILES:	CC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN6547
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.23

EN300-102853_2_1



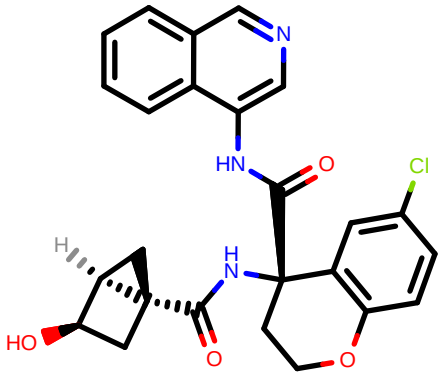
CID:	EN300-102853_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6nnnn6c5
RUN:	RUN8427
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.33

EN300-1932780_2_2



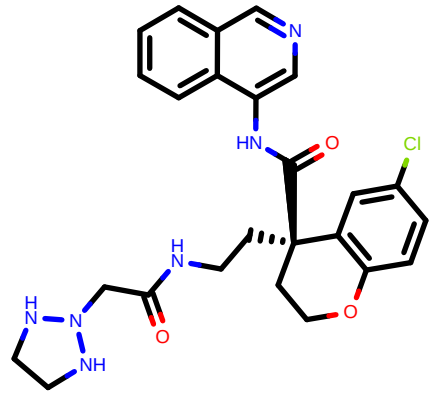
CID:	EN300-1932780_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C(F)F)O
RUN:	RUN3195
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.25

EN300-7433125_1_1



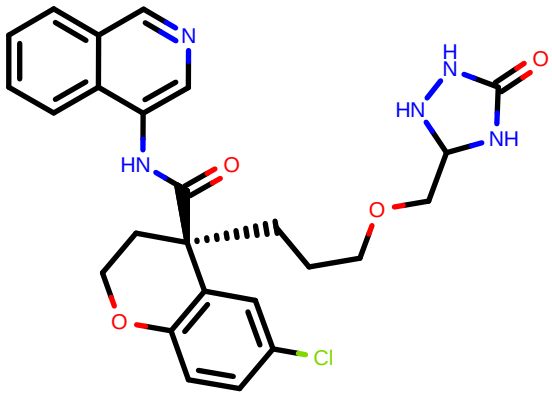
CID:	EN300-7433125_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@]56C[C@@H]5[C@@H](C6)O
RUN:	RUN4053
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.22

EN300-100916_3_1



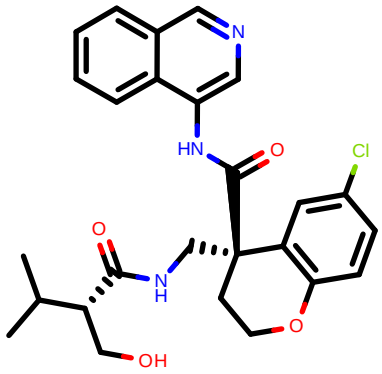
CID:	EN300-100916_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5nccn5
RUN:	RUN7604
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.27

EN300-73772_4_1



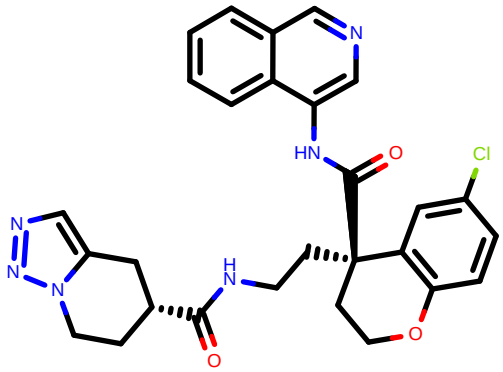
CID:	EN300-73772_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCc5[nH]c(=O)[nH]n5
RUN:	RUN308
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.34

EN300-153257_2_1



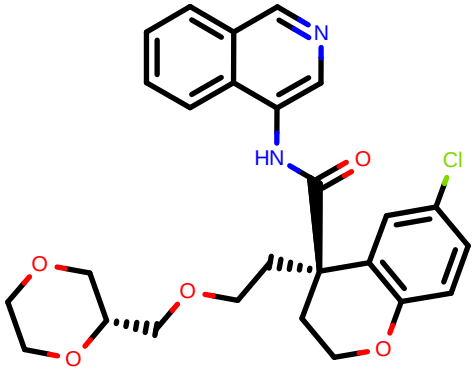
CID:	EN300-153257_2_1
SMILES:	CC(C)[C@@H](CO)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2451
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.32

EN300-7430501_3_1



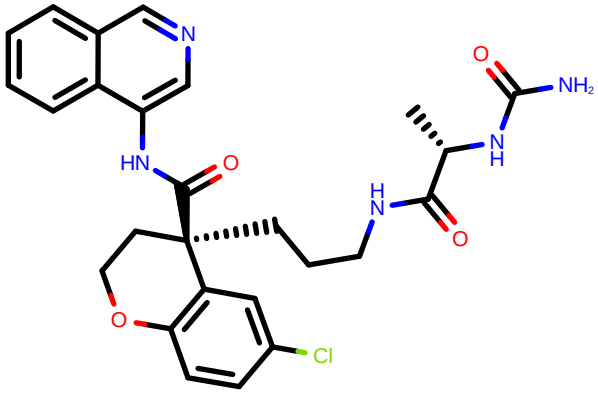
CID:	EN300-7430501_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCn6c(cnn6)C5
RUN:	RUN9406
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.32

EN300-139167_3_2



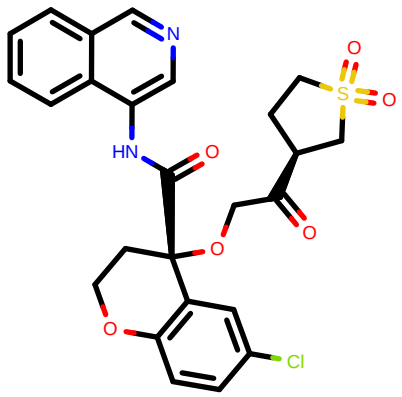
CID:	EN300-139167_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5COCCO5
RUN:	RUN680
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.32

EN300-00271_4_1



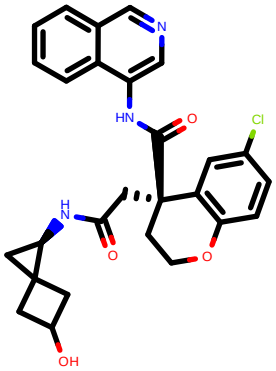
CID:	EN300-00271_4_1
SMILES:	C[C@@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN9948
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.39

EN300-226314_1_2



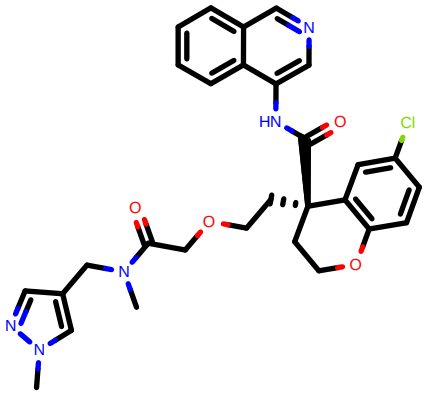
CID:	EN300-226314_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5CCS(=O)(=O)C5
RUN:	RUN277
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.30

EN300-624143_1_1



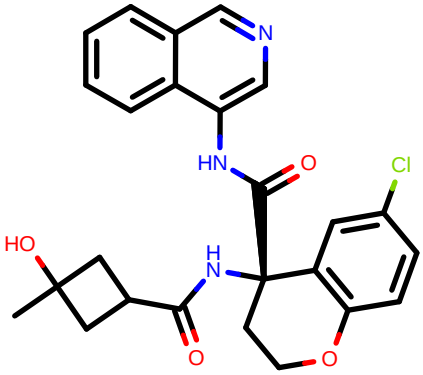
CID:	EN300-624143_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC56CC(C6)O
RUN:	RUN9616
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.23

EN300-65978_3_1



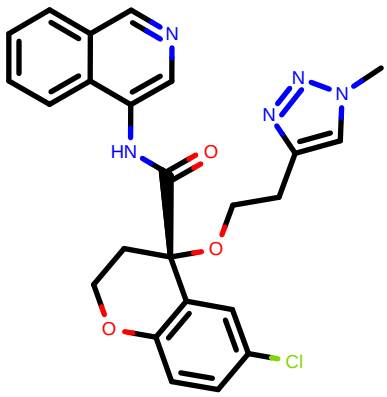
CID:	EN300-65978_3_1
SMILES:	Cn1cc(cn1)CN(C)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1731
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.52

EN300-247343_1_1



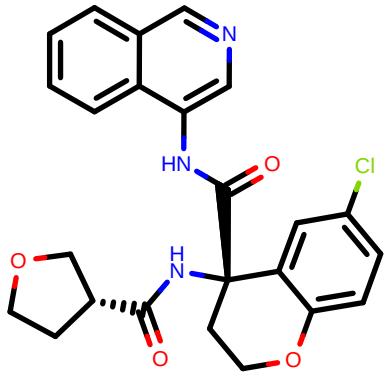
CID:	EN300-247343_1_1
SMILES:	CC1(CC(C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3434
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.25

EN300-1600786_1_1



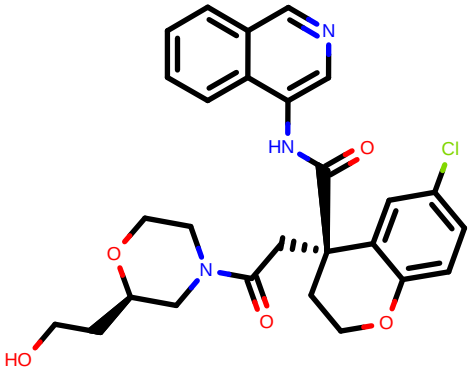
CID:	EN300-1600786_1_1
SMILES:	Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1032
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.21

EN300-53423_1_1



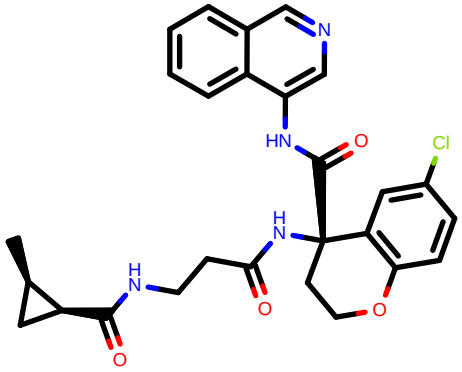
CID:	EN300-53423_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC5
RUN:	RUN5265
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.25

EN300-102007_1_1



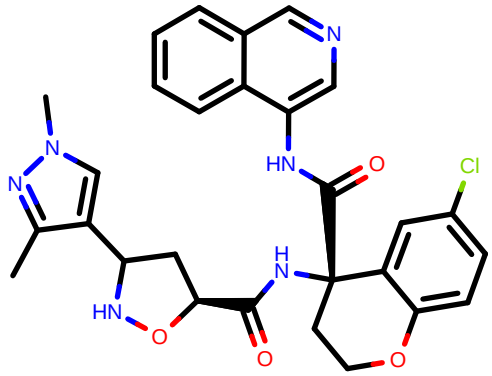
CID:	EN300-102007_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CCO
RUN:	RUN8596
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.33

EN300-36851_1_1



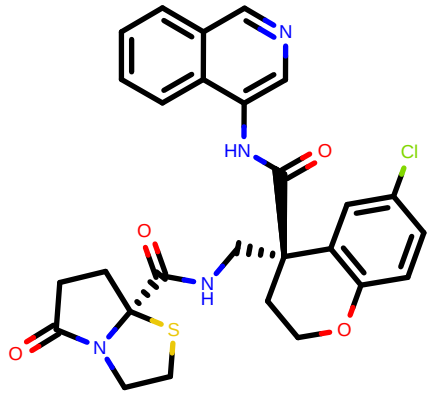
CID:	EN300-36851_1_1
SMILES:	C[C@@H]1C[C@@H]1C(=O)NCCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1181
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.29

EN300-92684_1_1



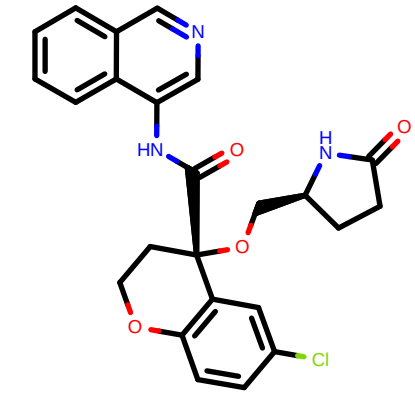
CID:	EN300-92684_1_1
SMILES:	Cc1c(cn(n1)C)C2=NO[C@@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7090
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.35

EN300-10334_2_1



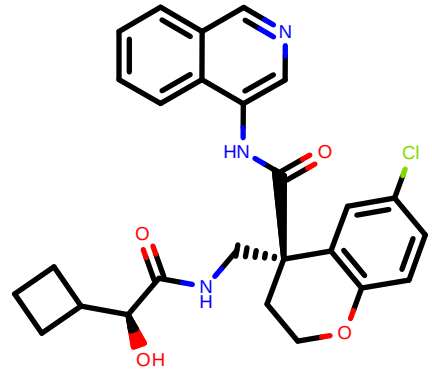
CID:	EN300-10334_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]56CCC(=O)N5CCS6
RUN:	RUN4310
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.33

EN300-195756_1_1



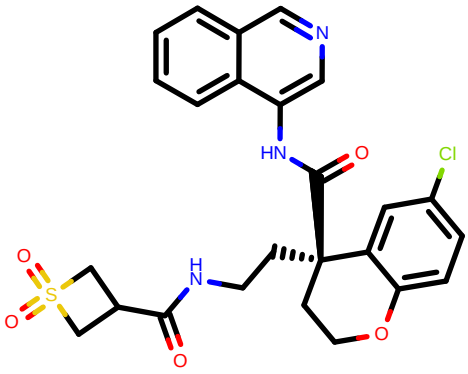
CID:	EN300-195756_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCC(=O)N5
RUN:	RUN2127
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.24

EN300-249764_2_2



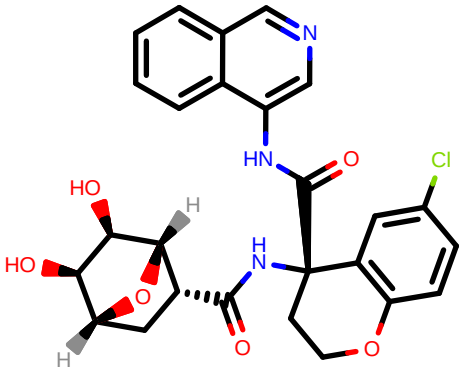
CID:	EN300-249764_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5CCC5)O
RUN:	RUN4318
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.27

EN300-261365_3_1



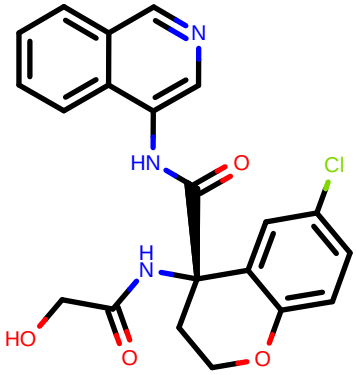
CID:	EN300-261365_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CS(=O)(=O)C5
RUN:	RUN10928
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.30

EN300-6764836_1_7



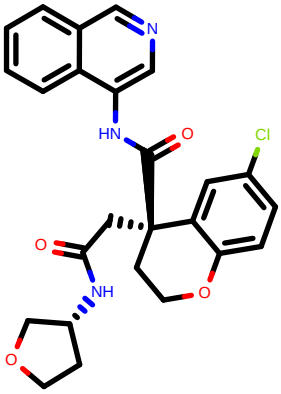
CID:	EN300-6764836_1_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6[C@H]([C@H](C5O6)O)O
RUN:	RUN5992
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.26

EN300-19242_1_1



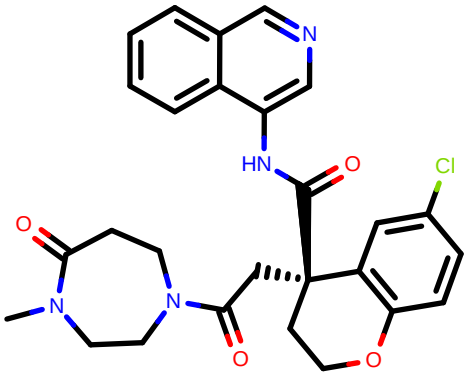
CID:	EN300-19242_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO
RUN:	RUN1780
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.17

EN300-171752_1_1



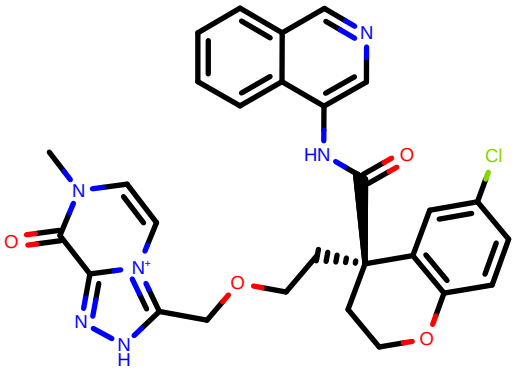
CID:	EN300-171752_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC5
RUN:	RUN10766
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.25

EN300-263395_1_1



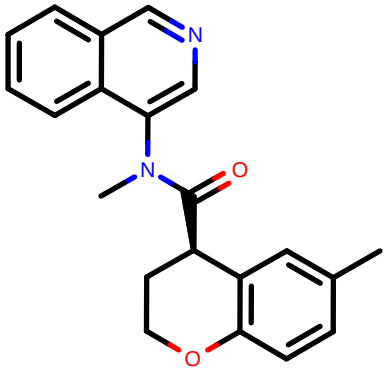
CID:	EN300-263395_1_1
SMILES:	CN1CCN(CCC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9324
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.31

EN300-379020_3_1



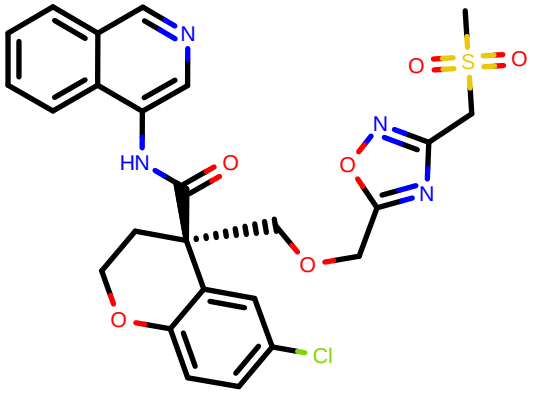
CID:	EN300-379020_3_1
SMILES:	Cn1ccn2c(nnc2c1=O)COCC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2398
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.33

MAK-UNK-3875bbc8-1_1



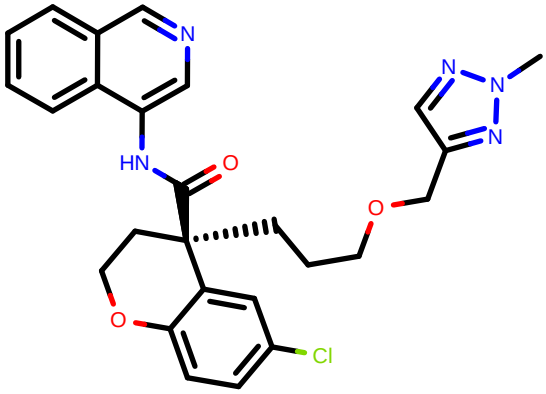
CID:	MAK-UNK-3875bbc8-1_1
SMILES:	Cc1ccc2c(c1)[C@@H](CCO2)C(=O)N(C)c3cncc4c3cccc4
RUN:	RUN32
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.09

EN300-94900_2_1



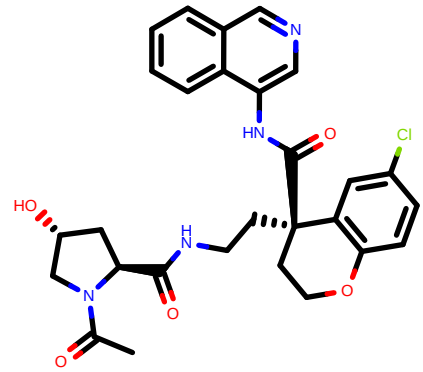
CID:	EN300-94900_2_1
SMILES:	CS(=O)(=O)Cc1nc(on1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN451
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.43

EN300-219020_4_1



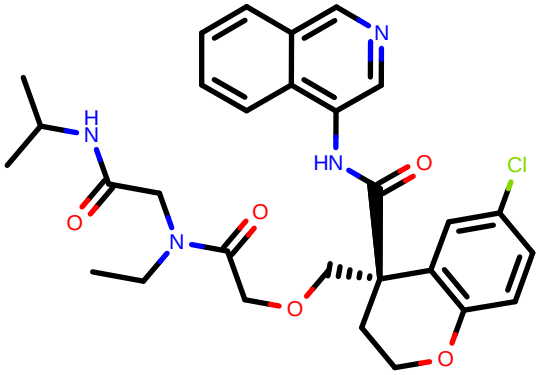
CID:	EN300-219020_4_1
SMILES:	Cn1ncc(n1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN547
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.31

EN300-1703718_3_1



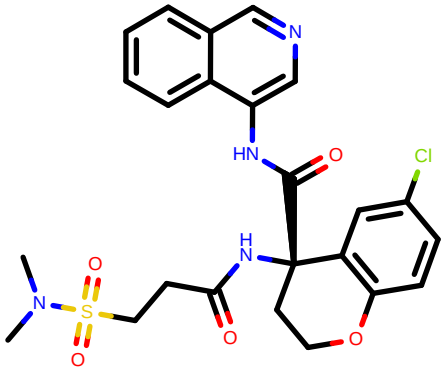
CID:	EN300-1703718_3_1
SMILES:	CC(=O)N1C[C@@H](C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN740
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.40

EN300-07936_2_1



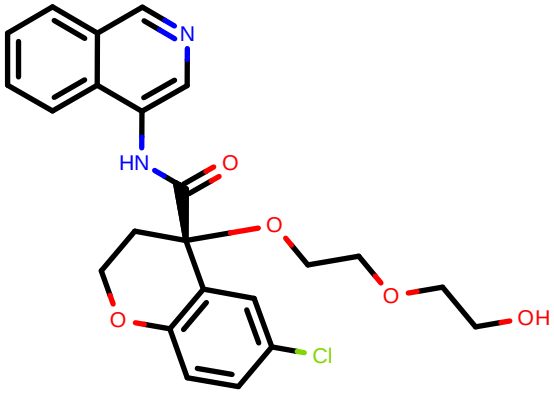
CID:	EN300-07936_2_1
SMILES:	CCN(CC(=O)NC(C)C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2615
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.40

EN300-50631_1_1



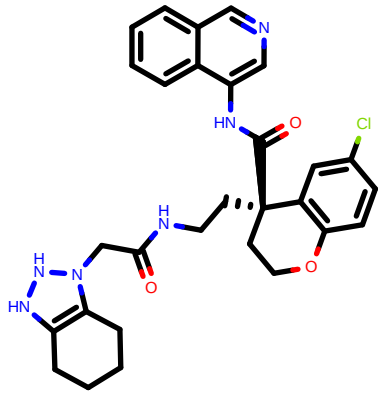
CID:	EN300-50631_1_1
SMILES:	CN(C)S(=O)(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3658
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.41

EN300-52467_1_1



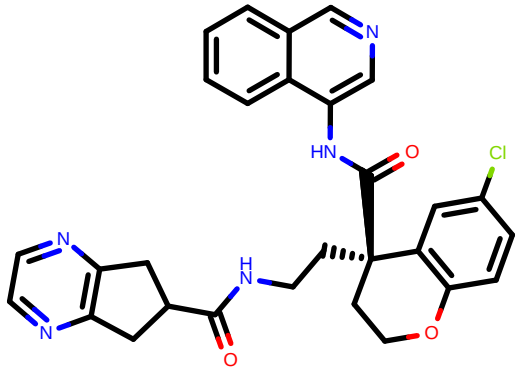
CID:	EN300-52467_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCO
RUN:	RUN904
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.31

EN300-223187_3_1



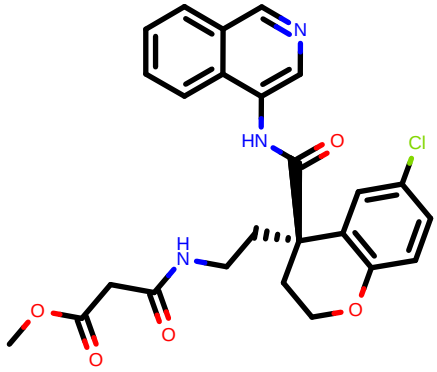
CID:	EN300-223187_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5c6c(nn5)CCCC6
RUN:	RUN10626
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.32

EN300-2011576_3_1



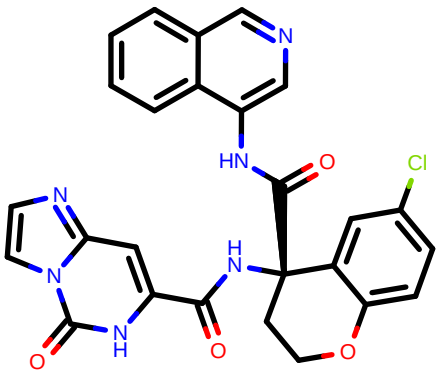
CID:	EN300-2011576_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5Cc6c(nccn6)C5
RUN:	RUN6924
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.33

EN300-20668_3_1



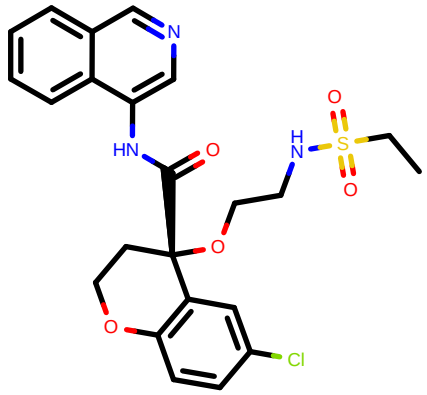
CID:	EN300-20668_3_1
SMILES:	COC(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5778
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.27

EN300-7440089_1_1



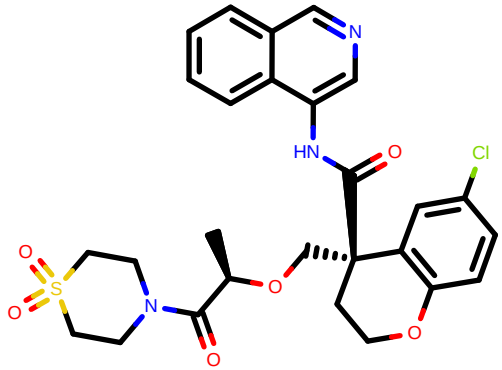
CID:	EN300-7440089_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6nccn6c(=O)[nH]5
RUN:	RUN5009
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.28

EN300-73582_1_1



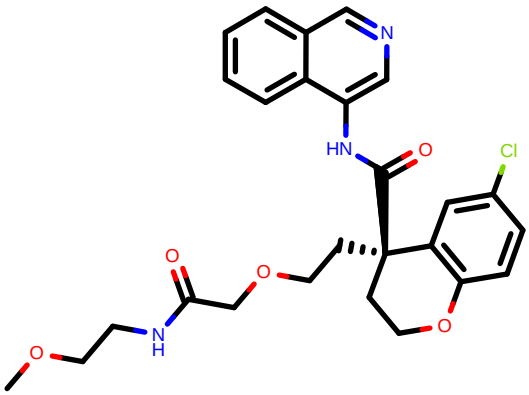
CID:	EN300-73582_1_1
SMILES:	CCS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1080
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.29

EN300-1265949_2_2



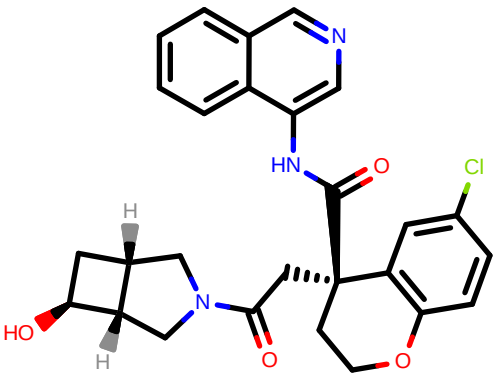
CID:	EN300-1265949_2_2
SMILES:	C[C@H](C(=O)N1CCS(=O)(=O)CC1)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1885
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.34

EN300-02015_3_1



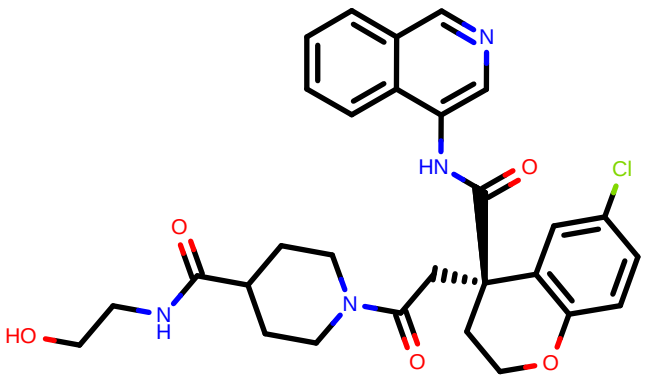
CID:	EN300-02015_3_1
SMILES:	COCCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN393
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.30

EN300-305294_1_6



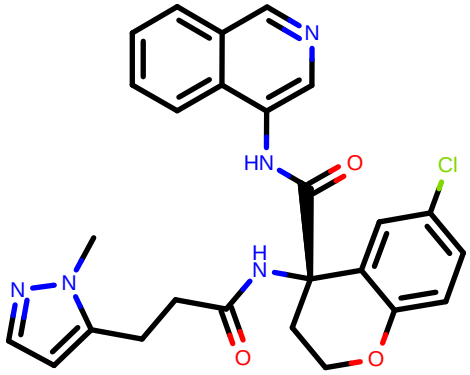
CID:	EN300-305294_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@@H]([C@H]6C5)O
RUN:	RUN3352
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.30

EN300-344753_1_1



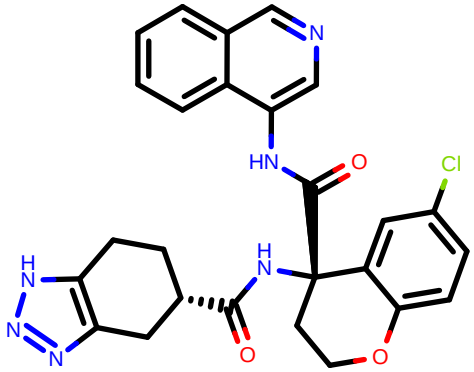
CID:	EN300-344753_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)C(=O)NCCO
RUN:	RUN8004
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.62

EN300-92662_1_1



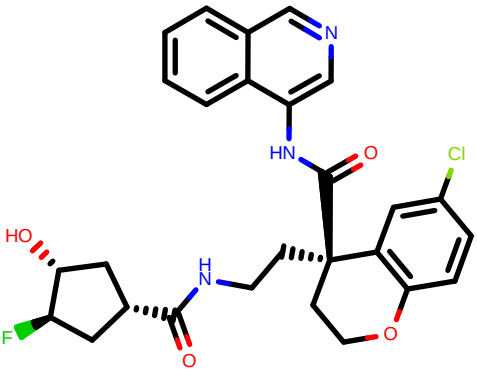
CID:	EN300-92662_1_1
SMILES:	Cn1c(ccn1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN537
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.28

EN300-185729_1_2



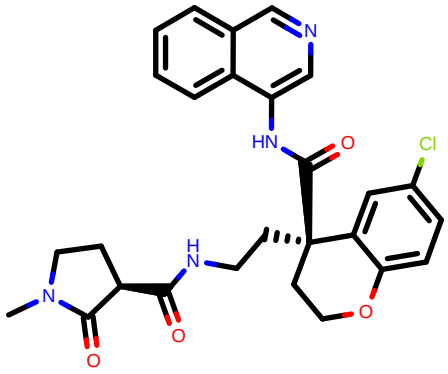
CID:	EN300-185729_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCc6c(nn[nH]6)C5
RUN:	RUN6259
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.31

EN300-7461217_3_2



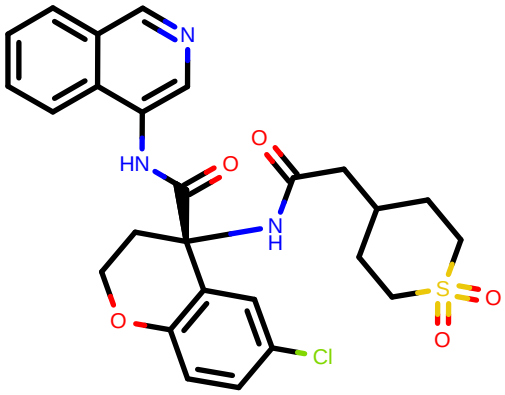
CID:	EN300-7461217_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5C[C@H]([C@@H](C5)F)O
RUN:	RUN10001
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.27

EN300-141695_3_2



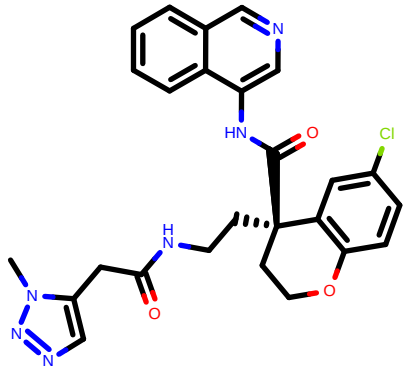
CID:	EN300-141695_3_2
SMILES:	CN1CC[C@H](C1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10982
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.35

EN300-250120_1_1



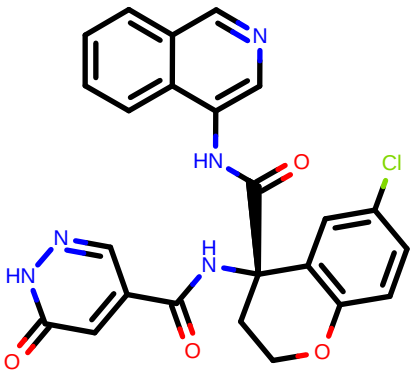
CID:	EN300-250120_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5CCS(=O)(=O)CC5
RUN:	RUN6435
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.29

EN300-6486855_3_1



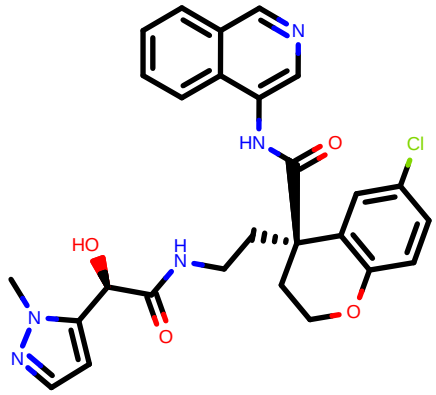
CID:	EN300-6486855_3_1
SMILES:	Cn1c(cnn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3004
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.34

EN300-159634_1_1



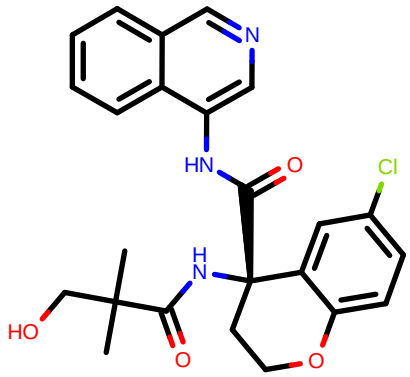
CID:	EN300-159634_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(=O)[nH]nc5
RUN:	RUN5428
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.19

EN300-6473273_3_2



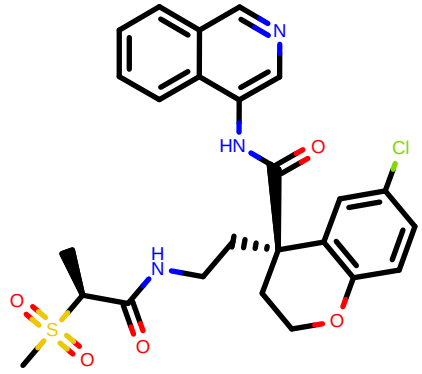
CID:	EN300-6473273_3_2
SMILES:	Cn1c(ccn1)[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1114
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.40

EN300-65050_1_1



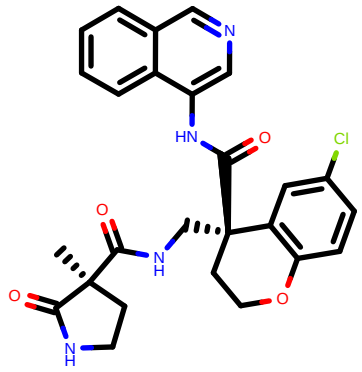
CID:	EN300-65050_1_1
SMILES:	CC(C)(CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2052
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.27

EN300-39405_3_1



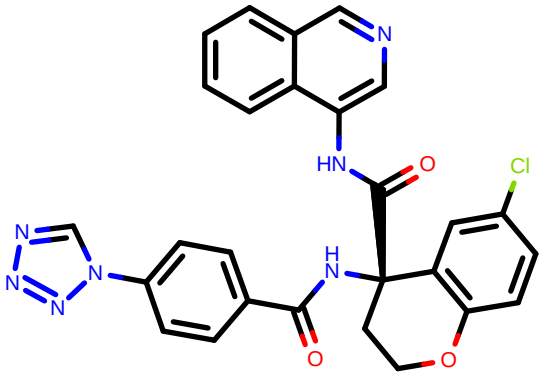
CID:	EN300-39405_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN4927
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.28

EN300-207959_2_1



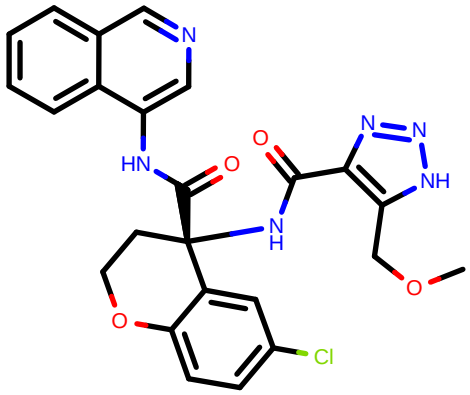
CID:	EN300-207959_2_1
SMILES:	C[C@@]1(CCNC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3379
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.38

EN300-06030_1_1



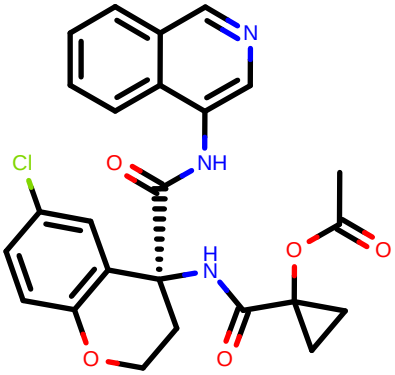
CID:	EN300-06030_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)n6cnnn6
RUN:	RUN8969
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.31

EN300-785910_1_1



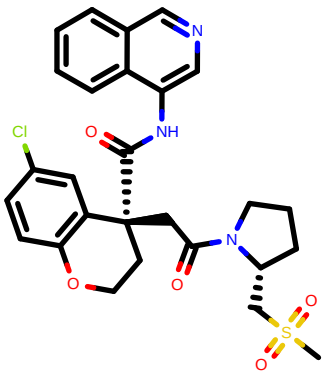
CID:	EN300-785910_1_1
SMILES:	COCc1c(nn[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5768
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.31

EN300-173023_1_1



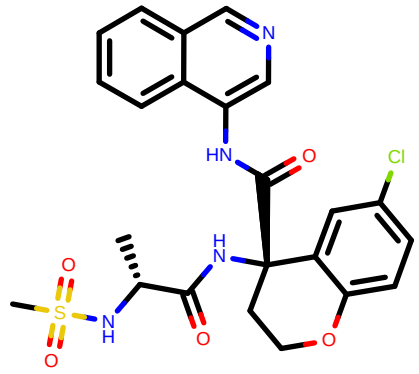
CID:	EN300-173023_1_1
SMILES:	CC(=O)OC1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4921
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.28

EN300-300294_1_1



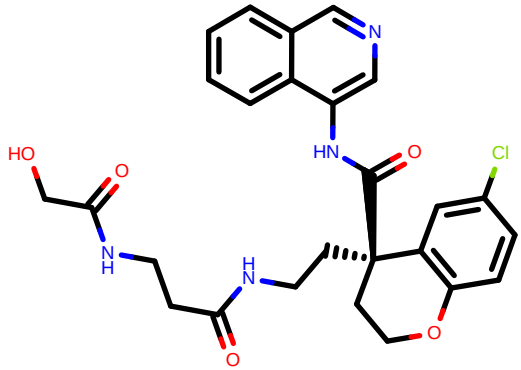
CID:	EN300-300294_1_1
SMILES:	CS(=O)(=O)C[C@H]1CCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8656
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.30

EN300-31210_1_2



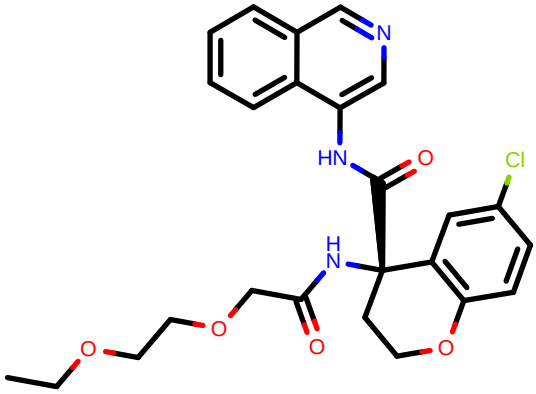
CID:	EN300-31210_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN3054
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.38

EN300-383904_3_1



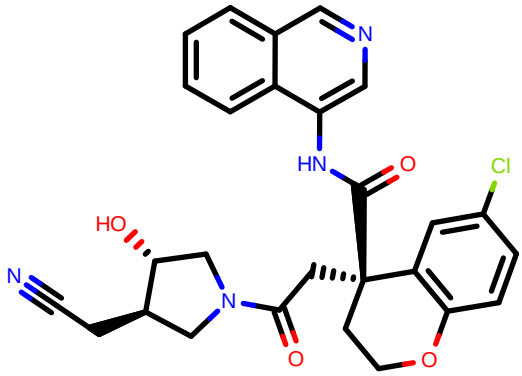
CID:	EN300-383904_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCNC(=O)CO
RUN:	RUN9698
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.36

EN300-54304_1_1



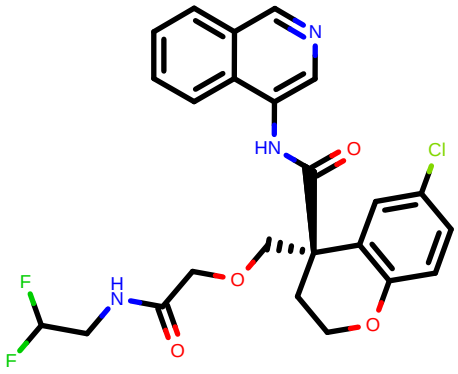
CID:	EN300-54304_1_1
SMILES:	CCOCCOCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2750
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.30

EN300-1719143_1_1



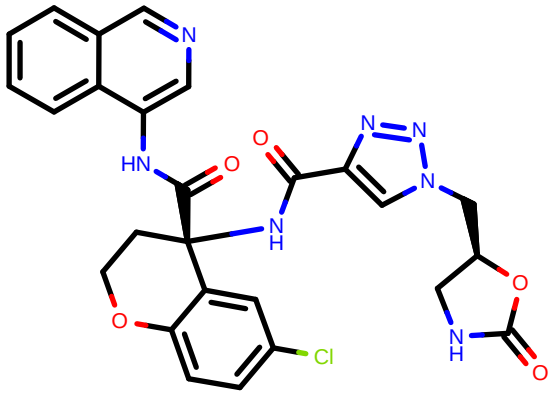
CID:	EN300-1719143_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NSC[C@H]([C@@H](CS)O)CC#N
RUN:	RUN8760
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.27

EN300-120586_2_1



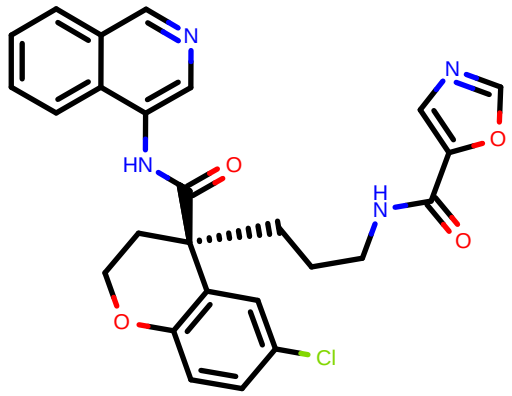
CID:	EN300-120586_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NCC(F)F
RUN:	RUN371
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.29

EN300-379219_1_1



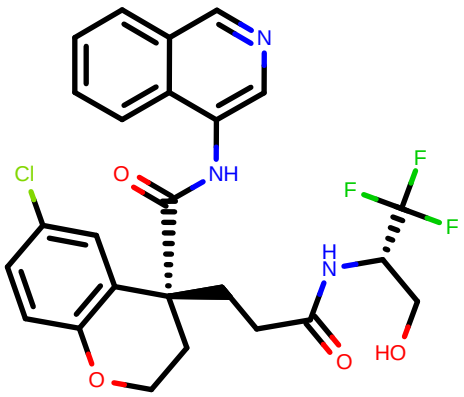
CID:	EN300-379219_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@H]6CNC(=O)O6
RUN:	RUN8670
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.29

EN300-25446_4_1



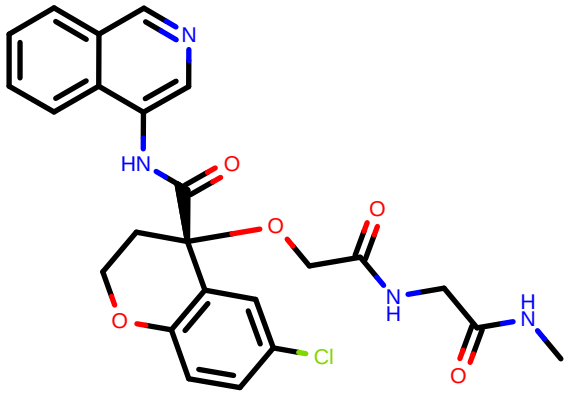
CID:	EN300-25446_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cnco5
RUN:	RUN8021
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.29

EN300-142130_2_1



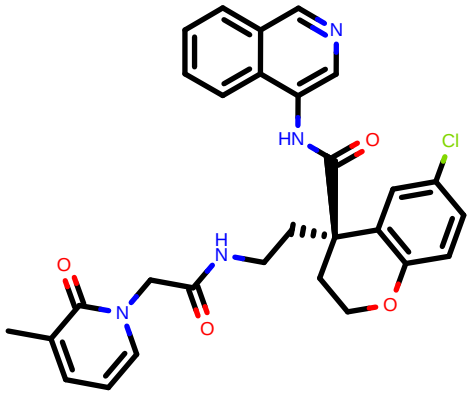
CID:	EN300-142130_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CO)C(F)(F)F
RUN:	RUN4028
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.40

EN300-23223_1_1



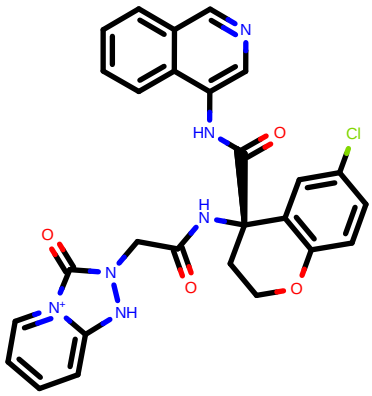
CID:	EN300-23223_1_1
SMILES:	CNC(=O)CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1152
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.27

EN300-126104_3_1



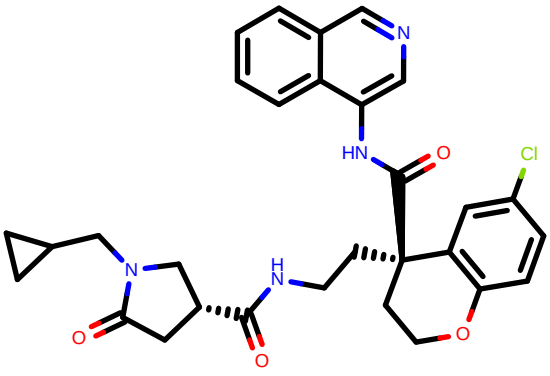
CID:	EN300-126104_3_1
SMILES:	Cc1cccn(c1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9614
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.32

EN300-27476_1_1



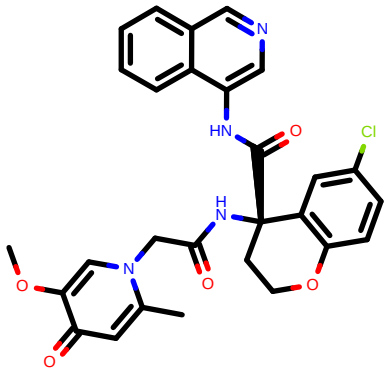
CID:	EN300-27476_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6ccccc6n5
RUN:	RUN8502
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.42

EN300-31969_3_1



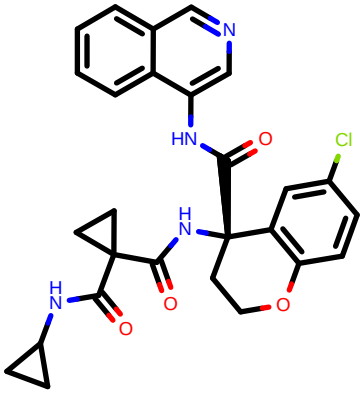
CID:	EN300-31969_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC(=O)N(C5)CC6CC6
RUN:	RUN1266
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.36

EN300-1271924_1_1



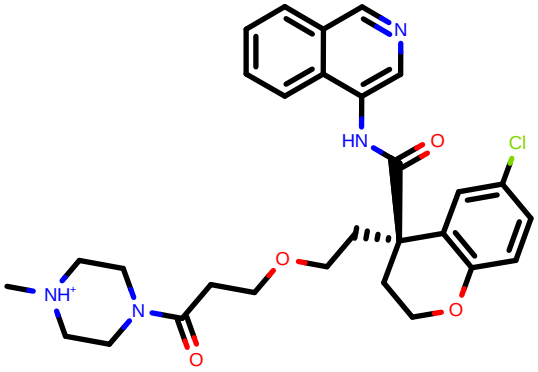
CID:	EN300-1271924_1_1
SMILES:	Cc1cc(=O)c(cn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)OC
RUN:	RUN8394
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.32

EN300-61636_1_1



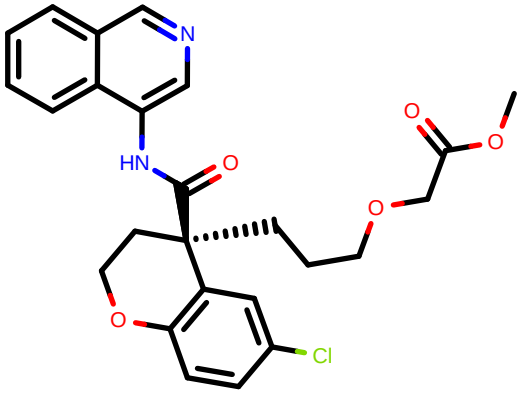
CID:	EN300-61636_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CC5)C(=O)NC6CC6
RUN:	RUN6251
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.33

EN300-178293_3_1



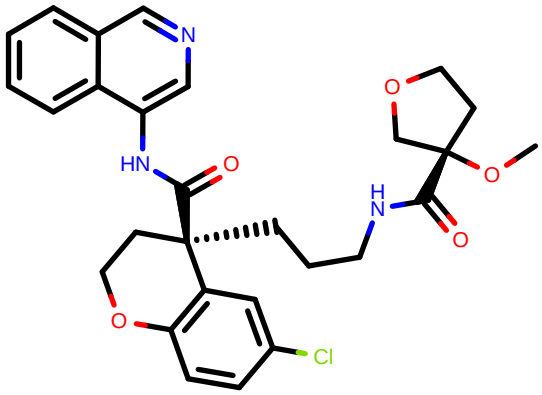
CID:	EN300-178293_3_1
SMILES:	CN1CCN(CC1)C(=O)CCOCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN844
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.45

EN300-19700_4_1



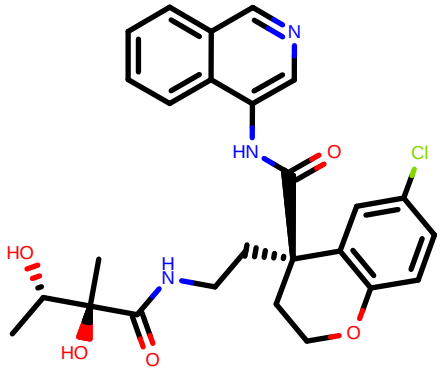
CID:	EN300-19700_4_1
SMILES:	COC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN420
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.27

EN300-174668_4_2



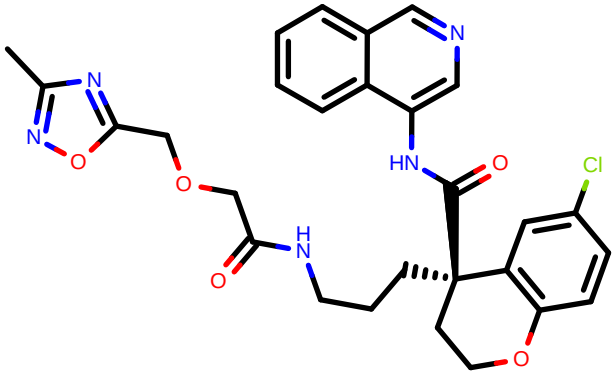
CID:	EN300-174668_4_2
SMILES:	CO[C@]1(CCOC1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10333
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.51

EN300-202922_3_3



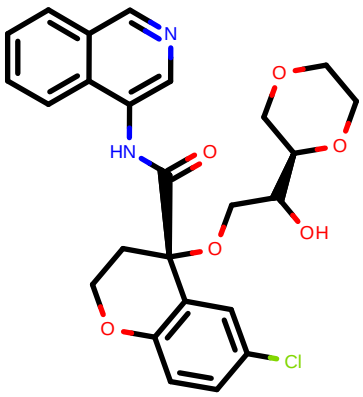
CID:	EN300-202922_3_3
SMILES:	C[C@@H]([C@](C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN5047
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.30

EN300-77006_4_1



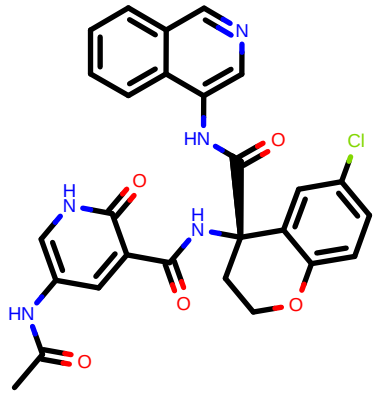
CID:	EN300-77006_4_1
SMILES:	Cc1nc(on1)COCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11251
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.33

EN300-6238494_1_2



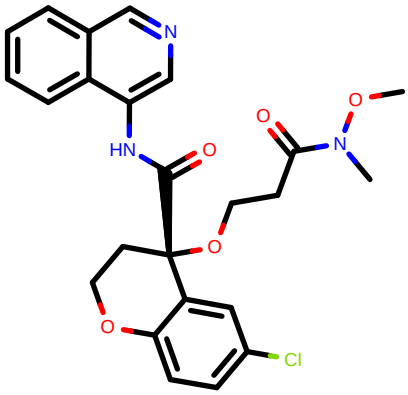
CID:	EN300-6238494_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[C@H]5COCCO5
RUN:	RUN309
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.31

EN300-307053_1_1



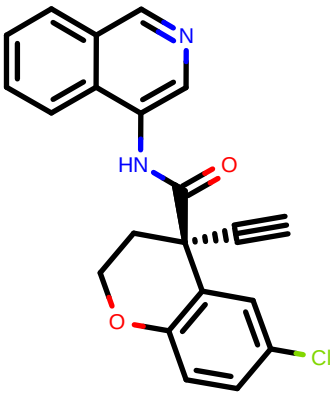
CID:	EN300-307053_1_1
SMILES:	CC(=O)Nc1cc(c(=O)[nH]c1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9071
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.27

EN300-174603_1_1



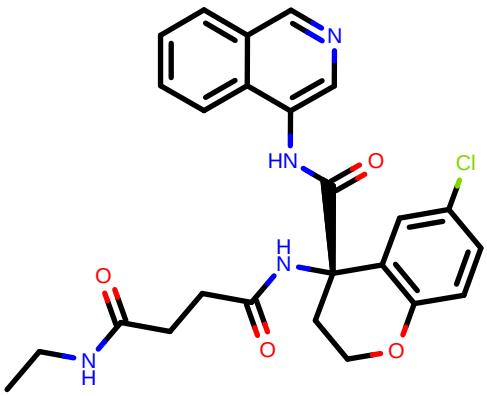
CID:	EN300-174603_1_1
SMILES:	CN(C(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN1272
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.23

PET-UNK-29afea89-1_1



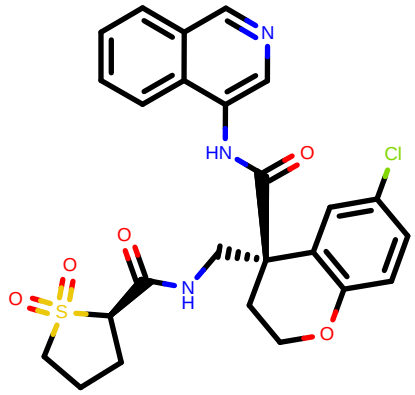
CID:	PET-UNK-29afea89-1_1
SMILES:	C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN40
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.10

EN300-68889_1_1



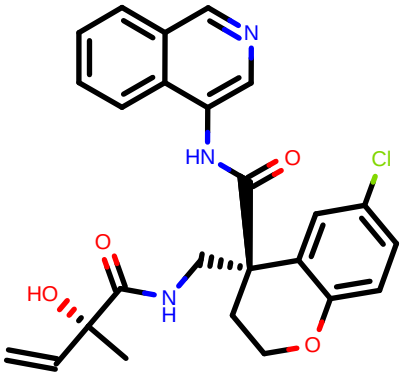
CID:	EN300-68889_1_1
SMILES:	CCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2566
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.25

EN300-88656_2_2



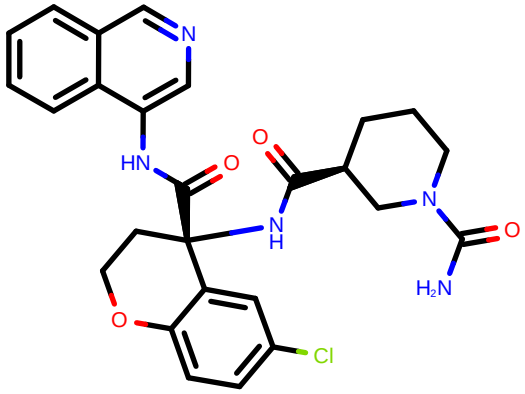
CID:	EN300-88656_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCS5(=O)=O
RUN:	RUN5309
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.29

EN300-248888_2_1



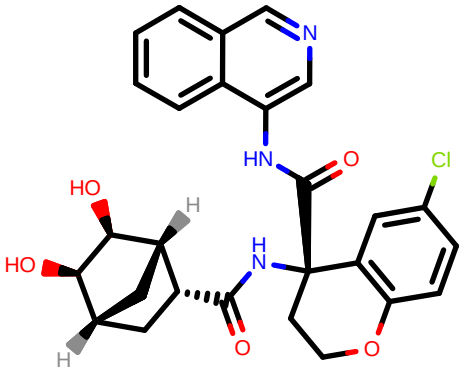
CID:	EN300-248888_2_1
SMILES:	C[C@@](C=C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4970
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.30

EN300-14767_1_2



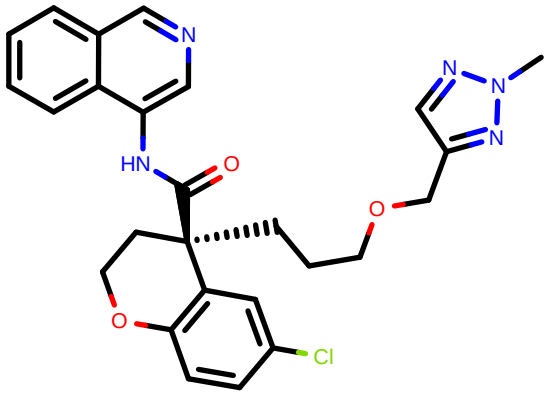
CID:	EN300-14767_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCN(C5)C(=O)N
RUN:	RUN4029
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.26

EN300-6744028_1_1



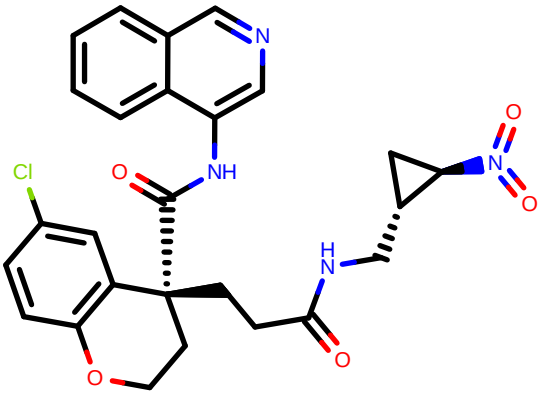
CID:	EN300-6744028_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CC6CC5[C@@H]([C@@H]6O)O
RUN:	RUN5644
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.32

EN300-219020_4_1



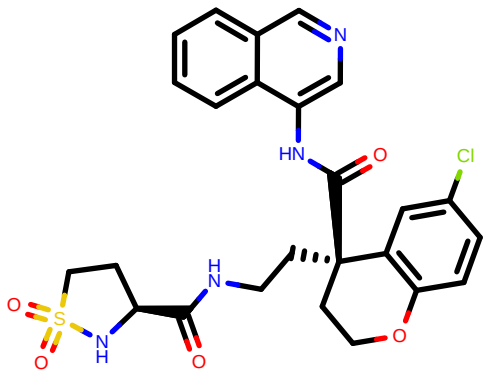
CID:	EN300-219020_4_1
SMILES:	Cn1ncc(n1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN555
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.32

EN300-7465222_2_1



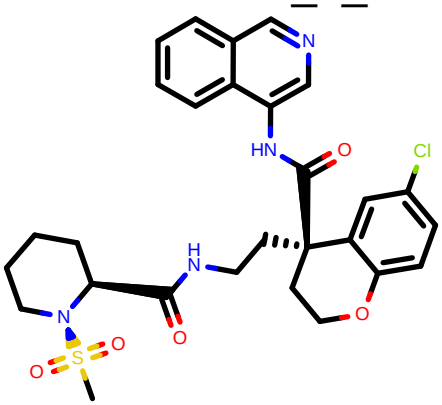
CID:	EN300-7465222_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H]5C[C@H]5N(=O)=O
RUN:	RUN4944
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.24

EN300-45049_3_1



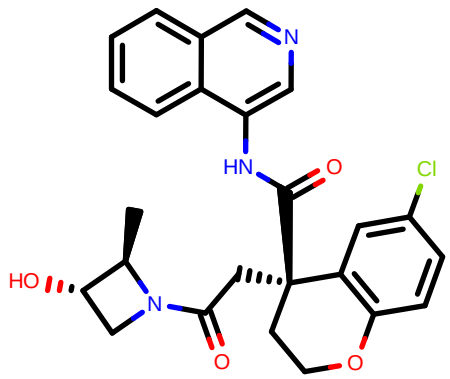
CID:	EN300-45049_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCS(=O)(=O)N5
RUN:	RUN9738
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.27

EN300-24014_3_2



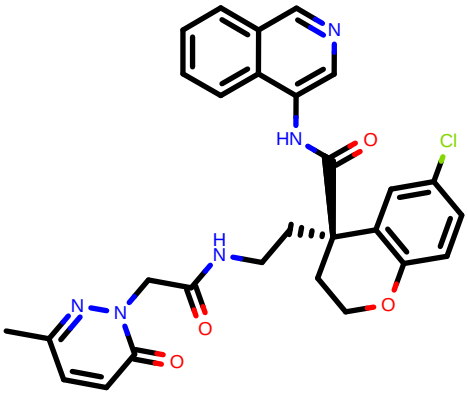
CID:	EN300-24014_3_2
SMILES:	CS(=O)(=O)N1CCCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6609
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.47

EN300-7471076_1_3



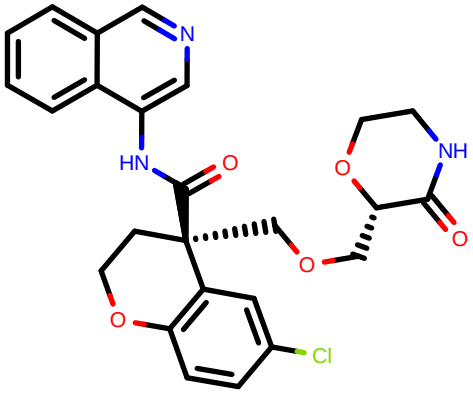
CID:	EN300-7471076_1_3
SMILES:	C[C@@H]1[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4035
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.26

EN300-69556_3_1



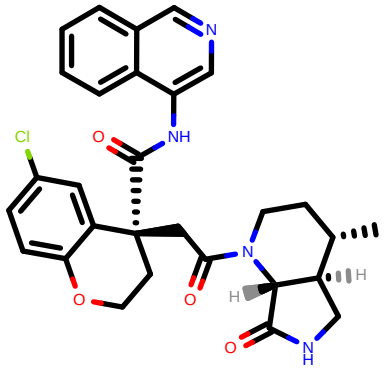
CID:	EN300-69556_3_1
SMILES:	Cc1ccc(=O)n(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8176
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.53

EN300-1706036_2_2



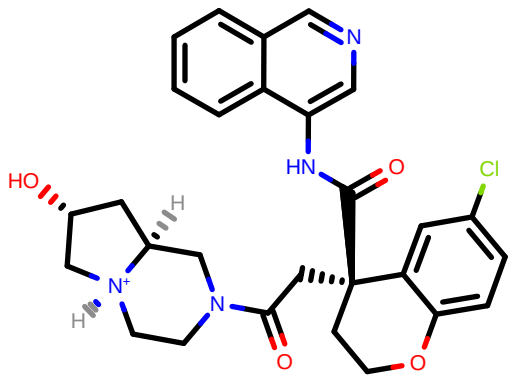
CID:	EN300-1706036_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C(=O)NCCO5
RUN:	RUN1645
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.29

EN300-6739879_1_2



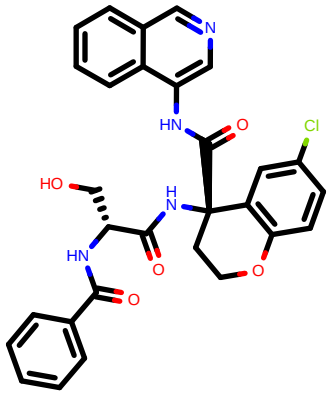
CID:	EN300-6739879_1_2
SMILES:	C[C@H]1CCN[C@@H]2[C@@H]1CNC2=O)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN10880
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.35

EN300-267855_1_1



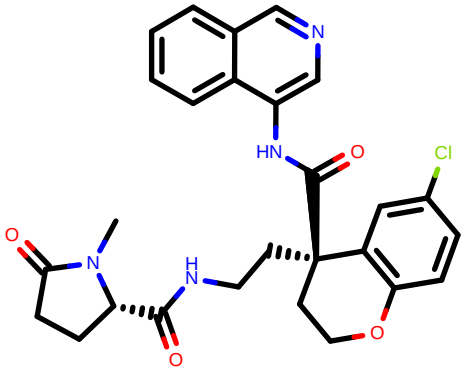
CID:	EN300-267855_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6C[C@@H](C[C@H]6C5)O
RUN:	RUN10834
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.32

EN300-50228_1_2



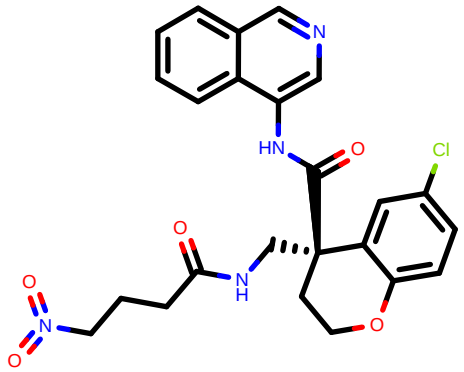
CID:	EN300-50228_1_2
SMILES:	c1ccc(cc1)C(=O)N[C@H](CO)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7634
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.35

EN300-132963_3_1



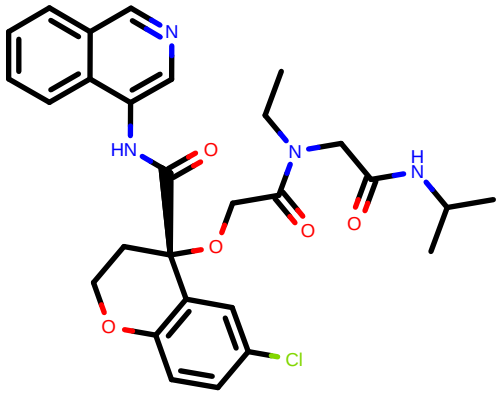
CID:	EN300-132963_3_1
SMILES:	CN1[C@@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6661
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.32

EN300-143449_2_1



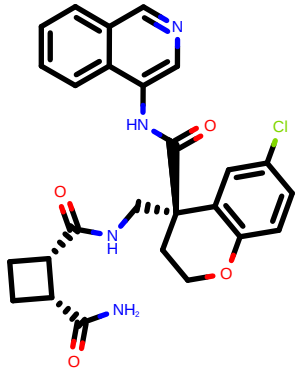
CID:	EN300-143449_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCN(=O)=O
RUN:	RUN2541
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.36

EN300-07936_1_1



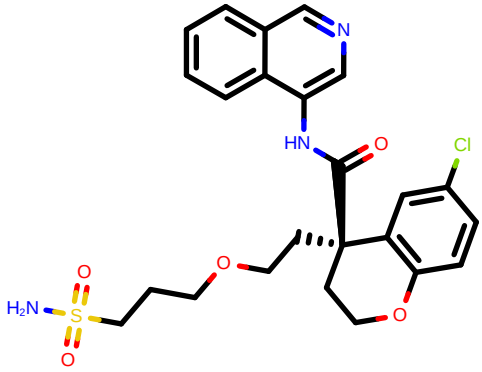
CID:	EN300-07936_1_1
SMILES:	CCN(CC(=O)NC(C)C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2628
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.36

EN300-217107_2_4



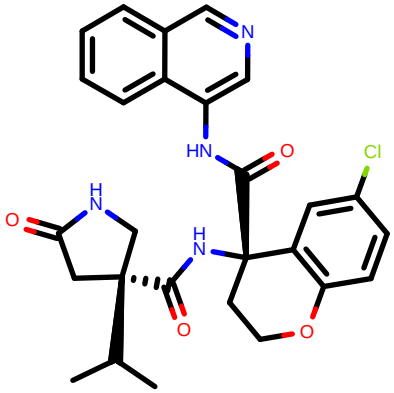
CID:	EN300-217107_2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC[C@H]5C(=O)N
RUN:	RUN2641
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.28

EN300-79588_3_1



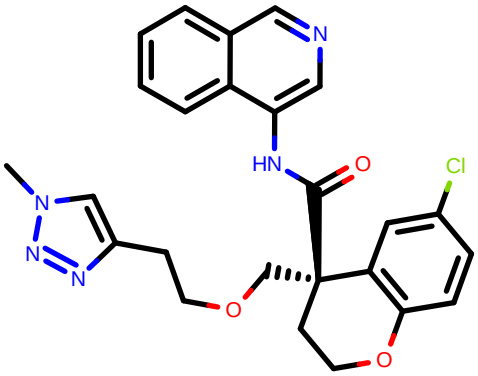
CID:	EN300-79588_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCCS(=O)(=O)N
RUN:	RUN2251
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.35

EN300-211203_1_2



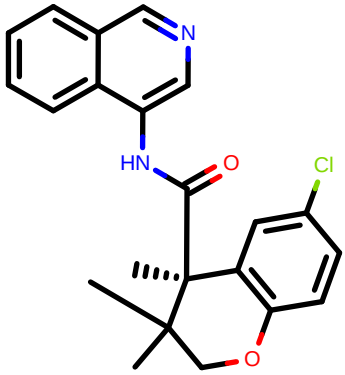
CID:	EN300-211203_1_2
SMILES:	CC(C)[C@]1(CC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4781
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.41

EN300-1600786_2_1



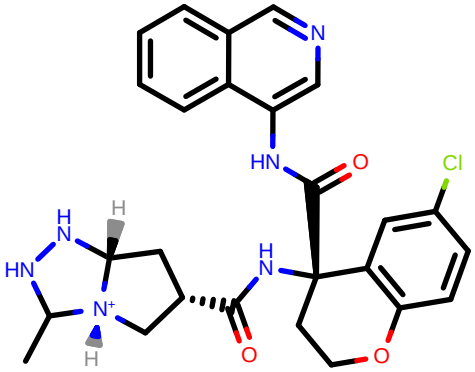
CID:	EN300-1600786_2_1
SMILES:	Cn1cc(nn1)CCOC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1781
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.32

DAR-DIA-0d514e7d-30_1



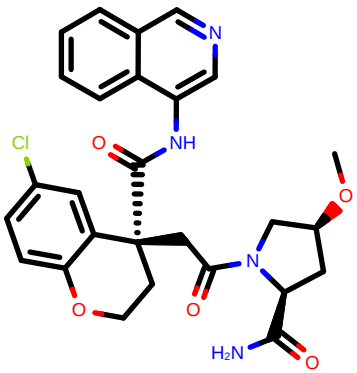
CID:	DAR-DIA-0d514e7d-30_1
SMILES:	C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN112
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.15

EN300-6729747_1_2



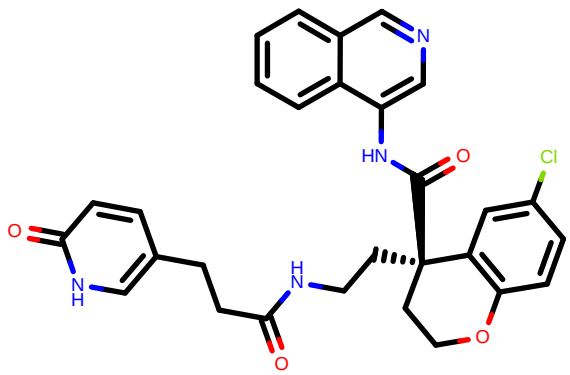
CID:	EN300-6729747_1_2
SMILES:	Cc1nnc2n1C[C@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7854
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.29

EN300-247497_1_1



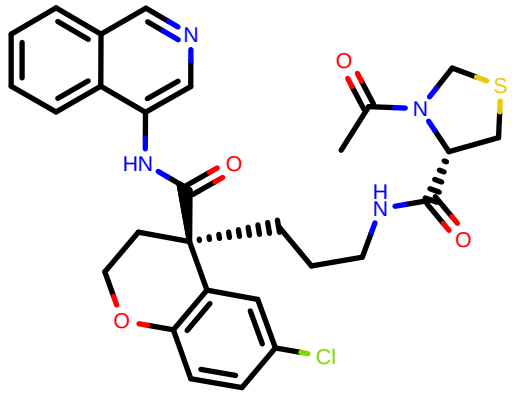
CID:	EN300-247497_1_1
SMILES:	CO[C@H]1C[C@H](N(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN9716
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.29

EN300-187385_3_1



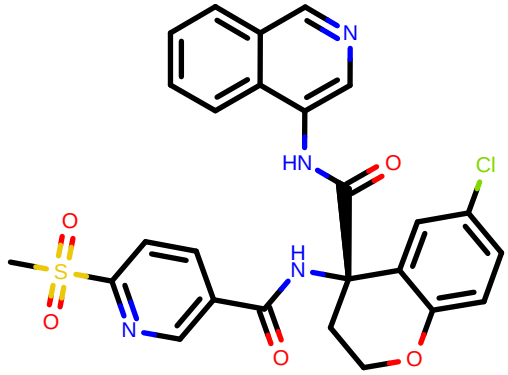
CID:	EN300-187385_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5ccc(=O)[nH]c5
RUN:	RUN11082
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.41

EN300-761220_4_1



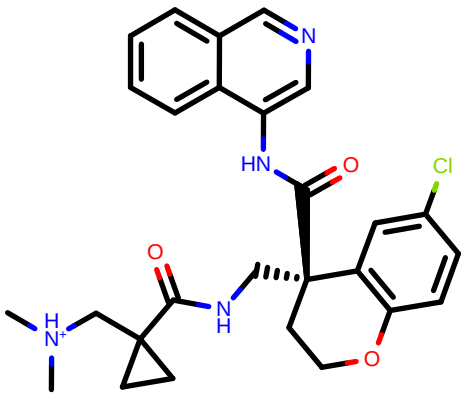
CID:	EN300-761220_4_1
SMILES:	CC(=O)N1CSC[C@@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10054
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.37

EN300-206769_1_1



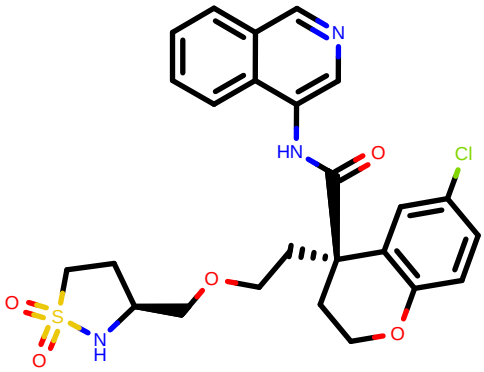
CID:	EN300-206769_1_1
SMILES:	CS(=O)(=O)c1ccc(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9083
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.28

EN300-205680_2_1



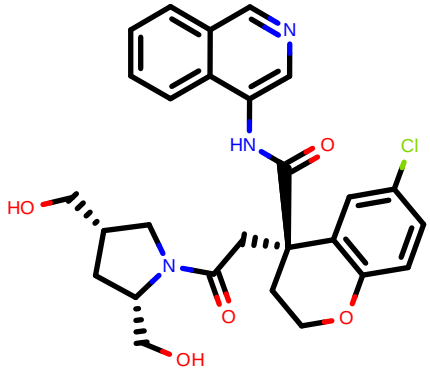
CID:	EN300-205680_2_1
SMILES:	CN(C)CC1(CC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5281
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.42

EN300-1699871_3_1



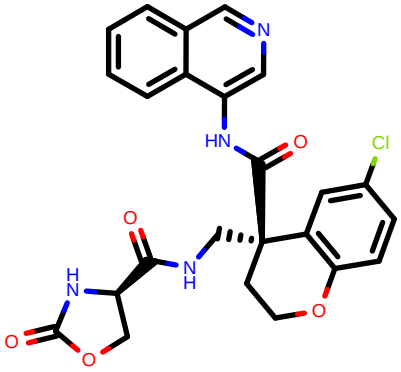
CID:	EN300-1699871_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)N5
RUN:	RUN1140
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.27

EN300-1212400_1_4



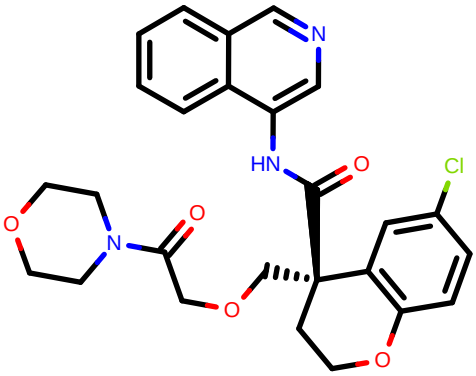
CID:	EN300-1212400_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C[C@H]5CO)CO
RUN:	RUN11298
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.34

EN300-305996_2_1



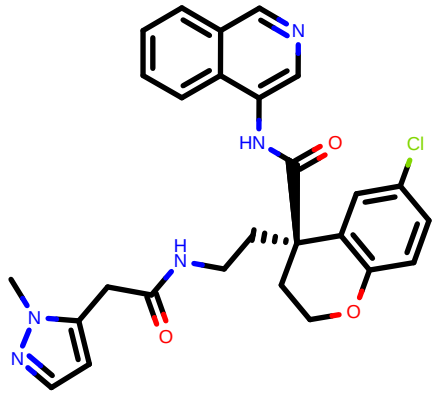
CID:	EN300-305996_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COC(=O)N5
RUN:	RUN4530
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.27

EN300-1241327_2_1



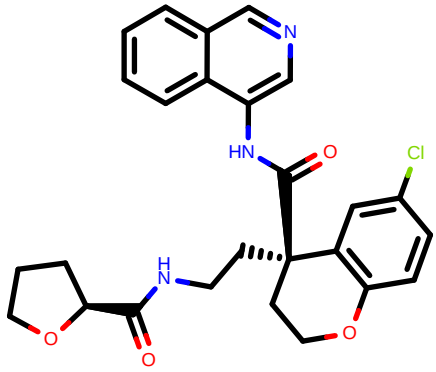
CID:	EN300-1241327_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCOCC5
RUN:	RUN403
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.24

EN300-114805_3_1



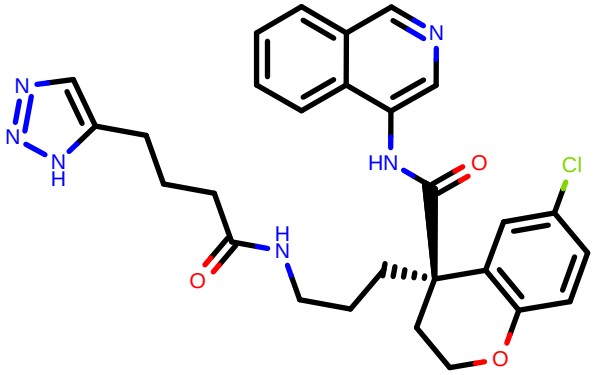
CID:	EN300-114805_3_1
SMILES:	Cn1c(ccn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2964
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.36

EN300-21009_3_1



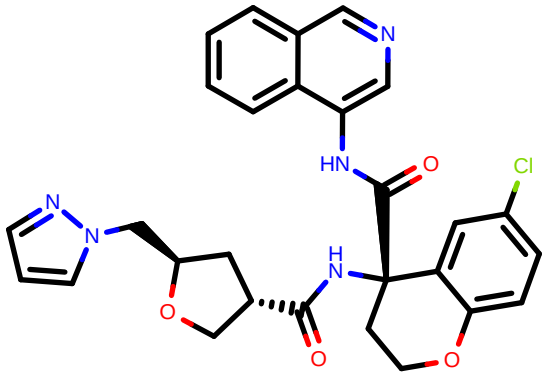
CID:	EN300-21009_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCO5
RUN:	RUN11202
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.26

EN300-156995_4_1



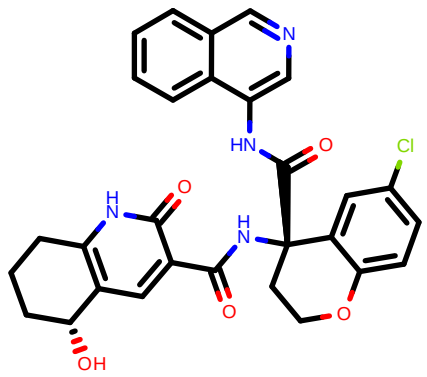
CID:	EN300-156995_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCCc5c[nH]nn5
RUN:	RUN11203
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.33

EN300-6494859_1_2



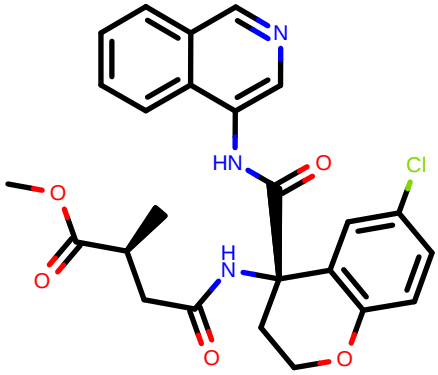
CID:	EN300-6494859_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@@H](OC5)Cn6cccn6
RUN:	RUN7598
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.38

EN300-238234_1_2



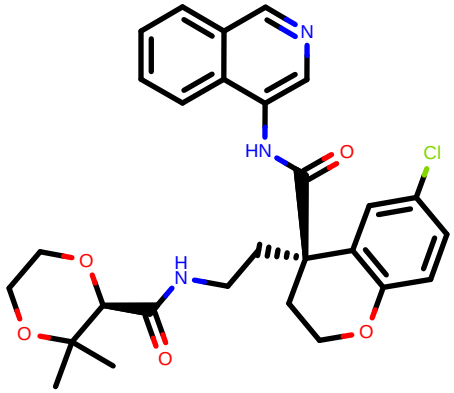
CID:	EN300-238234_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c[nH]c5=O)CCC[C@H]6O
RUN:	RUN9152
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.33

EN300-108413_1_1



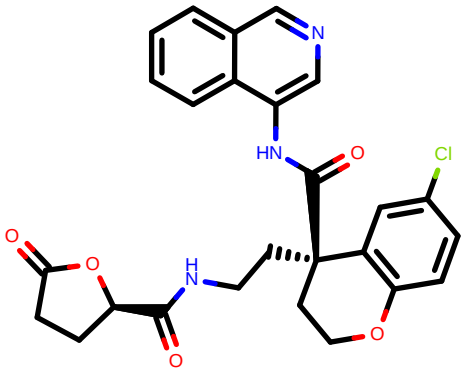
CID:	EN300-108413_1_1
SMILES:	C[C@@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN1517
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.29

EN300-1601684_3_1



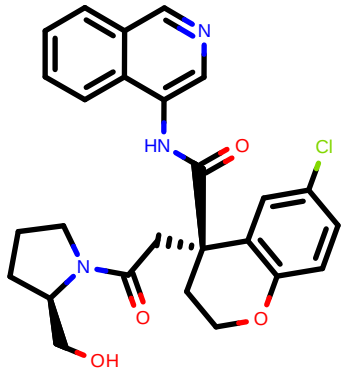
CID:	EN300-1601684_3_1
SMILES:	CC1([C@@H](OCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN5454
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.29

EN300-332606_3_1



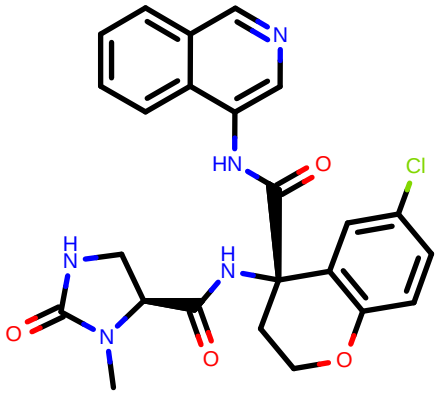
CID:	EN300-332606_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCC(=O)O5
RUN:	RUN10468
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.30

EN300-55109_1_1



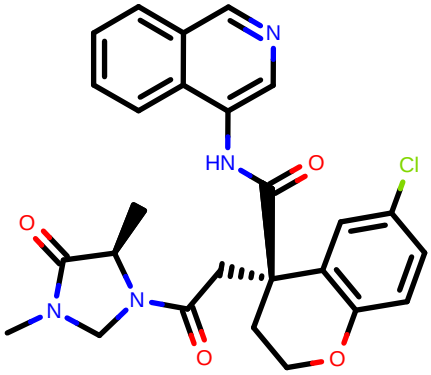
CID:	EN300-55109_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CO
RUN:	RUN10370
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.24

EN300-307008_1_1



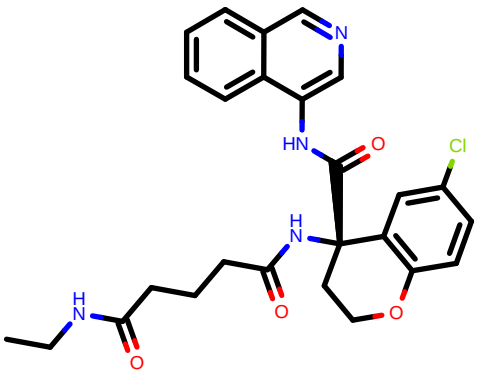
CID:	EN300-307008_1_1
SMILES:	CN1[C@@H](CNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8010
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.21

EN300-261410_1_1



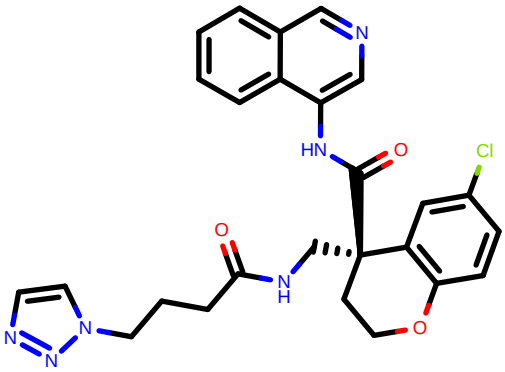
CID:	EN300-261410_1_1
SMILES:	C[C@@H]1C(=O)N(CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN10057
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.25

EN300-68635_1_1



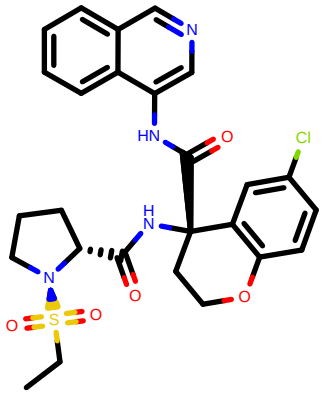
CID:	EN300-68635_1_1
SMILES:	CCNC(=O)CCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN649
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.31

EN300-124301_2_1



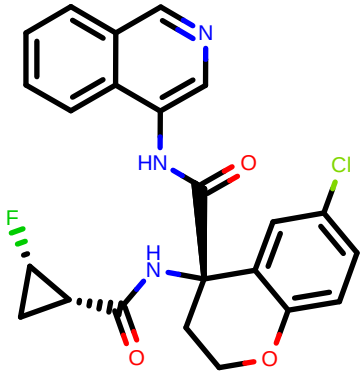
CID:	EN300-124301_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCCn5ccnn5
RUN:	RUN754
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.30

EN300-16091_1_1



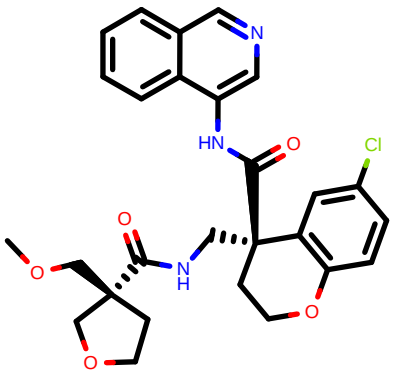
CID:	EN300-16091_1_1
SMILES:	CCS(=O)(=O)N1CCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5892
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.42

EN300-1654606_1_1



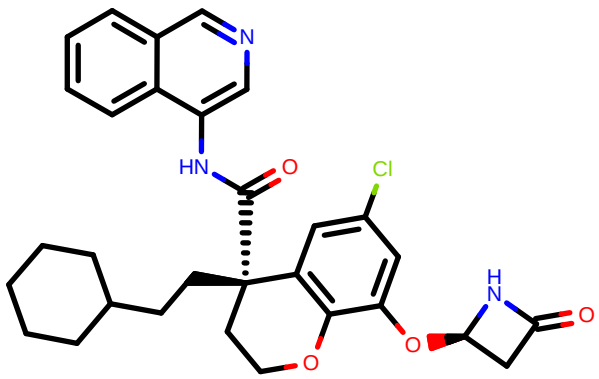
CID:	EN300-1654606_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H]5F
RUN:	RUN3374
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.21

EN300-248883_2_2



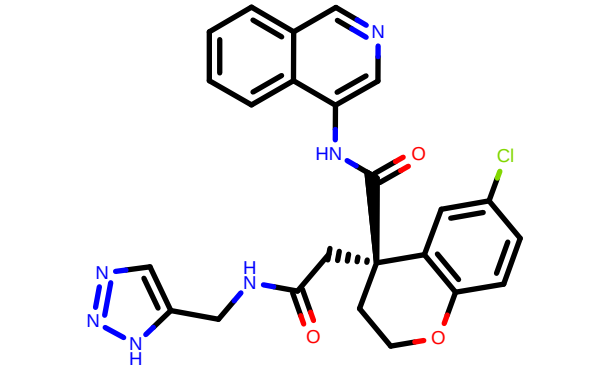
CID:	EN300-248883_2_2
SMILES:	COC[C@]1(CCOC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3495
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.36

VLA-UCB-05e51b3f-12_1



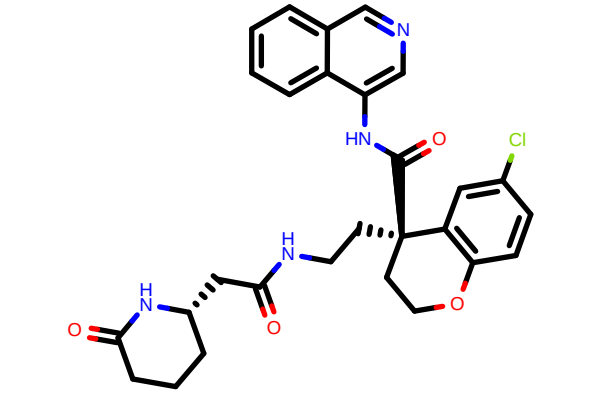
CID:	VLA-UCB-05e51b3f-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN241
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.33

EN300-98429_1_1



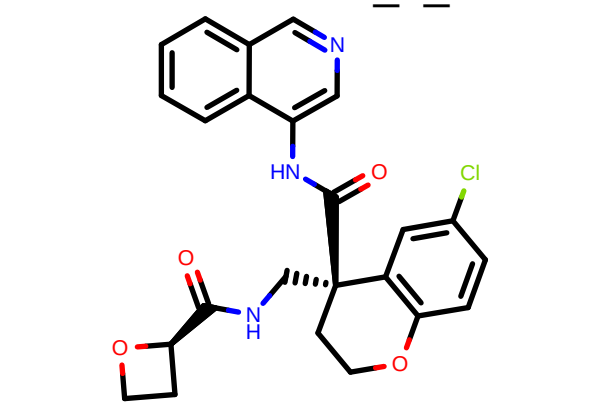
CID:	EN300-98429_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)NCc5c[nH]nn5
RUN:	RUN5958
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.26

EN300-210084_3_1



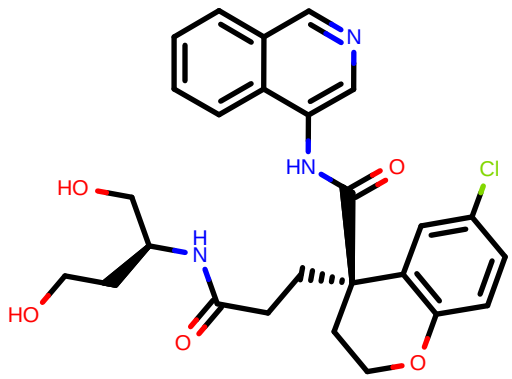
CID:	EN300-210084_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)C[C@@H]5CCCC(=O)N5
RUN:	RUN7808
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.36

EN300-85760_2_2



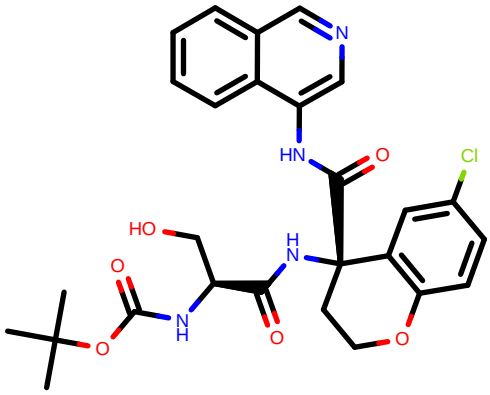
CID:	EN300-85760_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@H]5CCO5
RUN:	RUN4406
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.20

EN300-195790_2_1



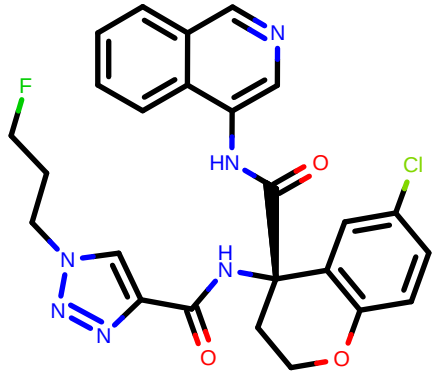
CID:	EN300-195790_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H](CCO)CO
RUN:	RUN10857
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.27

EN300-72109_1_1



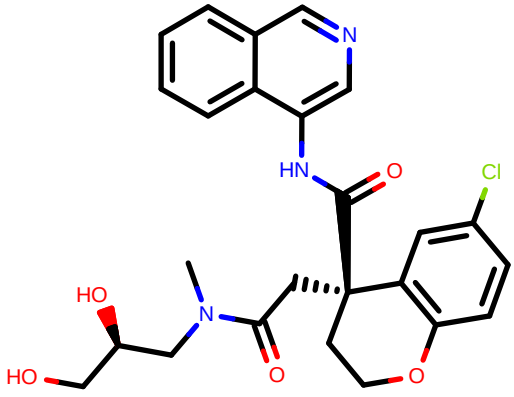
CID:	EN300-72109_1_1
SMILES:	CC(C)(C)OC(=O)N[C@@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7354
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.31

EN300-1704723_1_1



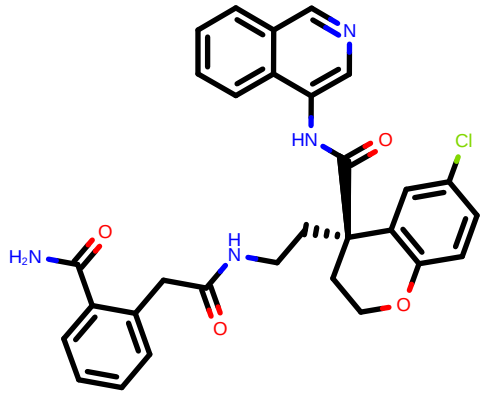
CID:	EN300-1704723_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)CCCF
RUN:	RUN6567
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.27

EN300-124376_1_1



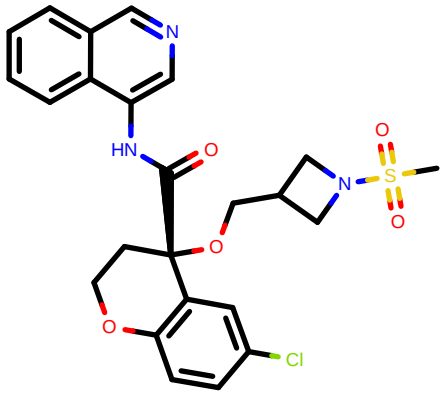
CID:	EN300-124376_1_1
SMILES:	CN(C[C@@H](CO)O)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10031
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.47

EN300-121144_3_1



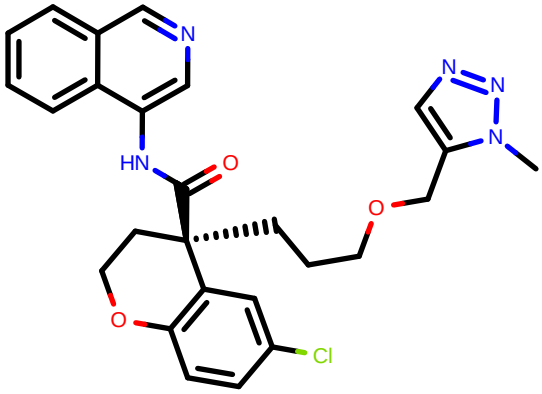
CID:	EN300-121144_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccccc5C(=O)N
RUN:	RUN6689
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.43

EN300-302290_1_1



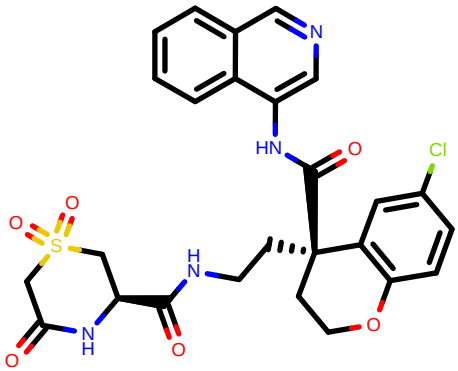
CID:	EN300-302290_1_1
SMILES:	CS(=O)(=O)N1CC(C1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN493
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.31

EN300-216673_4_1



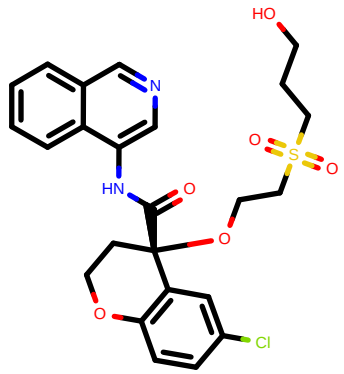
CID:	EN300-216673_4_1
SMILES:	Cn1c(cnn1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN300
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.34

EN300-754584_3_1



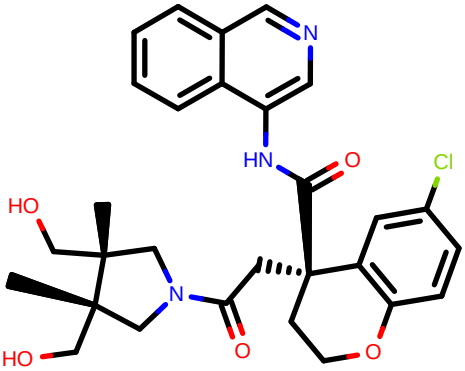
CID:	EN300-754584_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CS(=O)(=O)CC(=O)N5
RUN:	RUN9434
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.30

EN300-7456499_1_1



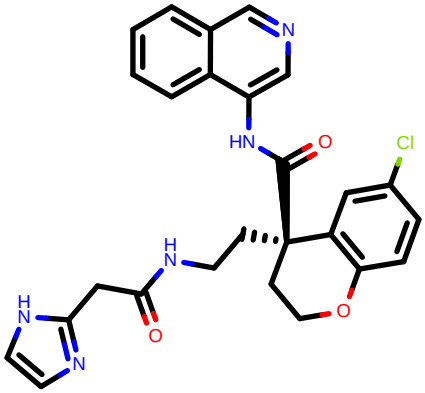
CID:	EN300-7456499_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCS(=O)(=O)CCCO
RUN:	RUN501
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.41

EN300-318058_1_1



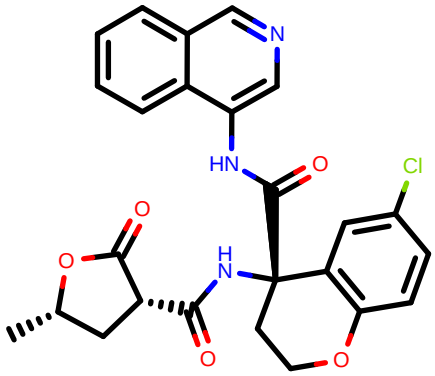
CID:	EN300-318058_1_1
SMILES:	C[C@@]1(CN(C[C@@]1(C)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN2582
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.32

EN300-220527_3_1



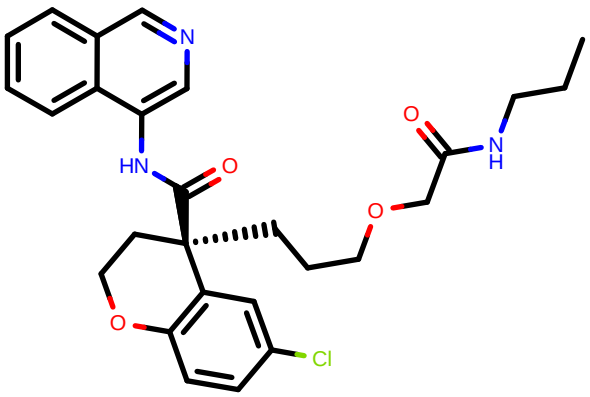
CID:	EN300-220527_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5[nH]ccn5
RUN:	RUN5247
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.31

EN300-7444533_1_4



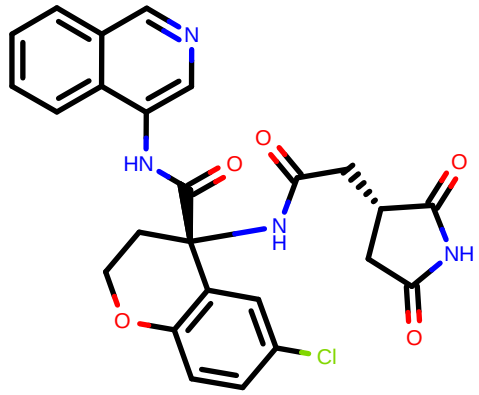
CID:	EN300-7444533_1_4
SMILES:	C[C@H]1C[C@H](C(=O)O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6523
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.25

EN300-17184_4_1



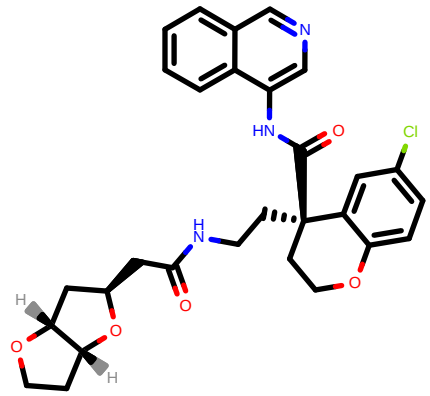
CID:	EN300-17184_4_1
SMILES:	C=CCNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1567
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.29

EN300-227055_1_2



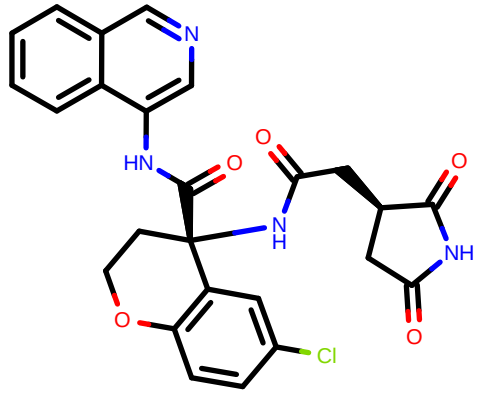
CID:	EN300-227055_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CC(=O)NC5=O
RUN:	RUN6224
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.29

EN300-7355519_3_5



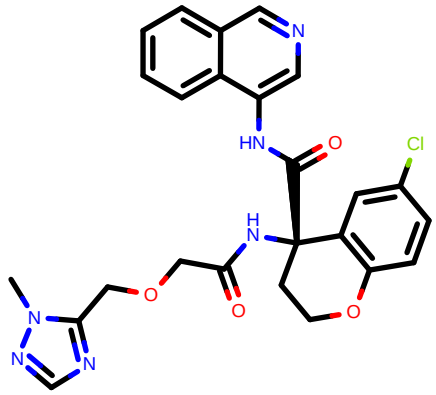
CID:	EN300-7355519_3_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5C[C@@H]6[C@H](OS)CCO6
RUN:	RUN4771
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.44

EN300-227055_1_1



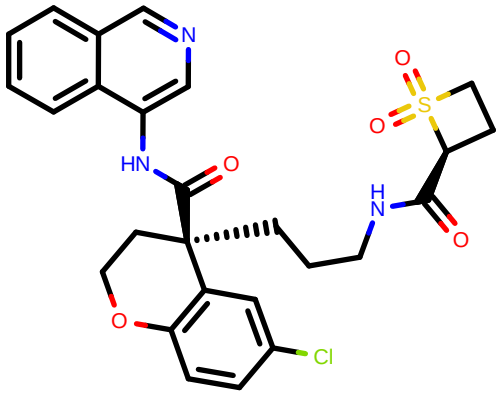
CID:	EN300-227055_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(=O)NC5=O
RUN:	RUN2942
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.27

EN300-213358_1_1



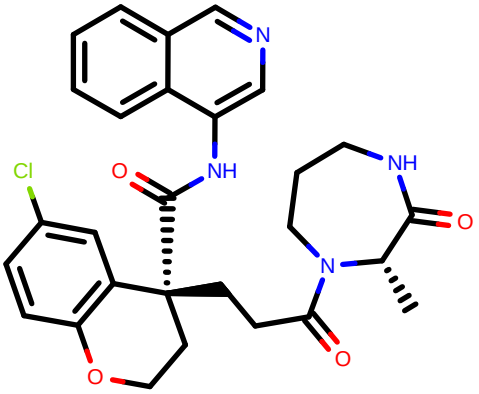
CID:	EN300-213358_1_1
SMILES:	Cn1c(ncn1)COCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN569
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.34

EN300-1387104_4_1



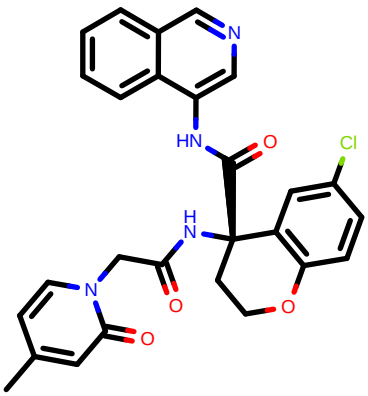
CID:	EN300-1387104_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCS5(=O)=O
RUN:	RUN9022
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.38

EN300-372748_2_1



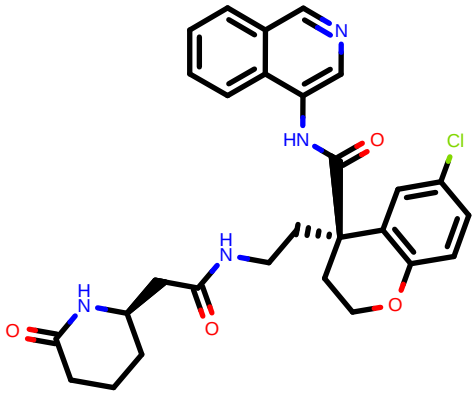
CID:	EN300-372748_2_1
SMILES:	C[C@H]1C(=O)NCCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN741
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.30

EN300-184446_1_1



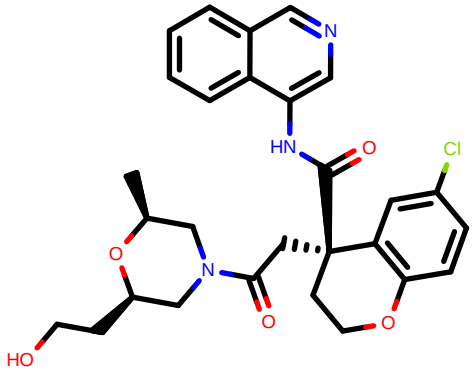
CID:	EN300-184446_1_1
SMILES:	Cc1ccn(c(=O)c1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3518
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.31

EN300-210084_3_2



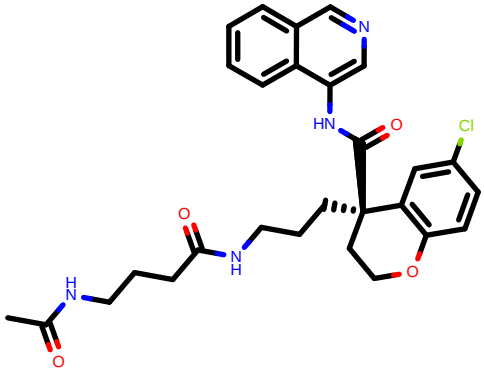
CID:	EN300-210084_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCC(=O)N5
RUN:	RUN8304
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.31

EN300-212814_1_4



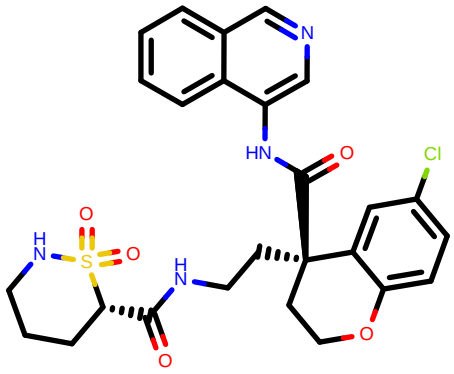
CID:	EN300-212814_1_4
SMILES:	C[C@H]1CN(C[C@H](O1)CCO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7912
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.28

EN300-18564_4_1



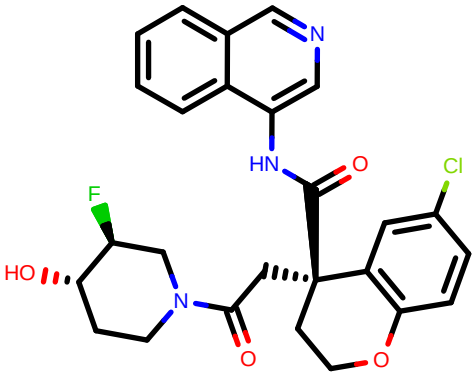
CID:	EN300-18564_4_1
SMILES:	CC(=O)NCCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN11109
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.30

EN300-1587757_3_1



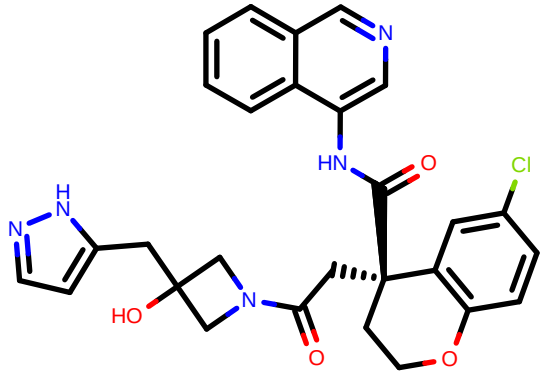
CID:	EN300-1587757_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCNS5(=O)=O
RUN:	RUN6014
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.37

EN300-741926_1_3



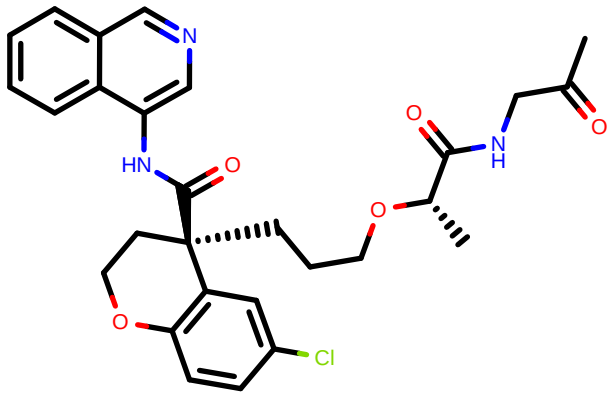
CID:	EN300-741926_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]([C@H](C5)F)O
RUN:	RUN2992
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.33

EN300-6489696_1_1



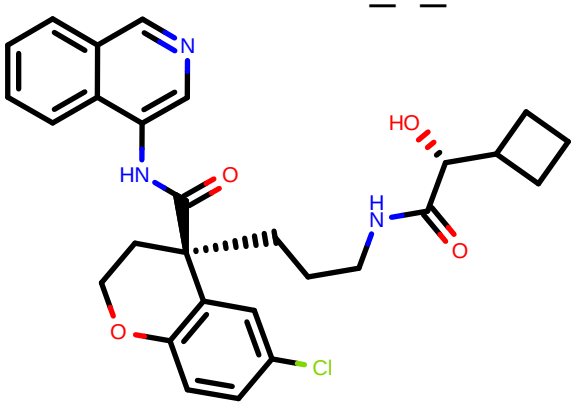
CID:	EN300-6489696_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(Cc6ccn[nH]6)O
RUN:	RUN9108
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.42

EN300-131093_4_1



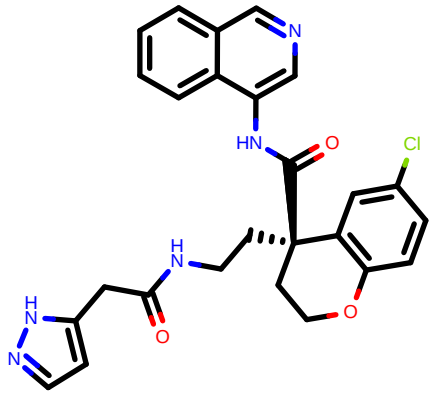
CID:	EN300-131093_4_1
SMILES:	C[C@@H](C(=O)NCC(=O)C)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2078
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.39

EN300-249764_4_1



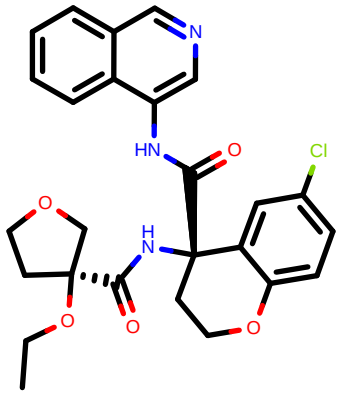
CID:	EN300-249764_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H](C5CCC5)O
RUN:	RUN10231
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.33

EN300-71405_3_1



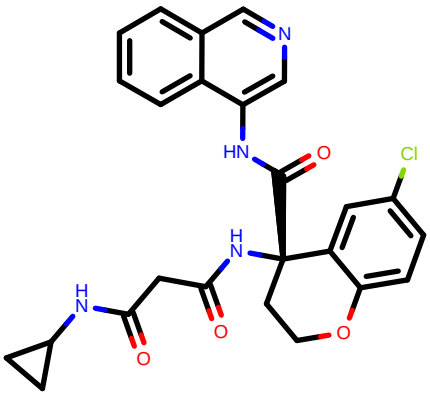
CID:	EN300-71405_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5ccn[nH]5
RUN:	RUN4623
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.28

EN300-259694_1_2



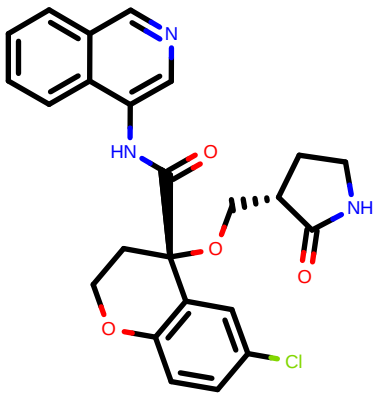
CID:	EN300-259694_1_2
SMILES:	CCO[C@]1(CCOC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4785
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.35

EN300-128464_1_1



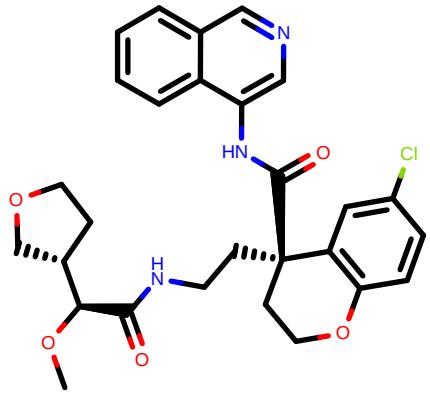
CID:	EN300-128464_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(=O)NC5CC5
RUN:	RUN3865
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.31

EN300-246248_1_1



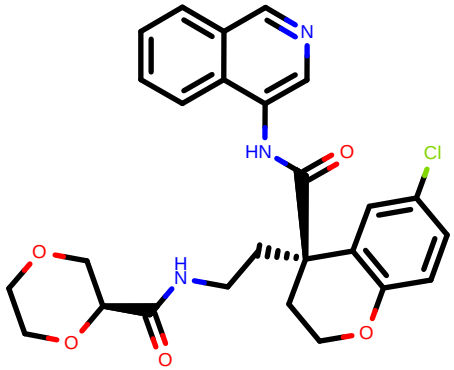
CID:	EN300-246248_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCNC5=O
RUN:	RUN2574
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.28

EN300-298552_3_3



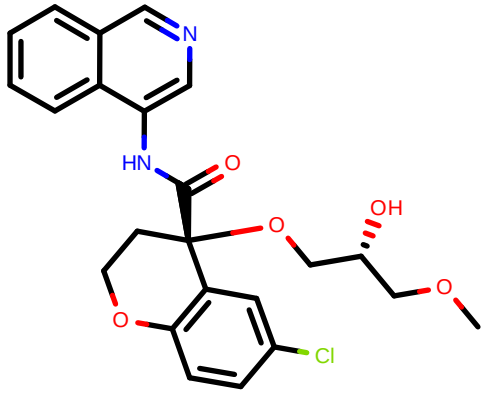
CID:	EN300-298552_3_3
SMILES:	CO[C@@H]([C@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4591
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.31

EN300-36158_3_1



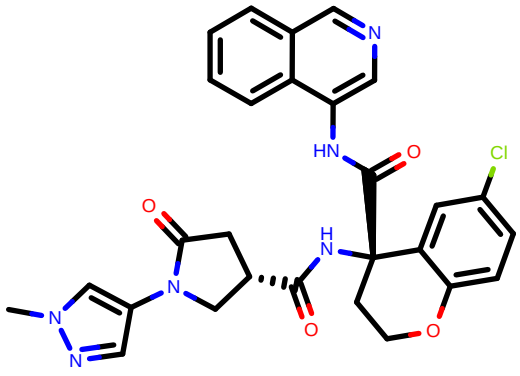
CID:	EN300-36158_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COCCO5
RUN:	RUN3532
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.33

EN300-1915260_1_2



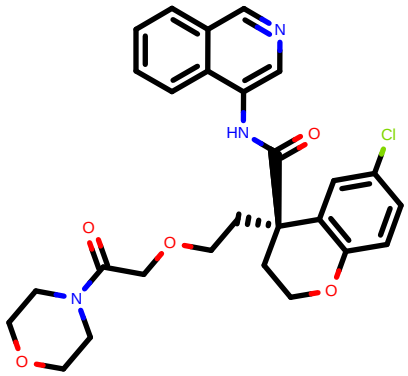
CID:	EN300-1915260_1_2
SMILES:	COC[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1480
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.34

EN300-92633_1_2



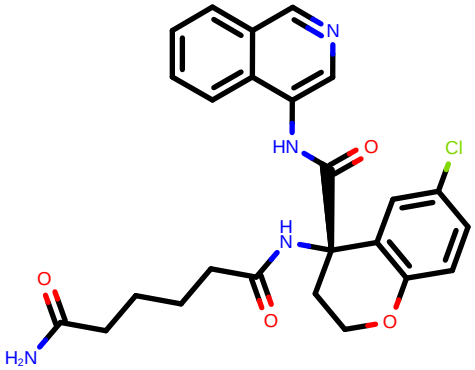
CID:	EN300-92633_1_2
SMILES:	Cn1cc(cn1)N2C[C@H](CC2=O)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8598
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.27

EN300-1241327_3_1



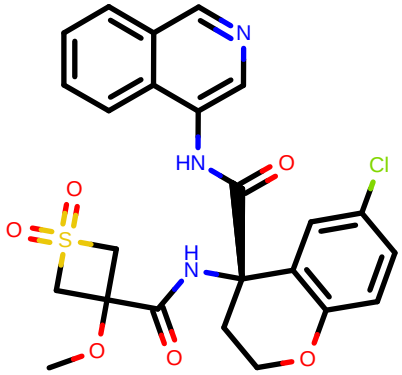
CID:	EN300-1241327_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N5CCOCC5
RUN:	RUN821
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.35

EN300-142412_1_1



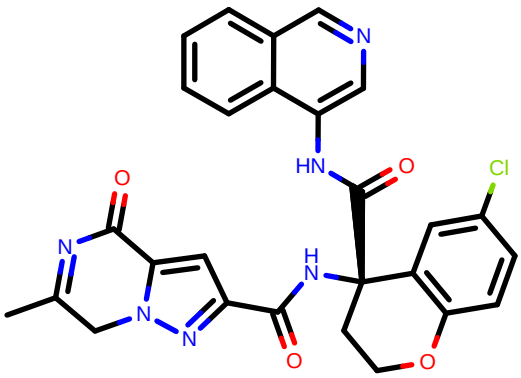
CID:	EN300-142412_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCCC(=O)N
RUN:	RUN2204
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.31

EN300-704025_1_1



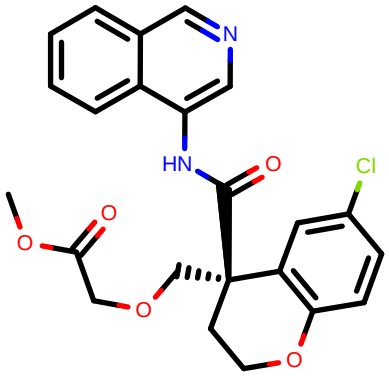
CID:	EN300-704025_1_1
SMILES:	COC1(CS(=O)(=O)C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5029
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.31

EN300-378276_1_1



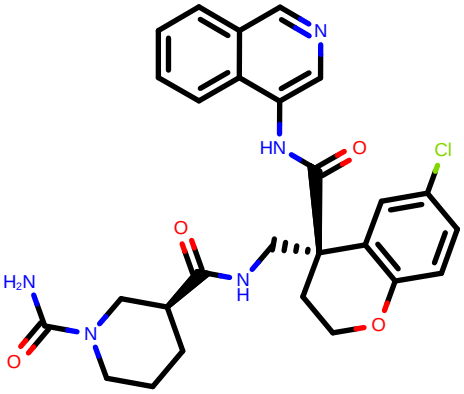
CID:	EN300-378276_1_1
SMILES:	Cc1cn2c(cc(n2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)c(=O)[nH]1
RUN:	RUN9026
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.32

EN300-19700_2_1



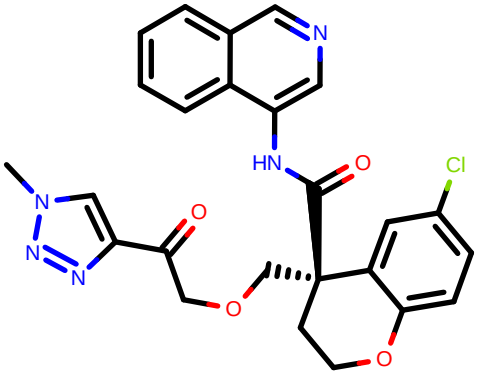
CID:	EN300-19700_2_1
SMILES:	COC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1406
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.20

EN300-14767_2_2



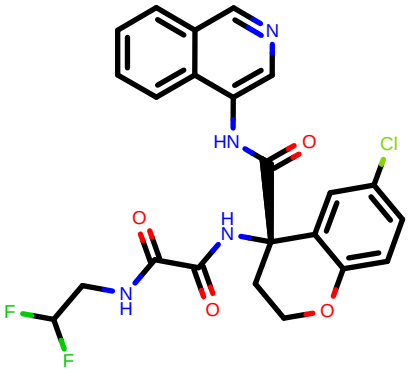
CID:	EN300-14767_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCN(C5)C(=O)N
RUN:	RUN1385
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.39

EN300-263153_2_1



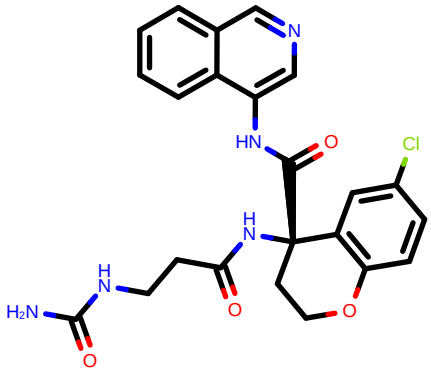
CID:	EN300-263153_2_1
SMILES:	Cn1cc(nn1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2267
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.33

EN300-128277_1_1



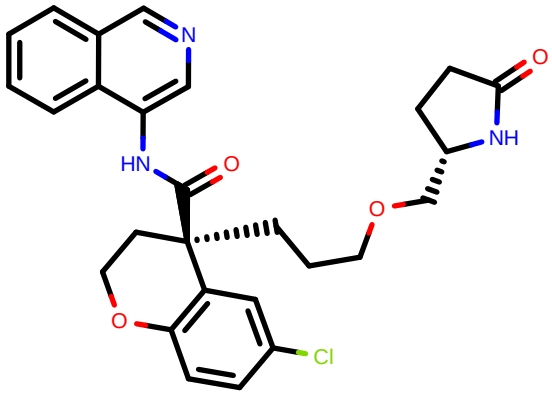
CID:	EN300-128277_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(=O)NCC(F)F
RUN:	RUN1157
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.27

EN300-10729_1_1



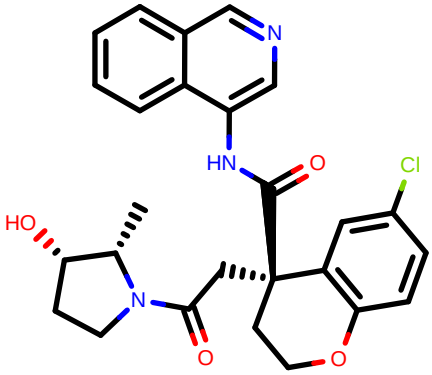
CID:	EN300-10729_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)N
RUN:	RUN1565
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.26

EN300-195756_4_1



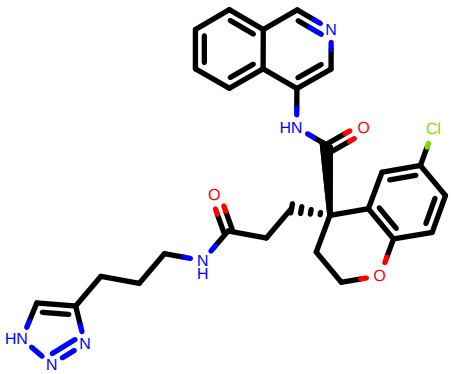
CID:	EN300-195756_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5CCC(=O)N5
RUN:	RUN1455
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.36

EN300-2008120_1_1



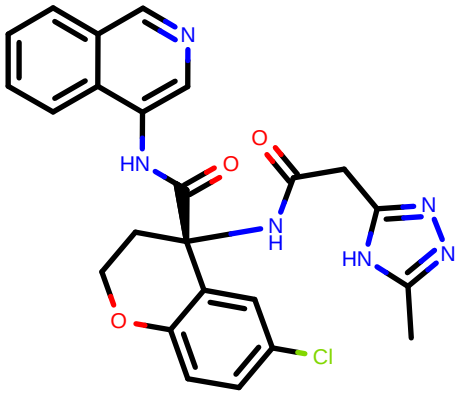
CID:	EN300-2008120_1_1
SMILES:	C[C@H]1[C@H](CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN9963
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.33

EN300-6493892_2_1



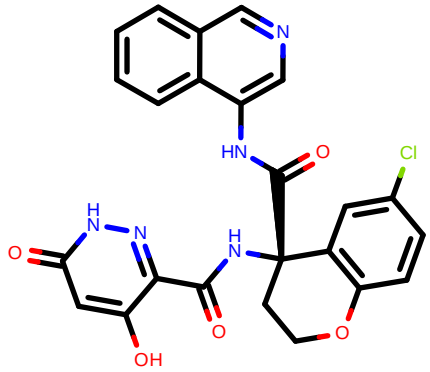
CID:	EN300-6493892_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCCc5c[nH]nn5
RUN:	RUN10689
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.29

EN300-119126_1_1



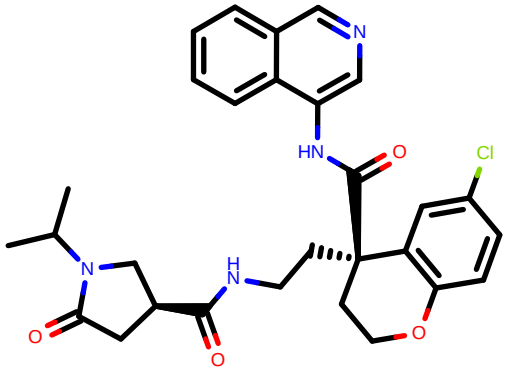
CID:	EN300-119126_1_1
SMILES:	Cc1[nH]c(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7070
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.21

EN300-111159_1_1



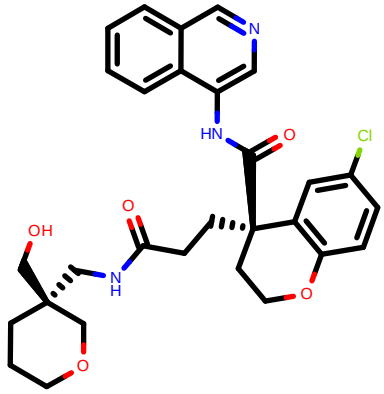
CID:	EN300-111159_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(cc(=O)[nH]n5)O
RUN:	RUN8346
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.23

EN300-33398_3_2



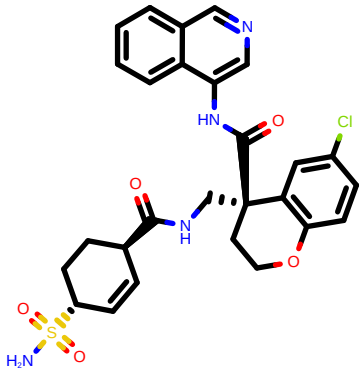
CID:	EN300-33398_3_2
SMILES:	CC(C)N1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9181
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.36

EN300-7500408_2_2



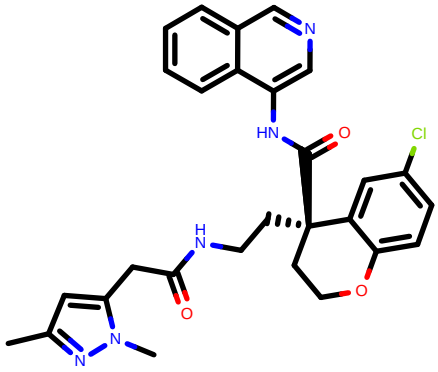
CID:	EN300-7500408_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@]5(CCCOC5)CO
RUN:	RUN11243
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.26

EN300-83864_2_1



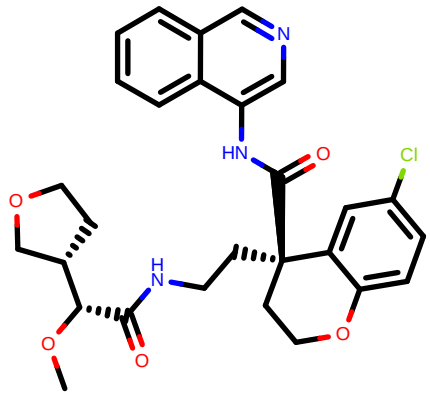
CID:	EN300-83864_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5CCC(CC5)S(=O)(=O)N
RUN:	RUN7383
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.35

EN300-6499639_3_1



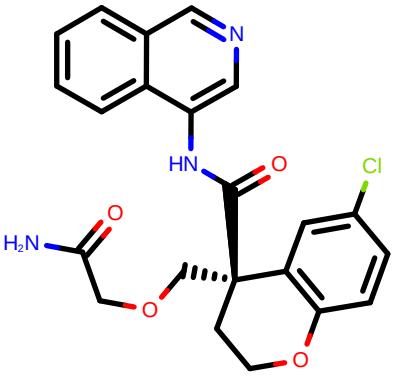
CID:	EN300-6499639_3_1
SMILES:	Cc1cc(n(n1)C)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3775
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.33

EN300-298552_3_4



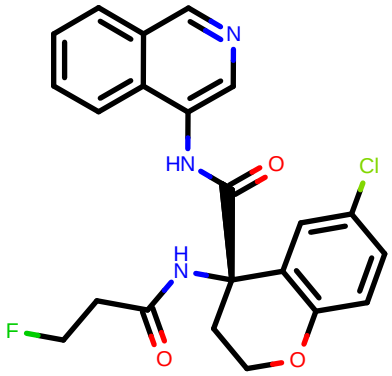
CID:	EN300-298552_3_4
SMILES:	CO[C@H]([C@H]1CCOC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3664
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.32

EN300-18249_2_1



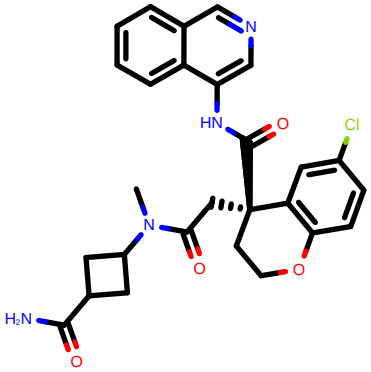
CID:	EN300-18249_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N
RUN:	RUN744
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.19

EN300-97758_1_1



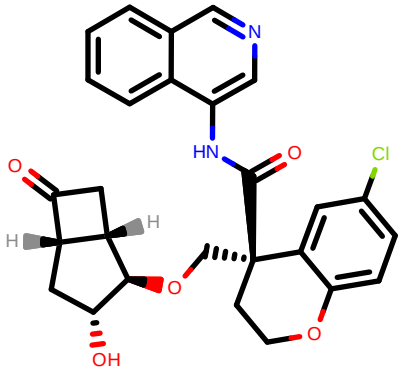
CID:	EN300-97758_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCF
RUN:	RUN1429
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.21

EN300-321459_1_1



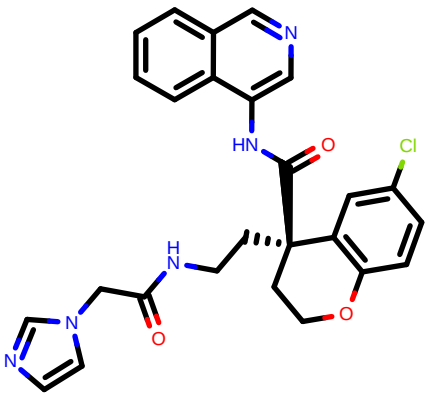
CID:	EN300-321459_1_1
SMILES:	CN(C(=O)C[C@@]1(c2c(ccc(c2)Cl)OCC1)C(=O)Nc3c4c(cnc3)cccc4)[C@H]5C[C@H](C5)C(=O)N
RUN:	RUN811
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.32

EN300-6481287_2_1



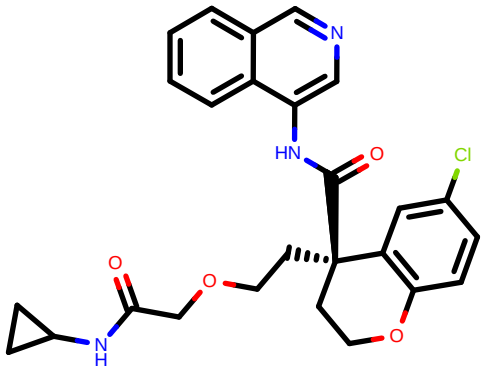
CID:	EN300-6481287_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5[C@@H](C[C@H]6[C@@H]5CC6=O)O
RUN:	RUN2442
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.24

EN300-38979_3_1



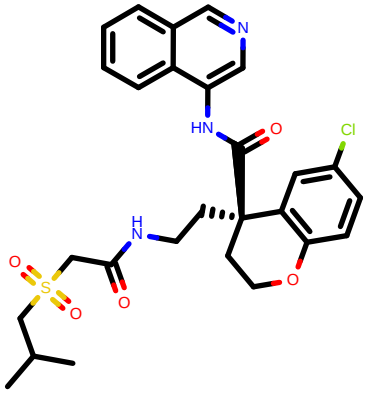
CID:	EN300-38979_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccnc5
RUN:	RUN1386
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.29

EN300-1253178_3_1



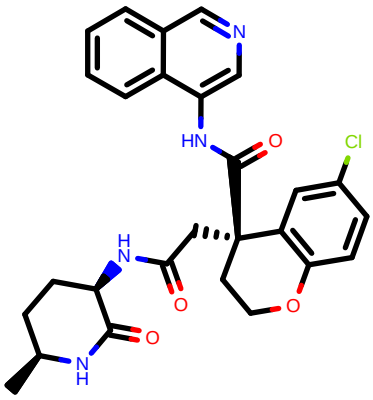
CID:	EN300-1253178_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC5CC5
RUN:	RUN1683
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.26

EN300-42243_3_1



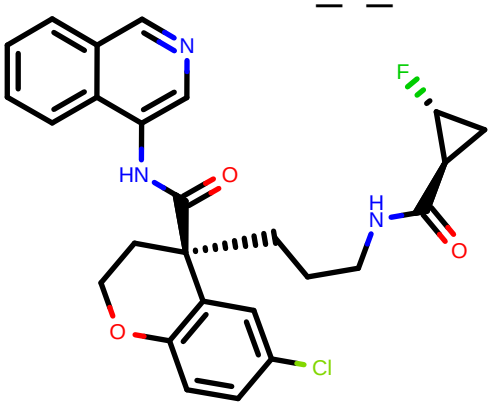
CID:	EN300-42243_3_1
SMILES:	CC(C)CS(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6808
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.45

EN300-201180_1_4



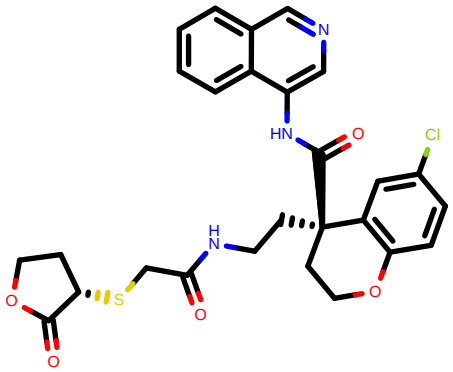
CID:	EN300-201180_1_4
SMILES:	C[C@H]1CC[C@H](C(=O)N1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8308
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.26

EN300-97300_4_3



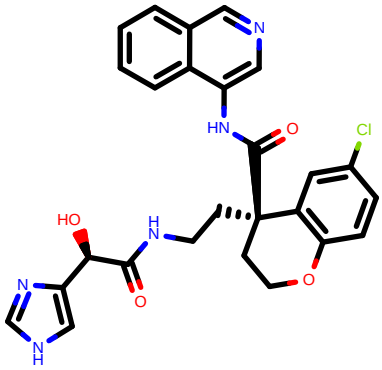
CID:	EN300-97300_4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5C[C@H]5F
RUN:	RUN10843
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.27

EN300-113218_3_2



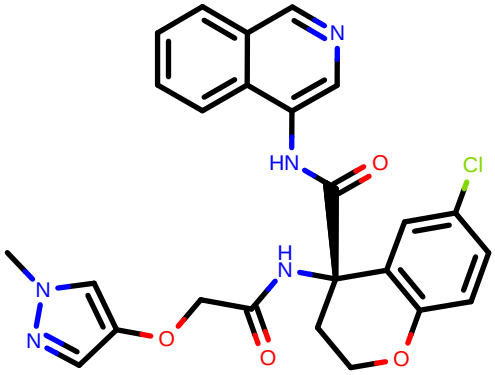
CID:	EN300-113218_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS[C@H]5CCOC5=O
RUN:	RUN8284
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.36

EN300-254121_3_1



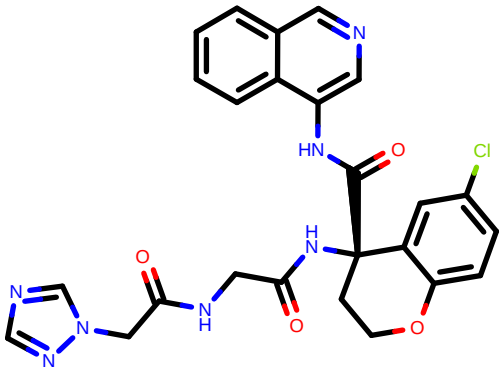
CID:	EN300-254121_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](c5cnc[nH]5)O
RUN:	RUN383
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.40

EN300-201553_1_1



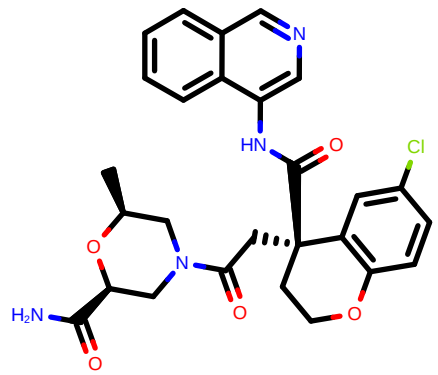
CID:	EN300-201553_1_1
SMILES:	Cn1cc(cn1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN806
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.26

EN300-52383_1_1



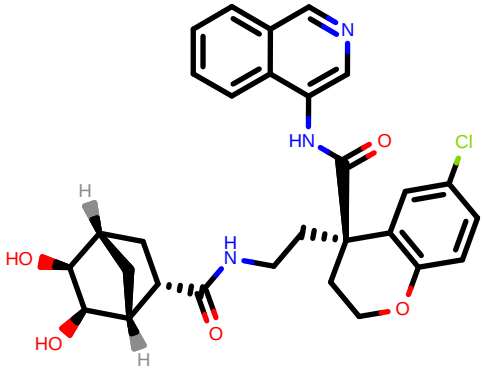
CID:	EN300-52383_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)Cn5cncn5
RUN:	RUN5193
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.34

EN300-295905_1_4



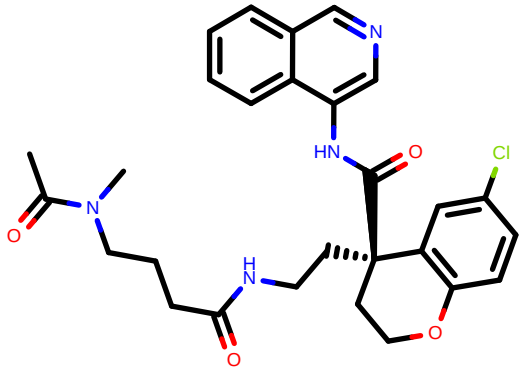
CID:	EN300-295905_1_4
SMILES:	C[C@H]1CN(C[C@H](O1)C(=O)N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN733
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.35

EN300-6744028_3_8



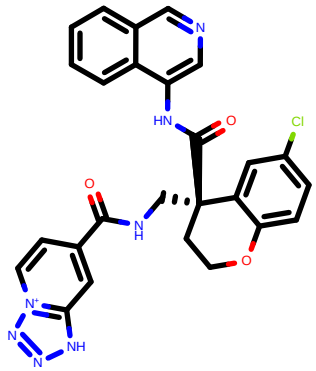
CID:	EN300-6744028_3_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC6CC5[C@H]([C@H]6O)O
RUN:	RUN10284
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.29

EN300-128750_3_1



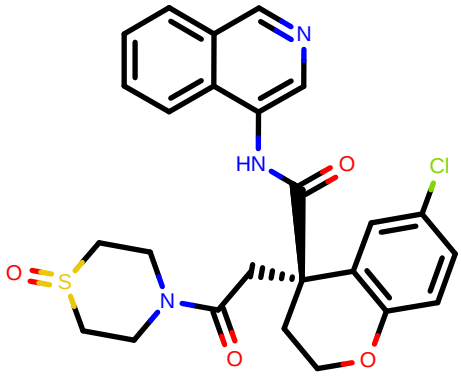
CID:	EN300-128750_3_1
SMILES:	CC(=O)N(C)CCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10202
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.33

EN300-305567_2_1



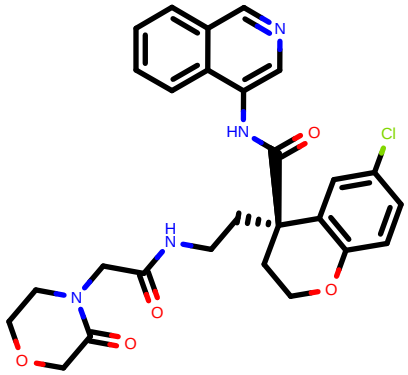
CID:	EN300-305567_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccn6c(c5)nnn6
RUN:	RUN8439
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.33

EN300-69588_1_1



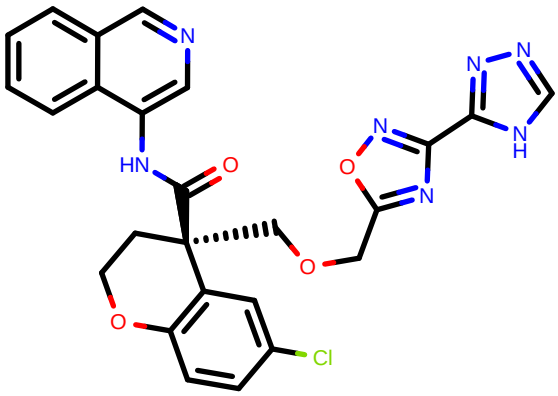
CID:	EN300-69588_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)CC5
RUN:	RUN7412
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.35

EN300-186943_3_1



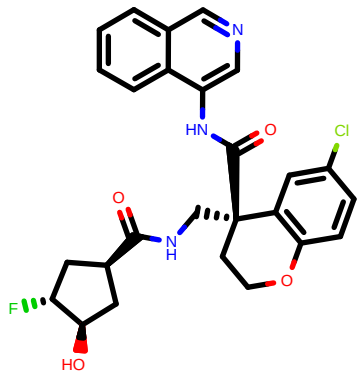
CID:	EN300-186943_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCOCC5=O
RUN:	RUN5774
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.28

EN300-92031_2_1



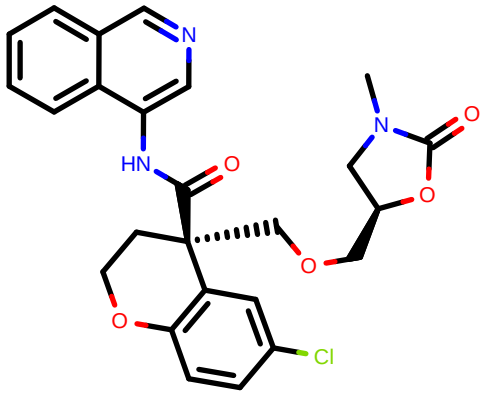
CID:	EN300-92031_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nc(no5)c6[nH]cnn6
RUN:	RUN2663
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.30

EN300-7461217_2_2



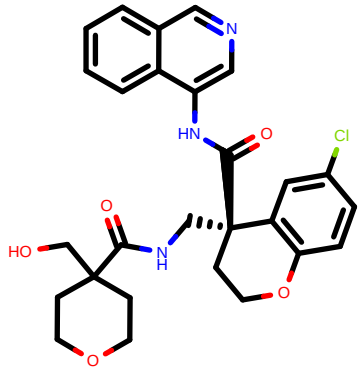
CID:	EN300-7461217_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5C[C@H](C@@H](C5)F)O
RUN:	RUN4490
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.21

EN300-222969_2_1



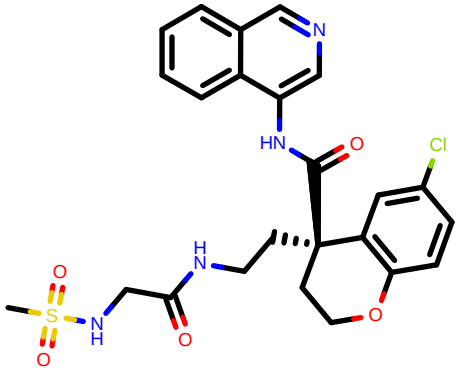
CID:	EN300-222969_2_1
SMILES:	CN1C[C@@H](OC1=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1701
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.33

EN300-244909_2_1



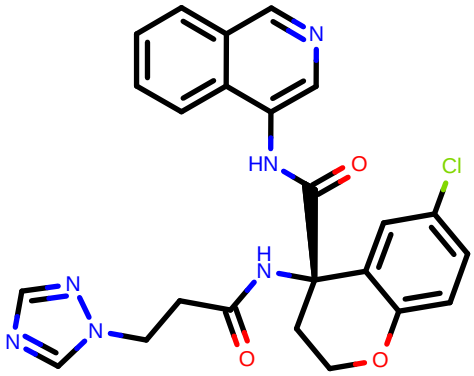
CID:	EN300-244909_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCOCC5)CO
RUN:	RUN2767
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.38

EN300-30419_3_1



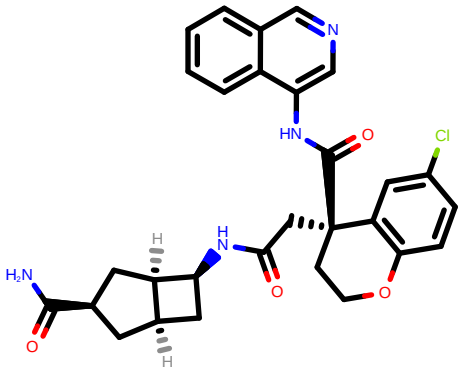
CID:	EN300-30419_3_1
SMILES:	CS(=O)(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7916
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.31

EN300-26147_1_1



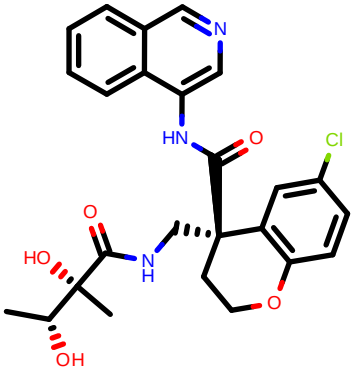
CID:	EN300-26147_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCn5cncn5
RUN:	RUN5652
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.24

EN300-1268016_1_6



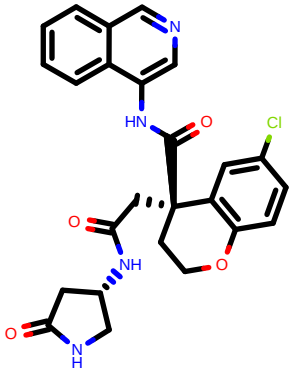
CID:	EN300-1268016_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@@H]6[C@H]5C[C@@H](C6)C(=O)N
RUN:	RUN994
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.38

EN300-202922_2_4



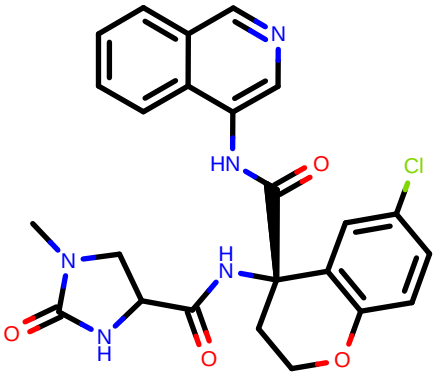
CID:	EN300-202922_2_4
SMILES:	C[C@H]([C@](C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN3778
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.29

EN300-127487_1_2



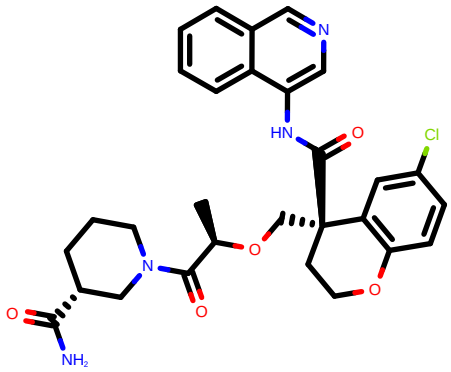
CID:	EN300-127487_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CC(=O)NC5
RUN:	RUN9540
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.26

EN300-226889_1_1



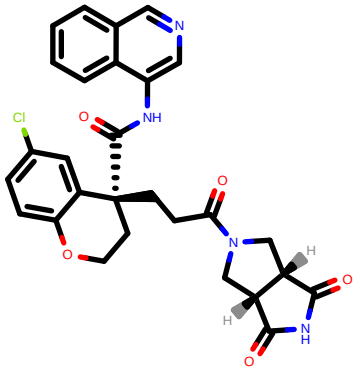
CID:	EN300-226889_1_1
SMILES:	Cn1cc([nH]c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2620
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.24

EN300-28177_2_4



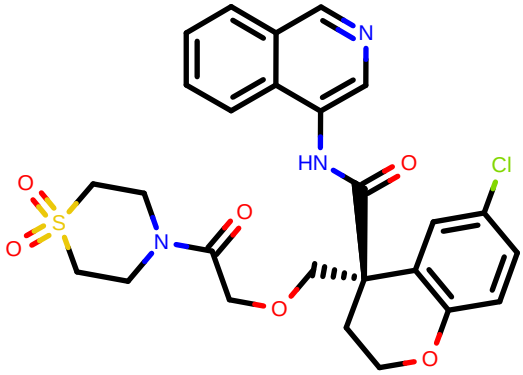
CID:	EN300-28177_2_4
SMILES:	C[C@H](C(=O)N1CCC[C@H](C1)C(=O)N)OC[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1342
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.30

EN300-246333_2_1



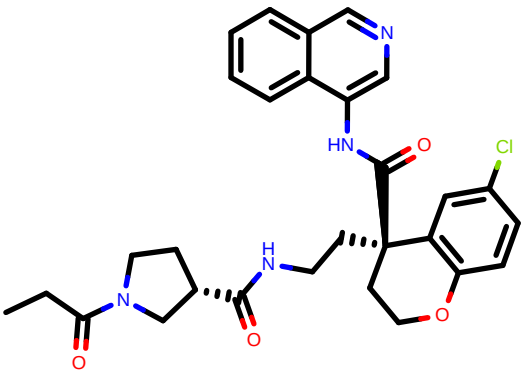
CID:	EN300-246333_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C[C@@H]6[C@H](C5)C(=O)NC6=O
RUN:	RUN5551
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.41

EN300-1265948_2_1



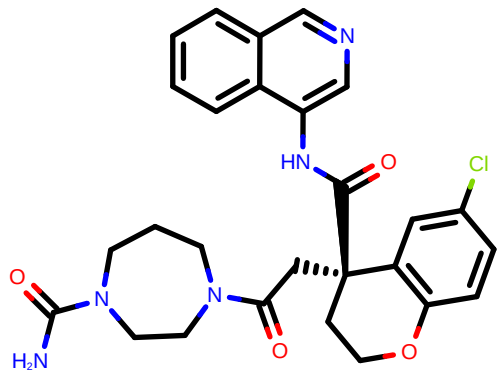
CID:	EN300-1265948_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCS(=O)(=O)CC5
RUN:	RUN2037
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.28

EN300-114133_3_1



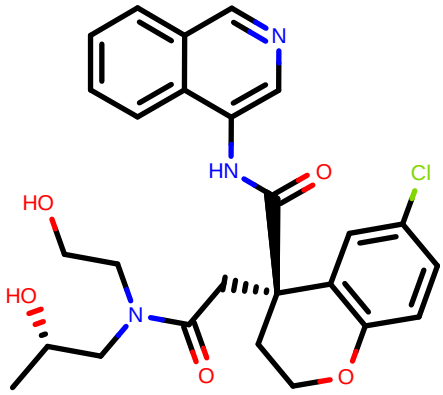
CID:	EN300-114133_3_1
SMILES:	CCC(=O)N1CC[C@@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1681
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.43

EN300-65063_1_1



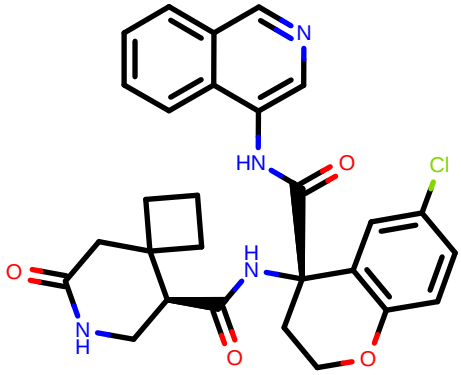
CID:	EN300-65063_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCN(CC5)C(=O)N
RUN:	RUN8520
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.27

EN300-214038_1_1



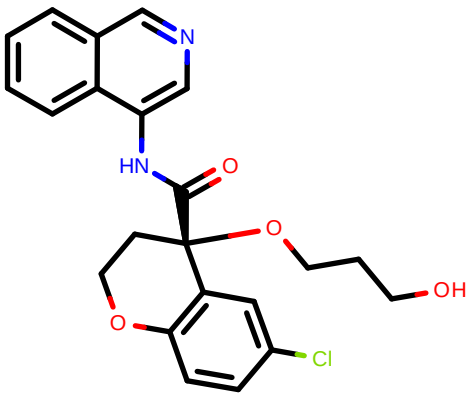
CID:	EN300-214038_1_1
SMILES:	C[C@@H](CN(CCO)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN7676
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.43

EN300-1704404_1_2



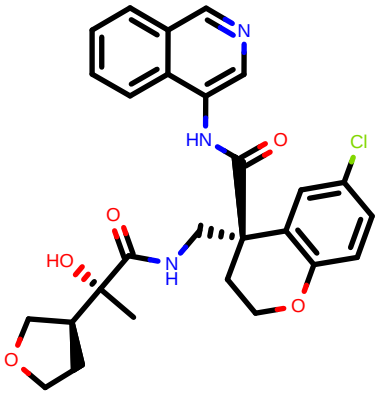
CID:	EN300-1704404_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)CC56CCC6
RUN:	RUN8102
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.35

EN300-221518_1_1



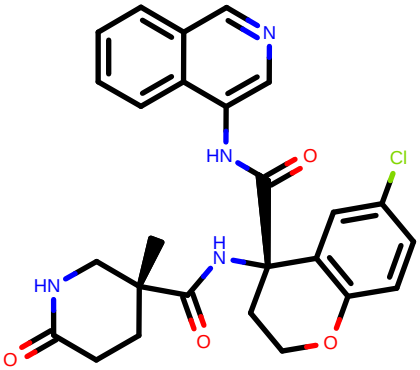
CID:	EN300-221518_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO
RUN:	RUN1000
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.19

EN300-217494_2_3



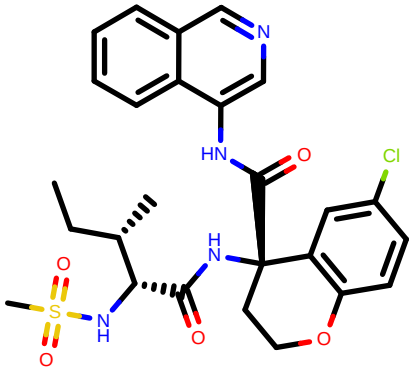
CID:	EN300-217494_2_3
SMILES:	C[C@@][[C@H]1CCOC1)(C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4042
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.34

EN300-195924_1_2



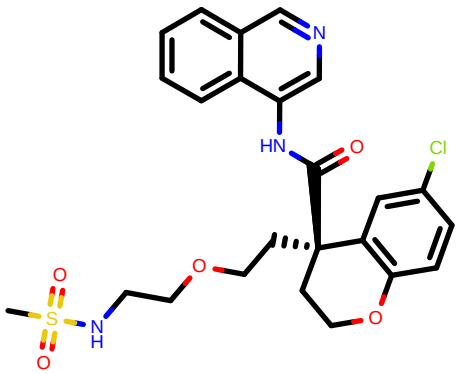
CID:	EN300-195924_1_2
SMILES:	C[C@]1(CCC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7026
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.32

EN300-76541_1_4



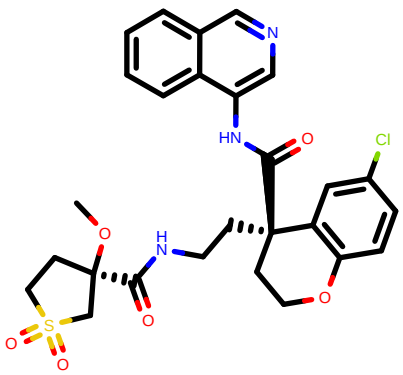
CID:	EN300-76541_1_4
SMILES:	CC[C@H](C)[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN5045
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.49

EN300-1238839_3_1



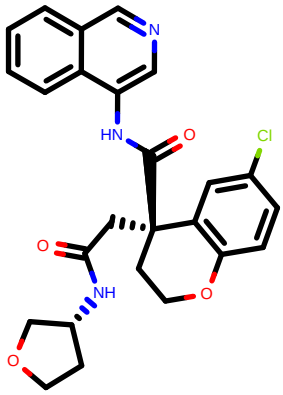
CID:	EN300-1238839_3_1
SMILES:	CS(=O)(=O)NCCOCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1100
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.37

EN300-385267_3_1



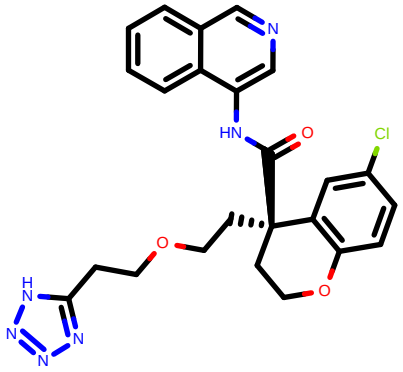
CID:	EN300-385267_3_1
SMILES:	CO[C@@]1(CCS(=O)(=O)C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10242
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.32

EN300-171752_1_1



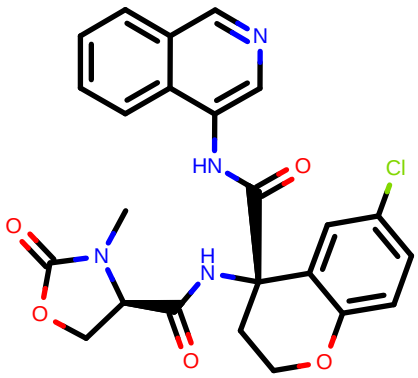
CID:	EN300-171752_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCOC5
RUN:	RUN10768
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.29

EN300-183231_3_1



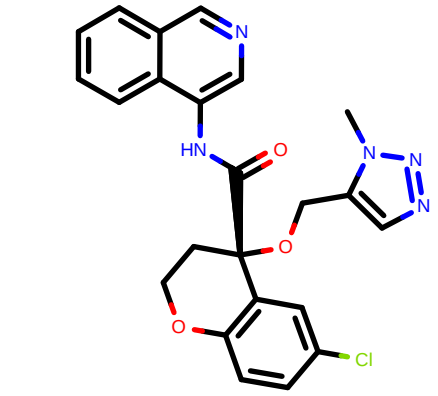
CID:	EN300-183231_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCCc5[nH]nnn5
RUN:	RUN2405
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.28

EN300-332838_1_2



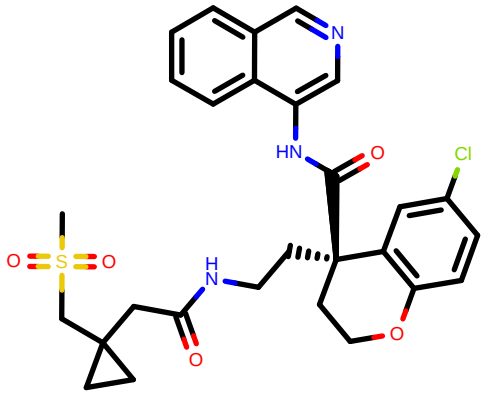
CID:	EN300-332838_1_2
SMILES:	CN1[C@H](COC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5636
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.29

EN300-216673_1_1



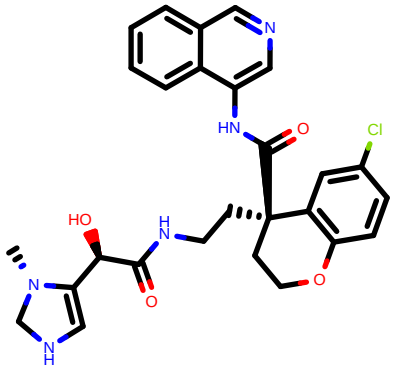
CID:	EN300-216673_1_1
SMILES:	Cn1c(cnn1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN564
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.24

EN300-97904_3_1



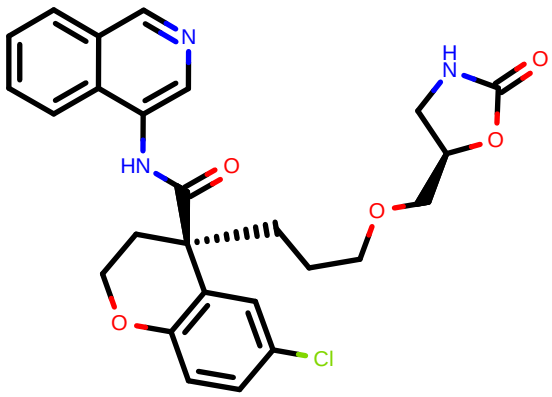
CID:	EN300-97904_3_1
SMILES:	CS(=O)(=O)CC1(CC1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5822
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.43

EN300-190283_3_2



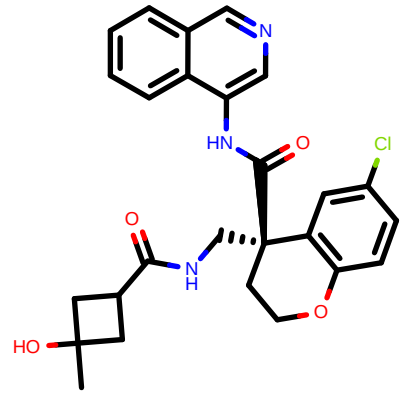
CID:	EN300-190283_3_2
SMILES:	Cn1cncc1[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN771
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.38

EN300-203293_4_2



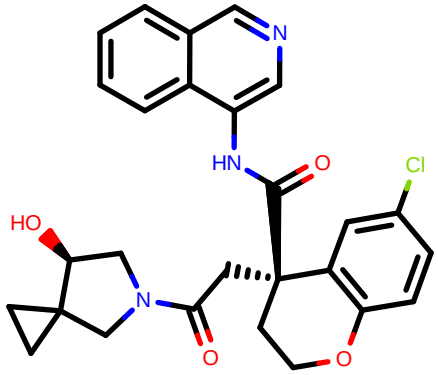
CID:	EN300-203293_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5CNC(=O)O5
RUN:	RUN1215
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.30

EN300-247343_2_1



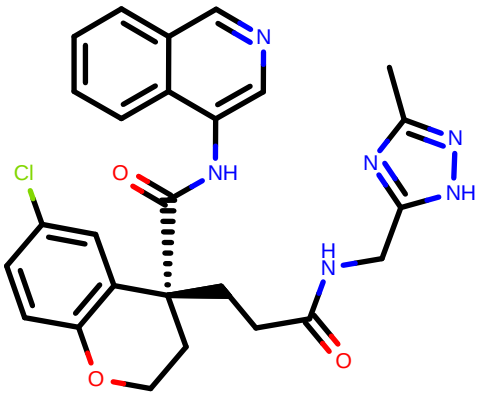
CID:	EN300-247343_2_1
SMILES:	CC1(CC(C1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6416
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.26

EN300-142333_1_1



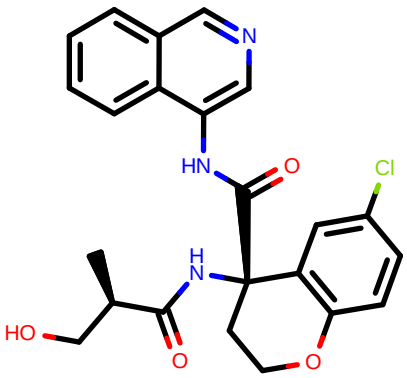
CID:	EN300-142333_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C6(C5)CC6)O
RUN:	RUN2508
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.34

EN300-70487_2_1



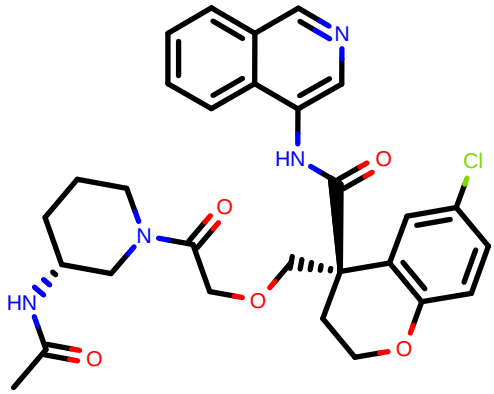
CID:	EN300-70487_2_1
SMILES:	Cc1[nH]c(nn1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3449
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.27

EN300-55072_1_2



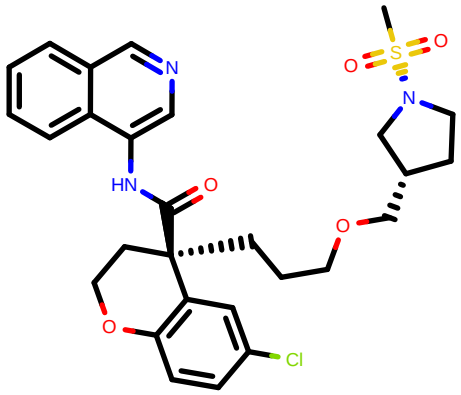
CID:	EN300-55072_1_2
SMILES:	C[C@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1493
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.26

EN300-48886_2_1



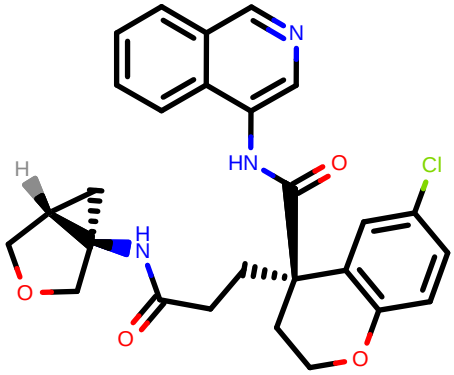
CID:	EN300-48886_2_1
SMILES:	CC(=O)N[C@@H]1CCCN(C1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2546
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.34

EN300-261986_4_1



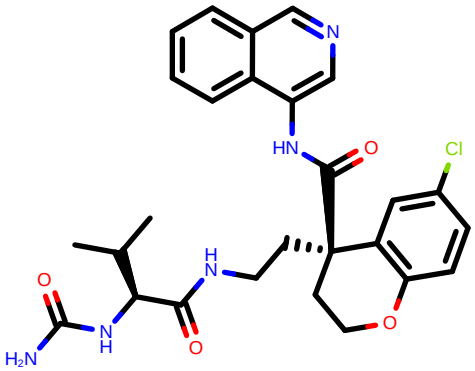
CID:	EN300-261986_4_1
SMILES:	CS(=O)(=O)N1CC[C@@H](C1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1327
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.49

EN300-367383_2_1



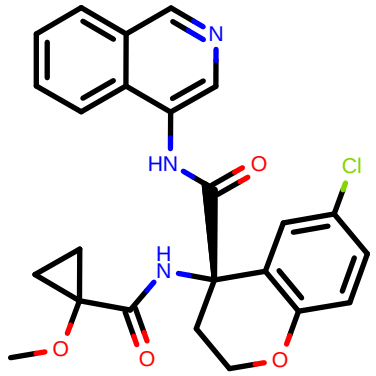
CID:	EN300-367383_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@]56C[C@H]5COC6
RUN:	RUN4844
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.27

EN300-87528_3_1



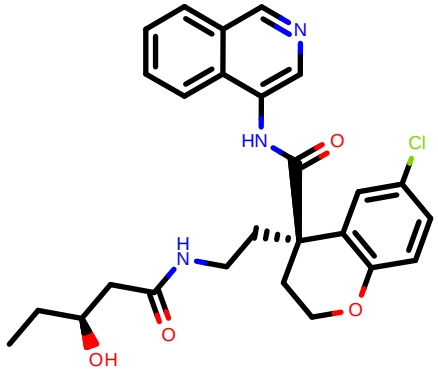
CID:	EN300-87528_3_1
SMILES:	CC(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN4987
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.43

EN300-182124_1_1



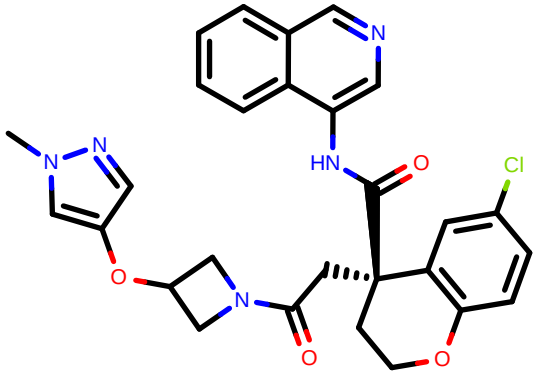
CID:	EN300-182124_1_1
SMILES:	COC1(CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2930
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.24

EN300-224741_3_1



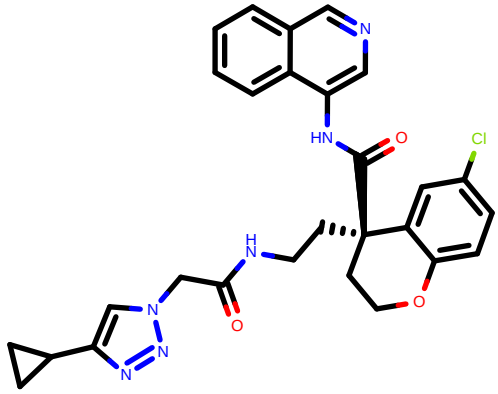
CID:	EN300-224741_3_1
SMILES:	CC[C@@H](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN6457
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.31

EN300-6762563_1_1



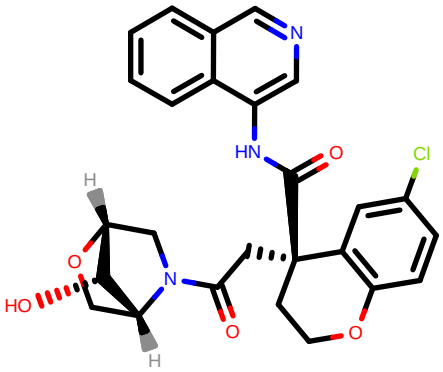
CID:	EN300-6762563_1_1
SMILES:	Cn1cc(cn1)OC2CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7544
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.35

EN300-107892_3_1



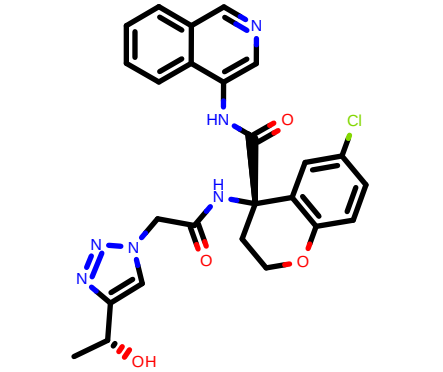
CID:	EN300-107892_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5cc(nn5)C6CC6
RUN:	RUN11220
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.33

EN300-6504714_1_1



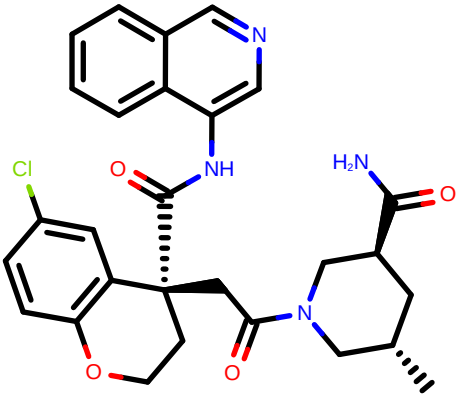
CID:	EN300-6504714_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@H]([C@H]5CO6)O
RUN:	RUN4847
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.28

EN300-109540_1_2



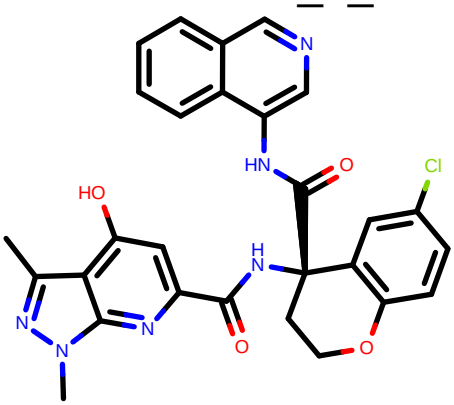
CID:	EN300-109540_1_2
SMILES:	C[C@H](c1cn(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6343
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.29

EN300-1724086_1_2



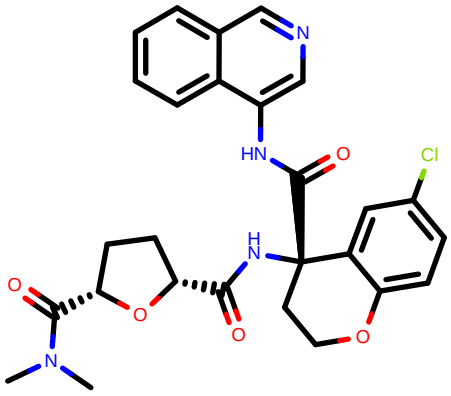
CID:	EN300-1724086_1_2
SMILES:	C[C@H]1C[C@@H](CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN423
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.23

EN300-74965_1_1



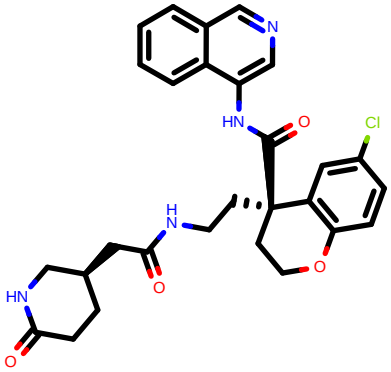
CID:	EN300-74965_1_1
SMILES:	Cc1c2c(=O)cc([nH]c2n(n1)C)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9122
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.28

EN300-314890_1_1



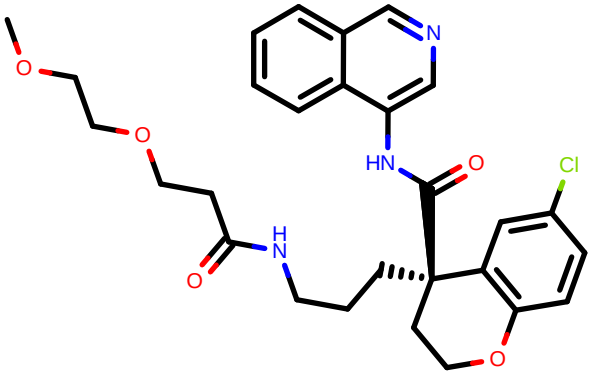
CID:	EN300-314890_1_1
SMILES:	CN(C)C(=O)[C@@H]1CC[C@@H](O1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5988
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.33

EN300-246992_3_2



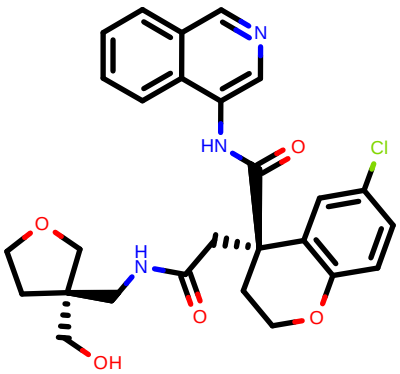
CID:	EN300-246992_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCC(=O)NC5
RUN:	RUN8612
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.35

EN300-55250_4_1



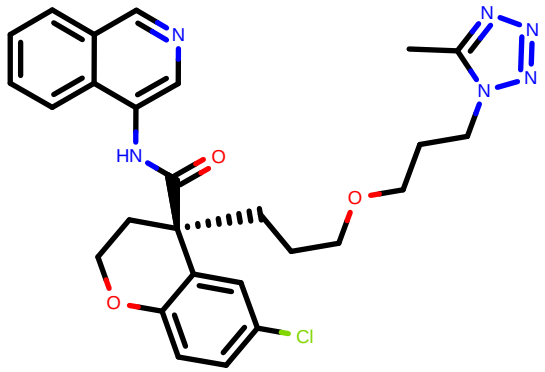
CID:	EN300-55250_4_1
SMILES:	COCCOCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10733
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.35

EN300-682529_1_2



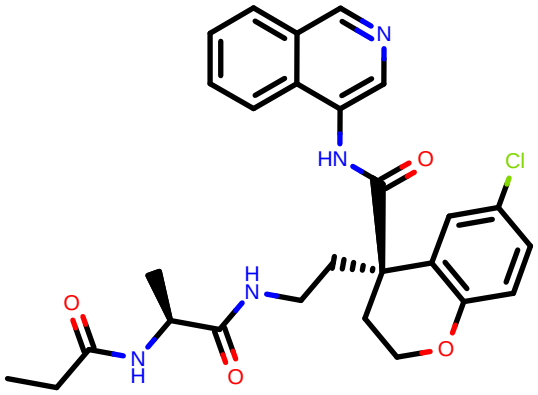
CID:	EN300-682529_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@]5(CCOC5)CO
RUN:	RUN9209
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.29

EN300-197715_4_1



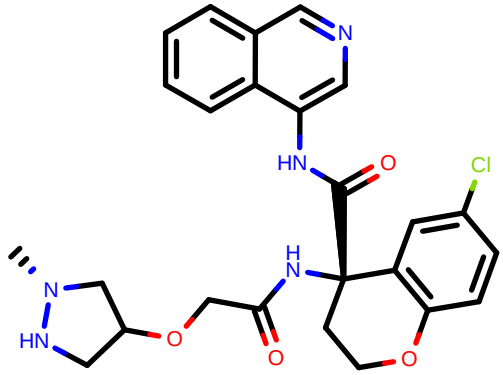
CID:	EN300-197715_4_1
SMILES:	Cc1nnnn1CCCOCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1543
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.39

EN300-31148_3_1



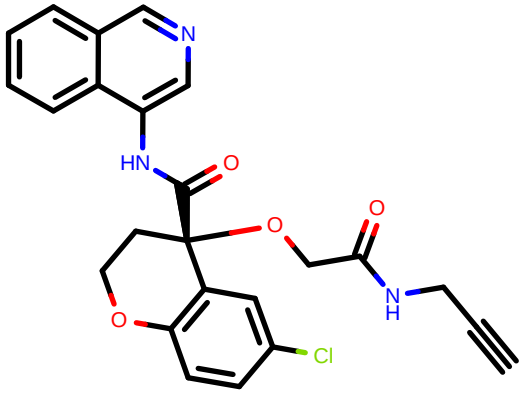
CID:	EN300-31148_3_1
SMILES:	CCC(=O)N[C@@H](C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4023
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.31

EN300-201553_1_1



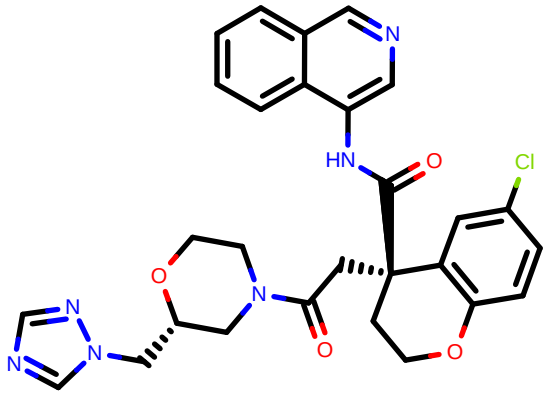
CID:	EN300-201553_1_1
SMILES:	Cn1cc(cn1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN814
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.25

EN300-1659582_1_1



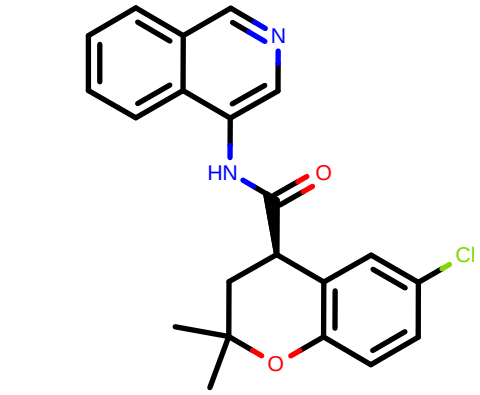
CID:	EN300-1659582_1_1
SMILES:	C#CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN469
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.23

EN300-80241_1_2



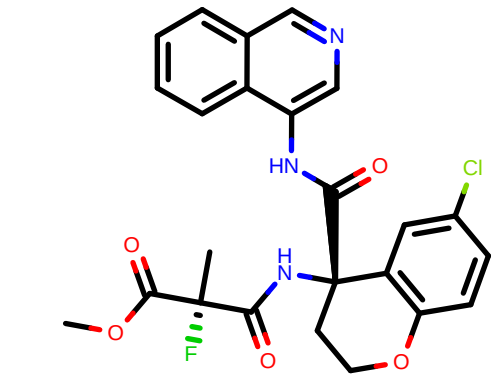
CID:	EN300-80241_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)Cn6cncn6
RUN:	RUN9542
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.36

ADA-UCB-dc2b944c-16_1



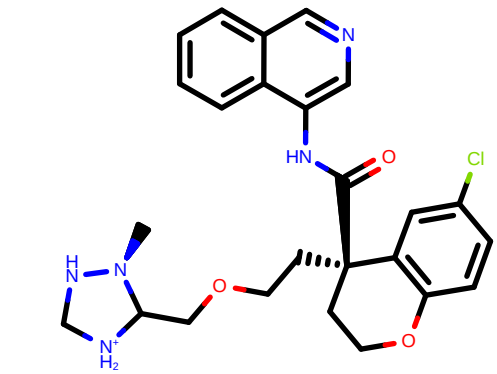
CID:	ADA-UCB-dc2b944c-16_1
SMILES:	CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C
RUN:	RUN43
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.10

EN300-7464289_1_1



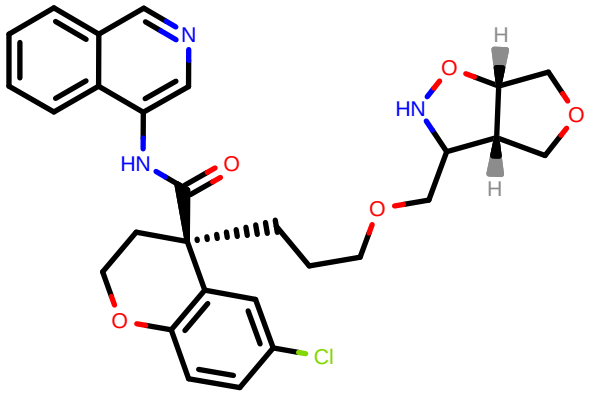
CID:	EN300-7464289_1_1
SMILES:	C[C@@](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(=O)OC)F
RUN:	RUN4845
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.24

EN300-87334_3_1



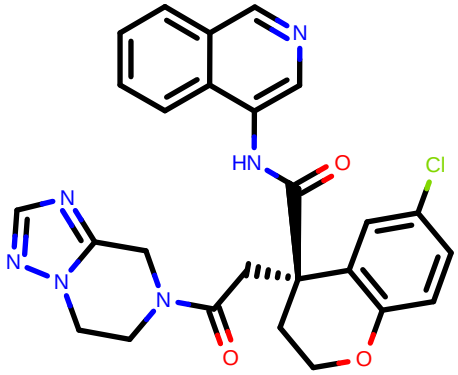
CID:	EN300-87334_3_1
SMILES:	Cn1c(ncn1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1300
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.26

EN300-7436306_4_1



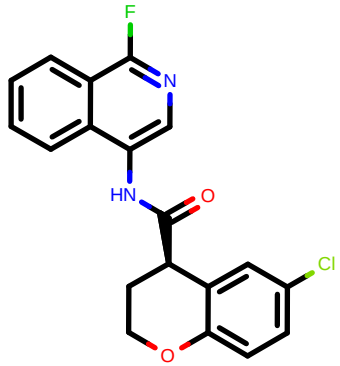
CID:	EN300-7436306_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5=NO[C@H]6[C@@H]5COC6
RUN:	RUN839
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.32

EN300-141224_1_1



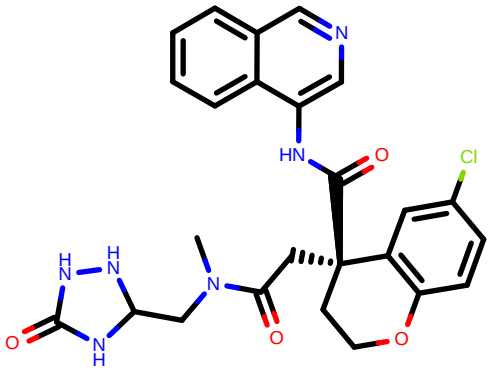
CID:	EN300-141224_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCn6c(ncn6)C5
RUN:	RUN5698
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.26

JOH-SUS-a69c159d-2_1



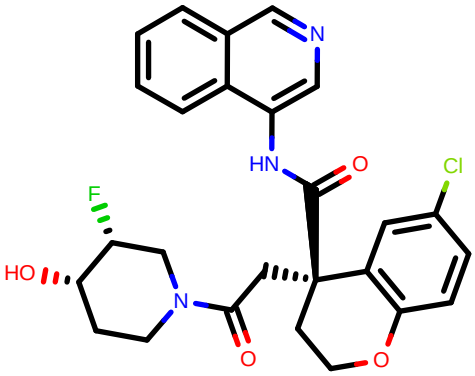
CID:	JOH-SUS-a69c159d-2_1
SMILES:	c1ccc2c(c1)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN50
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.03

EN300-1716006_1_1



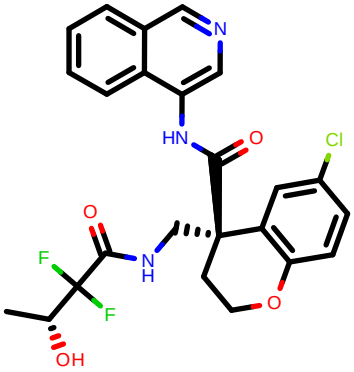
CID:	EN300-1716006_1_1
SMILES:	CN(Cc1[nH]c(=O)[nH]n1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5510
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.29

EN300-741926_1_1



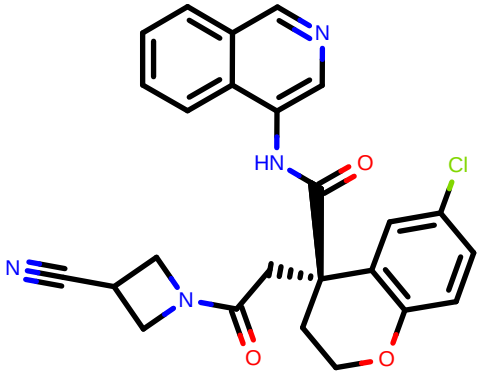
CID:	EN300-741926_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)F)O
RUN:	RUN3072
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.26

EN300-185398_2_2



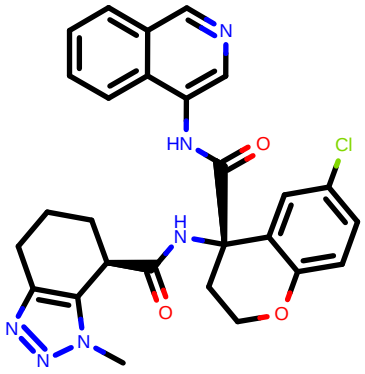
CID:	EN300-185398_2_2
SMILES:	C[C@H](C(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F)O
RUN:	RUN5693
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.23

EN300-206282_1_1



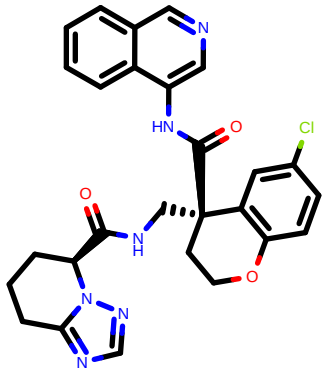
CID:	EN300-206282_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C#N
RUN:	RUN3172
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.22

EN300-1664865_1_2



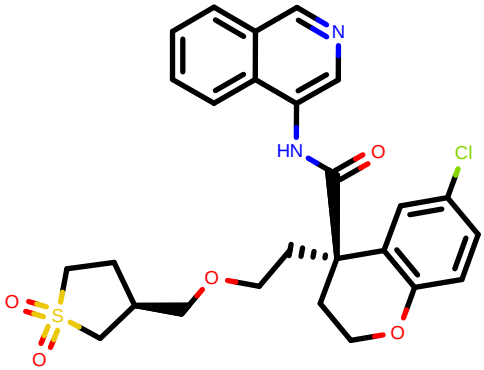
CID:	EN300-1664865_1_2
SMILES:	Cn1c2c(nn1)CCC[C@H]2C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7882
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.29

EN300-1273016_2_1



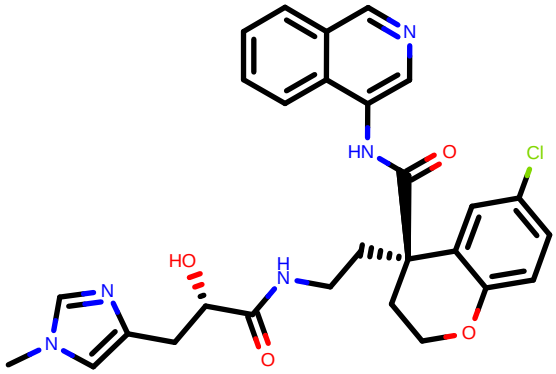
CID:	EN300-1273016_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCCc6n5ncn6
RUN:	RUN7507
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.23

EN300-1448603_3_1



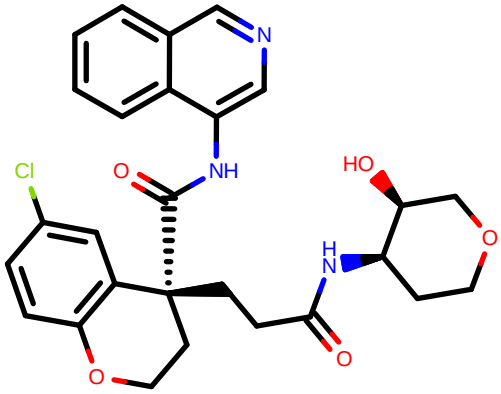
CID:	EN300-1448603_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CCS(=O)(=O)C5
RUN:	RUN2363
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.32

EN300-1725538_3_1



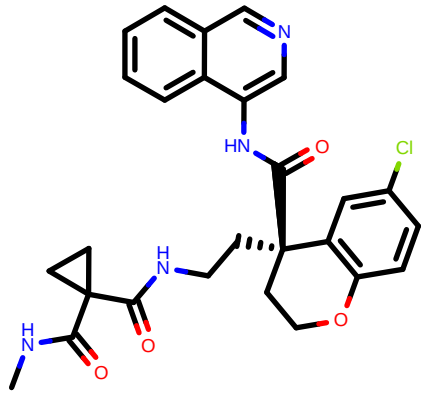
CID:	EN300-1725538_3_1
SMILES:	Cn1cc(nc1)C[C@@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN9971
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.30

EN300-321053_2_1



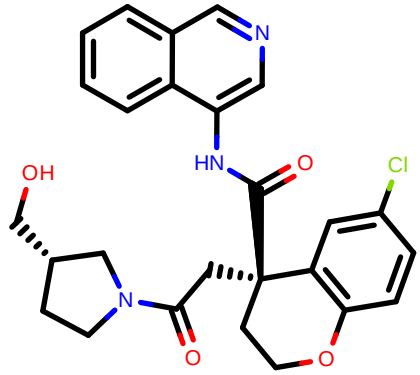
CID:	EN300-321053_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCOC[C@@H]5O
RUN:	RUN6282
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.29

EN300-66770_3_1



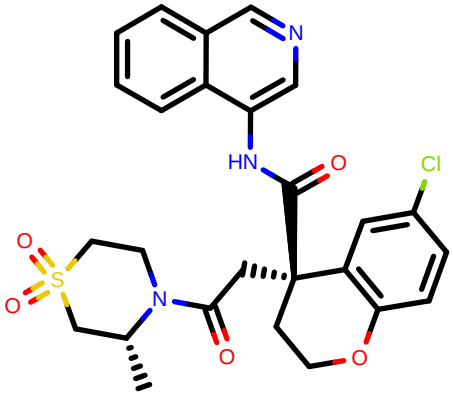
CID:	EN300-66770_3_1
SMILES:	CNC(=O)C1(CC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3791
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.34

EN300-256053_1_1



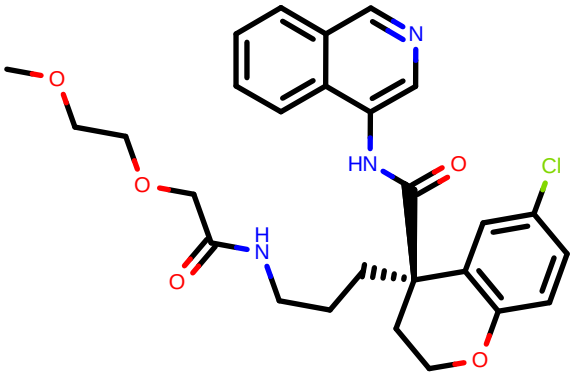
CID:	EN300-256053_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)CO
RUN:	RUN1450
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.27

EN300-171215_1_1



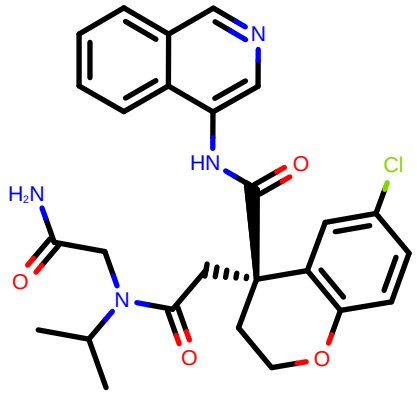
CID:	EN300-171215_1_1
SMILES:	C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10272
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.30

EN300-20375_4_1



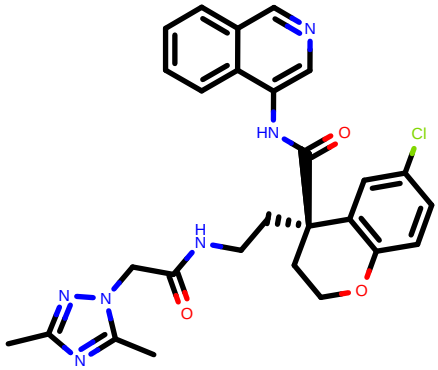
CID:	EN300-20375_4_1
SMILES:	COCCOCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN11017
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.33

EN300-35450_1_1



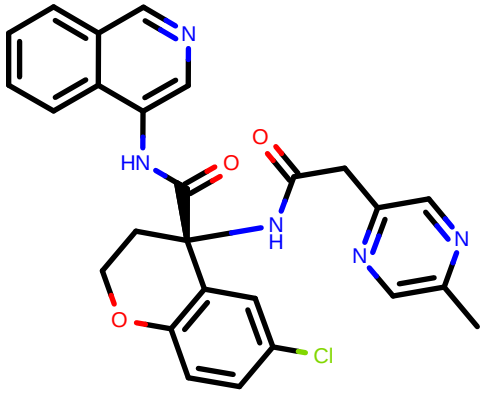
CID:	EN300-35450_1_1
SMILES:	CC(C)N(CC(=O)N)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8850
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.34

EN300-7423123_3_1



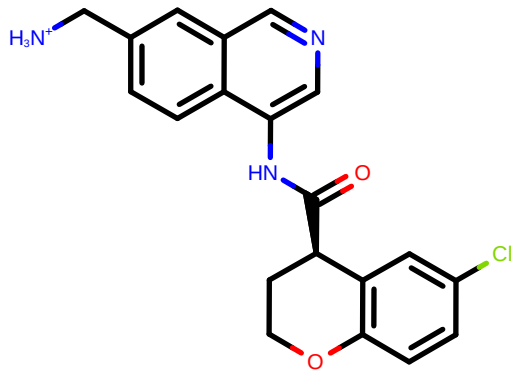
CID:	EN300-7423123_3_1
SMILES:	Cc1nc(n(n1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN11292
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.40

EN300-1709295_1_1



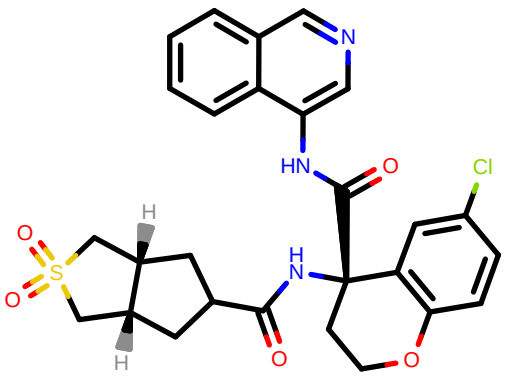
CID:	EN300-1709295_1_1
SMILES:	Cc1cnc(cn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5336
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.28

MAK-UNK-8be7dca9-5_1



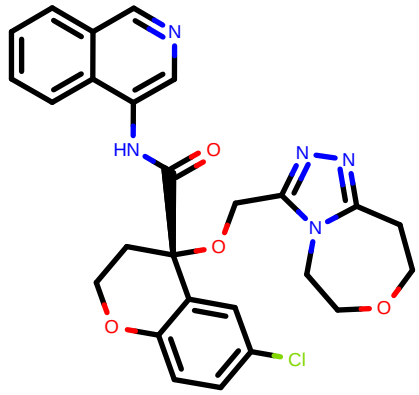
CID:	MAK-UNK-8be7dca9-5_1
SMILES:	c1cc2c(cc1CN)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN19
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.08

EN300-7438088_1_1



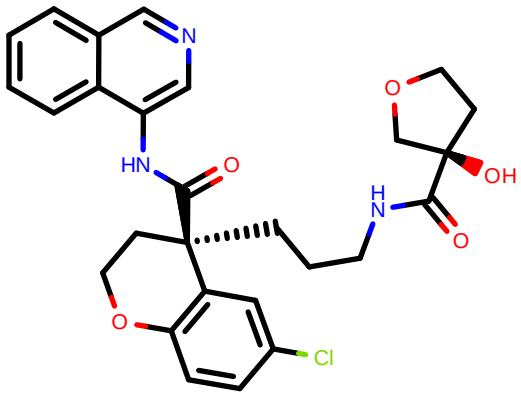
CID:	EN300-7438088_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C[C@@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN7106
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.41

EN300-310888_1_1



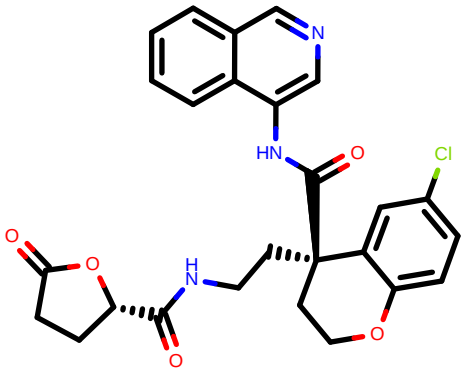
CID:	EN300-310888_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nnc6n5CCOCC6
RUN:	RUN1048
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.24

EN300-148421_4_2



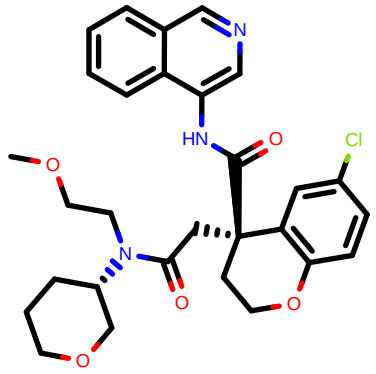
CID:	EN300-148421_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@]5(CCOC5)O
RUN:	RUN7885
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.51

EN300-359750_3_1



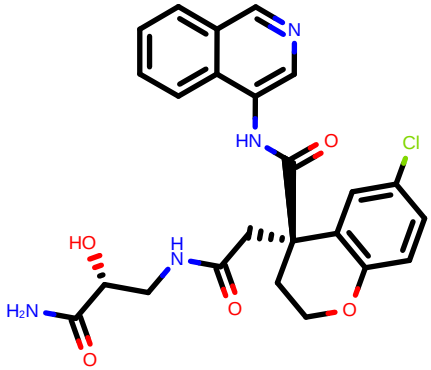
CID:	EN300-359750_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCC(=O)O5
RUN:	RUN5806
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.31

JAG-UCB-706446eb-5_2



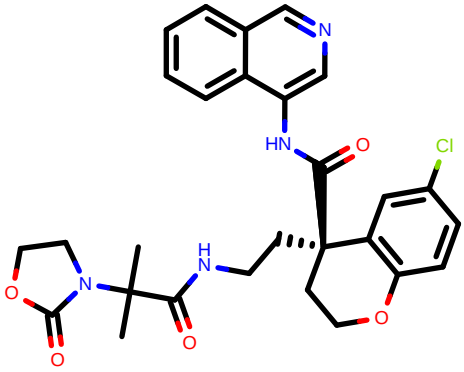
CID:	JAG-UCB-706446eb-5_2
SMILES:	COCCN([C@H]1CCCOC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN265
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.35

EN300-184355_1_2



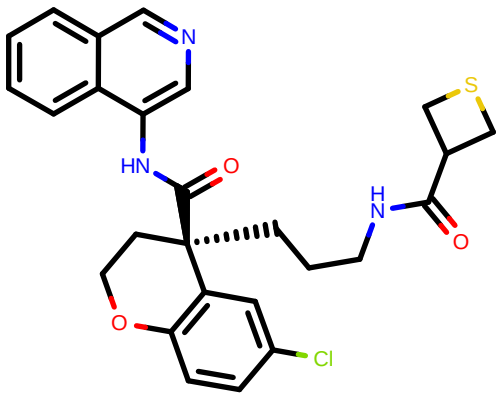
CID:	EN300-184355_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@H](C(=O)N)O
RUN:	RUN6018
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.39

EN300-96175_3_1



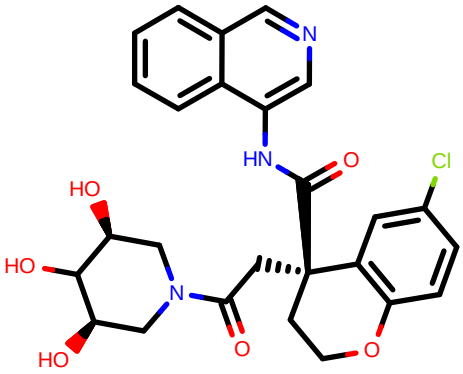
CID:	EN300-96175_3_1
SMILES:	CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N5CCOC5=O
RUN:	RUN3604
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.55

EN300-95094_4_1



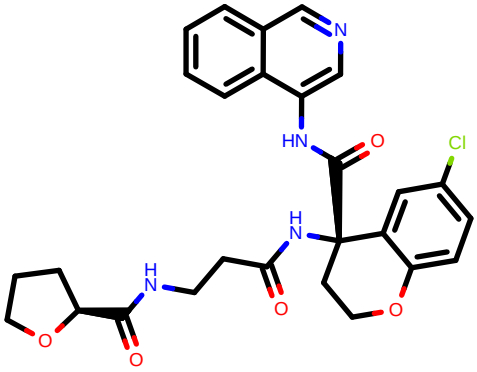
CID:	EN300-95094_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C5CSC5
RUN:	RUN11015
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.22

EN300-299920_1_1



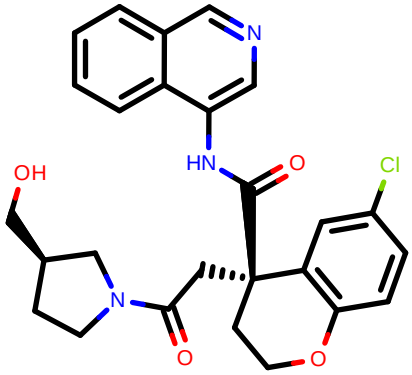
CID:	EN300-299920_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]([C@H]([C@H](C5)O)O)O
RUN:	RUN1769
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.35

EN300-86732_1_1



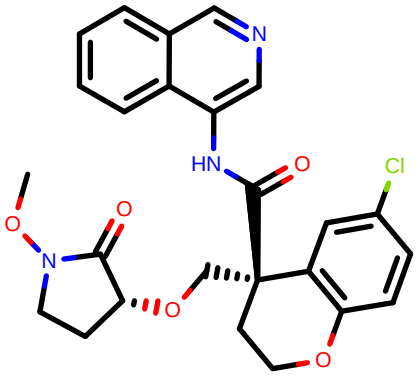
CID:	EN300-86732_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)[C@@H]5CCCO5
RUN:	RUN1932
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.26

EN300-256053_1_2



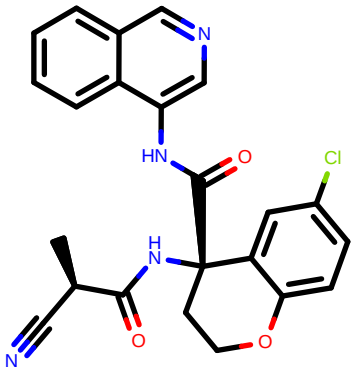
CID:	EN300-256053_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)CO
RUN:	RUN2612
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.26

EN300-302058_2_2



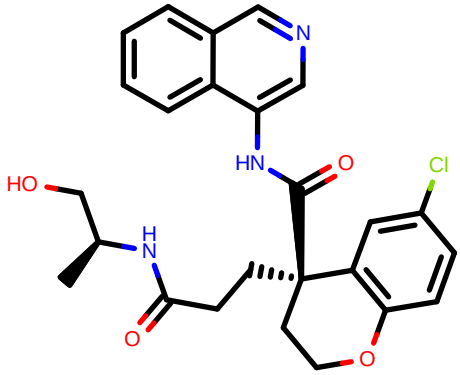
CID:	EN300-302058_2_2
SMILES:	CON1CC[C@H](C1=O)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2379
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.24

EN300-72730_1_2



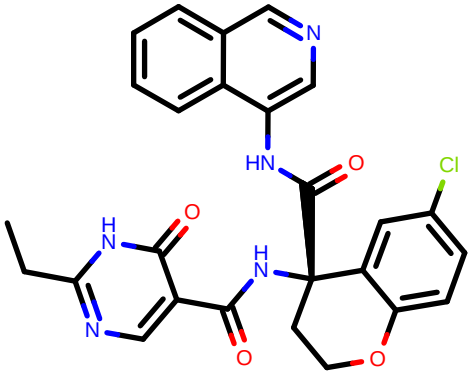
CID:	EN300-72730_1_2
SMILES:	C[C@H](C#N)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1261
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.20

EN300-86282_2_1



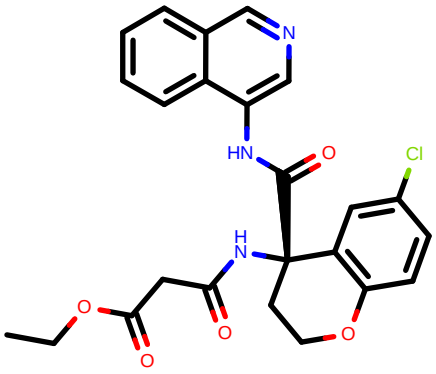
CID:	EN300-86282_2_1
SMILES:	C[C@@H](CO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1826
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.28

EN300-1273019_1_1



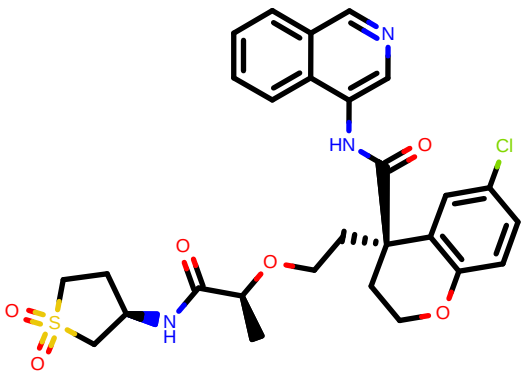
CID:	EN300-1273019_1_1
SMILES:	CCc1[nH]c(=O)c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8864
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.28

EN300-41828_1_1



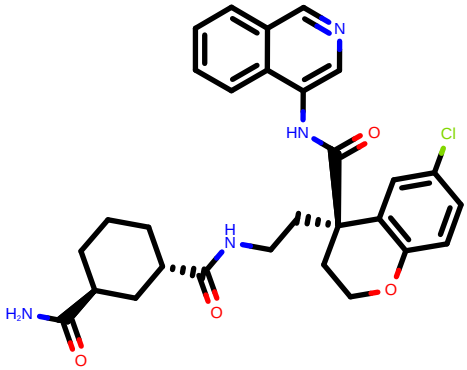
CID:	EN300-41828_1_1
SMILES:	CCOC(=O)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2834
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.22

EN300-23318_3_1



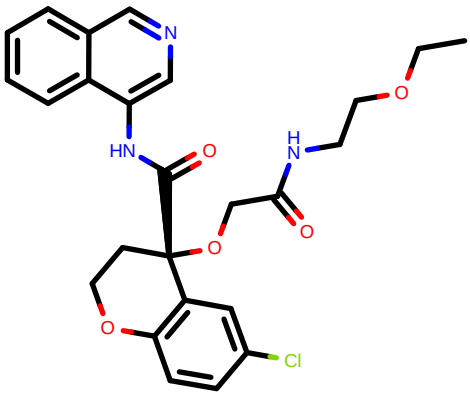
CID:	EN300-23318_3_1
SMILES:	C[C@@H](C(=O)N[C@@H]1CCS(=O)(=O)C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1444
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.42

EN300-90142_3_2



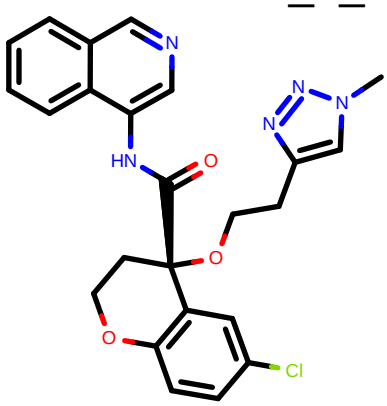
CID:	EN300-90142_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCC[C@@H](C5)C(=O)N
RUN:	RUN5978
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.35

EN300-103187_1_1



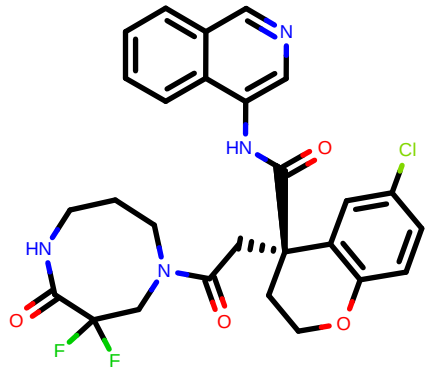
CID:	EN300-103187_1_1
SMILES:	CCOCCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1575
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.27

EN300-1600786_1_1



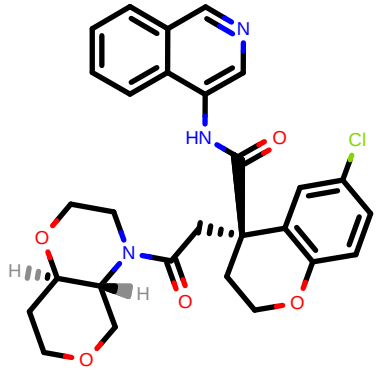
CID:	EN300-1600786_1_1
SMILES:	Cn1cc(nn1)CCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1024
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.23

EN300-1273202_1_1



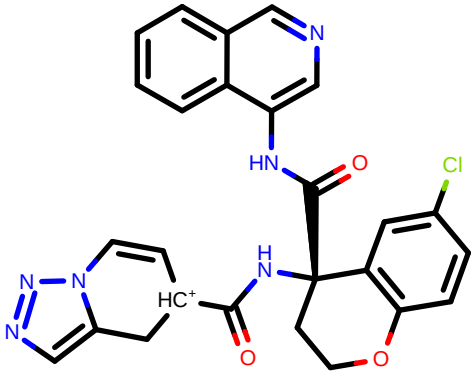
CID:	EN300-1273202_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCNC(=O)C(C5)(F)F
RUN:	RUN5550
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.31

EN300-1387243_1_1



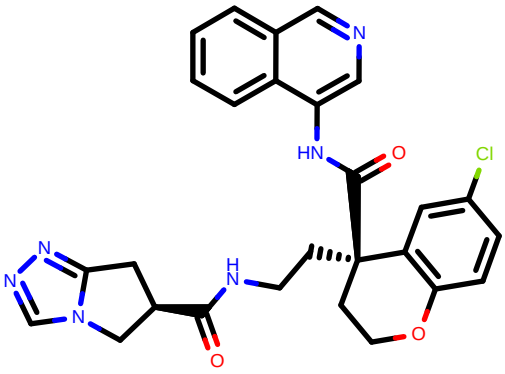
CID:	EN300-1387243_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H]6[C@H]5COCC6
RUN:	RUN7332
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.35

EN300-6743433_1_1



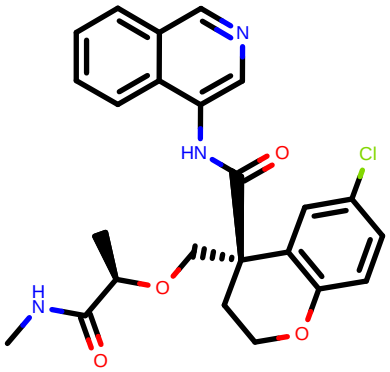
CID:	EN300-6743433_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn6c(c5)cnn6
RUN:	RUN8770
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.23

EN300-6745453_3_1



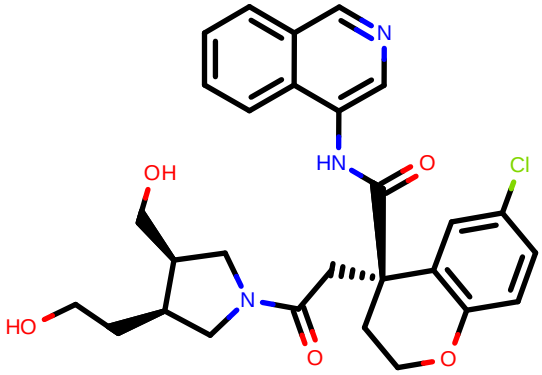
CID:	EN300-6745453_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5Cc6nncn6C5
RUN:	RUN10055
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.29

EN300-211482_2_2



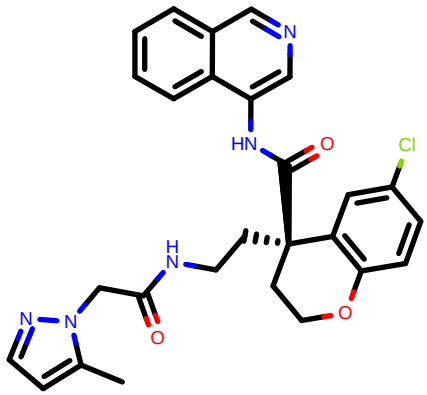
CID:	EN300-211482_2_2
SMILES:	C[C@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1542
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.25

EN300-1425608_1_4



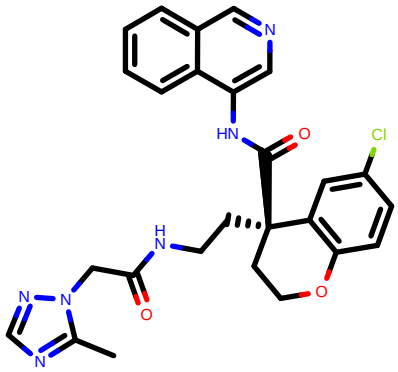
CID:	EN300-1425608_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]([C@H](C5)CO)CCO
RUN:	RUN351
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.33

EN300-83558_3_1



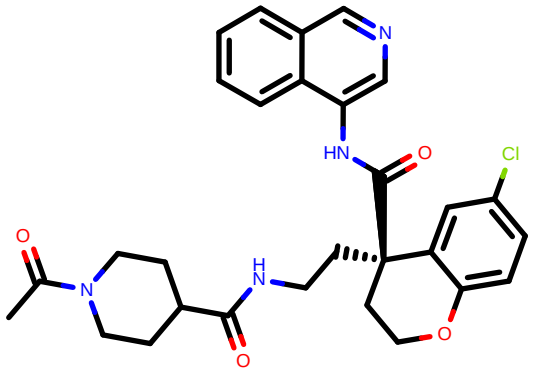
CID:	EN300-83558_3_1
SMILES:	Cc1ccnn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9482
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.29

EN300-7536177_3_1



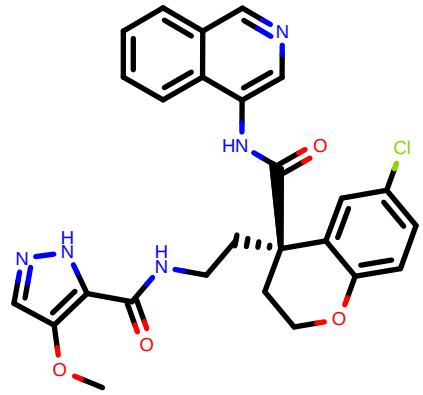
CID:	EN300-7536177_3_1
SMILES:	Cc1ncnn1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6709
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.39

EN300-18557_3_1



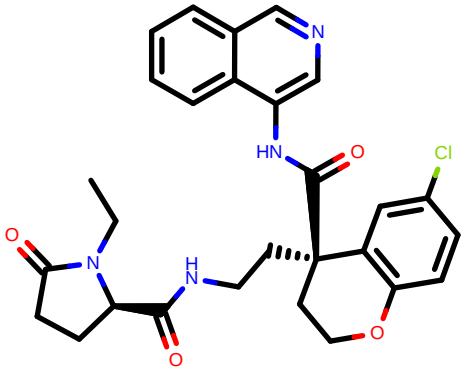
CID:	EN300-18557_3_1
SMILES:	CC(=O)N1CCC(CC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9678
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.36

EN300-7439284_3_1



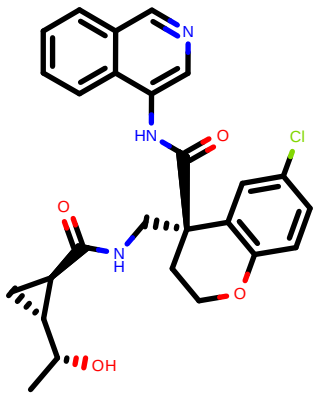
CID:	EN300-7439284_3_1
SMILES:	COc1cn[nH]c1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10328
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.29

EN300-718785_3_2



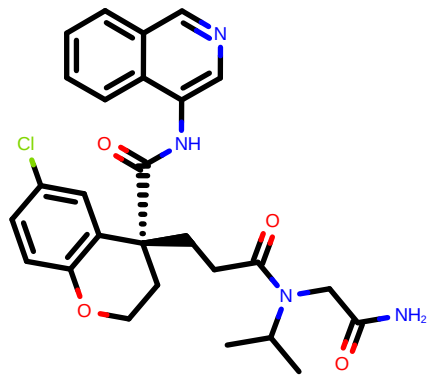
CID:	EN300-718785_3_2
SMILES:	CCN1[C@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5298
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.40

EN300-6729572_2_6



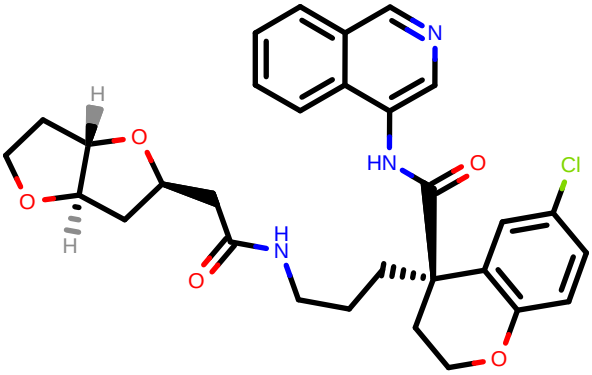
CID:	EN300-6729572_2_6
SMILES:	C[C@H]([C@@H]1C[C@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4906
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.24

EN300-35450_2_1



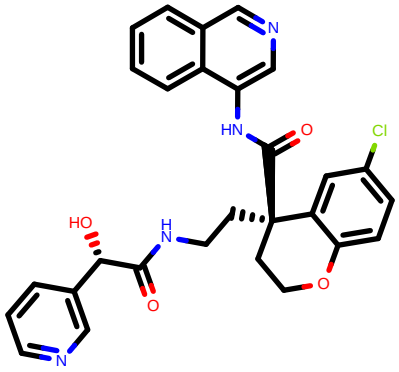
CID:	EN300-35450_2_1
SMILES:	CC(C)N(CC(=O)N)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8601
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.36

EN300-7355519_4_2



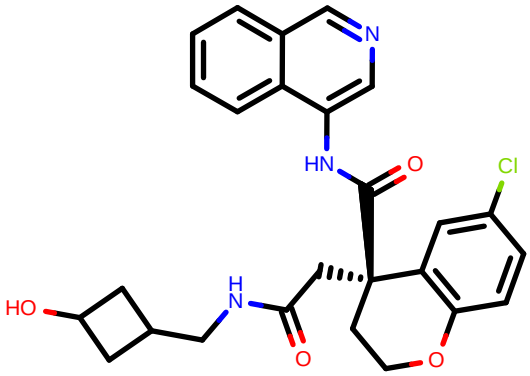
CID:	EN300-7355519_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C[C@H]5C[C@@H]6[C@@H](O5)CCO6
RUN:	RUN11089
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.40

EN300-134855_3_2



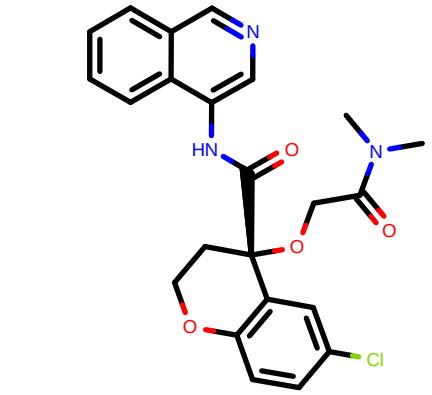
CID:	EN300-134855_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](c5cccnc5)O
RUN:	RUN8212
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.45

EN300-366299_1_1



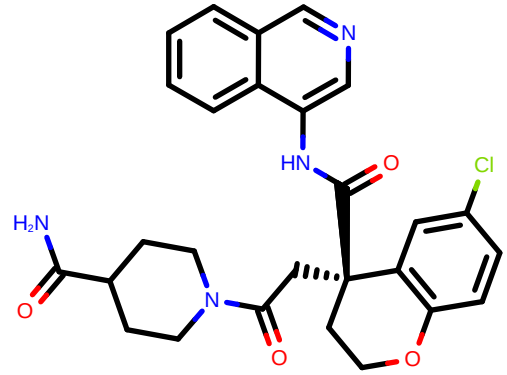
CID:	EN300-366299_1_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)CC(=O)NC[C@H]5C[C@@H](C5)O)cc1
RUN:	RUN5890
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.23

EN300-216063_1_1



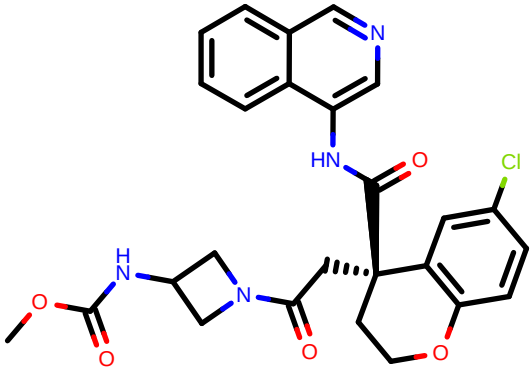
CID:	EN300-216063_1_1
SMILES:	CN(C)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN793
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.22

EN300-1265946_1_1



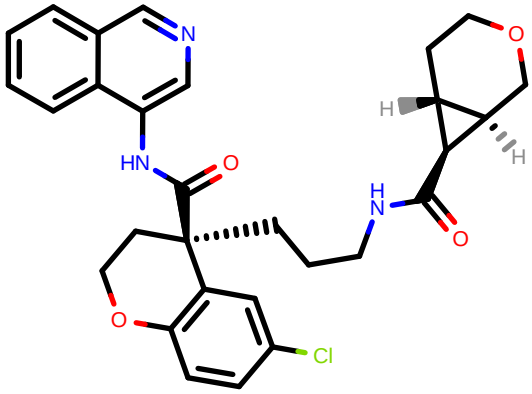
CID:	EN300-1265946_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)C(=O)N
RUN:	RUN4015
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.38

EN300-140383_1_1



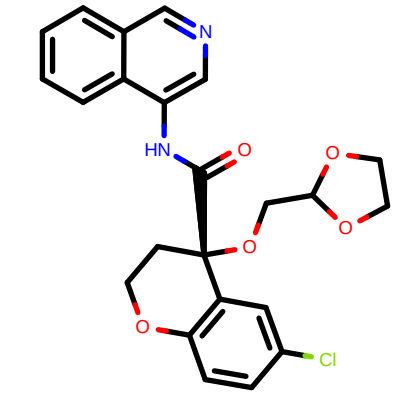
CID:	EN300-140383_1_1
SMILES:	COC(=O)NC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3807
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.25

EN300-1644723_4_8



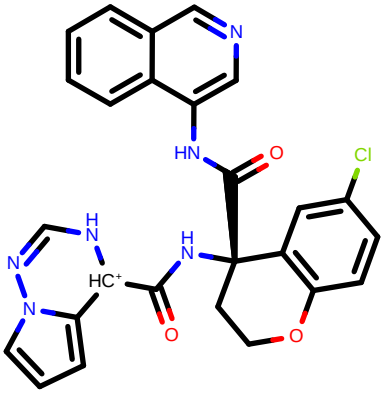
CID:	EN300-1644723_4_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5[C@H]6[C@H]5COCC6
RUN:	RUN10839
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.31

EN300-77092_1_1



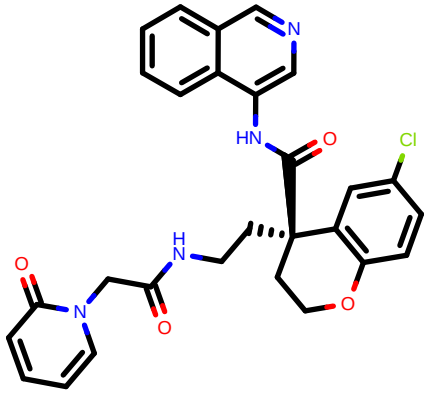
CID:	EN300-77092_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5OCCO5
RUN:	RUN2408
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.24

EN300-7426781_1_1



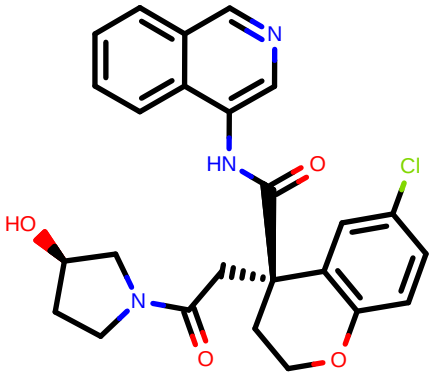
CID:	EN300-7426781_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c6cccn6ncn5
RUN:	RUN7862
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.23

EN300-11714_3_1



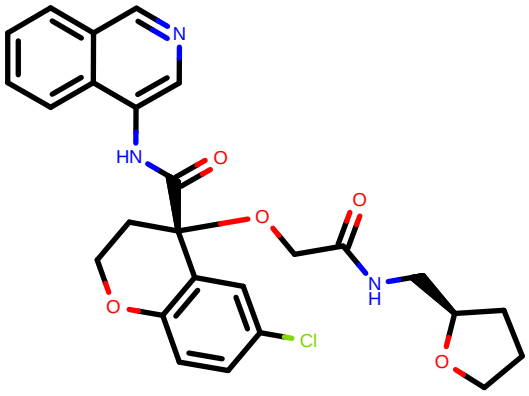
CID:	EN300-11714_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cn5ccccc5=O
RUN:	RUN9132
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.29

EN300-69313_1_1



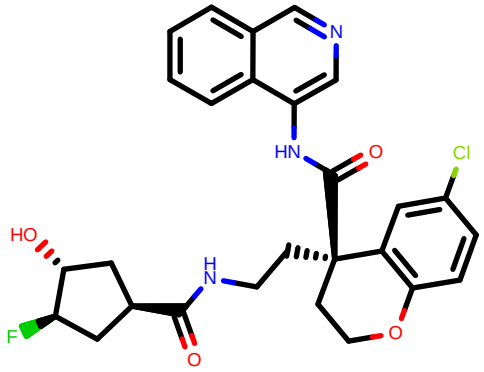
CID:	EN300-69313_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O
RUN:	RUN5191
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.31

EN300-01527_1_2



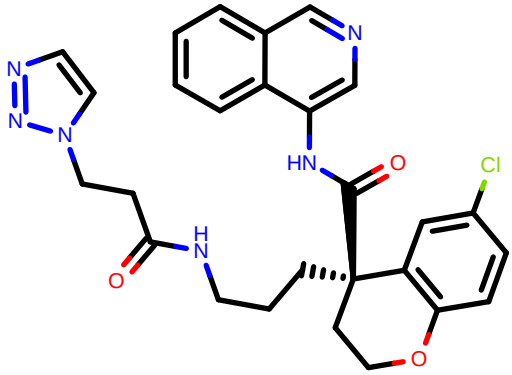
CID:	EN300-01527_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5CCCO5
RUN:	RUN1719
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.26

EN300-7461217_3_1



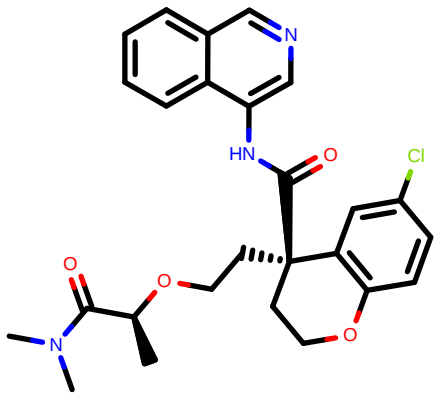
CID:	EN300-7461217_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@H]([C@@H](C5)F)O
RUN:	RUN7144
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.36

EN300-28871_4_1



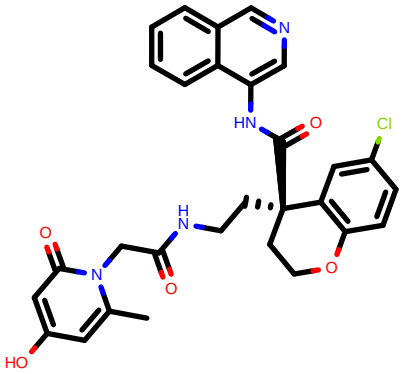
CID:	EN300-28871_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCn5ccnn5
RUN:	RUN9315
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.29

EN300-14458_3_1



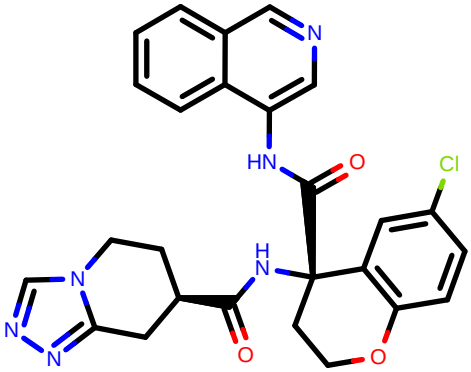
CID:	EN300-14458_3_1
SMILES:	C[C@@H](C(=O)N(C)C)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1524
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.26

EN300-102864_3_1



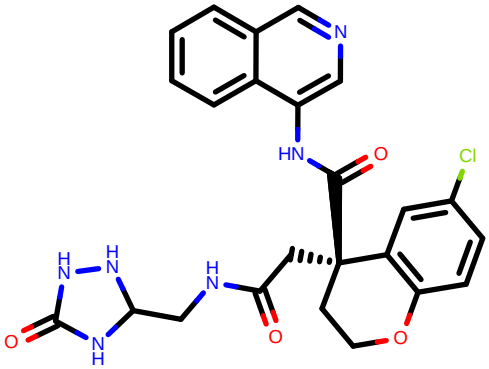
CID:	EN300-102864_3_1
SMILES:	Cc1cc(cc(=O)n1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3963
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.31

EN300-6474341_1_1



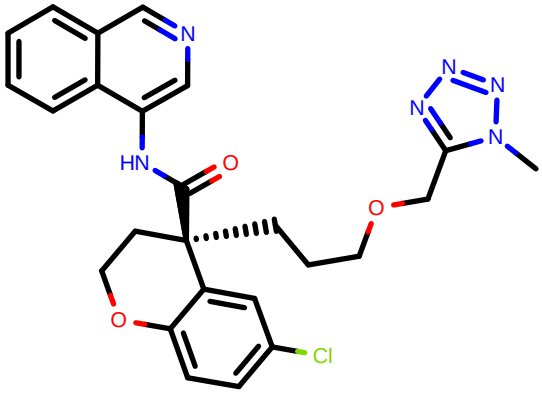
CID:	EN300-6474341_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCn6cnnc6C5
RUN:	RUN8262
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.30

EN300-98038_1_1



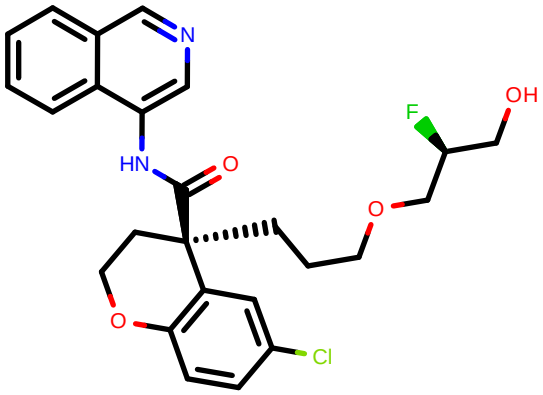
CID:	EN300-98038_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5[nH]c(=O)[nH]n5
RUN:	RUN5239
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.23

EN300-62574_4_1



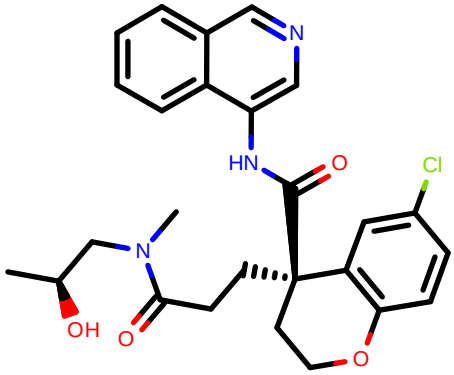
CID:	EN300-62574_4_1
SMILES:	Cn1c(nnn1)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN332
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.31

EN300-1600517_4_2



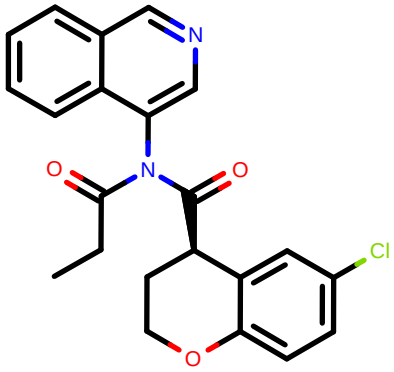
CID:	EN300-1600517_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H](CO)F
RUN:	RUN492
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.39

EN300-210254_2_1



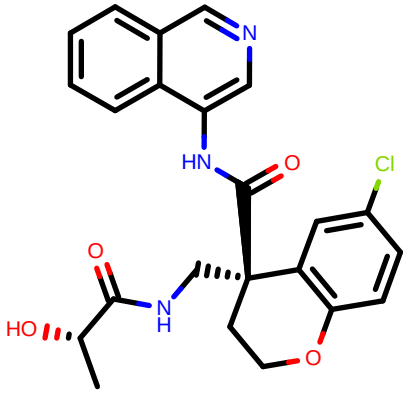
CID:	EN300-210254_2_1
SMILES:	C[C@@H](CN(C)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4456
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.29

VLA-UCB-50c39ae8-7_1



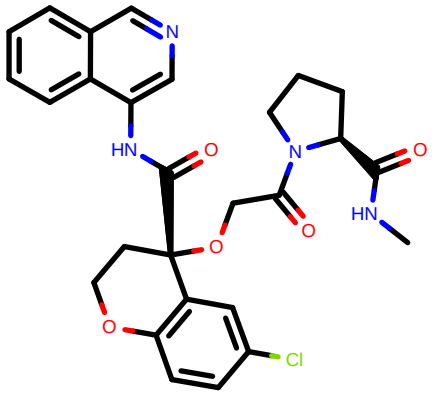
CID:	VLA-UCB-50c39ae8-7_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN147
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.19

EN300-19542_2_1



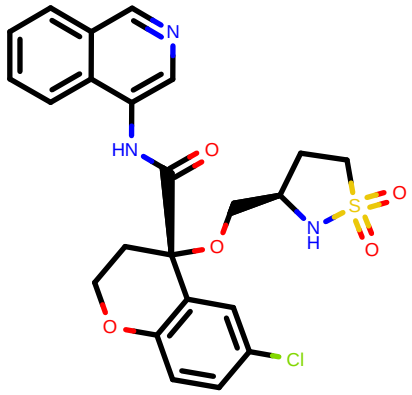
CID:	EN300-19542_2_1
SMILES:	C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2807
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.27

EN300-48902_1_1



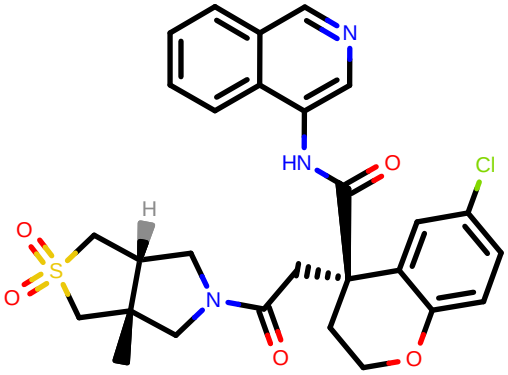
CID:	EN300-48902_1_1
SMILES:	CNC(=O)[C@@H]1CCCN1C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN365
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.32

EN300-1699871_1_2



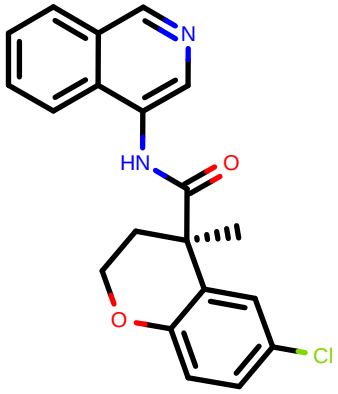
CID:	EN300-1699871_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCS(=O)(=O)N5
RUN:	RUN1224
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.27

EN300-748753_1_1



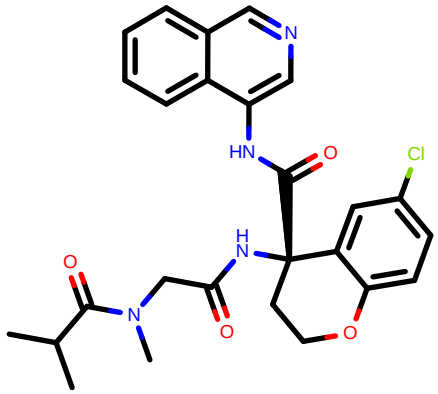
CID:	EN300-748753_1_1
SMILES:	C[C@]12CN(C[C@H]1CS(=O)(=O)C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2361
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.40

DAR-DIA-6a508060-10_2



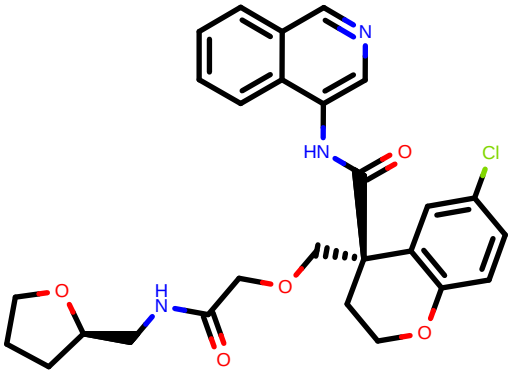
CID:	DAR-DIA-6a508060-10_2
SMILES:	C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.10

EN300-31145_1_1



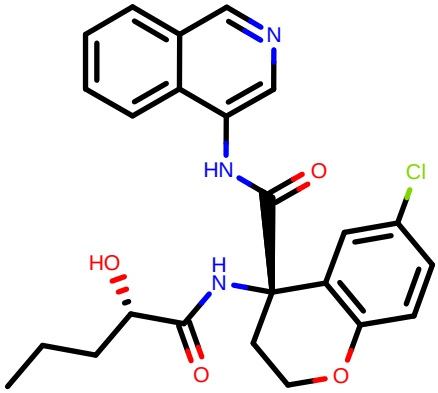
CID:	EN300-31145_1_1
SMILES:	CC(C)C(=O)N(C)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5181
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.34

EN300-01527_2_2



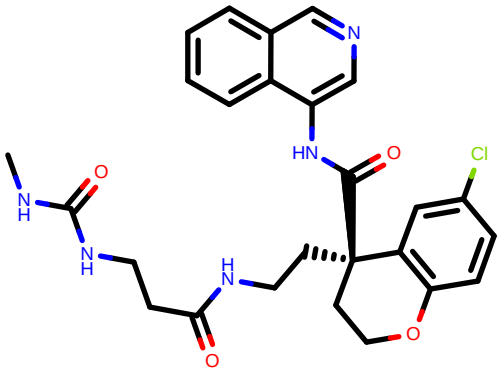
CID:	EN300-01527_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC[C@H]5CCCO5
RUN:	RUN594
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.32

EN300-316679_1_1



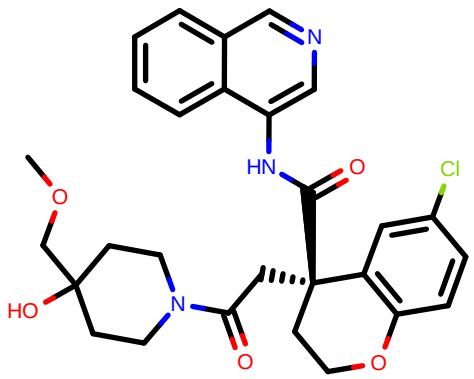
CID:	EN300-316679_1_1
SMILES:	CCC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3070
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.31

EN300-66494_3_1



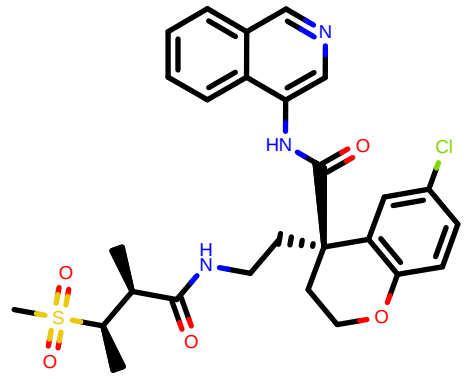
CID:	EN300-66494_3_1
SMILES:	CNC(=O)NCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7328
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.38

EN300-119366_1_1



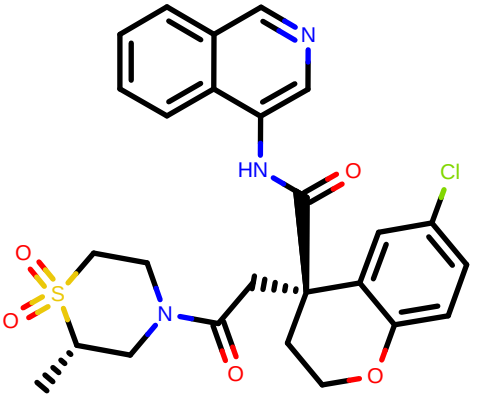
CID:	EN300-119366_1_1
SMILES:	COCC1(CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10876
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.34

EN300-182725_3_2



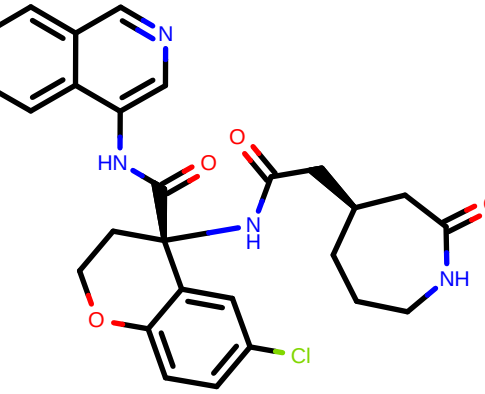
CID:	EN300-182725_3_2
SMILES:	C[C@H]([C@@H](C)S(=O)(=O)C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9390
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.33

EN300-137734_1_2



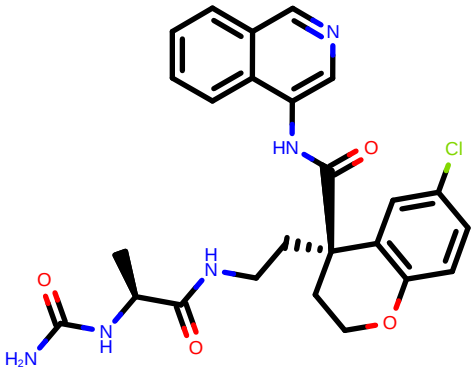
CID:	EN300-137734_1_2
SMILES:	C[C@H]1CN(CCS1(=O)=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3280
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.34

EN300-195590_1_1



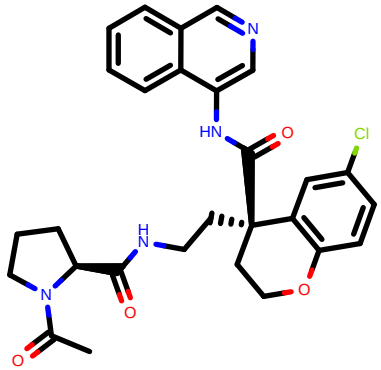
CID:	EN300-195590_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCCNC(=O)C5
RUN:	RUN2132
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.21

EN300-00271_3_1



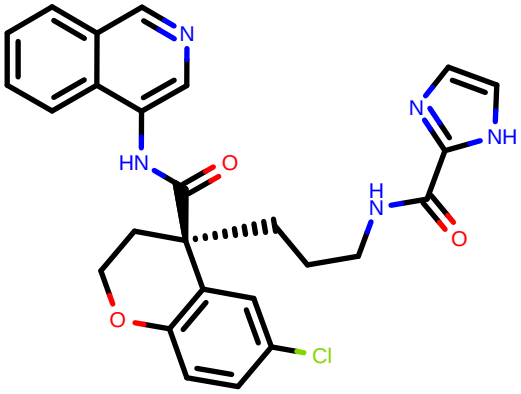
CID:	EN300-00271_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN2872
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.27

EN300-12587_3_2



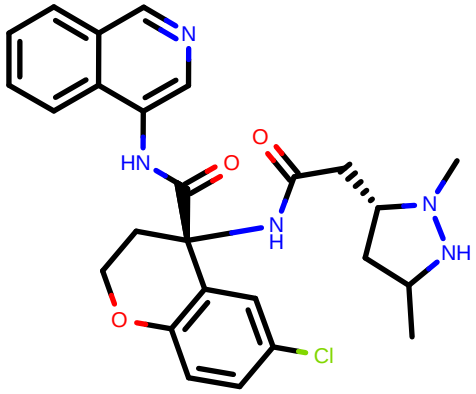
CID:	EN300-12587_3_2
SMILES:	CC(=O)N1CCC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3460
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.35

EN300-315836_4_1



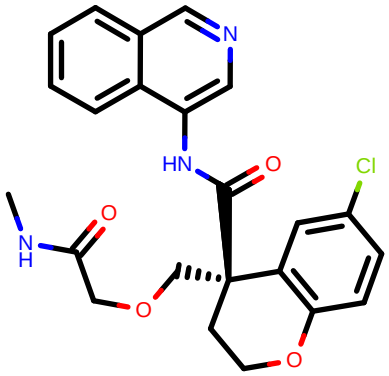
CID:	EN300-315836_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5[nH]ccn5
RUN:	RUN9683
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.35

EN300-6499639_1_1



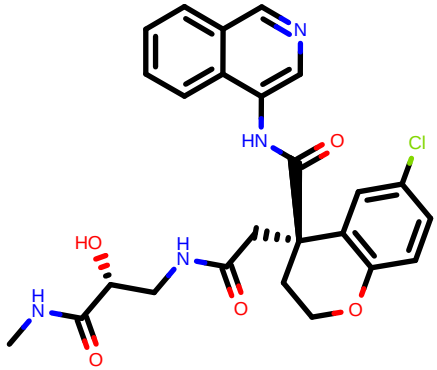
CID:	EN300-6499639_1_1
SMILES:	Cc1cc(n(n1)C)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4985
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.31

EN300-2977549_2_1



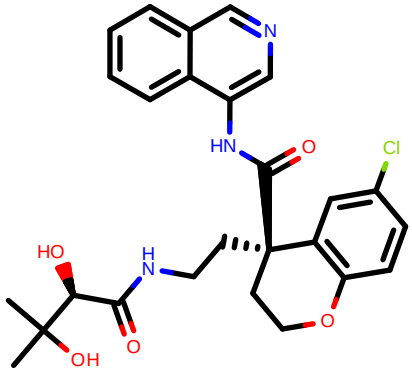
CID:	EN300-2977549_2_1
SMILES:	CNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1070
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.18

EN300-179352_1_1



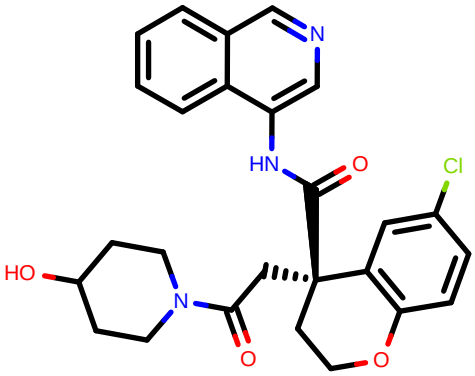
CID:	EN300-179352_1_1
SMILES:	CNC(=O)[C@@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN9027
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.32

EN300-299532_3_2



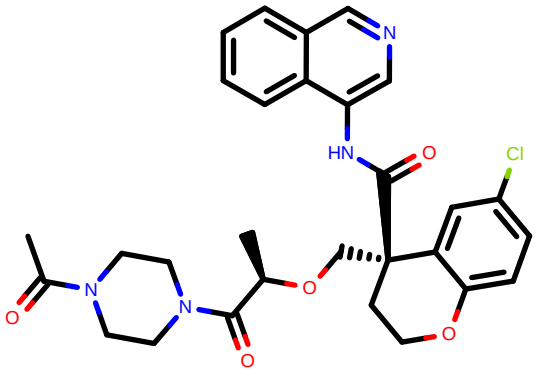
CID:	EN300-299532_3_2
SMILES:	CC(C)([C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN4699
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.37

EN300-379533_1_1



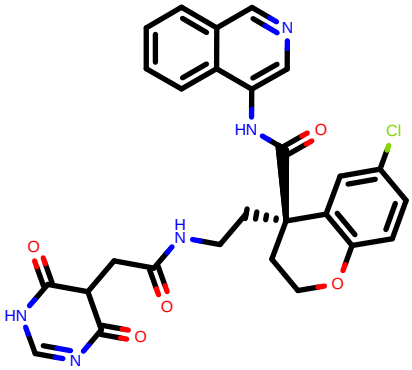
CID:	EN300-379533_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)O
RUN:	RUN6645
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.27

EN300-28106_2_2



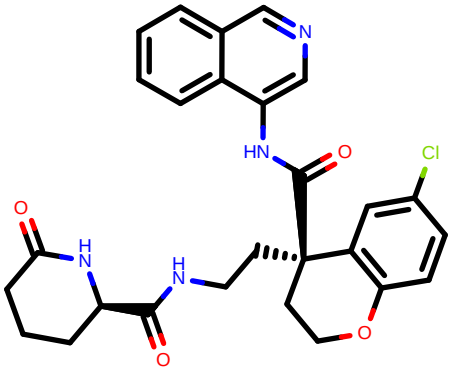
CID:	EN300-28106_2_2
SMILES:	C[C@H](C(=O)N1CCN(CC1)C(=O)C)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1621
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.39

EN300-86205_3_1



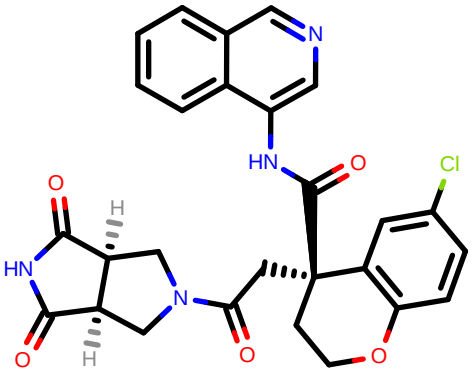
CID:	EN300-86205_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5c(=O)[nH]cnc5O
RUN:	RUN5770
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.39

EN300-146491_3_1



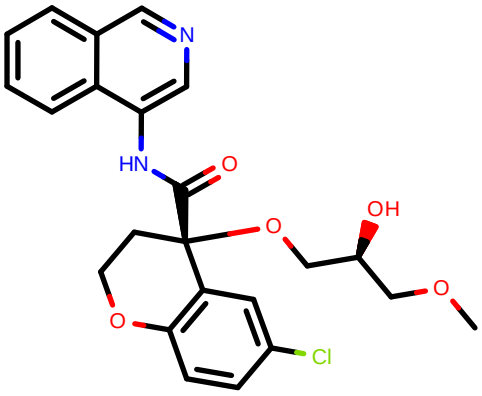
CID:	EN300-146491_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCC(=O)N5
RUN:	RUN5314
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.25

EN300-246333_1_1



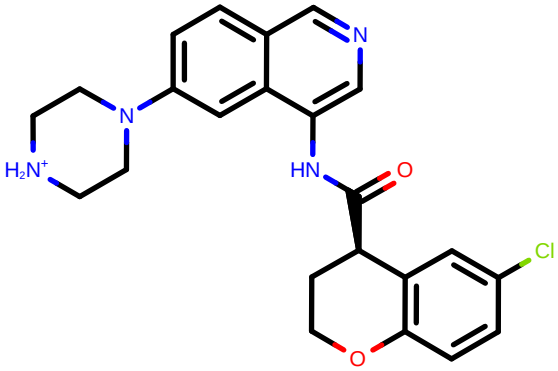
CID:	EN300-246333_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6[C@H](C5)C(=O)NC6=O
RUN:	RUN11044
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.43

EN300-1915260_1_1



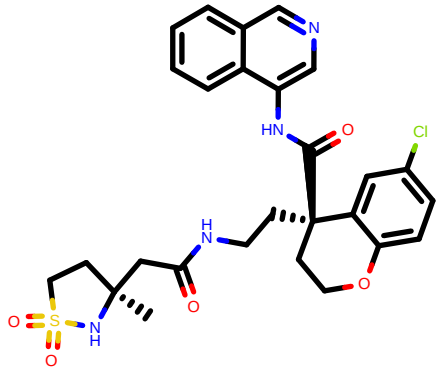
CID:	EN300-1915260_1_1
SMILES:	COC[C@@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1863
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.37

MAK-UNK-8be7dca9-4_1



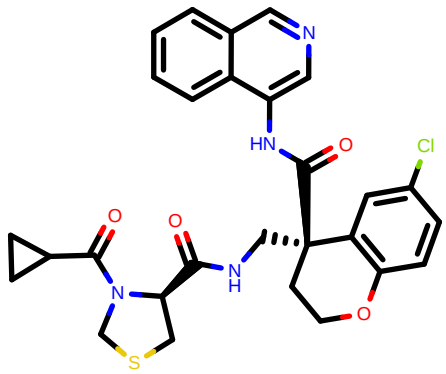
CID:	MAK-UNK-8be7dca9-4_1
SMILES:	c1cc2cncc(c2cc1N3CCNCC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN56
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.08

EN300-385235_3_2



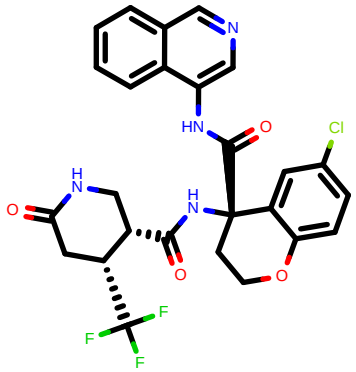
CID:	EN300-385235_3_2
SMILES:	C[C@]1(CCS(=O)(=O)N1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9336
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.36

EN300-18928_2_2



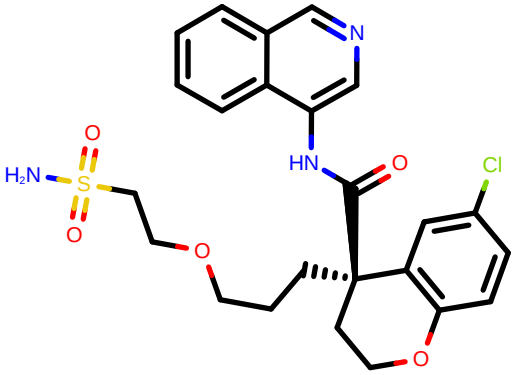
CID:	EN300-18928_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CSCN5C(=O)C6CC6
RUN:	RUN2963
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.35

EN300-208959_1_4



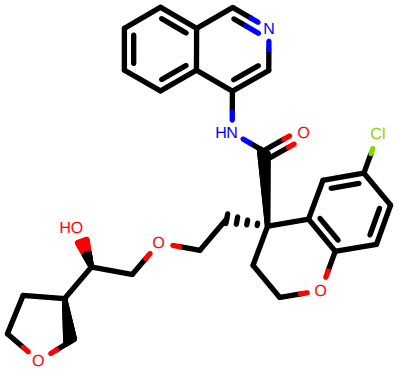
CID:	EN300-208959_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CNC(=O)C[C@H]5C(F)(F)F
RUN:	RUN7594
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.30

EN300-270710_4_1



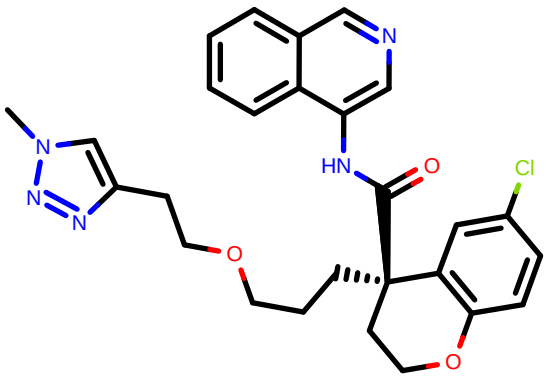
CID:	EN300-270710_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCS(=O)(=O)N
RUN:	RUN991
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.34

EN300-1911992_3_1



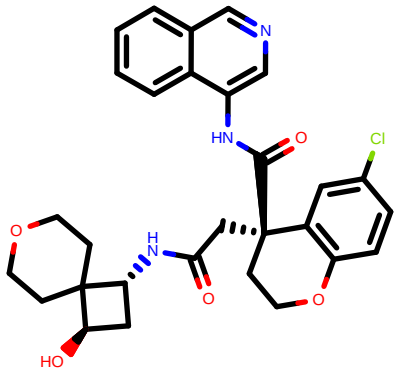
CID:	EN300-1911992_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]([C@@H]5CCOC5)O
RUN:	RUN481
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.32

EN300-1600786_4_1



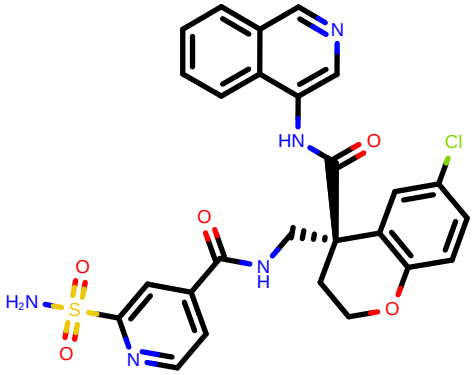
CID:	EN300-1600786_4_1
SMILES:	Cn1cc(nn1)CCOCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1918
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.31

EN300-640503_1_1



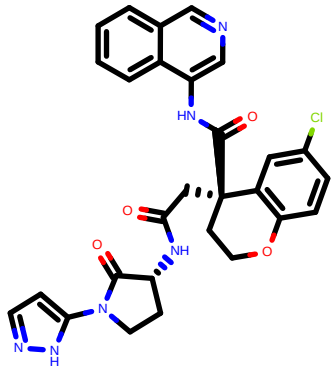
CID:	EN300-640503_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H](C56CCOCC6)O
RUN:	RUN8934
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.30

EN300-141628_2_1



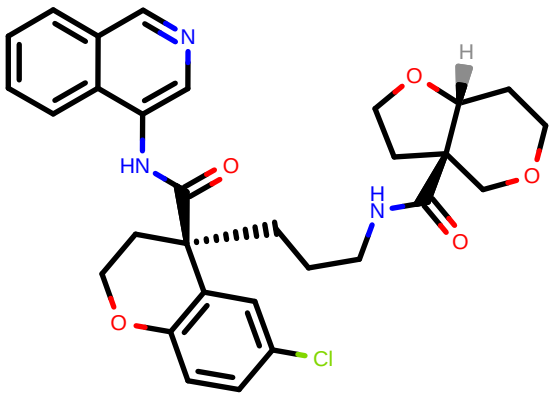
CID:	EN300-141628_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccnc(c5)S(=O)(=O)N
RUN:	RUN8103
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.46

EN300-7547467_1_1



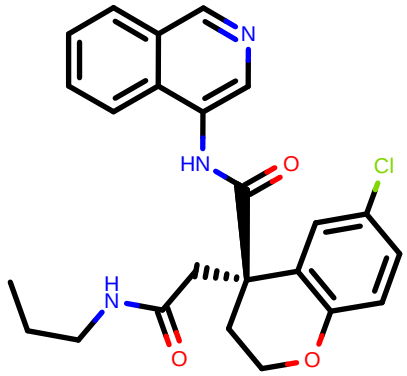
CID:	EN300-7547467_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCN(C5=O)c6ccn[nH]6
RUN:	RUN10472
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.34

EN300-341337_4_1



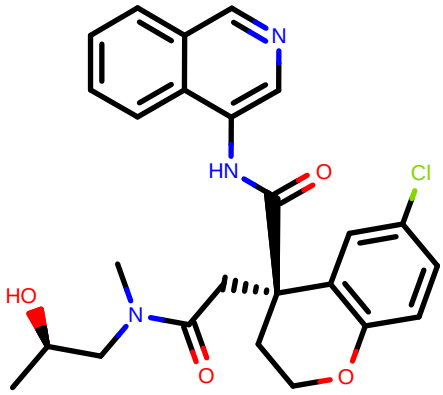
CID:	EN300-341337_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@]56CCO[C@@H]5CCOC6
RUN:	RUN9739
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.33

EN300-21409_1_1



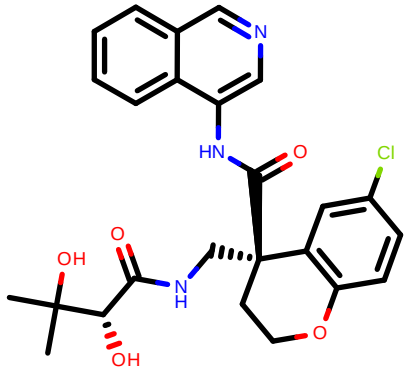
CID:	EN300-21409_1_1
SMILES:	C#CCNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10938
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.18

EN300-209068_1_1



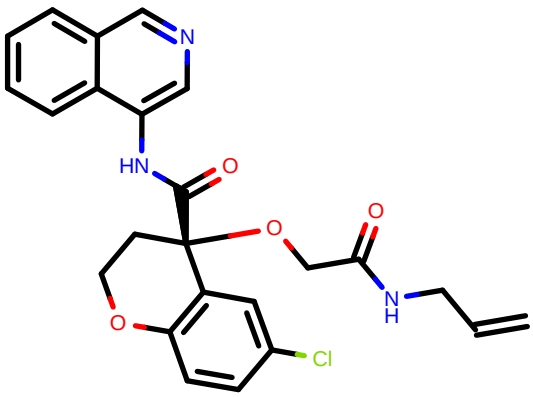
CID:	EN300-209068_1_1
SMILES:	C[C@H](CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN8616
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.33

EN300-299532_2_2



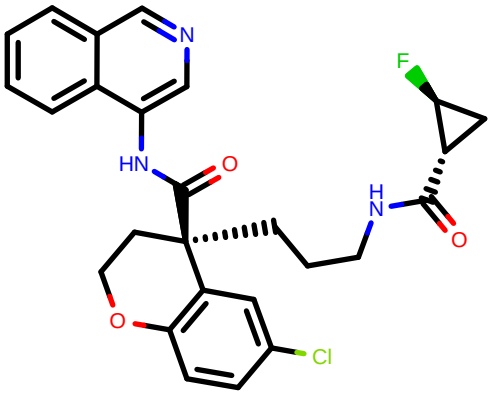
CID:	EN300-299532_2_2
SMILES:	CC(C)([C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN3738
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.39

EN300-17184_1_1



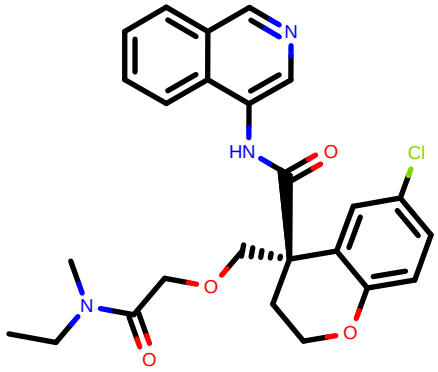
CID:	EN300-17184_1_1
SMILES:	C=CCNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN445
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.25

EN300-97300_4_2



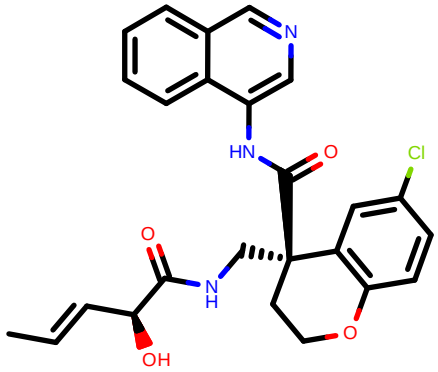
CID:	EN300-97300_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5C[C@@H]5F
RUN:	RUN10851
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.27

EN300-1253122_2_1



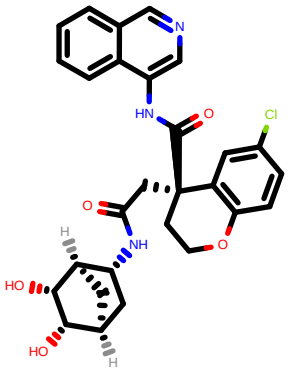
CID:	EN300-1253122_2_1
SMILES:	CCN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1446
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.23

EN300-300217_2_2



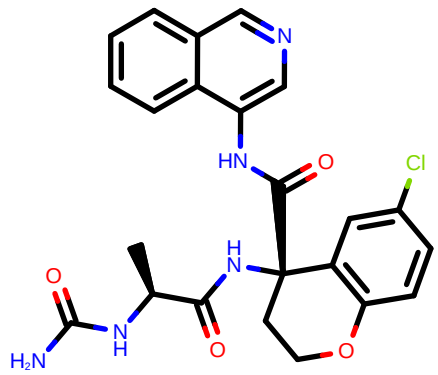
CID:	EN300-300217_2_2
SMILES:	C/C=C/[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4902
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.34

EN300-6763291_1_7



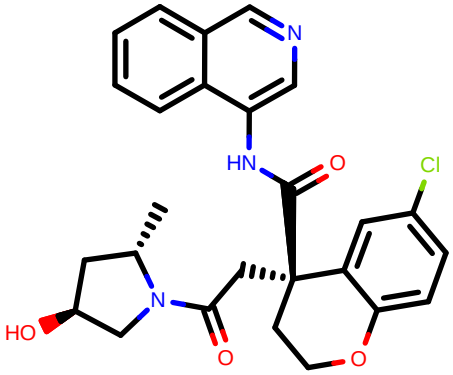
CID:	EN300-6763291_1_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC6CCS[C@H]([C@H]6O)O
RUN:	RUN9236
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.30

EN300-152705_1_1



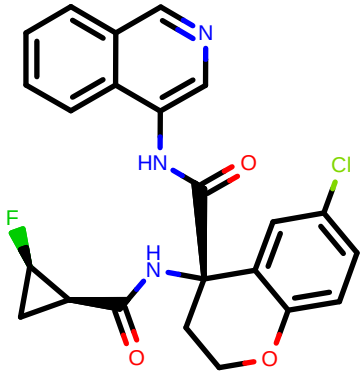
CID:	EN300-152705_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN3278
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.25

EN300-173562_1_2



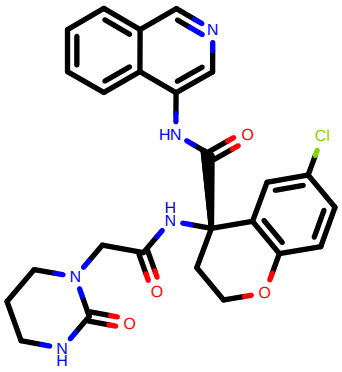
CID:	EN300-173562_1_2
SMILES:	C[C@H]1C[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7688
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.27

EN300-6953121_1_1



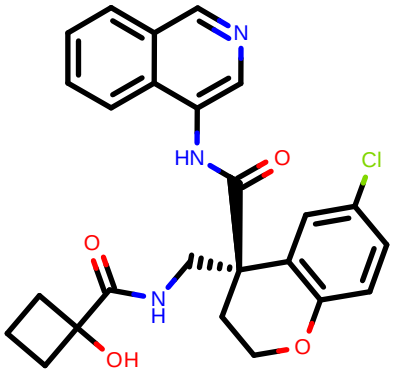
CID:	EN300-6953121_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5C[C@H]5F
RUN:	RUN2770
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.21

EN300-36096_1_1



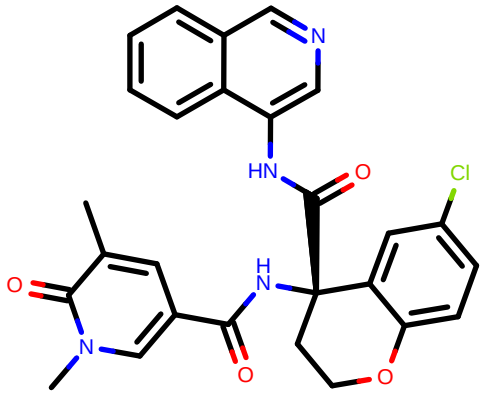
CID:	EN300-36096_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCNC5=O
RUN:	RUN7950
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.27

EN300-52009_2_1



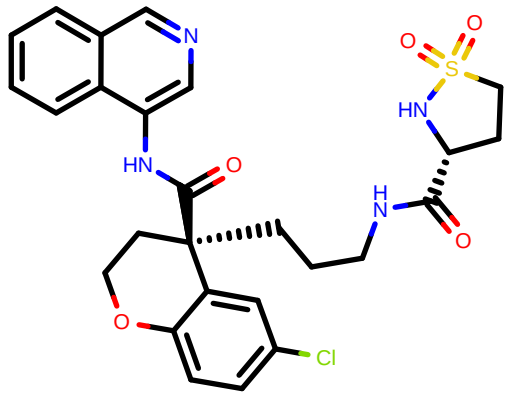
CID:	EN300-52009_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCC5)O
RUN:	RUN5541
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.25

EN300-1703340_1_1



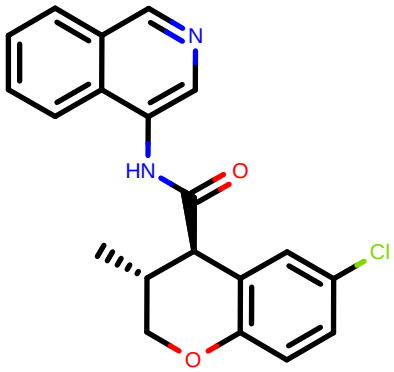
CID:	EN300-1703340_1_1
SMILES:	Cc1cc(cn(c1=O)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5117
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.24

EN300-45049_4_2



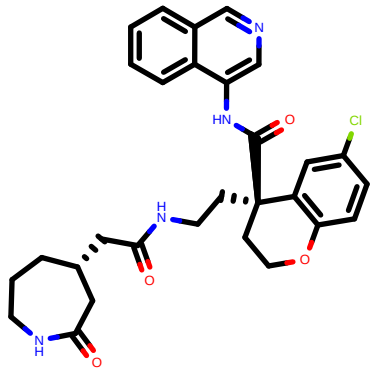
CID:	EN300-45049_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCS(=O)(=O)N5
RUN:	RUN9573
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.32

MAT-POS-8a69d52e-4_2



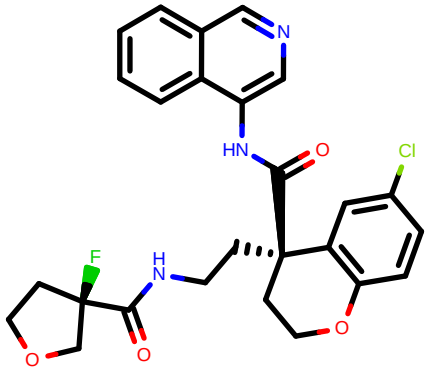
CID:	MAT-POS-8a69d52e-4_2
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN13
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.05

EN300-195590_3_2



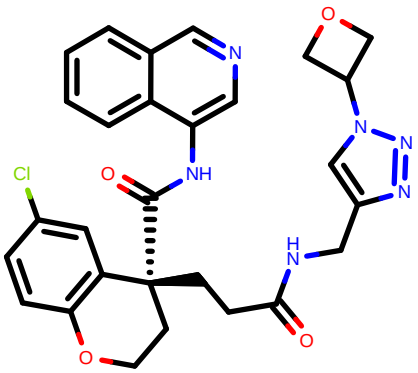
CID:	EN300-195590_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@H]5CCCNC(=O)C5
RUN:	RUN5590
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.36

EN300-188356_3_2



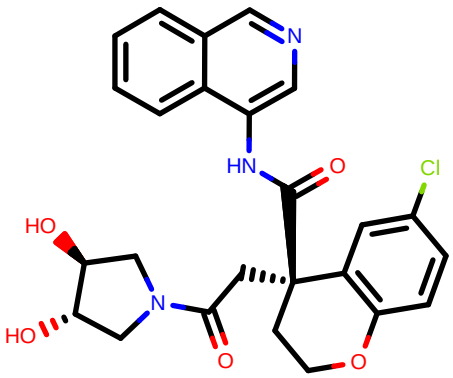
CID:	EN300-188356_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOC5)F
RUN:	RUN3528
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.34

EN300-1709745_2_1



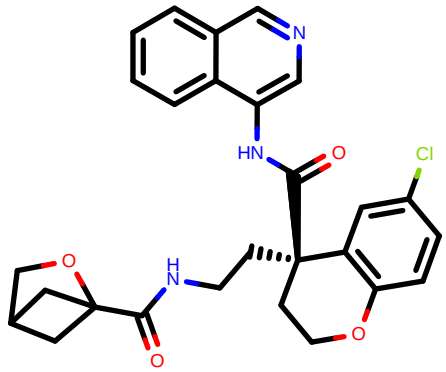
CID:	EN300-1709745_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cn(nn5)C6COC6
RUN:	RUN10375
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.22

EN300-96037_1_1



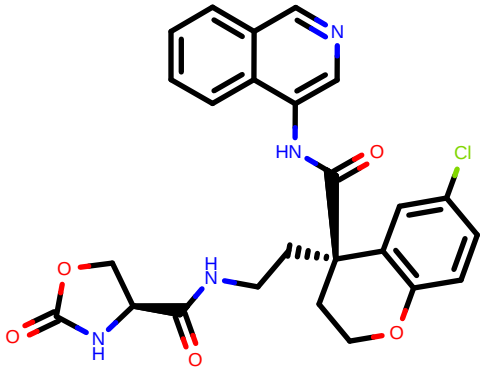
CID:	EN300-96037_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]([C@H](C5)O)O
RUN:	RUN4903
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.33

EN300-2007648_3_1



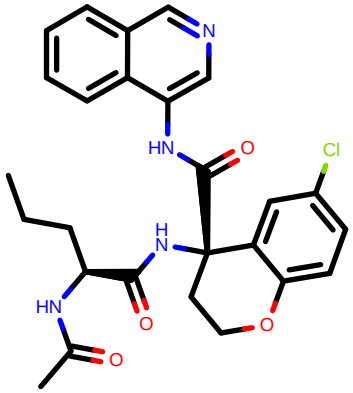
CID:	EN300-2007648_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C56CC(C5)CO6
RUN:	RUN11162
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.25

EN300-126389_3_1



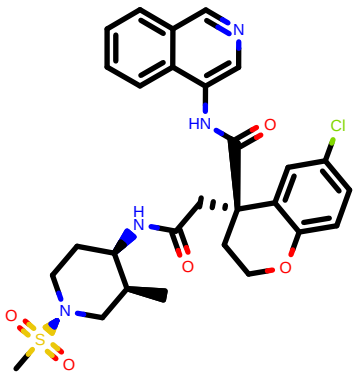
CID:	EN300-126389_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5COC(=O)N5
RUN:	RUN8404
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.29

EN300-51801_1_1



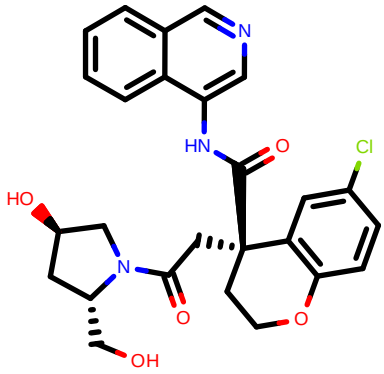
CID:	EN300-51801_1_1
SMILES:	CCC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN5468
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.26

EN300-94479_1_4



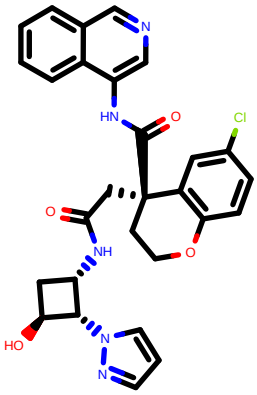
CID:	EN300-94479_1_4
SMILES:	C[C@H]1CN(CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN10660
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.38

EN300-153245_1_1



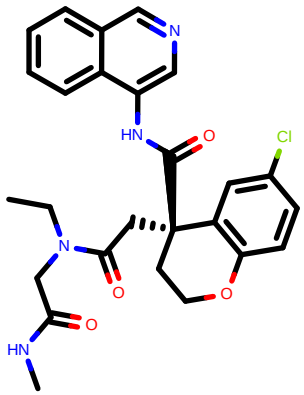
CID:	EN300-153245_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@H]5CO)O
RUN:	RUN10778
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.34

EN300-260696_1_6



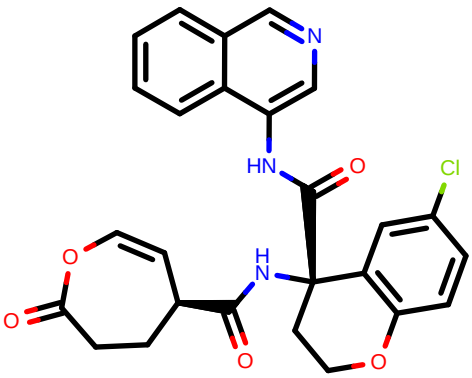
CID:	EN300-260696_1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@@H][C@H]5n6cccn6)O
RUN:	RUN2438
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.40

EN300-39007_1_1



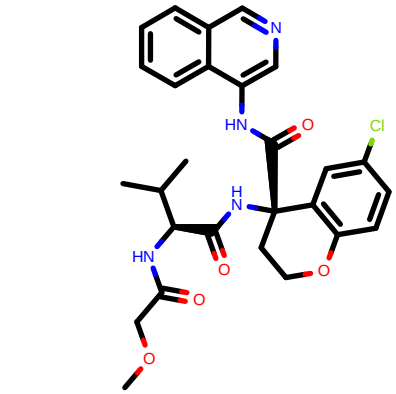
CID:	EN300-39007_1_1
SMILES:	CCN(CC(=O)NC)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9522
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.30

EN300-2011083_1_2



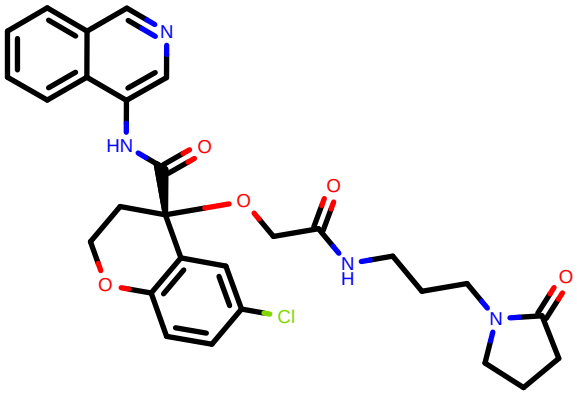
CID:	EN300-2011083_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCC(=O)OCC5
RUN:	RUN3314
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.28

EN300-83918_1_1



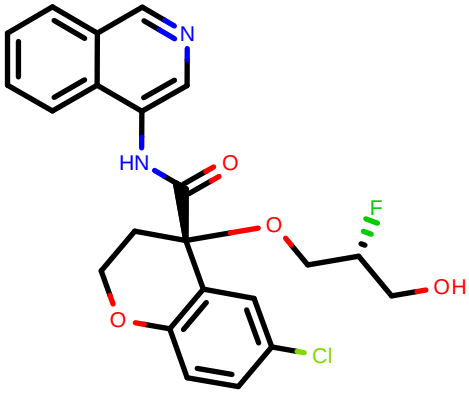
CID:	EN300-83918_1_1
SMILES:	CC(C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)COC
RUN:	RUN6707
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.26

EN300-08259_1_1



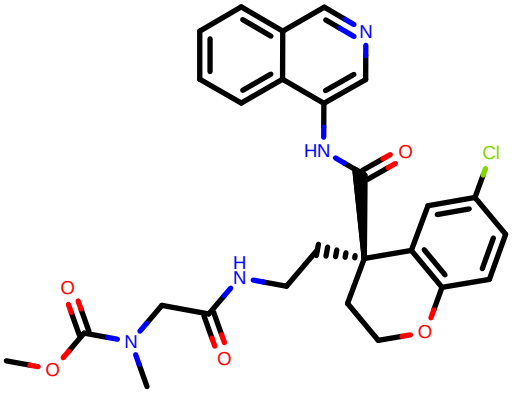
CID:	EN300-08259_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCN5CCCC5=O
RUN:	RUN2223
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.37

EN300-1600517_1_1



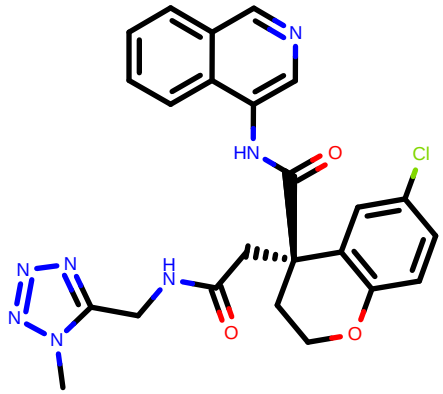
CID:	EN300-1600517_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](CO)F
RUN:	RUN2268
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.32

EN300-39005_3_1



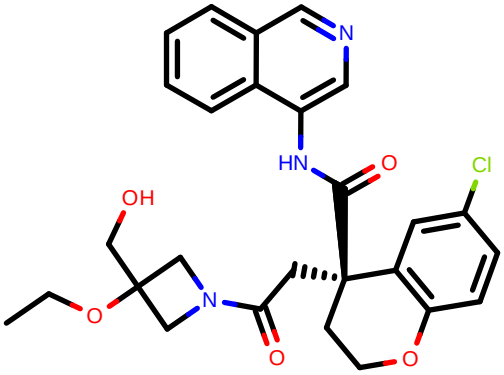
CID:	EN300-39005_3_1
SMILES:	CN(CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)OC
RUN:	RUN4527
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.39

EN300-156212_1_1



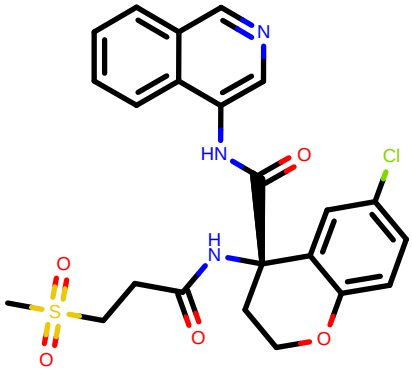
CID:	EN300-156212_1_1
SMILES:	Cn1c(nnn1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7976
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.26

EN300-7432898_1_1



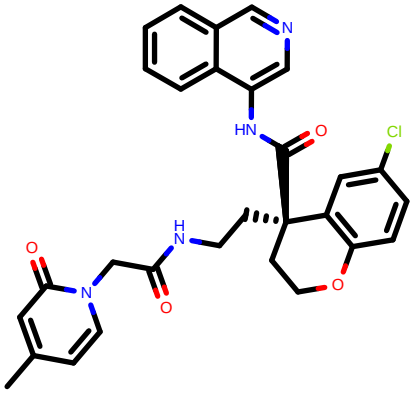
CID:	EN300-7432898_1_1
SMILES:	CCOC1(CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN6361
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.38

EN300-31387_1_1



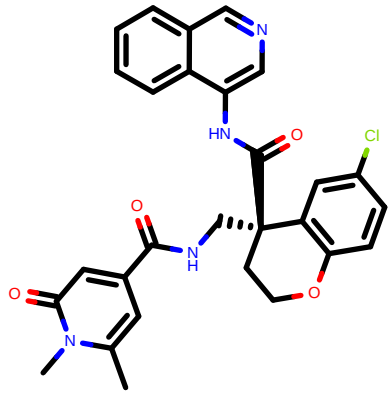
CID:	EN300-31387_1_1
SMILES:	CS(=O)(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2810
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.33

EN300-184446_3_1



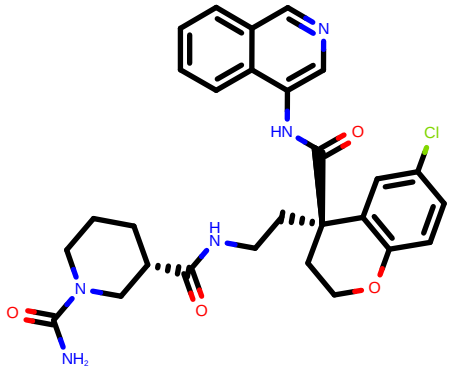
CID:	EN300-184446_3_1
SMILES:	Cc1ccn(c(=O)c1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9224
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.32

EN300-4287199_2_1



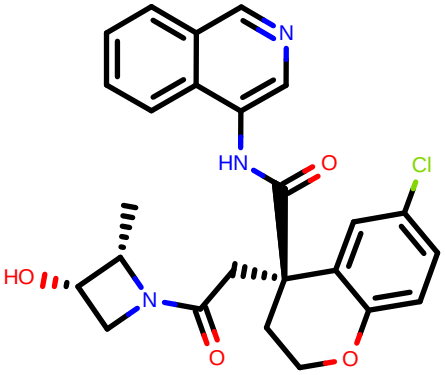
CID:	EN300-4287199_2_1
SMILES:	Cc1cc(cc(=O)n1C)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8407
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.34

EN300-14767_3_2



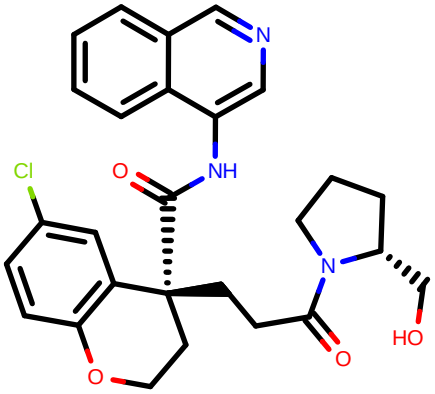
CID:	EN300-14767_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCN(C5)C(=O)N
RUN:	RUN3891
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.33

EN300-7471076_1_4



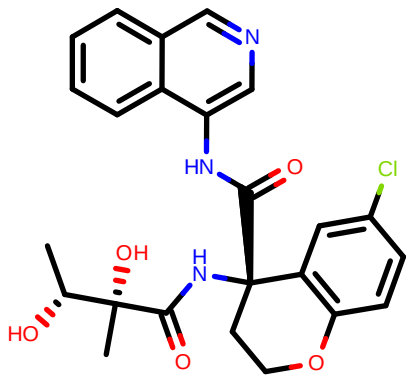
CID:	EN300-7471076_1_4
SMILES:	C[C@H]1[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2137
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.31

EN300-54891_2_1



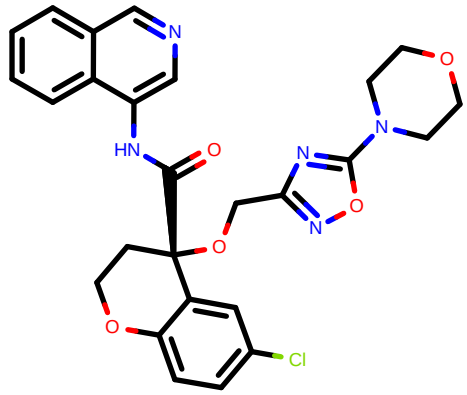
CID:	EN300-54891_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@@H]5CO
RUN:	RUN3177
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.25

EN300-202922_1_4



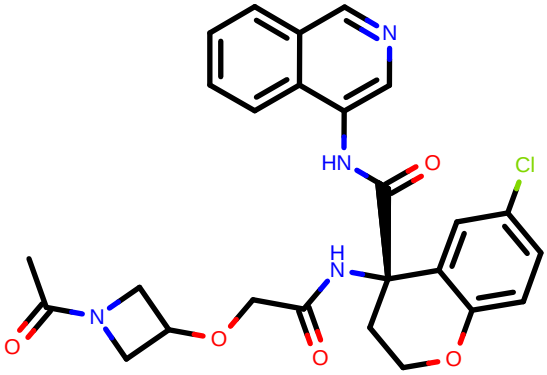
CID:	EN300-202922_1_4
SMILES:	C[C@H]([C@](C)(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN1357
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.42

EN300-1608590_1_1



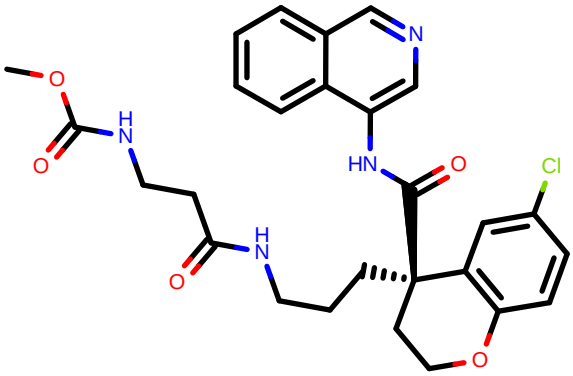
CID:	EN300-1608590_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nc(on5)N6CCOCC6
RUN:	RUN1615
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.24

EN300-259004_1_1



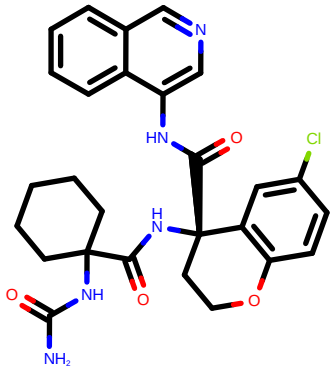
CID:	EN300-259004_1_1
SMILES:	CC(=O)N1CC(C1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3258
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.33

EN300-71558_4_1



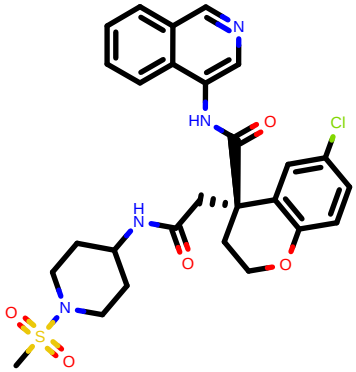
CID:	EN300-71558_4_1
SMILES:	COC(=O)NCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9565
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.31

EN300-78368_1_1



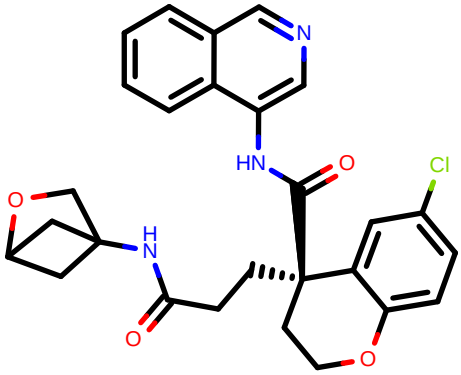
CID:	EN300-78368_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCCCC5)NC(=O)N
RUN:	RUN6599
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.39

EN300-34705_1_1



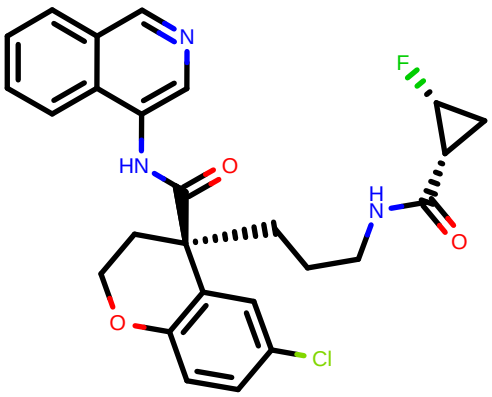
CID:	EN300-34705_1_1
SMILES:	CS(=O)(=O)N1CCC(CC1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11174
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.40

EN300-6734977_2_1



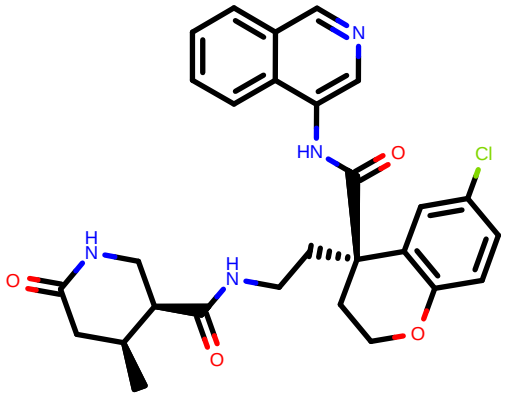
CID:	EN300-6734977_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC56CC(C5)OC6
RUN:	RUN7233
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.25

EN300-6953121_4_1



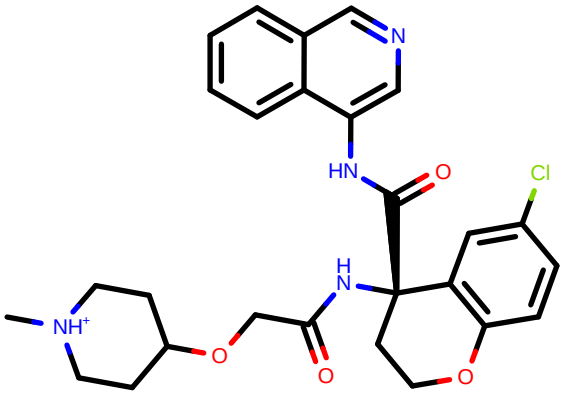
CID:	EN300-6953121_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5C[C@H]5F
RUN:	RUN10867
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.31

EN300-95698_3_4



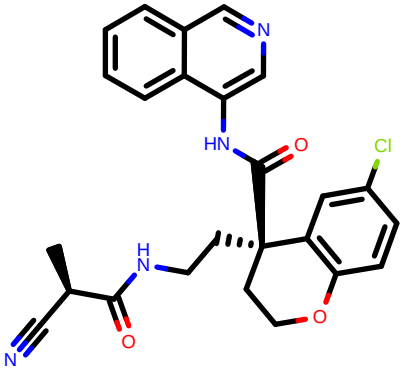
CID:	EN300-95698_3_4
SMILES:	C[C@H]1CC(=O)NC[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10143
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.35

EN300-237224_1_1



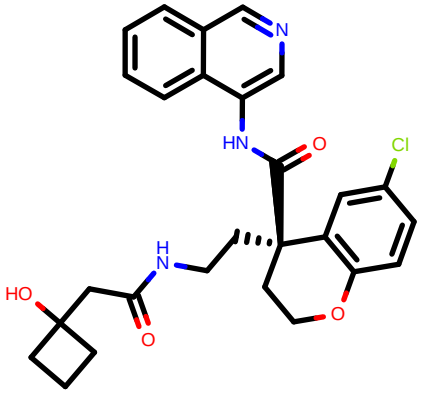
CID:	EN300-237224_1_1
SMILES:	CN1CCC(CC1)OCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5608
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.27

EN300-72730_3_2



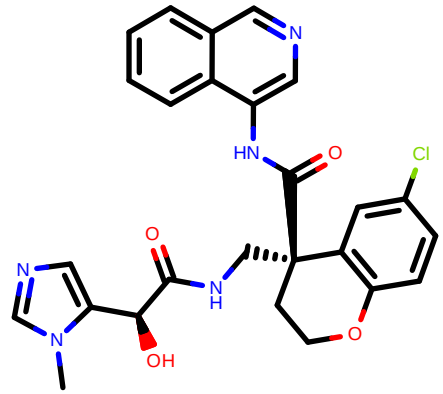
CID:	EN300-72730_3_2
SMILES:	C[C@H](C#N)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6441
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.26

EN300-246423_3_1



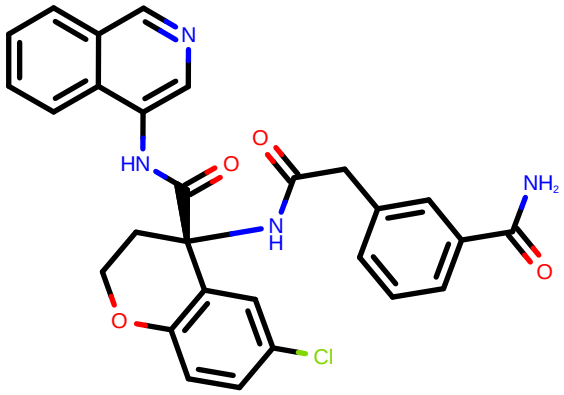
CID:	EN300-246423_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CCC5)O
RUN:	RUN5842
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.29

EN300-190283_2_1



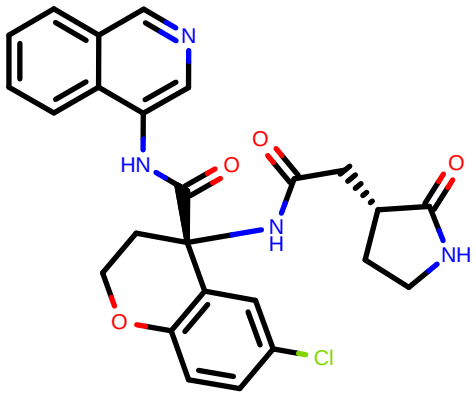
CID:	EN300-190283_2_1
SMILES:	Cn1cncc1[C@@H](C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5126
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.36

EN300-1179673_1_1



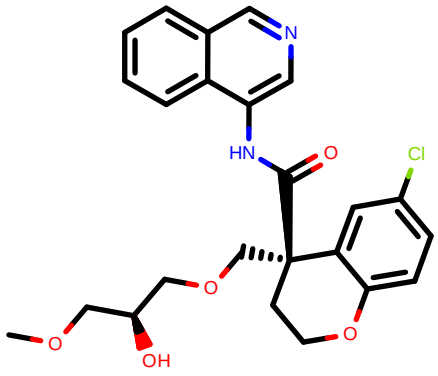
CID:	EN300-1179673_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cccc(c5)C(=O)N
RUN:	RUN7370
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.24

EN300-343474_1_2



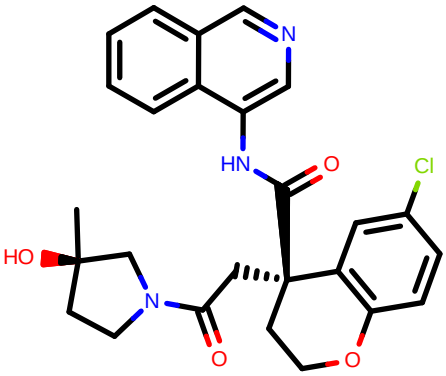
CID:	EN300-343474_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCNC5=O
RUN:	RUN3406
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.27

EN300-1915260_2_1



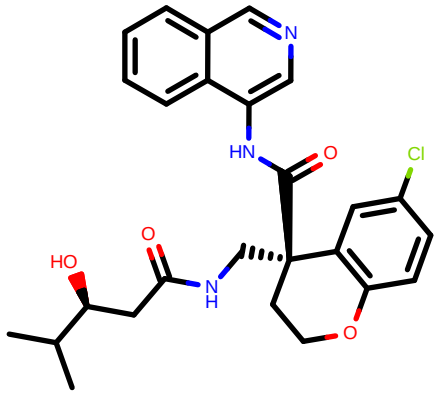
CID:	EN300-1915260_2_1
SMILES:	COC[C@@H](COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN934
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.42

EN300-99161_1_2



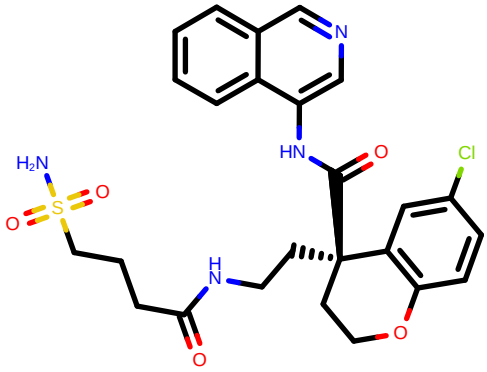
CID:	EN300-99161_1_2
SMILES:	C[C@]1(CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3536
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.35

EN300-155498_2_1



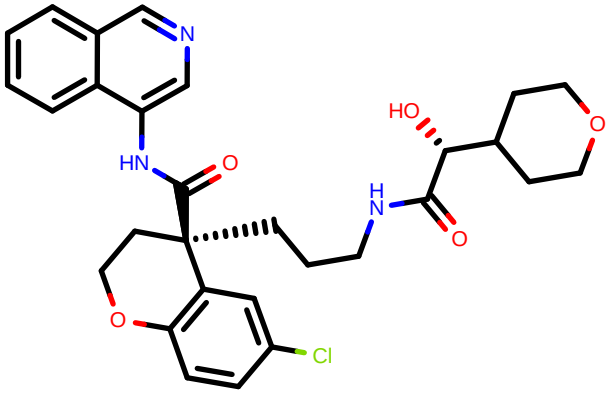
CID:	EN300-155498_2_1
SMILES:	CC(=C)[C@H](CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3742
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.35

EN300-39504_3_1



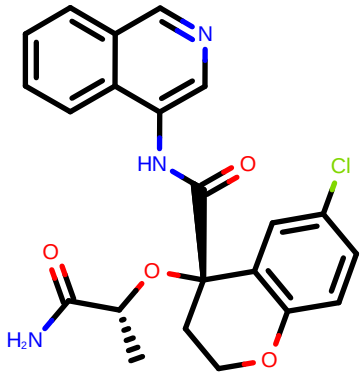
CID:	EN300-39504_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCS(=O)(=O)N
RUN:	RUN3735
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.40

EN300-7443878_4_1



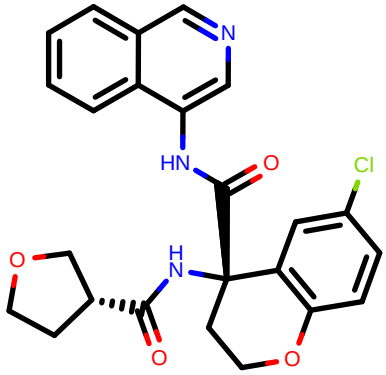
CID:	EN300-7443878_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H](C5CCOCC5)O
RUN:	RUN10257
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.34

EN300-17381_1_2



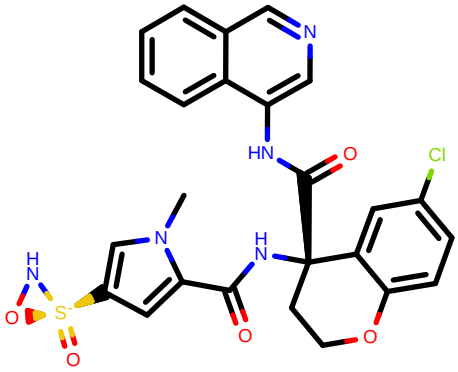
CID:	EN300-17381_1_2
SMILES:	C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN817
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.21

EN300-697519_1_1



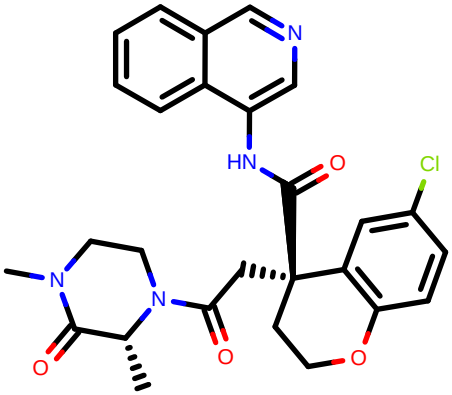
CID:	EN300-697519_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC5
RUN:	RUN5261
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.30

EN300-24102_1_1



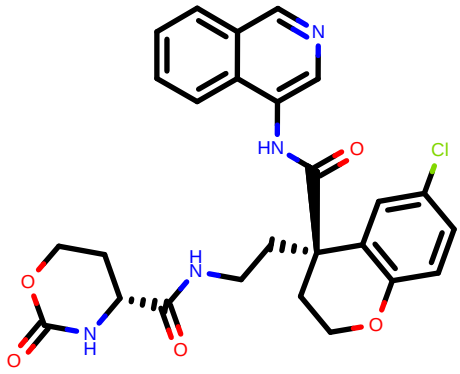
CID:	EN300-24102_1_1
SMILES:	Cn1cc(cc1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)N
RUN:	RUN9101
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.30

EN300-155764_1_1



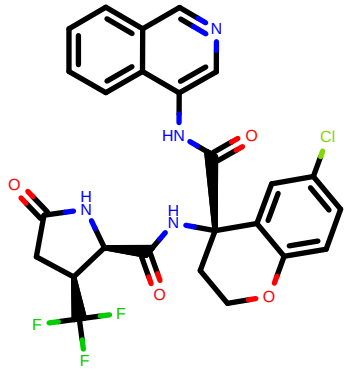
CID:	EN300-155764_1_1
SMILES:	C[C@@H]1C(=O)N(CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN6685
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.34

EN300-249804_3_2



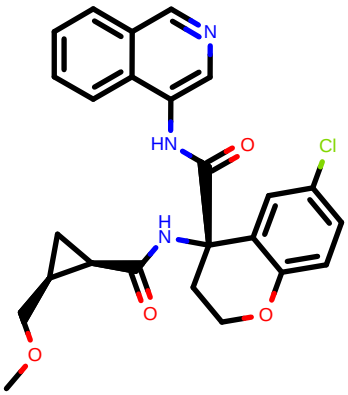
CID:	EN300-249804_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC(=O)N5
RUN:	RUN10131
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.29

EN300-169955_1_4



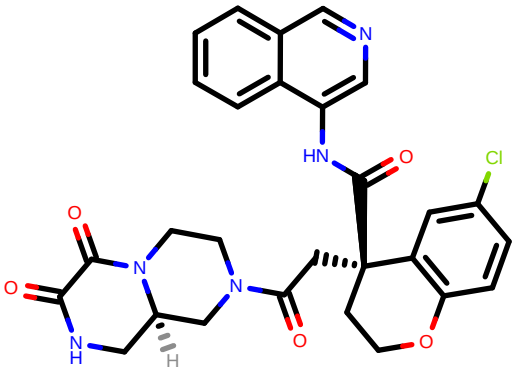
CID:	EN300-169955_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5[C@H](CC(=O)N5)C(F)(F)F
RUN:	RUN7418
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.26

EN300-705381_1_1



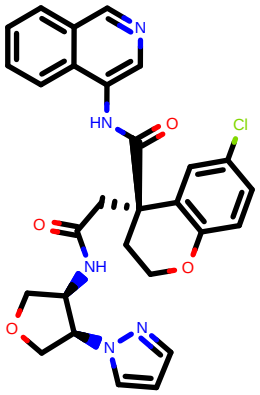
CID:	EN300-705381_1_1
SMILES:	COC[C@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1692
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.29

EN300-100768_1_1



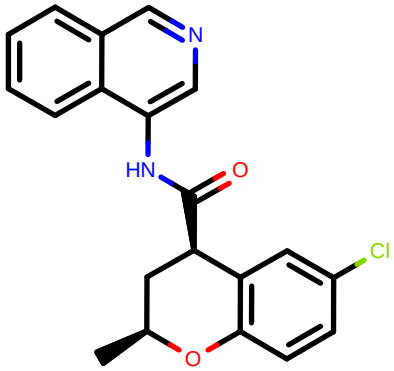
CID:	EN300-100768_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@H](C5)CNC(=O)C6=O
RUN:	RUN1122
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.40

EN300-1086925_1_1



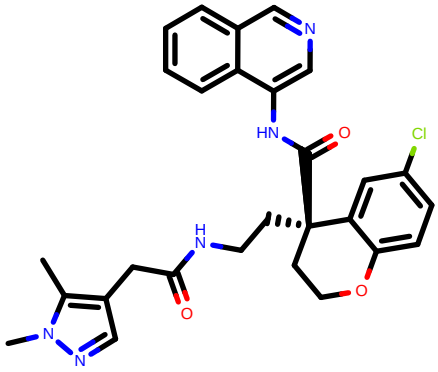
CID:	EN300-1086925_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5n6cccn6
RUN:	RUN4571
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.30

EDJ-MED-e4b030d8-3_1



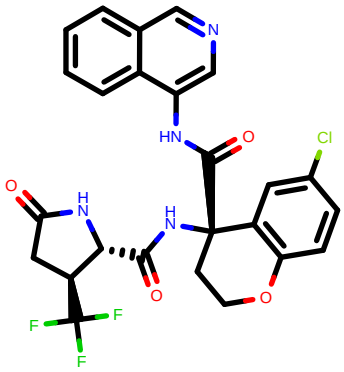
CID:	EDJ-MED-e4b030d8-3_1
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN22
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.09

EN300-219437_3_1



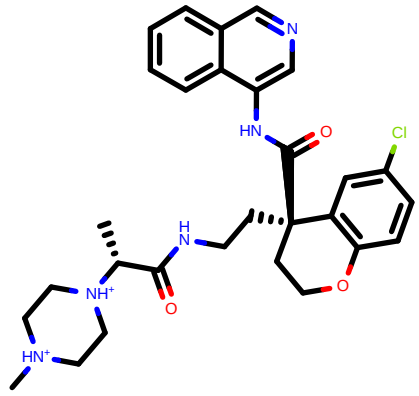
CID:	EN300-219437_3_1
SMILES:	Cc1c(cnn1C)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7768
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.36

EN300-169955_1_3



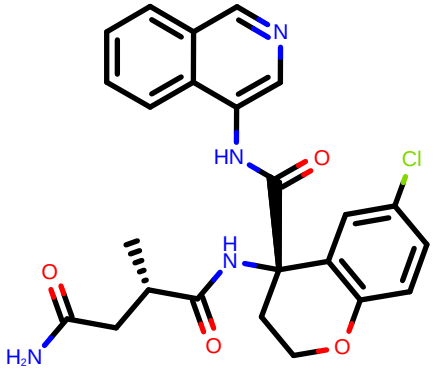
CID:	EN300-169955_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5[C@H](CC(=O)N5)C(F)(F)F
RUN:	RUN7618
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.32

EN300-45384_3_2



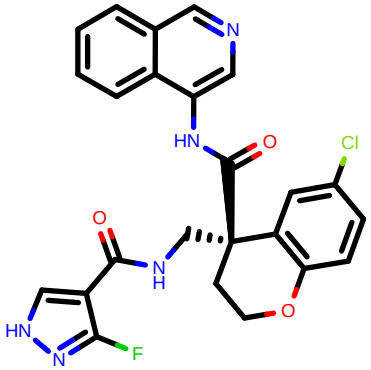
CID:	EN300-45384_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N5CCN(CC5)C
RUN:	RUN10804
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.38

EN300-202757_1_1



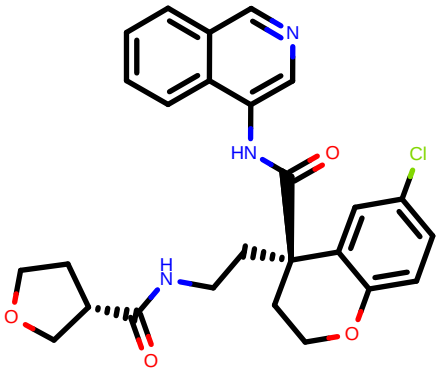
CID:	EN300-202757_1_1
SMILES:	C[C@@H](CC(=O)N)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2196
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.27

EN300-7121836_2_1



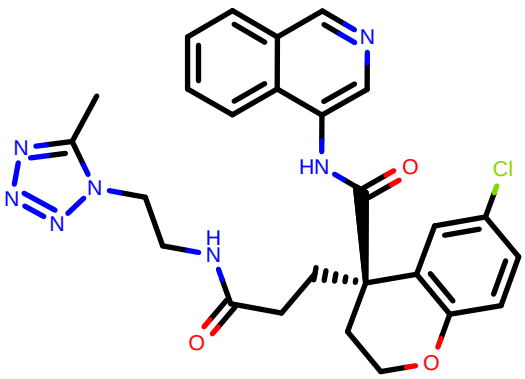
CID:	EN300-7121836_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]c5F
RUN:	RUN6552
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.21

EN300-53423_3_2



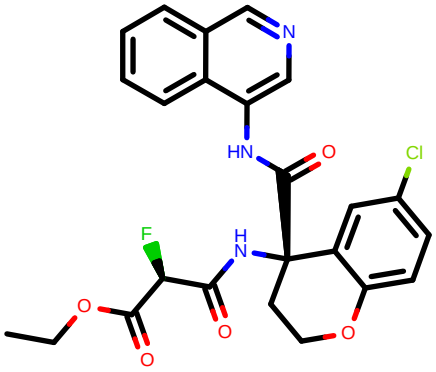
CID:	EN300-53423_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCOC5
RUN:	RUN3967
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.28

EN300-77343_2_1



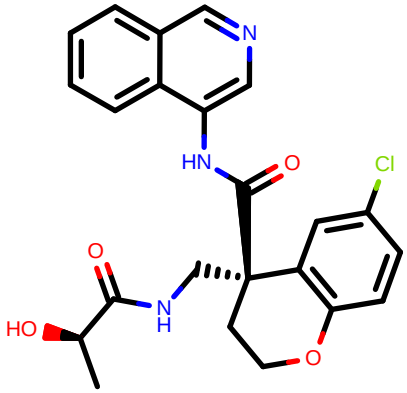
CID:	EN300-77343_2_1
SMILES:	Cc1nnnn1CCNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8441
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.30

EN300-123398_1_2



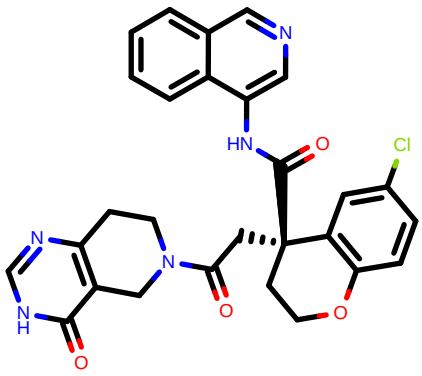
CID:	EN300-123398_1_2
SMILES:	CCOC(=O)[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)F
RUN:	RUN2790
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.26

EN300-77464_2_1



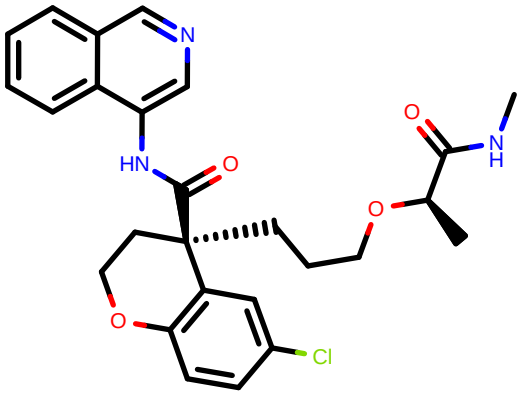
CID:	EN300-77464_2_1
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2032
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.22

EN300-175474_1_1



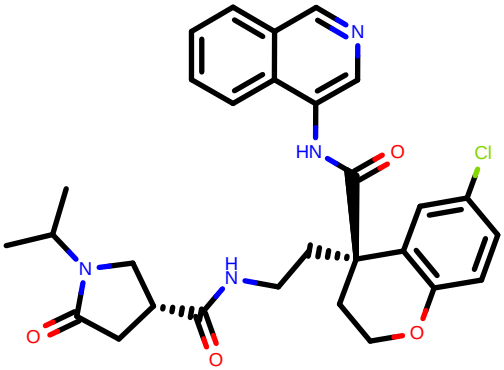
CID:	EN300-175474_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c(c(=O)[nH]cn6)C5
RUN:	RUN9165
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.42

EN300-211482_4_2



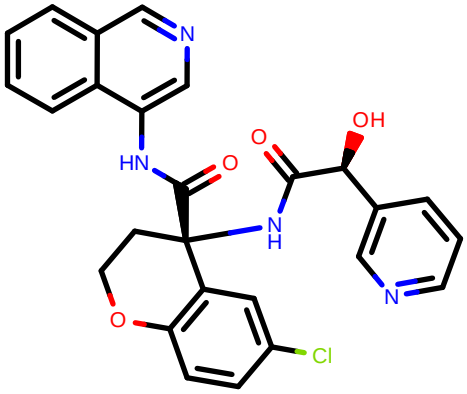
CID:	EN300-211482_4_2
SMILES:	C[C@H](C(=O)NC)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN364
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.34

EN300-33398_3_1



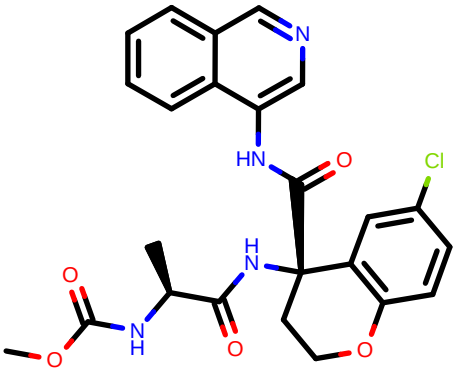
CID:	EN300-33398_3_1
SMILES:	CC(C)N1C[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2908
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.50

EN300-134855_1_2



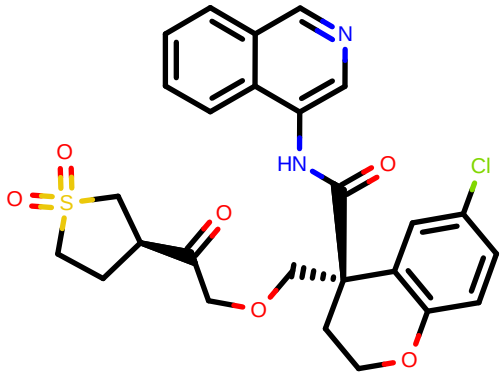
CID:	EN300-134855_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](c5cccnc5)O
RUN:	RUN6279
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.25

EN300-120068_1_1



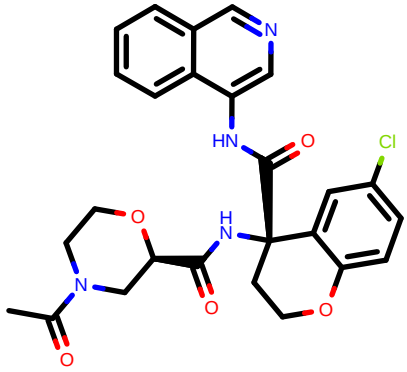
CID:	EN300-120068_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)OC
RUN:	RUN4345
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.24

EN300-226314_2_2



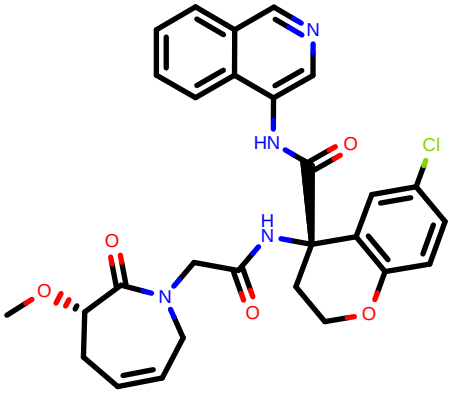
CID:	EN300-226314_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)[C@H]5CCS(=O)(=O)C5
RUN:	RUN459
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.44

EN300-100689_1_2



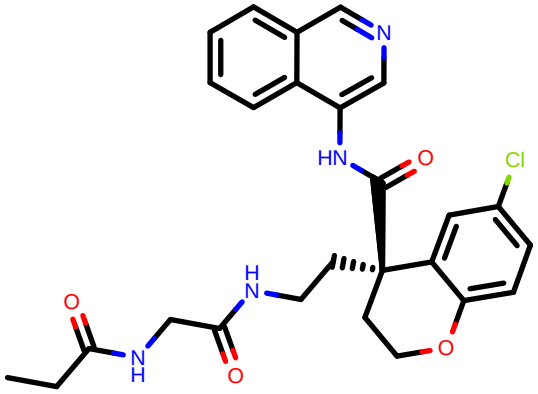
CID:	EN300-100689_1_2
SMILES:	CC(=O)N1CCO[C@H](C1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5776
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.25

EN300-259847_1_2



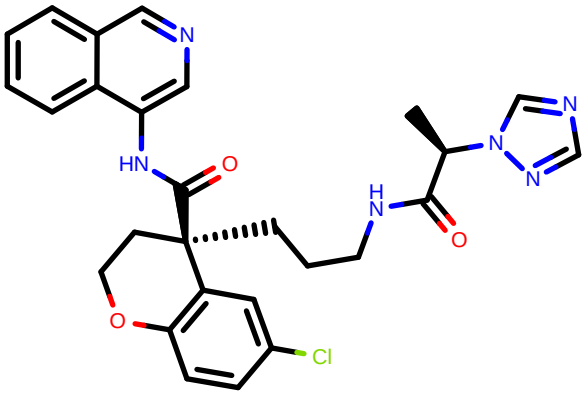
CID:	EN300-259847_1_2
SMILES:	CO[C@H]1CCCCN(C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4697
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.30

EN300-31099_3_1



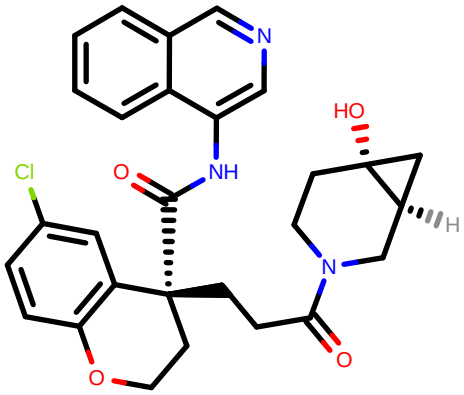
CID:	EN300-31099_3_1
SMILES:	CCC(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2896
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.29

EN300-30397_4_2



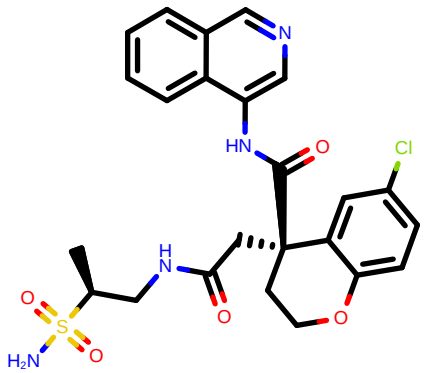
CID:	EN300-30397_4_2
SMILES:	C[C@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cncn5
RUN:	RUN10985
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.36

EN300-303908_2_1



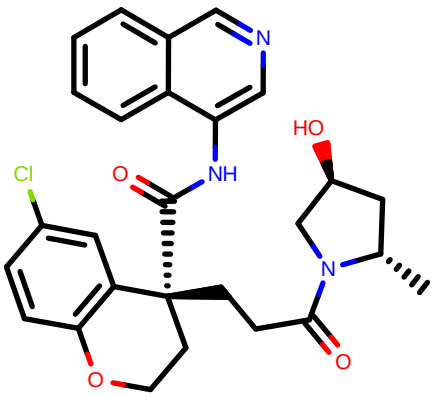
CID:	EN300-303908_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@]6(C[C@H]6C5)O
RUN:	RUN6258
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.30

EN300-123623_1_1



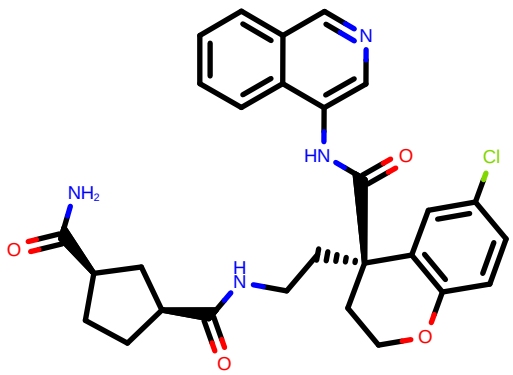
CID:	EN300-123623_1_1
SMILES:	C[C@@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N
RUN:	RUN6665
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.28

EN300-173562_2_2



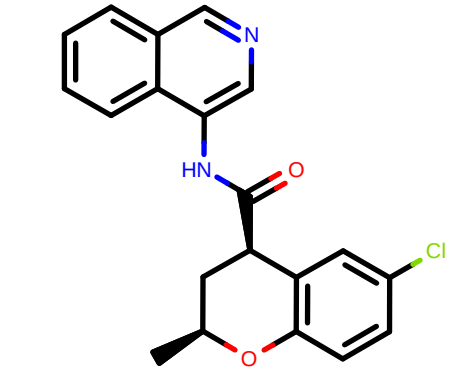
CID:	EN300-173562_2_2
SMILES:	C[C@H]1C[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4792
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.27

EN300-370753_3_1



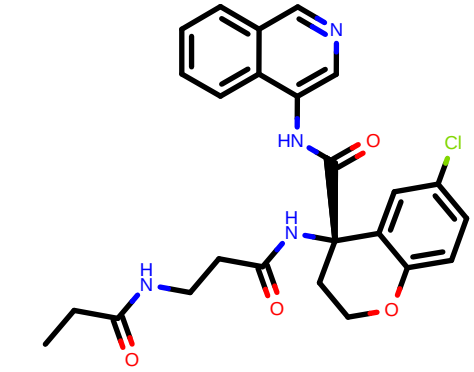
CID:	EN300-370753_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC[C@H](C5)C(=O)N
RUN:	RUN3763
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.26

MAT-POS-8a69d52e-1_4



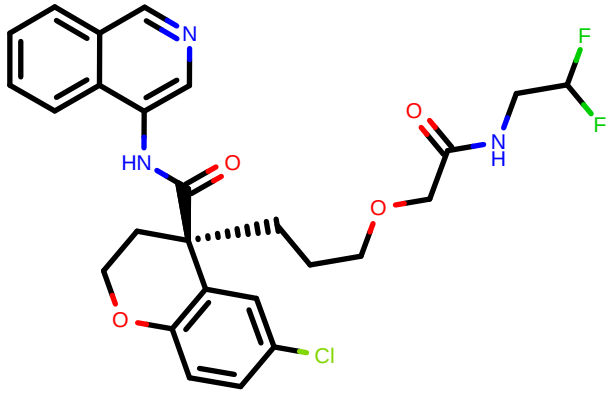
CID:	MAT-POS-8a69d52e-1_4
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN21
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.09

EN300-31186_1_1



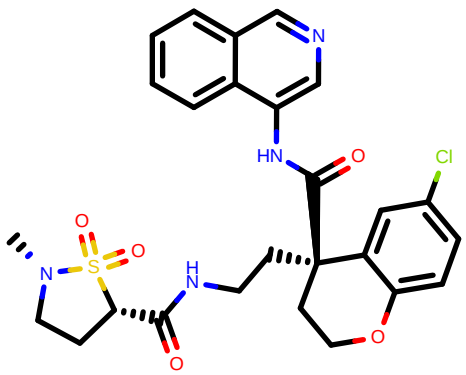
CID:	EN300-31186_1_1
SMILES:	CCC(=O)NCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2476
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.31

EN300-120586_4_1



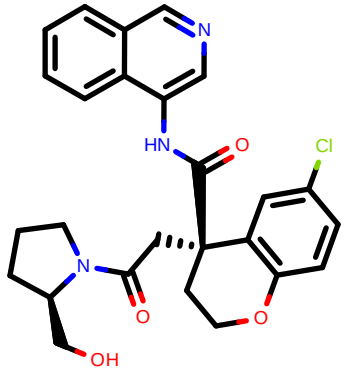
CID:	EN300-120586_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)NCC(F)F
RUN:	RUN1878
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.32

EN300-255496_3_2



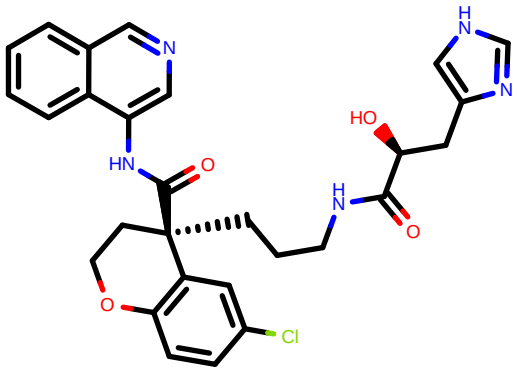
CID:	EN300-255496_3_2
SMILES:	CN1CC[C@H](S1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6573
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.38

EN300-378343_1_1



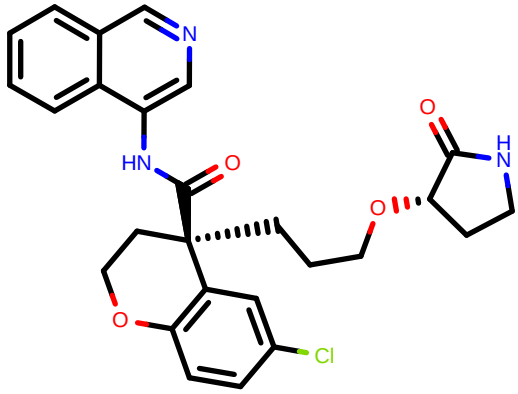
CID:	EN300-378343_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC=C[C@@H]5CO
RUN:	RUN10380
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.24

EN300-6503811_4_1



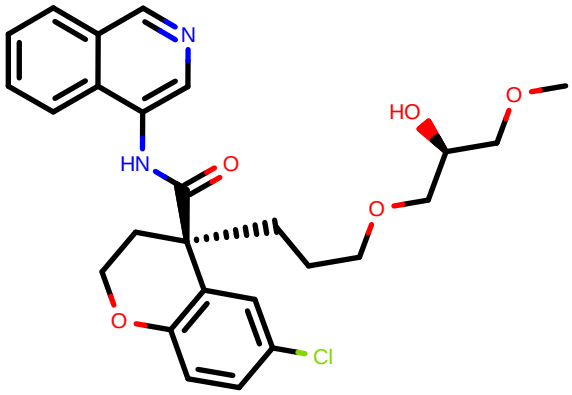
CID:	EN300-6503811_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H](Cc5cnc[nH]5)O
RUN:	RUN9851
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.40

EN300-6736413_4_2



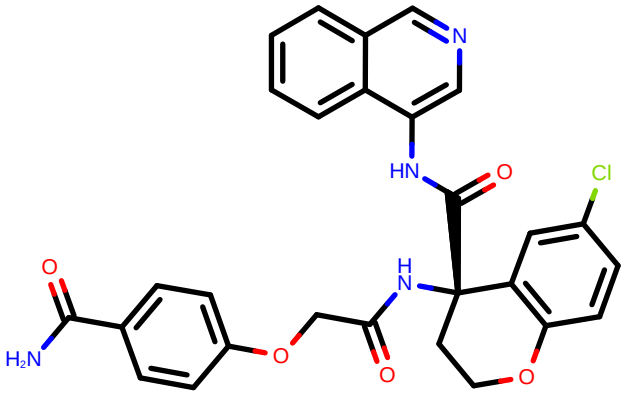
CID:	EN300-6736413_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@H]5CCNC5=O
RUN:	RUN1974
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.26

EN300-1915260_4_1



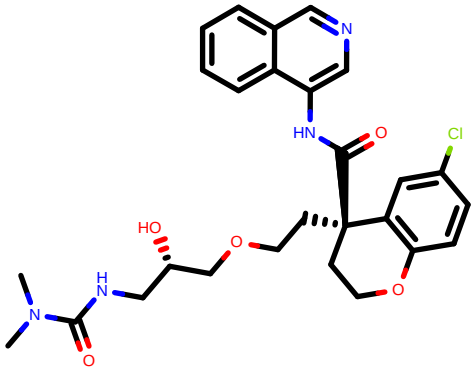
CID:	EN300-1915260_4_1
SMILES:	COC[C@@H](COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN714
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.42

EN300-55498_1_1



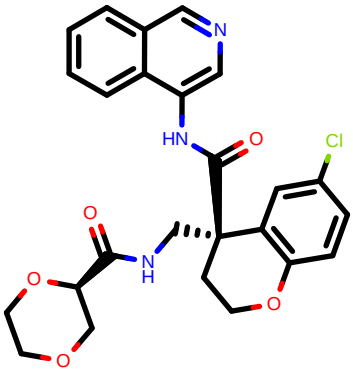
CID:	EN300-55498_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)COc5ccc(cc5)C(=O)N
RUN:	RUN5049
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.36

EN300-6501360_3_1



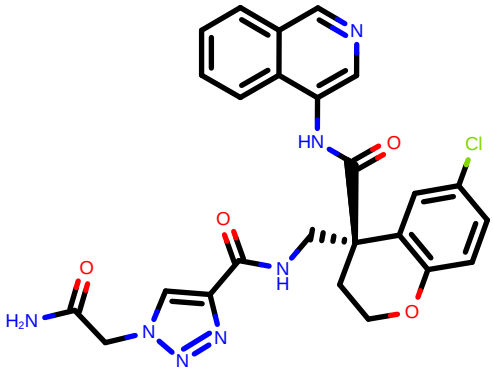
CID:	EN300-6501360_3_1
SMILES:	CN(C)C(=O)NC[C@@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2468
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.49

EN300-36158_2_2



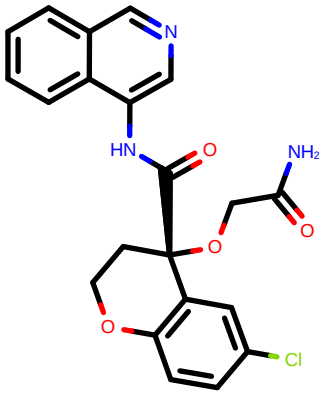
CID:	EN300-36158_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCCO5
RUN:	RUN5993
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.23

EN300-52380_2_1



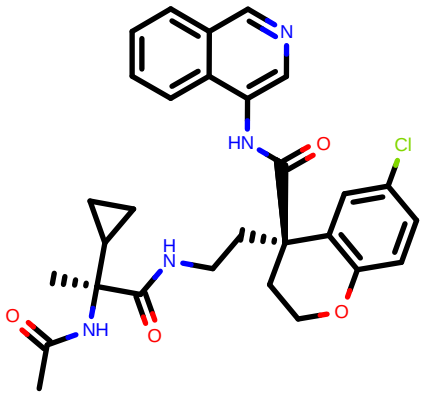
CID:	EN300-52380_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)CC(=O)N
RUN:	RUN6197
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.33

EN300-18249_1_1



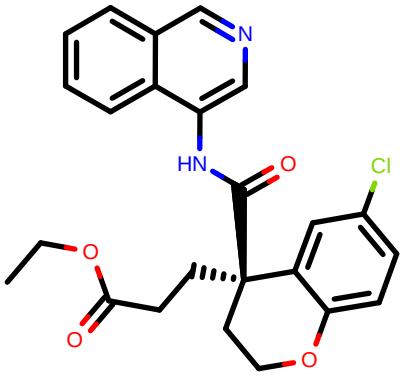
CID:	EN300-18249_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)N
RUN:	RUN1128
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.16

EN300-67073_3_1



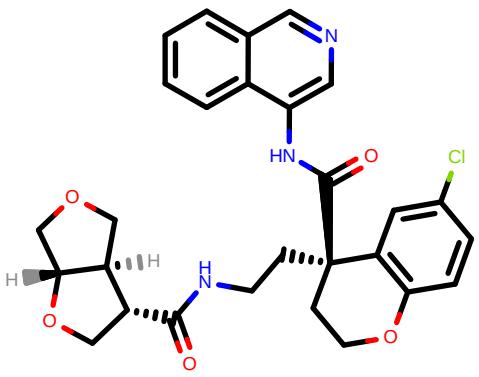
CID:	EN300-67073_3_1
SMILES:	CC(=O)N[C@@](C)(C1CC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3204
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.44

JAG-UCB-706446eb-4_1



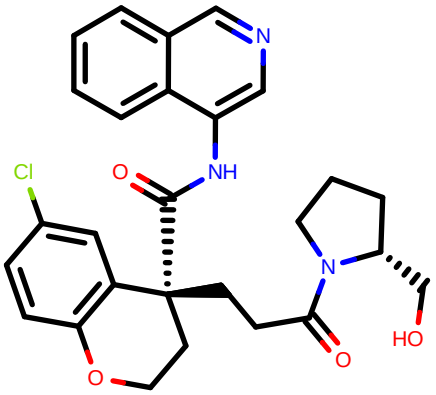
CID:	JAG-UCB-706446eb-4_1
SMILES:	CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.21

EN300-6482296_3_7



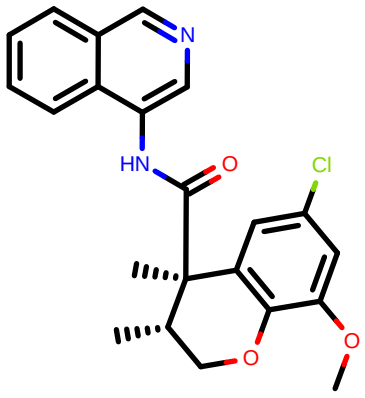
CID:	EN300-6482296_3_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CO[C@H]6[C@H]5COC6
RUN:	RUN8889
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.29

EN300-55109_2_1



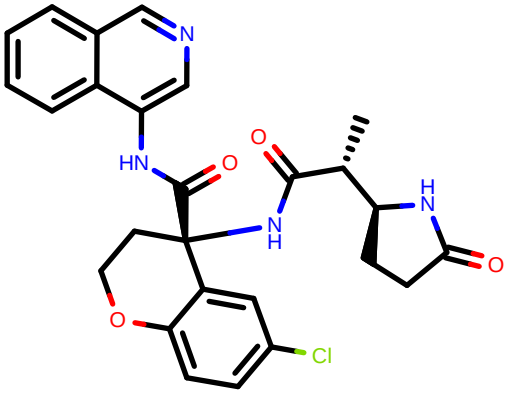
CID:	EN300-55109_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@@H]5CO
RUN:	RUN3181
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.26

DAR-DIA-0d514e7d-25_1



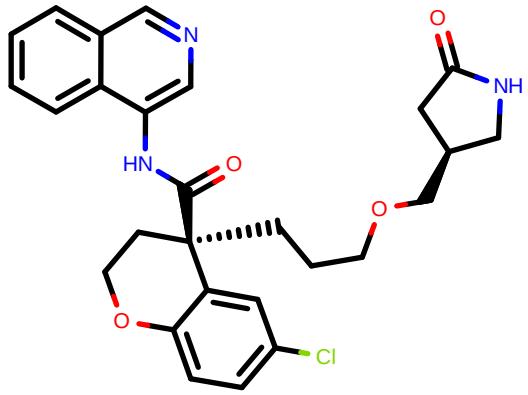
CID:	DAR-DIA-0d514e7d-25_1
SMILES:	C[C@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN73
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.13

EN300-249421_1_2



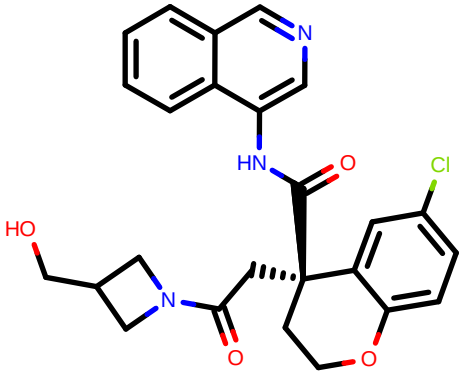
CID:	EN300-249421_1_2
SMILES:	C[C@H]([C@@H]1CCC(=O)N1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6243
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.21

EN300-246747_4_2



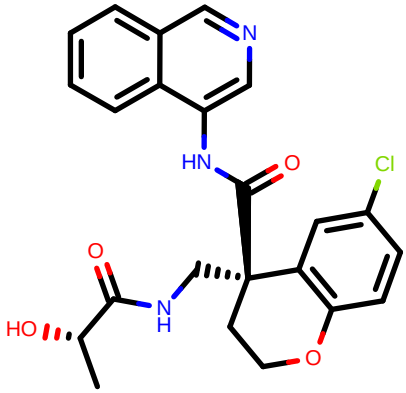
CID:	EN300-246747_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5CC(=O)NC5
RUN:	RUN895
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.39

EN300-7370063_1_1



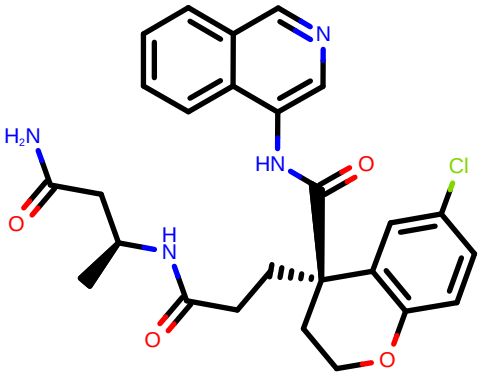
CID:	EN300-7370063_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CO
RUN:	RUN2713
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.24

EN300-91905_2_1



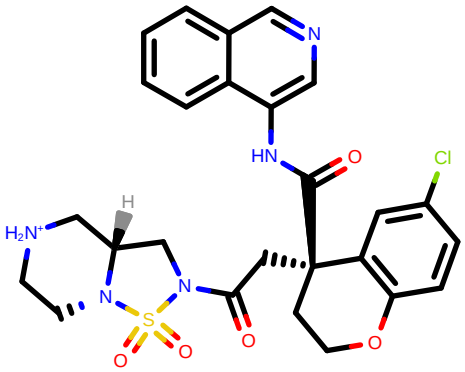
CID:	EN300-91905_2_1
SMILES:	C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2802
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.23

EN300-84785_2_1



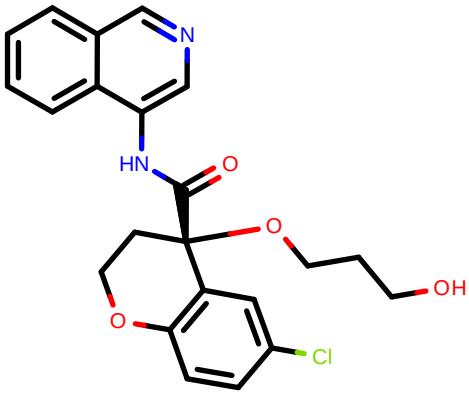
CID:	EN300-84785_2_1
SMILES:	C[C@@H](CC(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2589
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.25

EN300-717233_1_2



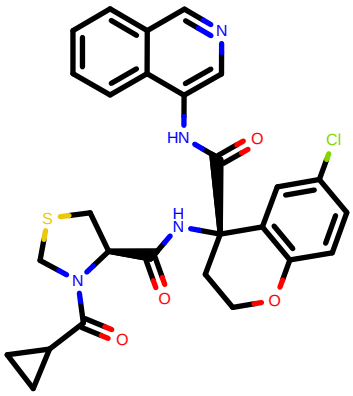
CID:	EN300-717233_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CNCCN6S5(=O)=O
RUN:	RUN10950
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.49

EN300-221518_1_1



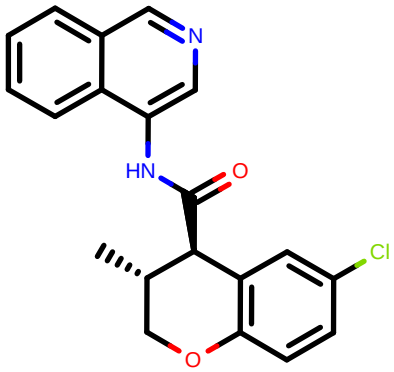
CID:	EN300-221518_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCO
RUN:	RUN984
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.19

EN300-18928_1_1



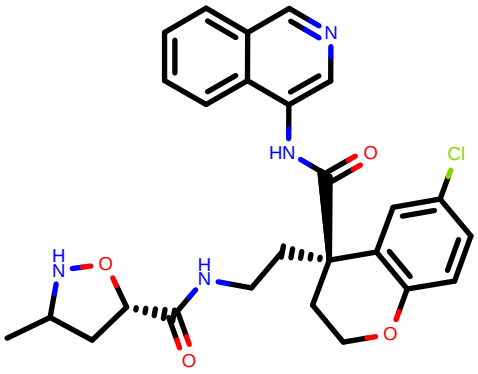
CID:	EN300-18928_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CSCN5C(=O)C6CC6
RUN:	RUN7922
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.31

EDJ-MED-e4b030d8-11_1



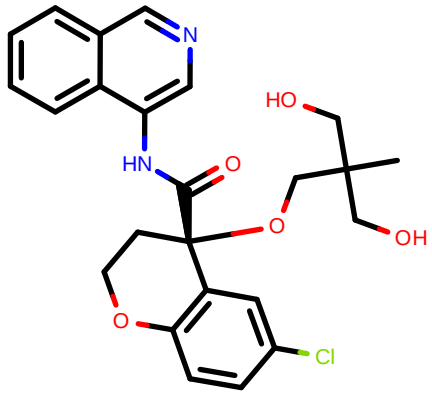
CID:	EDJ-MED-e4b030d8-11_1
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN12
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.06

EN300-92447_3_1



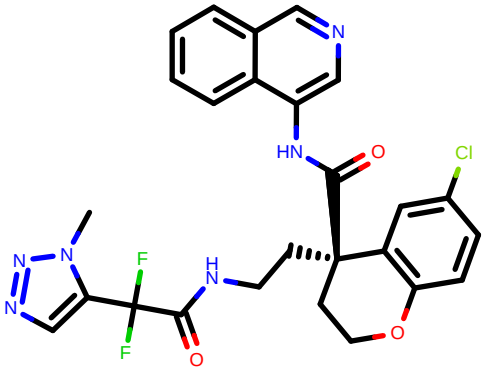
CID:	EN300-92447_3_1
SMILES:	CC1=NO[C@@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10940
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.30

EN300-218116_1_1



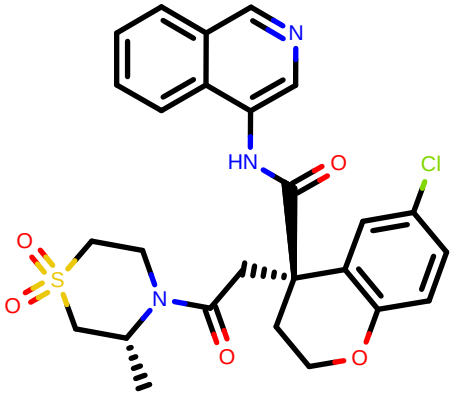
CID:	EN300-218116_1_1
SMILES:	CC(CO)(CO)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2207
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.30

EN300-1726073_3_1



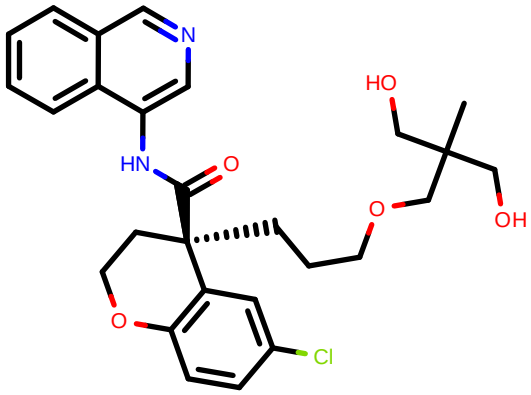
CID:	EN300-1726073_3_1
SMILES:	Cn1c(cnn1)C(C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(F)F
RUN:	RUN1705
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.34

EN300-6497238_1_1



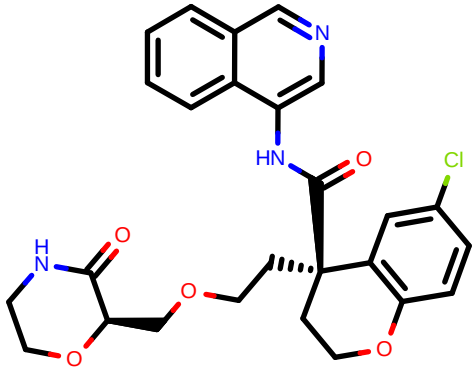
CID:	EN300-6497238_1_1
SMILES:	C[C@@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10270
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.37

EN300-218116_4_1



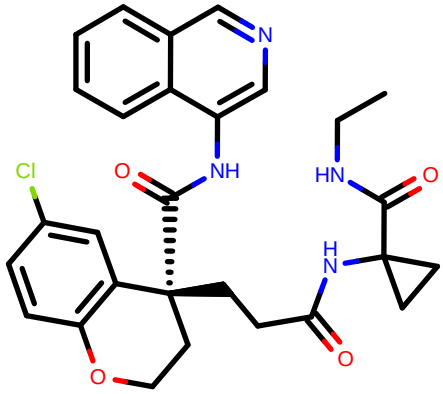
CID:	EN300-218116_4_1
SMILES:	CC(CO)(CO)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN348
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.46

EN300-1706036_3_1



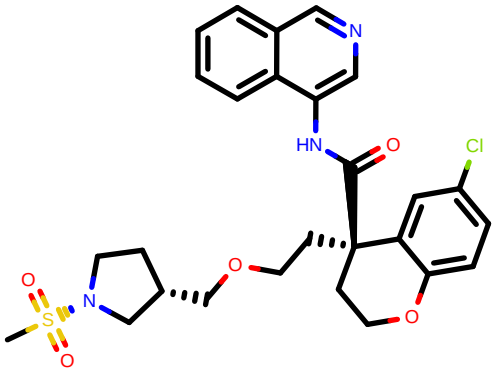
CID:	EN300-1706036_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C(=O)NCCO5
RUN:	RUN1028
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.33

EN300-6735698_2_1



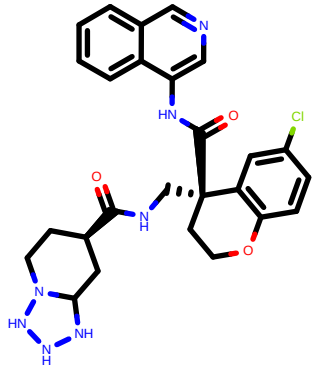
CID:	EN300-6735698_2_1
SMILES:	CCNC(=O)C1(CC1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4120
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.26

EN300-261986_3_1



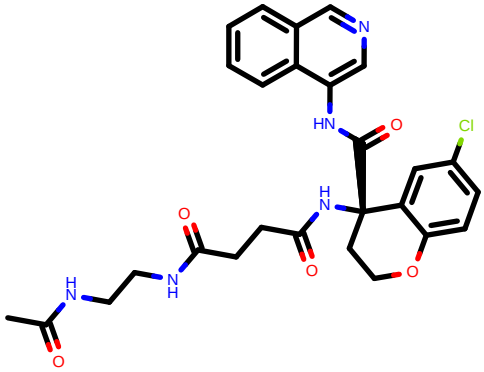
CID:	EN300-261986_3_1
SMILES:	CS(=O)(=O)N1CC[C@@H](C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN473
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.36

EN300-1653482_2_1



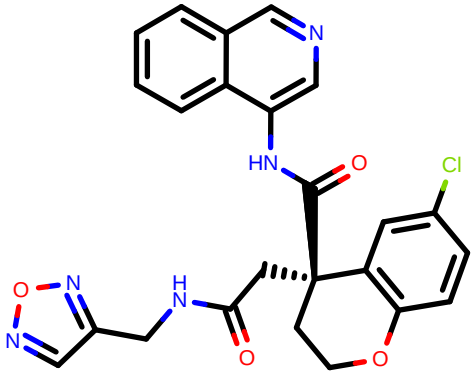
CID:	EN300-1653482_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCn6c(nnn6)C5
RUN:	RUN6444
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.33

EN300-73507_1_1



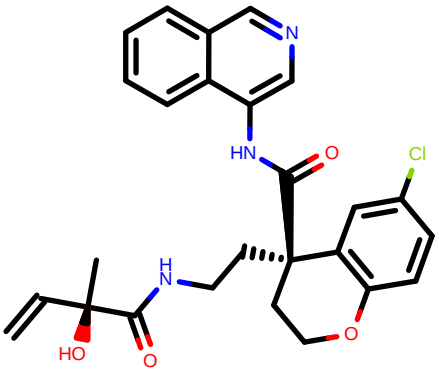
CID:	EN300-73507_1_1
SMILES:	CC(=O)NCCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5189
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.30

EN300-1068239_1_1



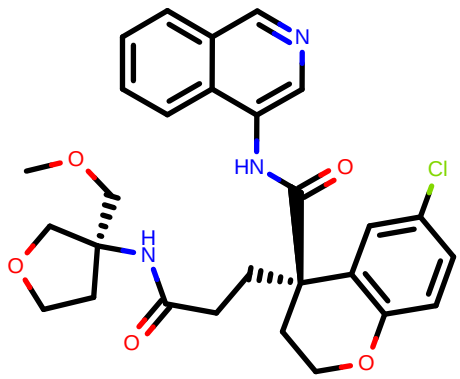
CID:	EN300-1068239_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5cnon5
RUN:	RUN9768
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.24

EN300-248888_3_1



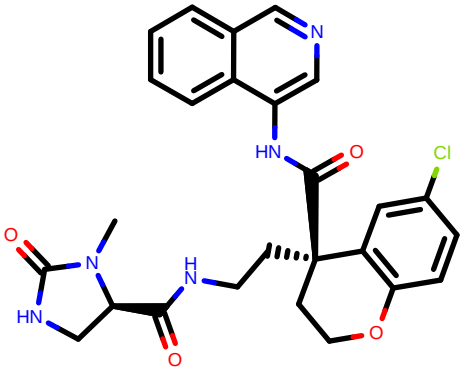
CID:	EN300-248888_3_1
SMILES:	C[C@@](C=C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN763
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.35

EN300-250501_2_1



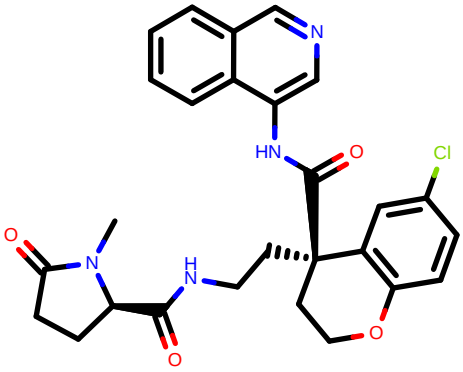
CID:	EN300-250501_2_1
SMILES:	COC[C@@]1(CCOC1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6191
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.37

EN300-307008_3_2



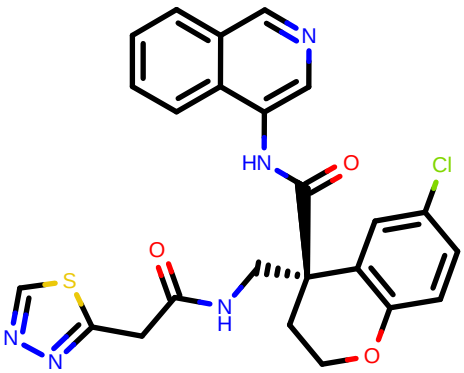
CID:	EN300-307008_3_2
SMILES:	CN1[C@H](CNC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9500
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.26

EN300-132963_3_2



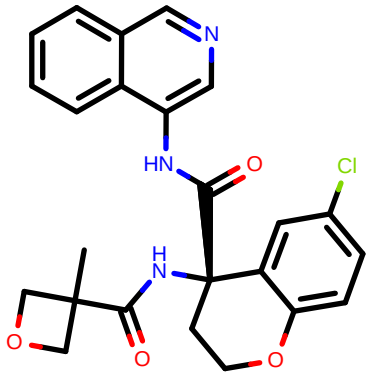
CID:	EN300-132963_3_2
SMILES:	CN1[C@H](CCC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5322
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.27

EN300-6488240_2_1



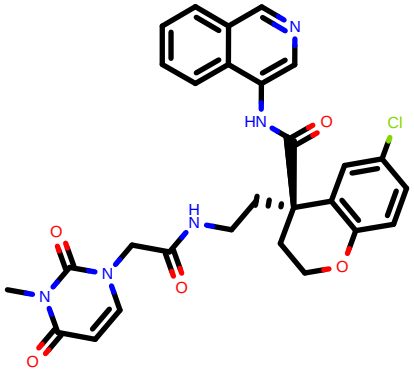
CID:	EN300-6488240_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5nncs5
RUN:	RUN2692
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.25

EN300-78753_1_1



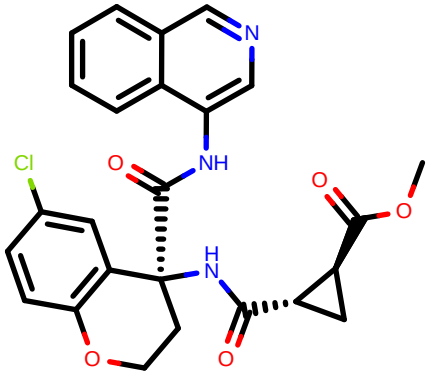
CID:	EN300-78753_1_1
SMILES:	CC1(COC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2060
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.24

EN300-36690_3_1



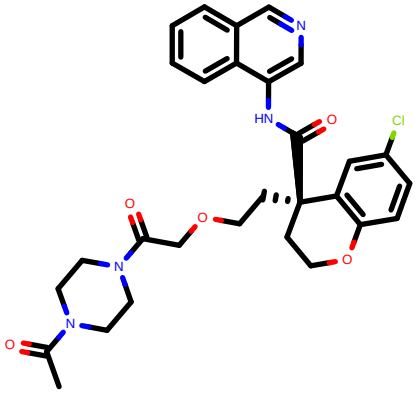
CID:	EN300-36690_3_1
SMILES:	Cn1c(=O)ccn(c1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7524
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.42

EN300-66764_1_2



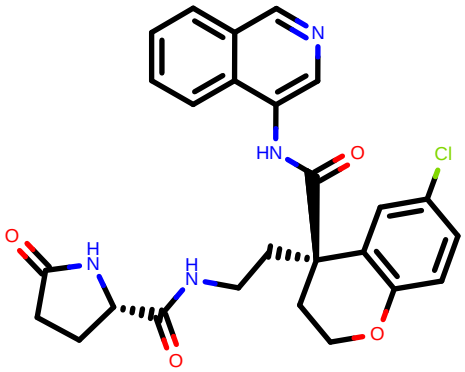
CID:	EN300-66764_1_2
SMILES:	COC(=O)[C@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5692
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.28

EN300-1724771_3_1



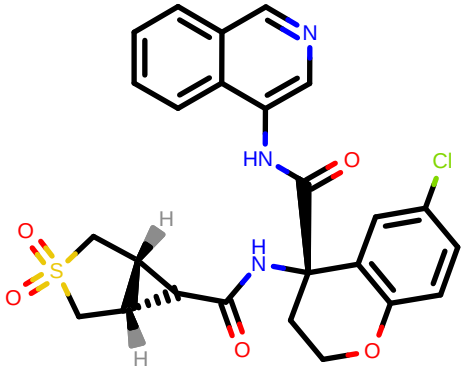
CID:	EN300-1724771_3_1
SMILES:	CC(=O)N1CCN(CC1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1603
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.30

EN300-72896_3_1



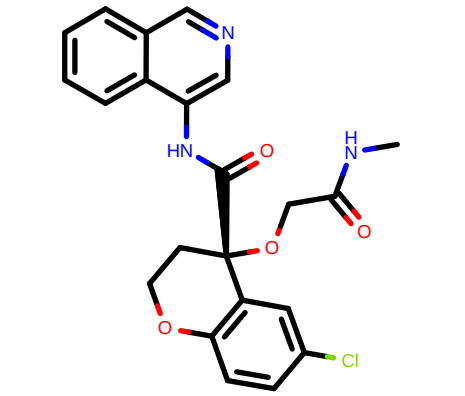
CID:	EN300-72896_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCC(=O)N5
RUN:	RUN7760
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.27

EN300-6779469_1_2



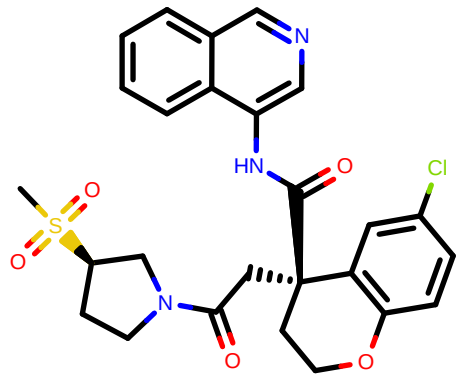
CID:	EN300-6779469_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5[C@H]6[C@@H]5CS(=O)(=O)C6
RUN:	RUN6120
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.30

EN300-2977549_1_1



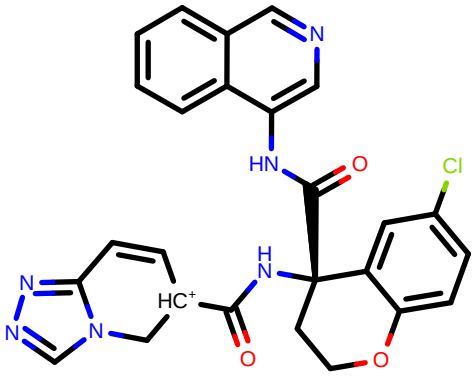
CID:	EN300-2977549_1_1
SMILES:	CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1056
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.18

EN300-200609_1_1



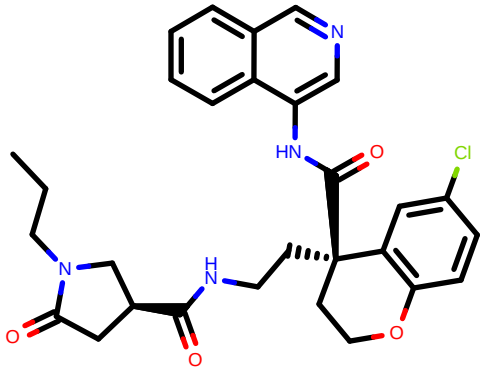
CID:	EN300-200609_1_1
SMILES:	CS(=O)(=O)[C@@H]1CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5023
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.63

EN300-60837_1_1



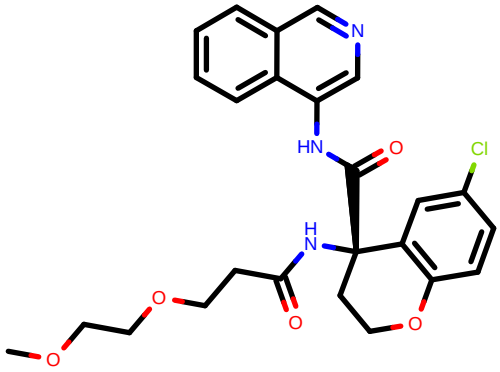
CID:	EN300-60837_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc6nncn6c5
RUN:	RUN8790
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.35

EN300-253443_3_2



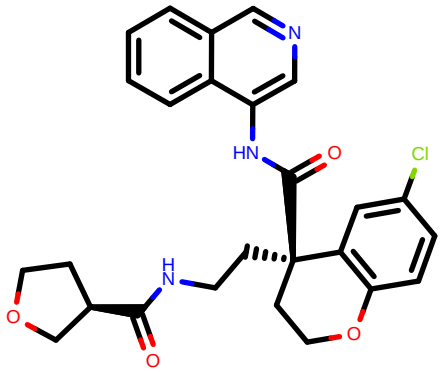
CID:	EN300-253443_3_2
SMILES:	CCCN1C[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4691
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.37

EN300-55250_1_1



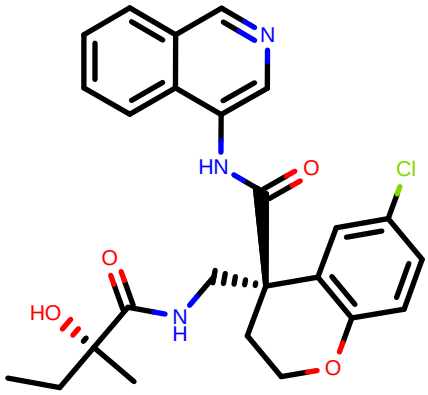
CID:	EN300-55250_1_1
SMILES:	COCCOCCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3522
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.26

EN300-697519_3_1



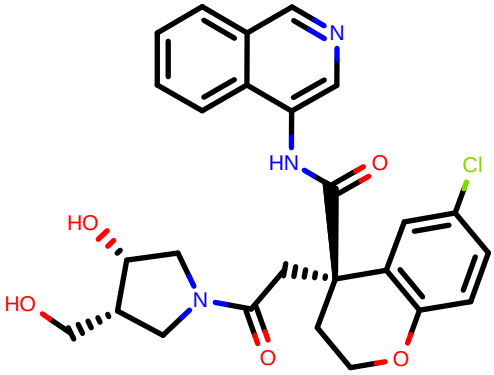
CID:	EN300-697519_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCOC5
RUN:	RUN8052
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.28

EN300-104746_2_2



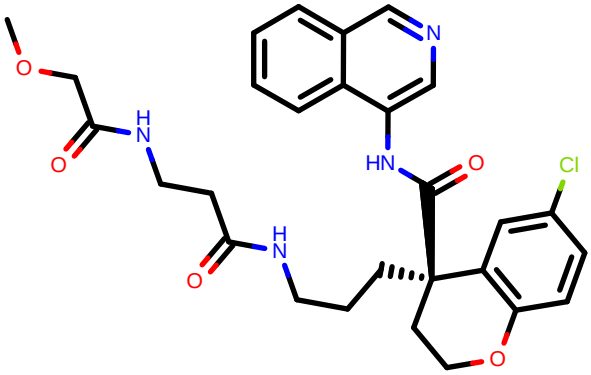
CID:	EN300-104746_2_2
SMILES:	CC[C@](C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5234
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.26

EN300-248521_1_1



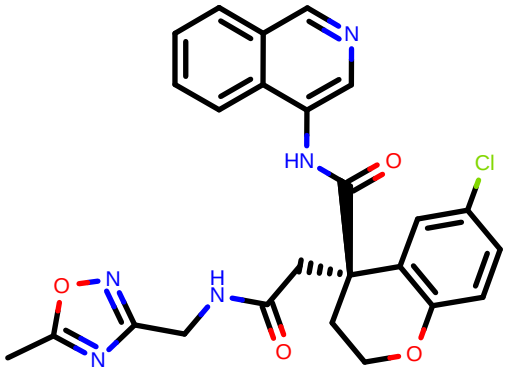
CID:	EN300-248521_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H](C5)O)CO
RUN:	RUN3380
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.40

EN300-31242_4_1



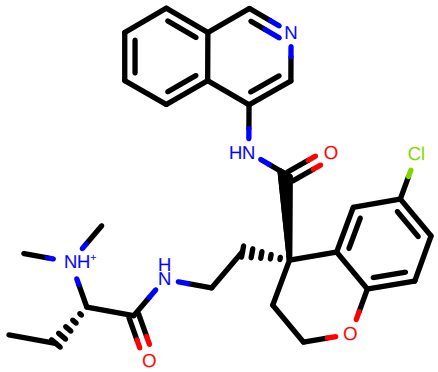
CID:	EN300-31242_4_1
SMILES:	COCC(=O)NCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9527
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.34

EN300-78727_1_1



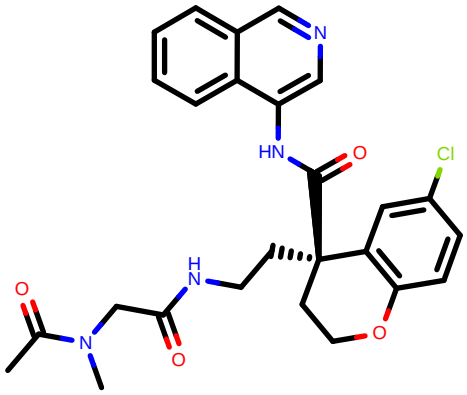
CID:	EN300-78727_1_1
SMILES:	Cc1nc(no1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6110
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.23

EN300-223964_3_1



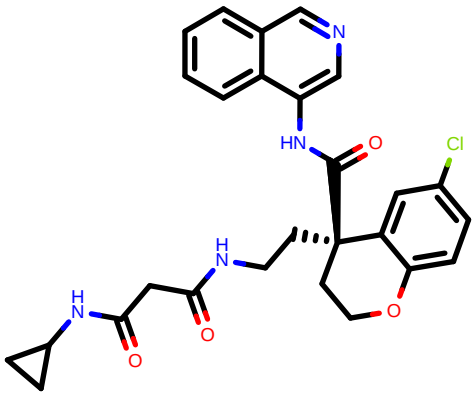
CID:	EN300-223964_3_1
SMILES:	CC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C)C
RUN:	RUN590
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.33

EN300-33657_3_1



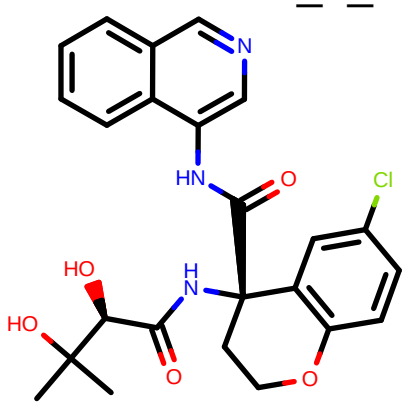
CID:	EN300-33657_3_1
SMILES:	CC(=O)N(C)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4447
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.34

EN300-128464_3_1



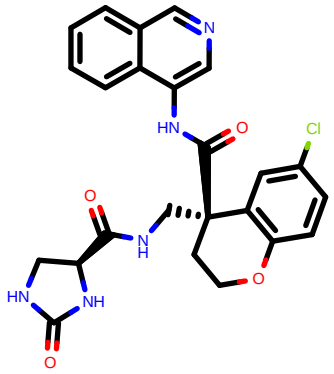
CID:	EN300-128464_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)NC5CC5
RUN:	RUN6828
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.39

EN300-299532_1_2



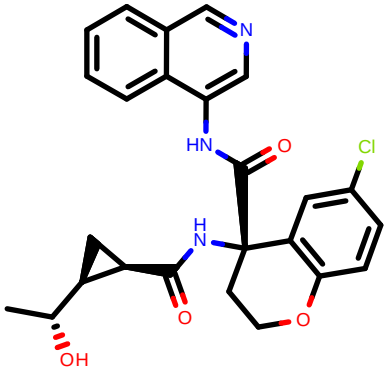
CID:	EN300-299532_1_2
SMILES:	CC(C)([C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)O
RUN:	RUN1644
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.22

EN300-66461_2_1



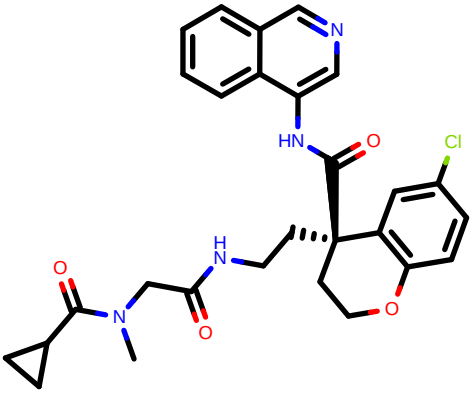
CID:	EN300-66461_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CNC(=O)N5
RUN:	RUN6656
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.24

EN300-6729572_1_8



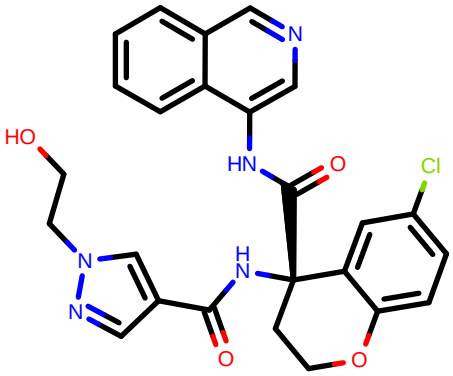
CID:	EN300-6729572_1_8
SMILES:	C[C@H]([C@H]1C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2946
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.30

EN300-31146_3_1



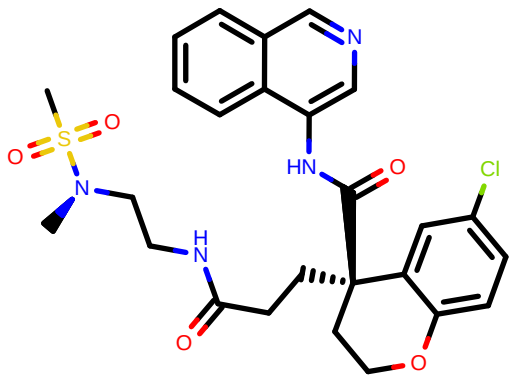
CID:	EN300-31146_3_1
SMILES:	CN(CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)C5CC5
RUN:	RUN4995
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.38

EN300-761209_1_1



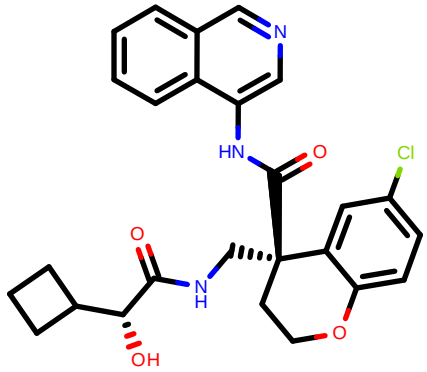
CID:	EN300-761209_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn(c5)CCO
RUN:	RUN6914
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.25

EN300-6478561_2_1



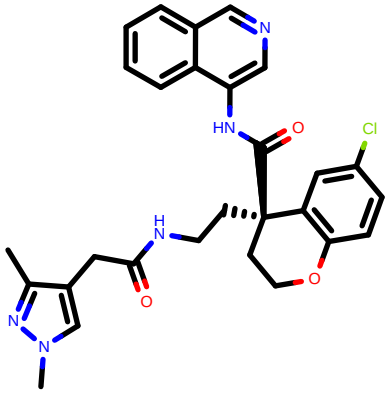
CID:	EN300-6478561_2_1
SMILES:	CN(CCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN11333
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.28

EN300-249764_2_1



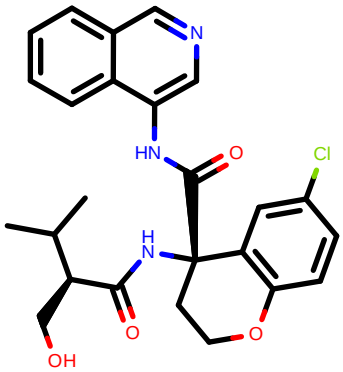
CID:	EN300-249764_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](C5CCC5)O
RUN:	RUN3719
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.33

EN300-245061_3_1



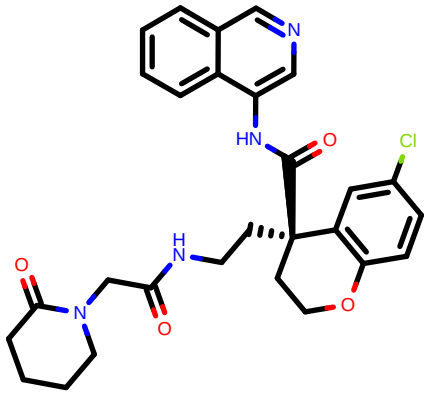
CID:	EN300-245061_3_1
SMILES:	Cc1c(cn(n1)C)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10344
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.37

EN300-153257_1_2



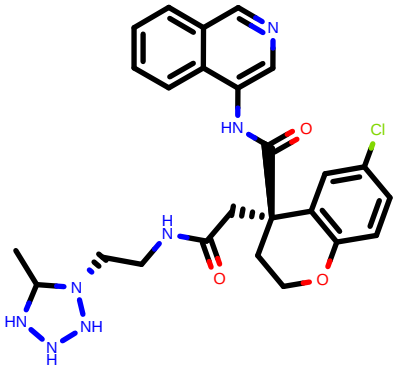
CID:	EN300-153257_1_2
SMILES:	CC(C)[C@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3418
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.28

EN300-36111_3_1



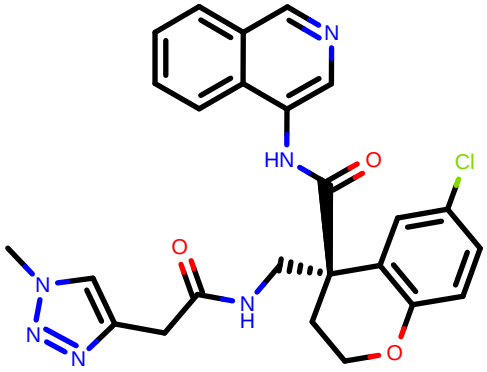
CID:	EN300-36111_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCCCC5=O
RUN:	RUN6461
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.31

EN300-77343_1_1



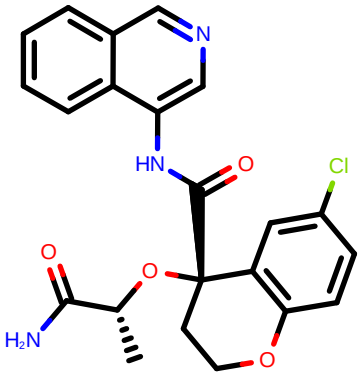
CID:	EN300-77343_1_1
SMILES:	Cc1nnnn1CCNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9676
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.31

EN300-1073264_2_1



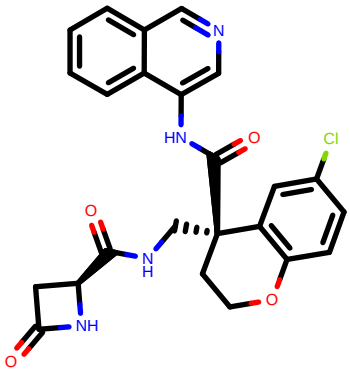
CID:	EN300-1073264_2_1
SMILES:	Cn1cc(nn1)CC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3567
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.30

EN300-17381_1_2



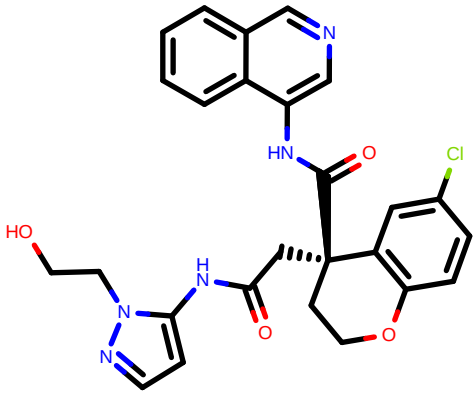
CID:	EN300-17381_1_2
SMILES:	C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN809
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.20

EN300-103219_2_1



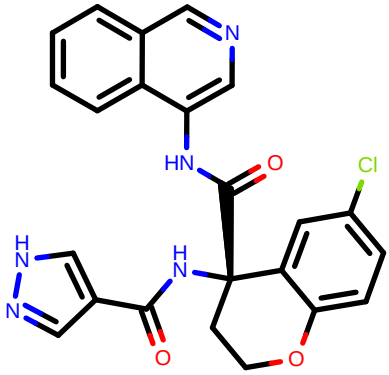
CID:	EN300-103219_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC(=O)N5
RUN:	RUN6272
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.23

EN300-134536_1_1



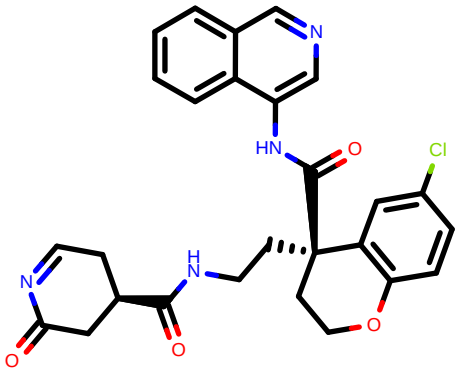
CID:	EN300-134536_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ccnn5CCO
RUN:	RUN5670
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.28

EN300-41863_1_1



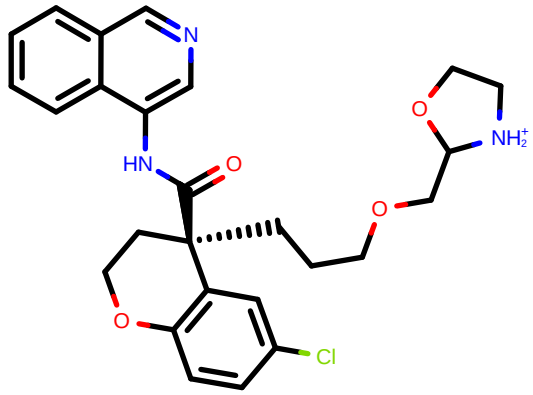
CID:	EN300-41863_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c[nH]nc5
RUN:	RUN2322
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.18

EN300-107493_3_1



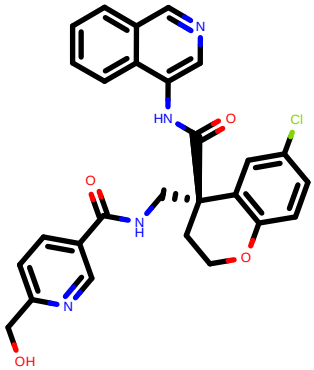
CID:	EN300-107493_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCNC(=O)C5
RUN:	RUN10906
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.23

EN300-317555_4_1



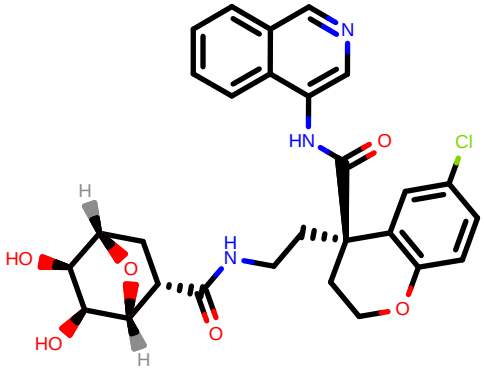
CID:	EN300-317555_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5=NCCO5
RUN:	RUN500
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.26

EN300-146051_2_1



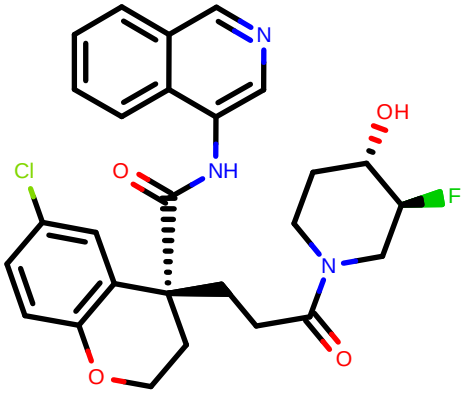
CID:	EN300-146051_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(nc5)CO
RUN:	RUN8395
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.25

EN300-6764836_3_2



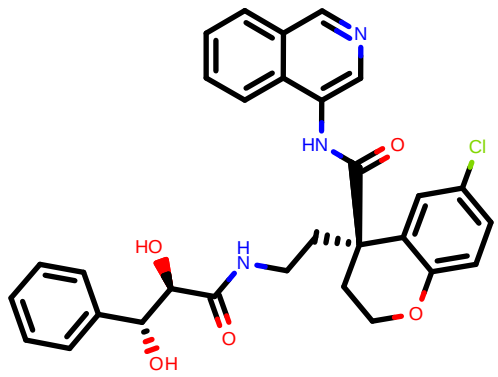
CID:	EN300-6764836_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC6[C@@H][C@@H](C5O6)O)O
RUN:	RUN9772
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.28

EN300-741926_2_3



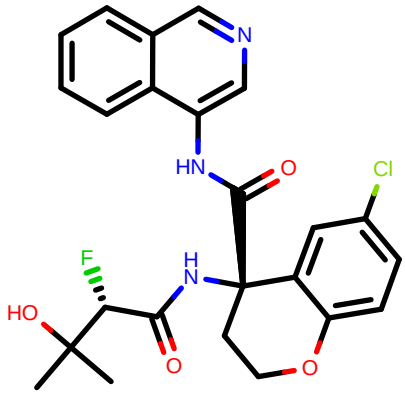
CID:	EN300-741926_2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H][C@H](C5)F)O
RUN:	RUN1219
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.28

EN300-2923949_3_4



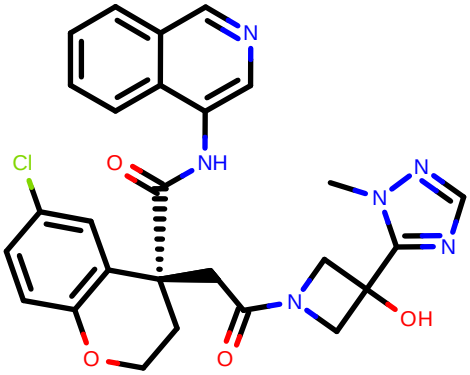
CID:	EN300-2923949_3_4
SMILES:	c1ccc(cc1)[C@H]([C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O
RUN:	RUN10636
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.39

EN300-264744_1_1



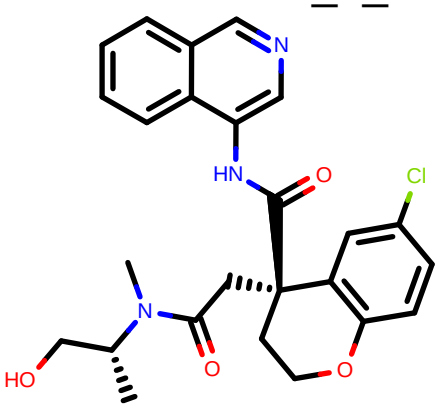
CID:	EN300-264744_1_1
SMILES:	CC(C)([C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)F)O
RUN:	RUN2890
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.21

EN300-381149_1_1



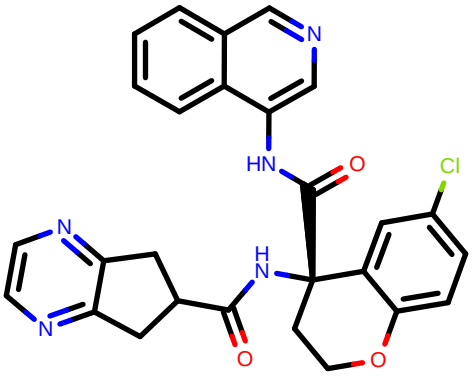
CID:	EN300-381149_1_1
SMILES:	Cn1c(ncn1)C2(CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)O
RUN:	RUN9634
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.31

EN300-205110_1_1



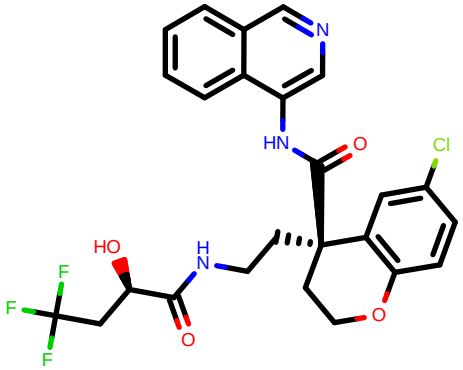
CID:	EN300-205110_1_1
SMILES:	C[C@H](CO)N(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8988
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.30

EN300-2011576_1_1



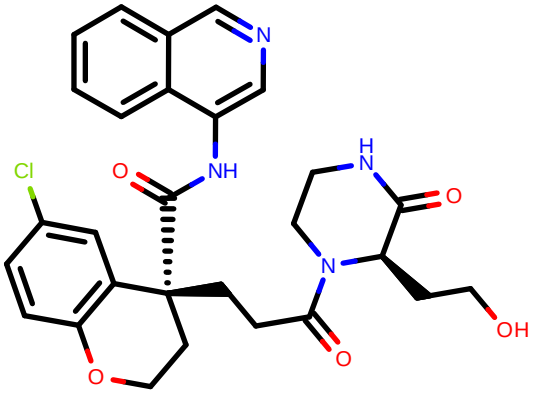
CID:	EN300-2011576_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5Cc6c(nccn6)C5
RUN:	RUN8310
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.26

EN300-1932013_3_1



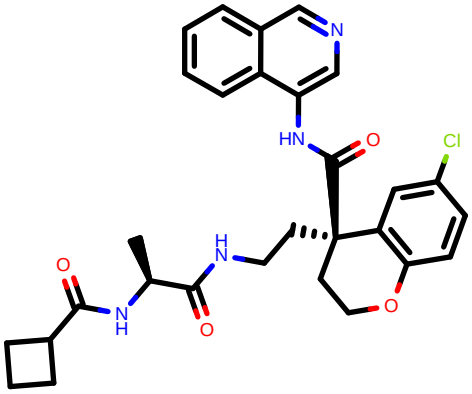
CID:	EN300-1932013_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H](CC(F)(F)F)O
RUN:	RUN3408
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.46

EN300-1587691_2_2



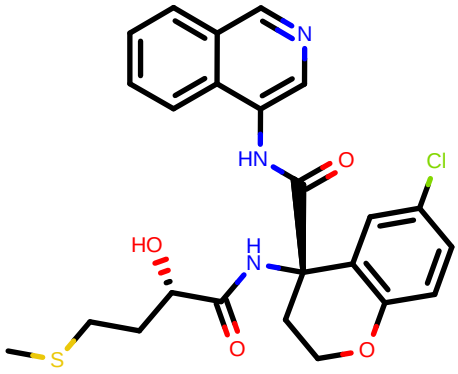
CID:	EN300-1587691_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCNC(=O)[C@H]5CCO
RUN:	RUN7657
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.37

EN300-66082_3_1



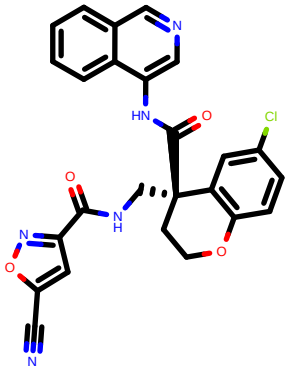
CID:	EN300-66082_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCC5
RUN:	RUN10027
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.42

EN300-103144_1_1



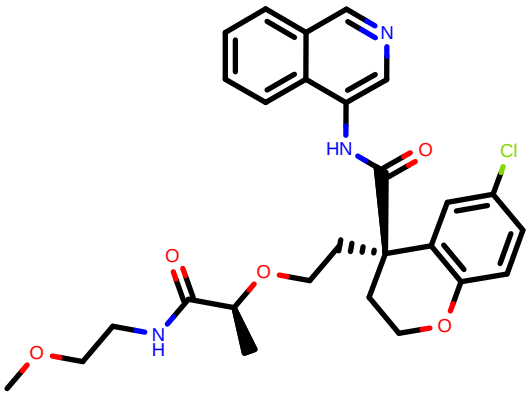
CID:	EN300-103144_1_1
SMILES:	CSCC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2036
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.27

EN300-1178005_2_1



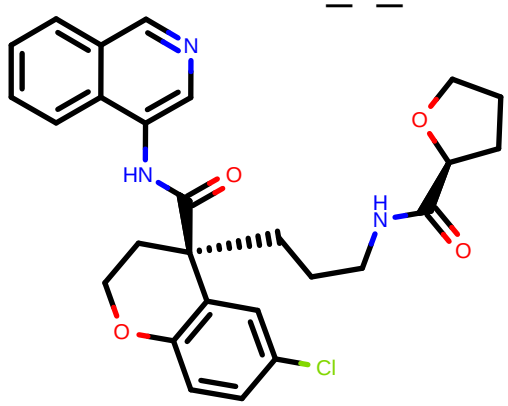
CID:	EN300-1178005_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(on5)C#N
RUN:	RUN8307
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.25

EN300-23317_3_1



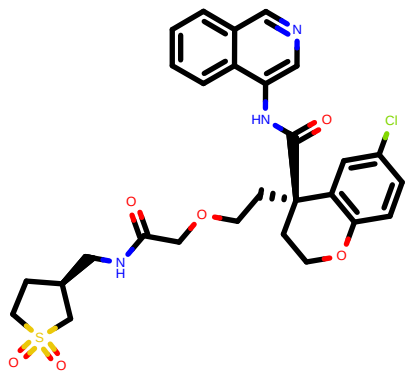
CID:	EN300-23317_3_1
SMILES:	C[C@@H](C(=O)NCCOC)OCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN924
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.37

EN300-21009_4_1



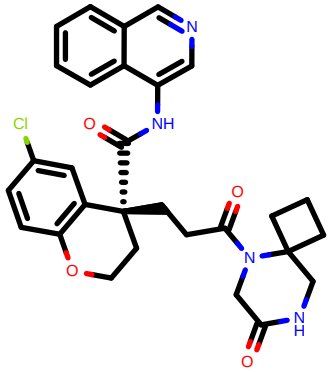
CID:	EN300-21009_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCCO5
RUN:	RUN10529
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.29

EN300-47606_3_1



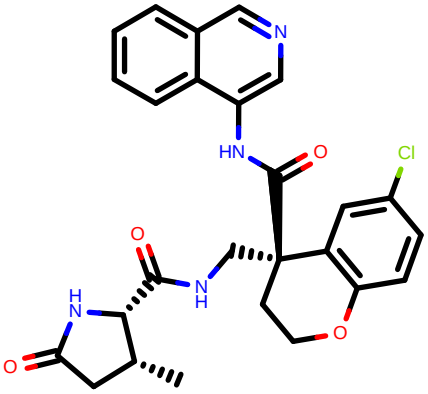
CID:	EN300-47606_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)NC[C@@H]5CCS(=O)(=O)C5
RUN:	RUN1771
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.37

EN300-7349829_2_1



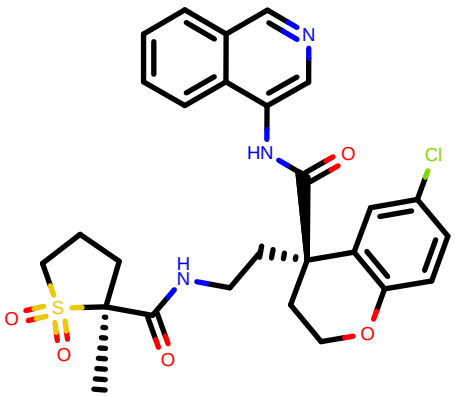
CID:	EN300-7349829_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(=O)NCC56CCC6
RUN:	RUN6043
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.29

EN300-155362_2_1



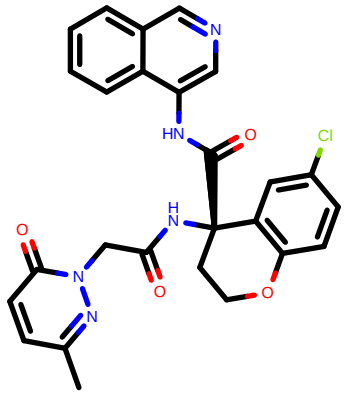
CID:	EN300-155362_2_1
SMILES:	C[C@@H]1CC(=O)N[C@@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7203
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.25

EN300-373476_3_2



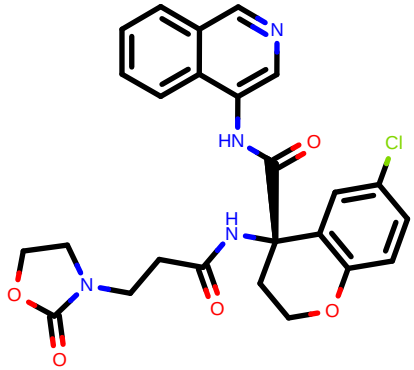
CID:	EN300-373476_3_2
SMILES:	C[C@]1(CCCS1(=O)=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6429
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.35

EN300-69556_1_1



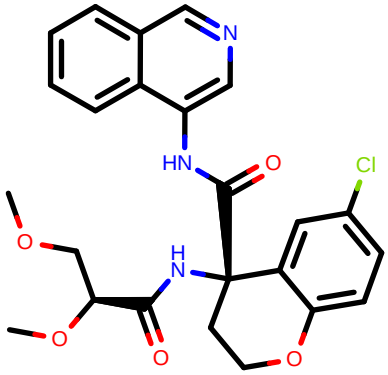
CID:	EN300-69556_1_1
SMILES:	Cc1ccc(=O)n(n1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5756
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.34

EN300-53918_1_1



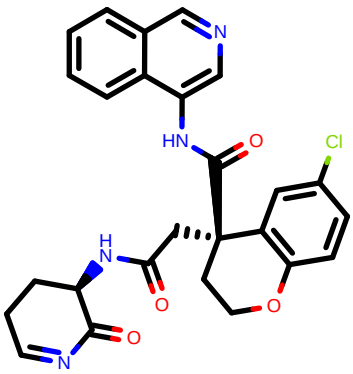
CID:	EN300-53918_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCN5CCOC5=O
RUN:	RUN2700
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.26

EN300-305282_1_1



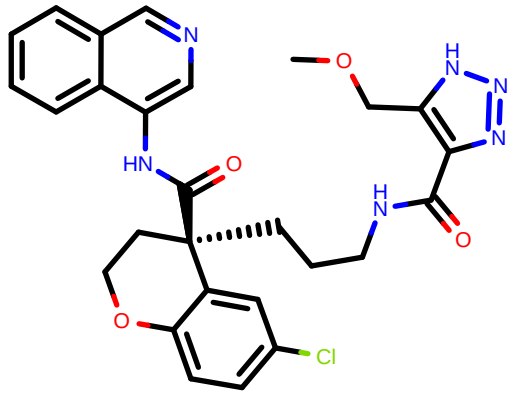
CID:	EN300-305282_1_1
SMILES:	COC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN2866
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.38

EN300-60035_1_1



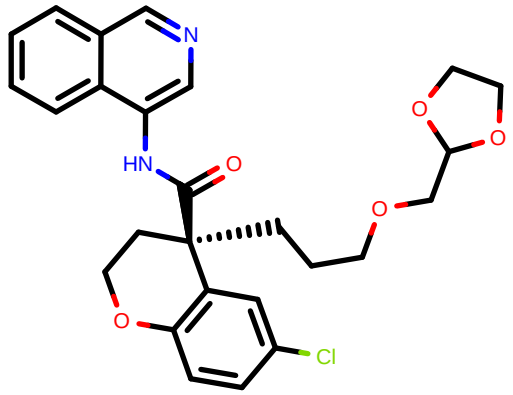
CID:	EN300-60035_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCNC5=O
RUN:	RUN11224
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.29

EN300-785910_4_1



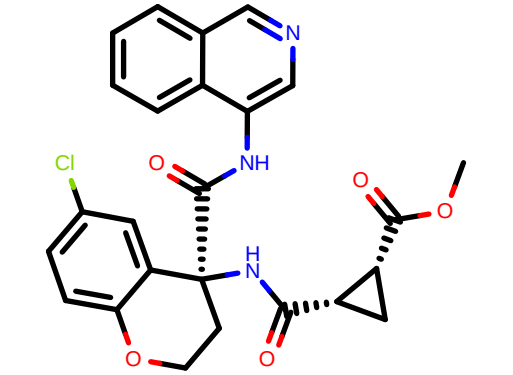
CID:	EN300-785910_4_1
SMILES:	COCc1c(nn[nH]1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9223
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.33

EN300-77092_4_1



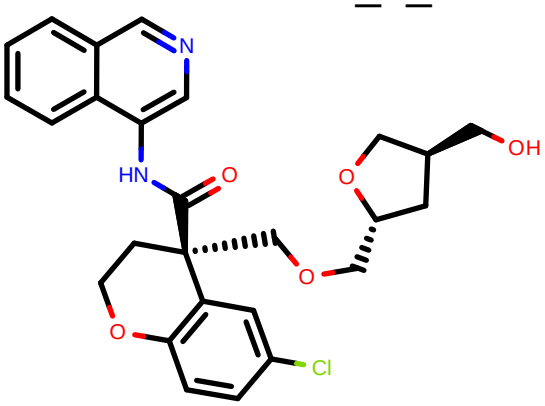
CID:	EN300-77092_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5OCCO5
RUN:	RUN651
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.38

EN300-384027_1_1



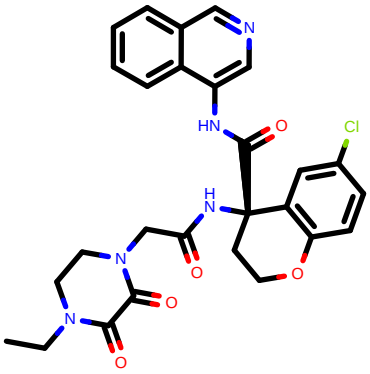
CID:	EN300-384027_1_1
SMILES:	COC(=O)[C@@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3749
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.20

EN300-6494158_2_2



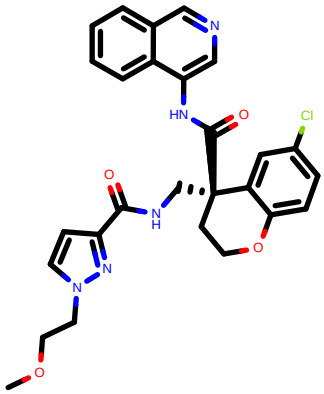
CID:	EN300-6494158_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C[C@@H](CO5)CO
RUN:	RUN2414
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.38

EN300-39961_1_1



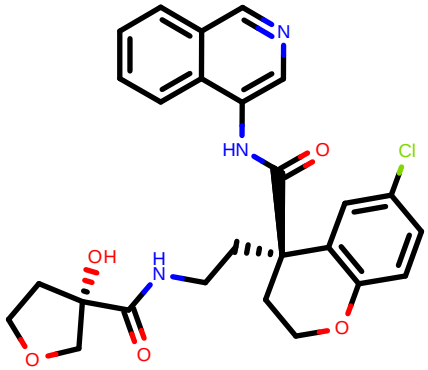
CID:	EN300-39961_1_1
SMILES:	CCN1CCN(C(=O)C1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3358
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.37

EN300-160277_2_1



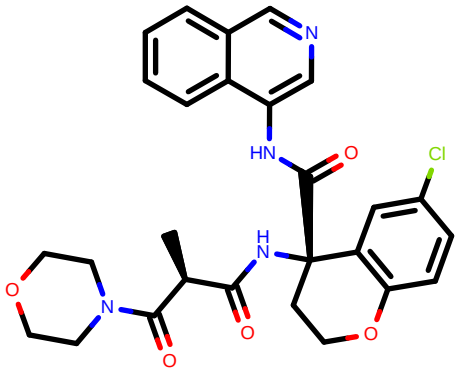
CID:	EN300-160277_2_1
SMILES:	COCCn1ccc(n1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5965
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.29

EN300-148421_3_1



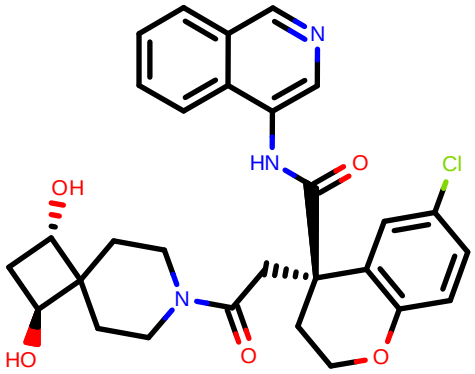
CID:	EN300-148421_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@]5(CCOC5)O
RUN:	RUN7196
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.34

EN300-2855057_1_1



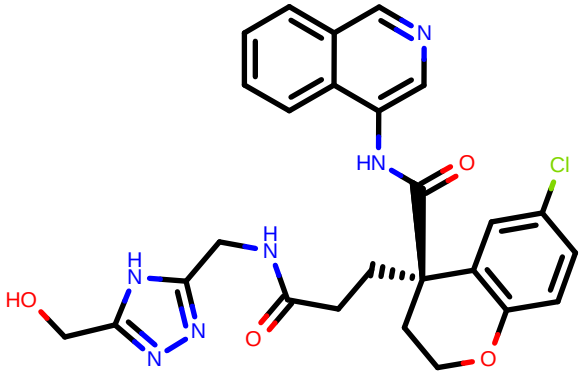
CID:	EN300-2855057_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)N5CCOCC5
RUN:	RUN6247
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.27

EN300-7448078_1_2



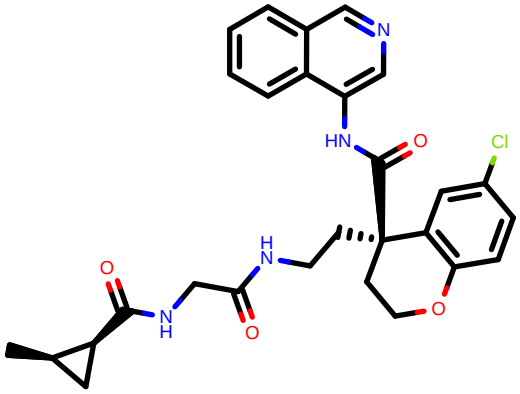
CID:	EN300-7448078_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC6(CC5)[C@H](C[C@@H]6O)O
RUN:	RUN9266
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.33

EN300-312662_2_1



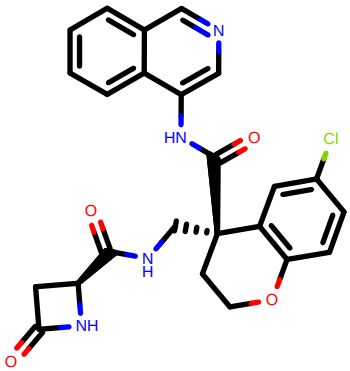
CID:	EN300-312662_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5[nH]c(nn5)CO
RUN:	RUN10679
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.26

EN300-30768_3_1



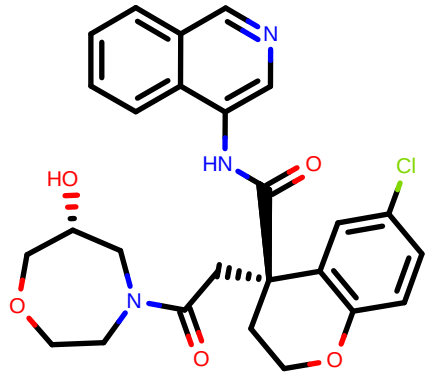
CID:	EN300-30768_3_1
SMILES:	C[C@@H]1C[C@@H]1C(=O)NCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3436
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.29

EN300-101505_2_1



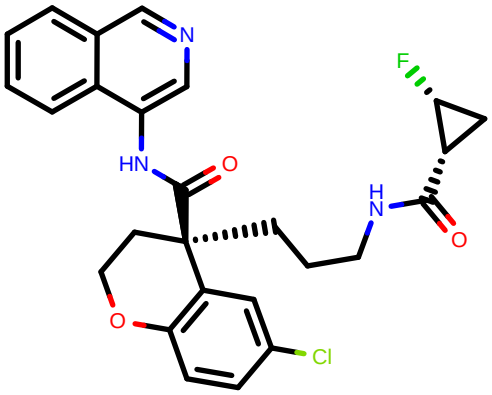
CID:	EN300-101505_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CC(=O)N5
RUN:	RUN6268
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.23

EN300-233951_1_1



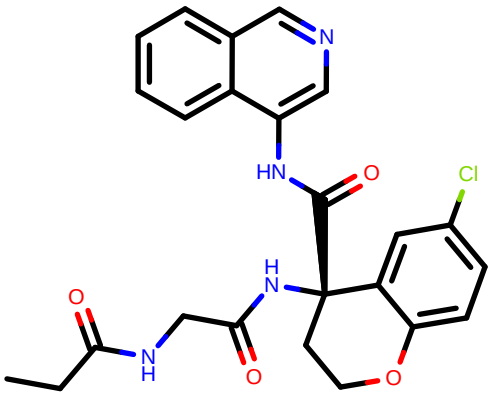
CID:	EN300-233951_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H](C5)O
RUN:	RUN10642
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.43

EN300-97300_4_4



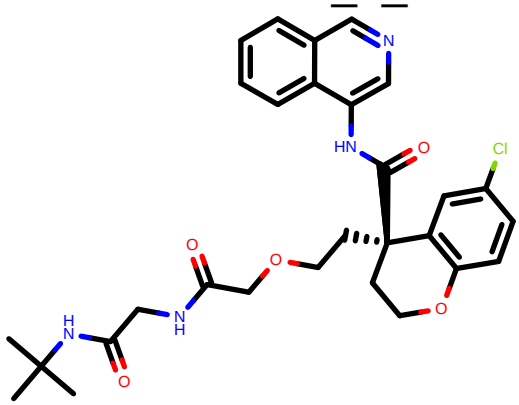
CID:	EN300-97300_4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5C[C@H]5F
RUN:	RUN10869
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.32

EN300-31099_1_1



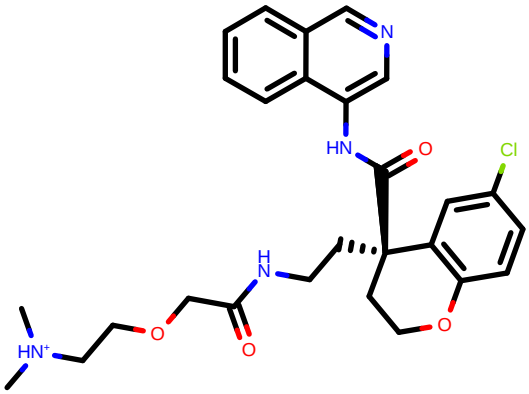
CID:	EN300-31099_1_1
SMILES:	CCC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3618
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.26

EN300-48760_3_1



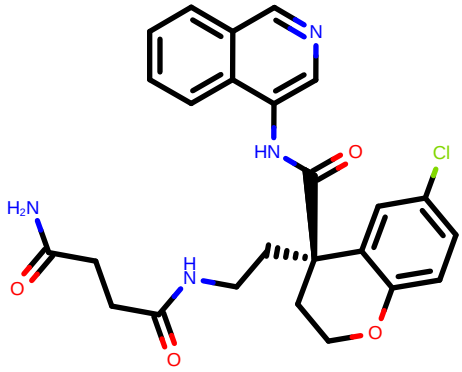
CID:	EN300-48760_3_1
SMILES:	CC(C)(C)NC(=O)CNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1164
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.30

EN300-1865348_3_1



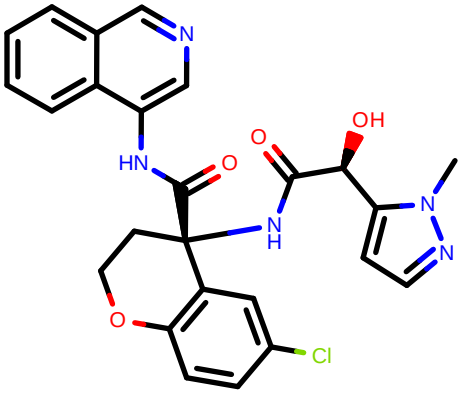
CID:	EN300-1865348_3_1
SMILES:	CN(C)CCOCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3228
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.64

EN300-178515_3_1



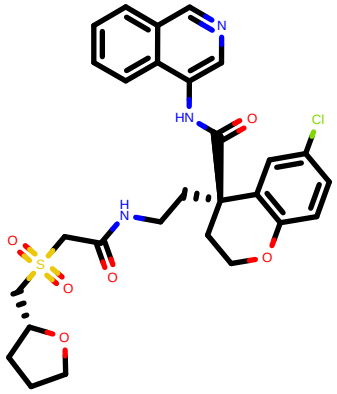
CID:	EN300-178515_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCC(=O)N
RUN:	RUN6082
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.27

EN300-6473273_1_1



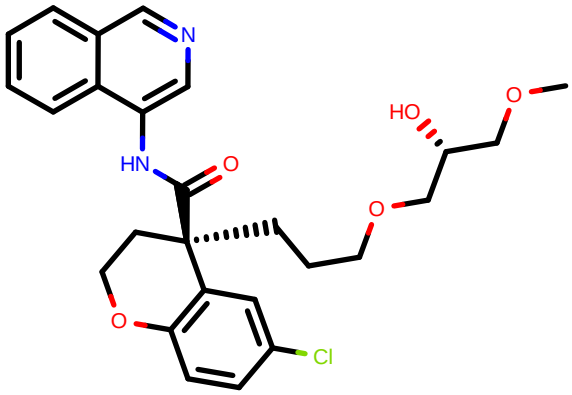
CID:	EN300-6473273_1_1
SMILES:	Cn1c(ccn1)[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7430
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.29

EN300-67023_3_2



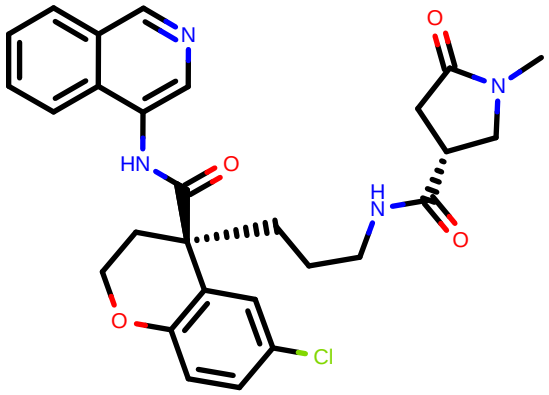
CID:	EN300-67023_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CS(=O)(=O)C[C@H]5CCCO5
RUN:	RUN8720
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.47

EN300-1915260_4_2



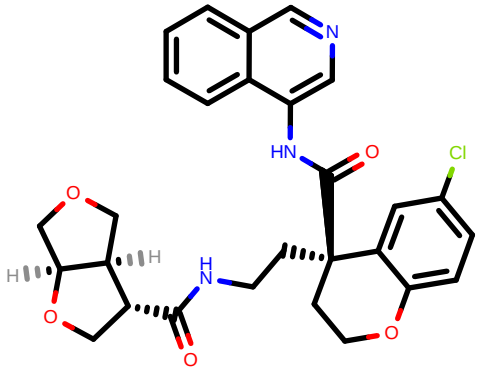
CID:	EN300-1915260_4_2
SMILES:	COC[C@H](COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN579
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.40

EN300-33601_4_1



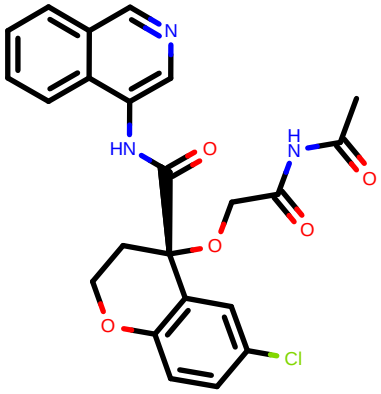
CID:	EN300-33601_4_1
SMILES:	CN1C[C@@H](CC1=O)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9657
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.35

EN300-6482296_3_5



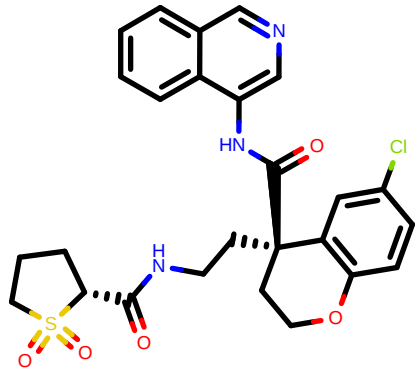
CID:	EN300-6482296_3_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CO[C@@H]6[C@H]5COC6
RUN:	RUN9975
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.32

EN300-249475_1_1



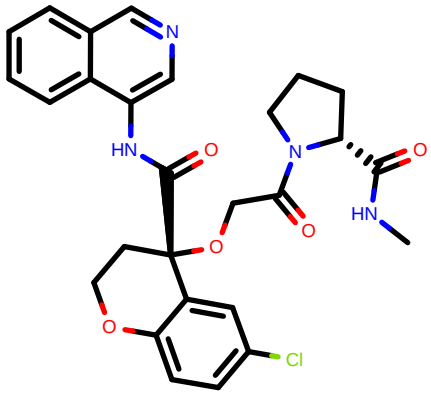
CID:	EN300-249475_1_1
SMILES:	CC(=O)NC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN896
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.23

EN300-88656_3_2



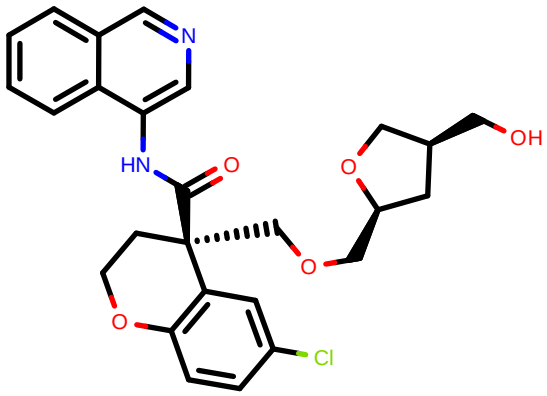
CID:	EN300-88656_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCS5(=O)=O
RUN:	RUN8922
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.29

EN300-48902_1_2



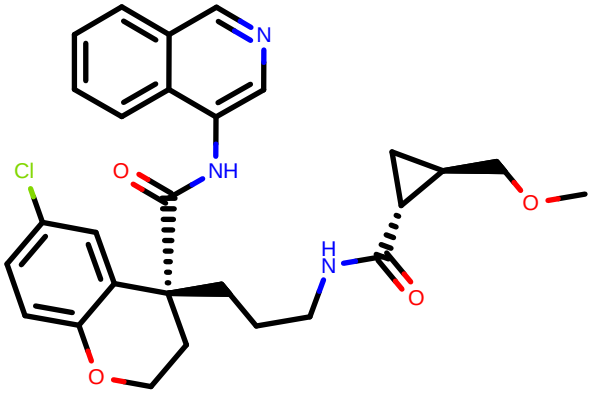
CID:	EN300-48902_1_2
SMILES:	CNC(=O)[C@H]1CCCN1C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1544
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.41

EN300-6494158_2_1



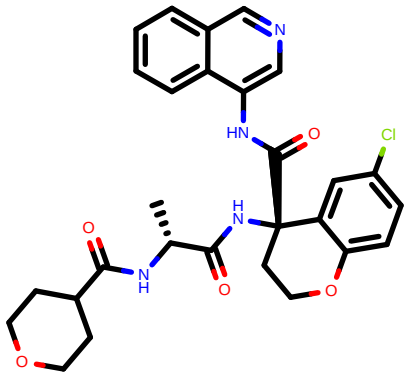
CID:	EN300-6494158_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5C[C@@H](CO5)CO
RUN:	RUN2435
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.31

EN300-705386_4_1



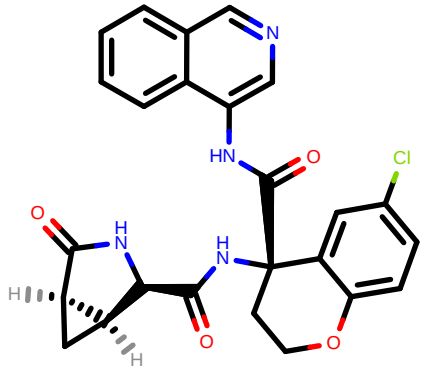
CID:	EN300-705386_4_1
SMILES:	COC[C@@H]1C[C@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9631
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.29

EN300-73102_1_2



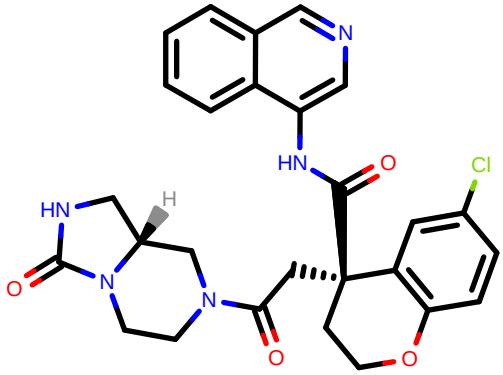
CID:	EN300-73102_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCOCC5
RUN:	RUN6112
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.35

EN300-6766359_1_1



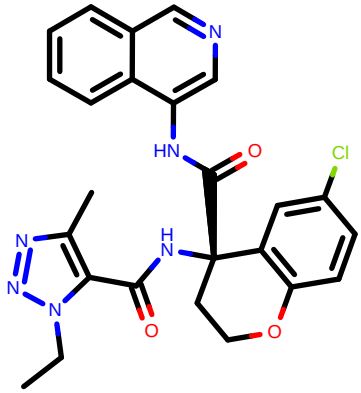
CID:	EN300-6766359_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5[C@H]6C[C@H]6C(=O)N5
RUN:	RUN7822
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.24

EN300-100765_1_1



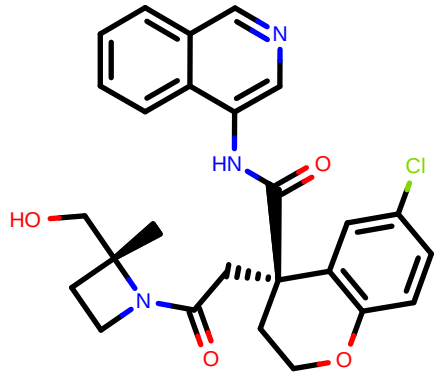
CID:	EN300-100765_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@@H](C5)CNC6=O
RUN:	RUN3608
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.42

EN300-217526_1_1



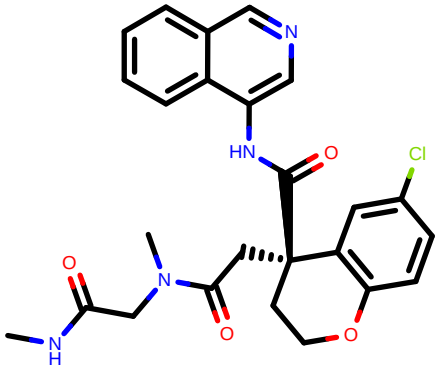
CID:	EN300-217526_1_1
SMILES:	CCn1c(c(nn1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5936
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.27

EN300-1717630_1_1



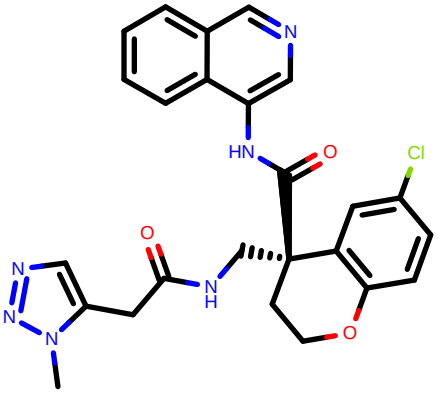
CID:	EN300-1717630_1_1
SMILES:	C[C@@]1(CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN4883
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.29

EN300-34491_1_1



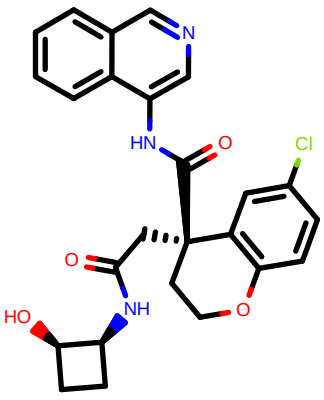
CID:	EN300-34491_1_1
SMILES:	CNC(=O)CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10366
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.28

EN300-6486855_2_1



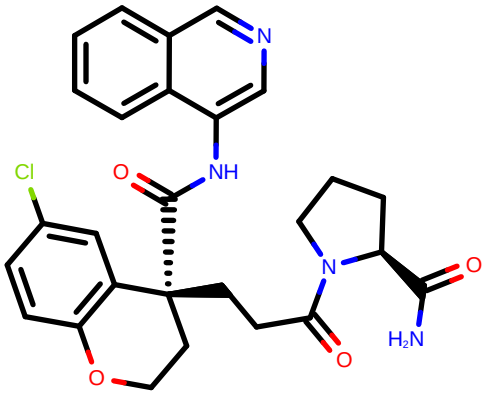
CID:	EN300-6486855_2_1
SMILES:	Cn1c(cnn1)CC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6141
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.30

EN300-129424_1_4



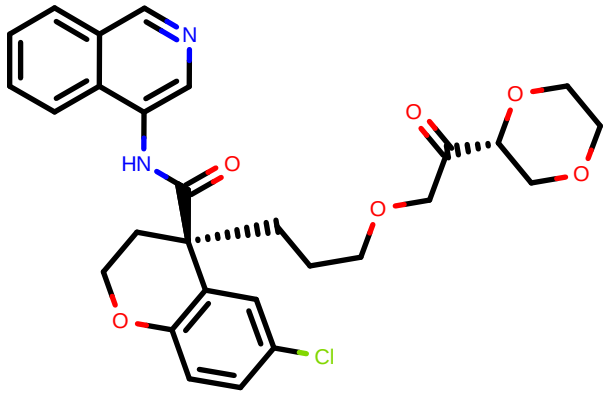
CID:	EN300-129424_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CC[C@H]5O
RUN:	RUN10121
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.24

EN300-07127_2_2



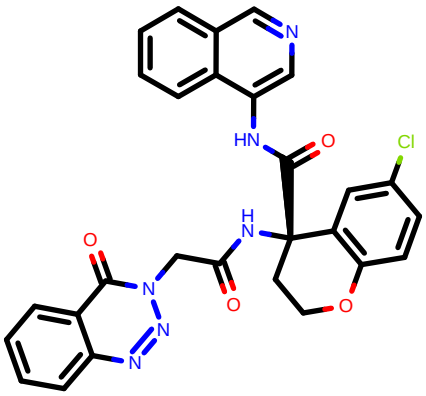
CID:	EN300-07127_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@H]5C(=O)N
RUN:	RUN3353
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.28

EN300-6238494_4_2



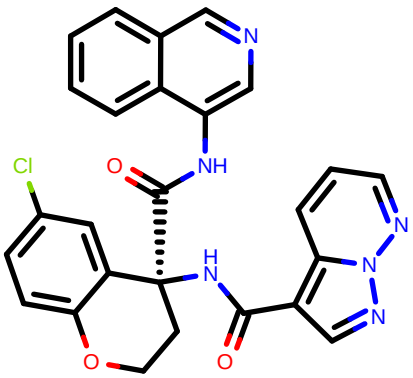
CID:	EN300-6238494_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)[C@H]5COCCO5
RUN:	RUN1127
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.38

EN300-21813_1_1



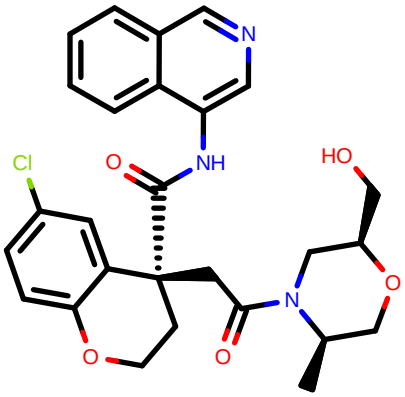
CID:	EN300-21813_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)c6ccccc6nn5
RUN:	RUN6407
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.33

EN300-114593_1_1



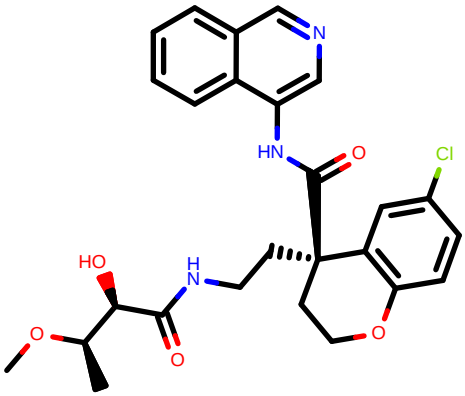
CID:	EN300-114593_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn6c5cccn6
RUN:	RUN7038
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.28

EN300-109920_1_1



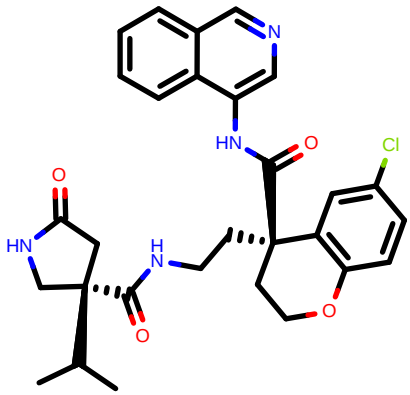
CID:	EN300-109920_1_1
SMILES:	C[C@@H]1CO[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN9754
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.46

EN300-220194_3_4



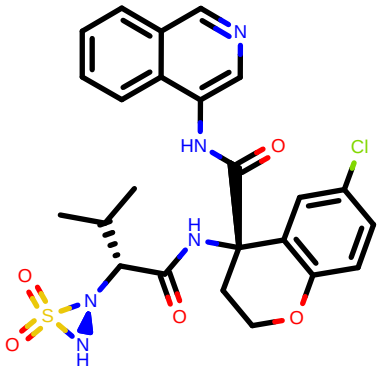
CID:	EN300-220194_3_4
SMILES:	C[C@H]([C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN4915
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.30

EN300-211203_3_1



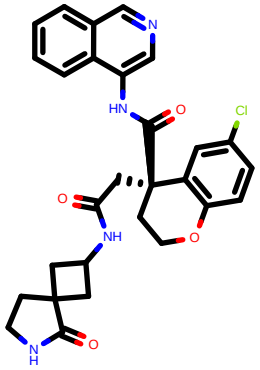
CID:	EN300-211203_3_1
SMILES:	CC(C)[C@@]1(CC(=O)NC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3680
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.33

EN300-2803713_1_1



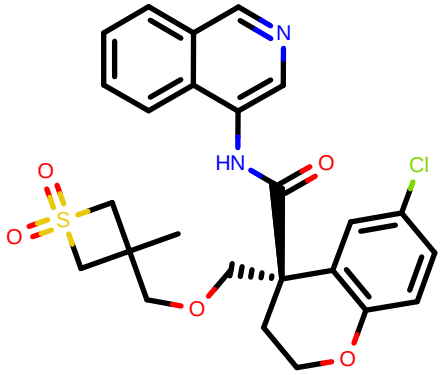
CID:	EN300-2803713_1_1
SMILES:	CC(C)[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)N
RUN:	RUN4609
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.39

EN300-743350_1_1



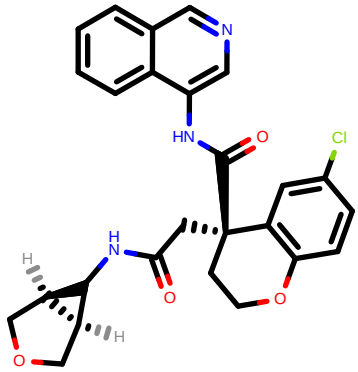
CID:	EN300-743350_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC6(C5)CCNC6=O
RUN:	RUN10067
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.28

EN300-1705754_2_1



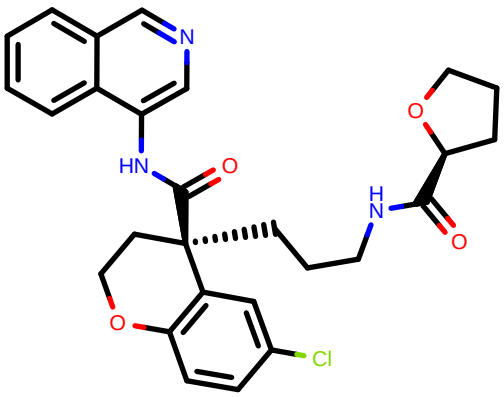
CID:	EN300-1705754_2_1
SMILES:	CC1(CS(=O)(=O)C1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2456
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.24

EN300-192482_1_1



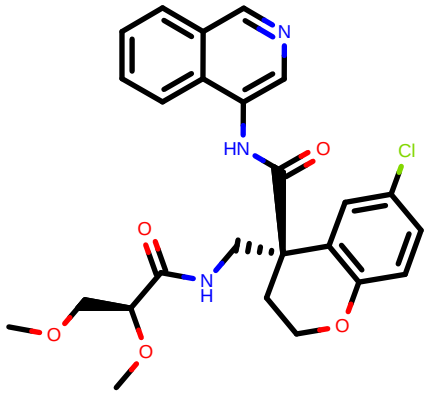
CID:	EN300-192482_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5[C@H]6[C@@H]5COC6
RUN:	RUN7888
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.25

EN300-104395_4_1



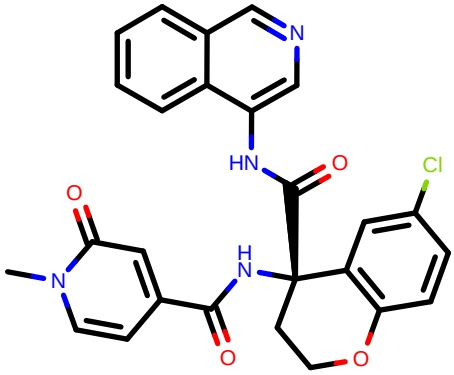
CID:	EN300-104395_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCCO5
RUN:	RUN10531
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.33

EN300-305282_2_1



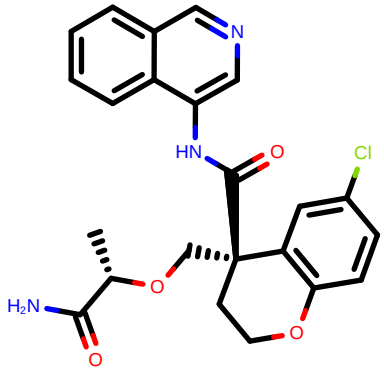
CID:	EN300-305282_2_1
SMILES:	COC[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN1329
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.30

EN300-30480_1_1



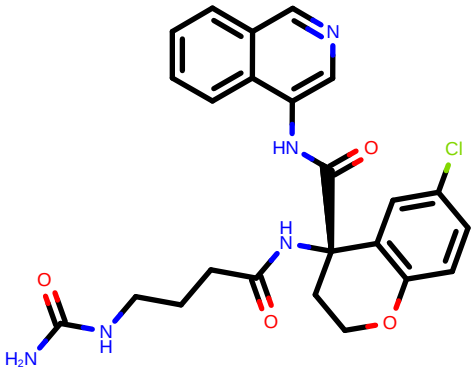
CID:	EN300-30480_1_1
SMILES:	Cn1ccc(cc1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4745
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.24

EN300-17381_2_1



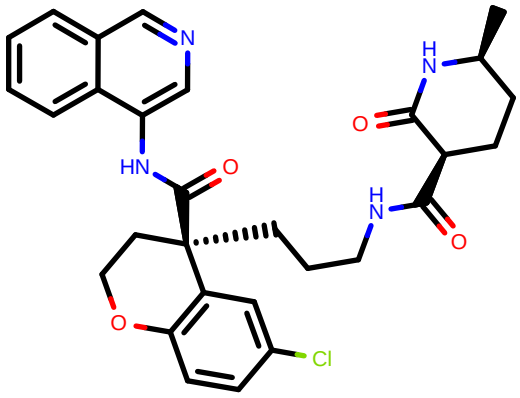
CID:	EN300-17381_2_1
SMILES:	C[C@@H](C(=O)N)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN894
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.20

EN300-05620_1_1



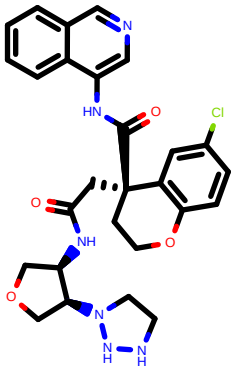
CID:	EN300-05620_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCNC(=O)N
RUN:	RUN577
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.25

EN300-6505003_4_4



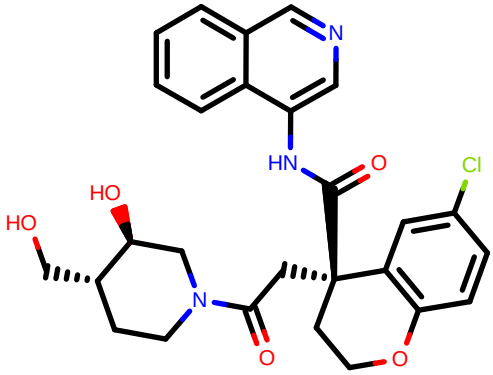
CID:	EN300-6505003_4_4
SMILES:	C[C@H]1CC[C@H](C(=O)N1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10505
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.37

EN300-1273248_1_1



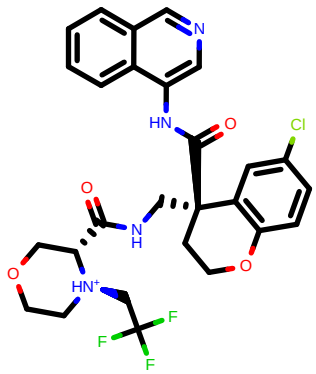
CID:	EN300-1273248_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5n6ccnn6
RUN:	RUN11186
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.32

EN300-95639_1_3



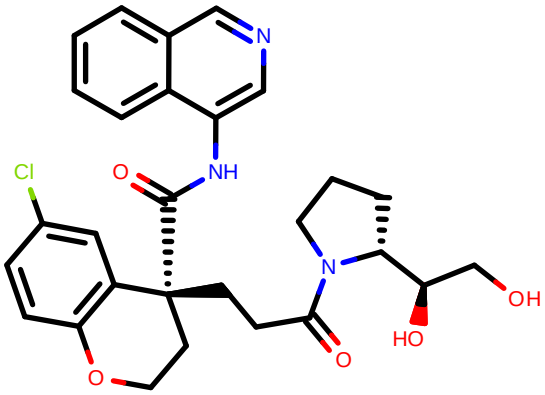
CID:	EN300-95639_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]([C@H](C5)O)CO
RUN:	RUN447
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.34

EN300-201551_2_2



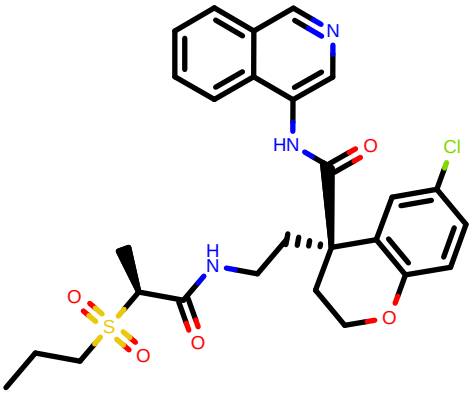
CID:	EN300-201551_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCCN5CC(F)(F)F
RUN:	RUN3770
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.44

EN300-7459540_2_1



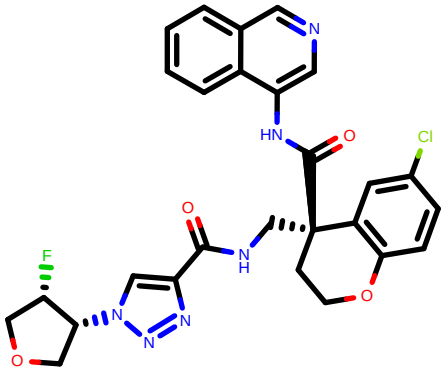
CID:	EN300-7459540_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@@H]5[C@@H](CO)O
RUN:	RUN9387
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.43

EN300-52768_3_1



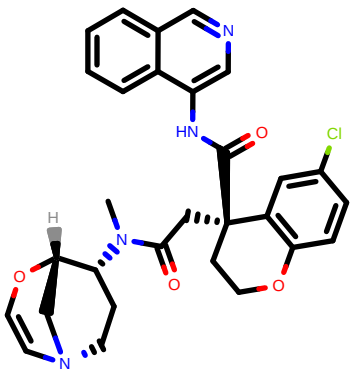
CID:	EN300-52768_3_1
SMILES:	CCCS(=O)(=O)[C@@H](C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7340
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.51

EN300-6759512_2_1



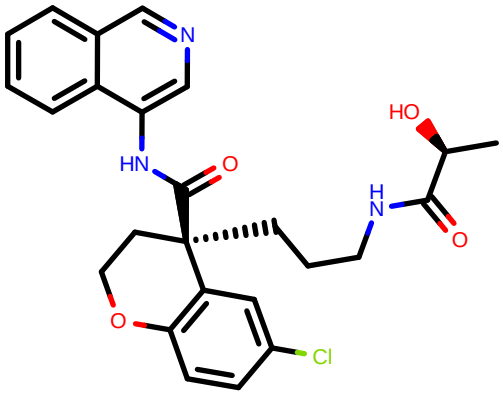
CID:	EN300-6759512_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)[C@@H]6COC[C@@H]6F
RUN:	RUN6991
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.28

EN300-159953_1_1



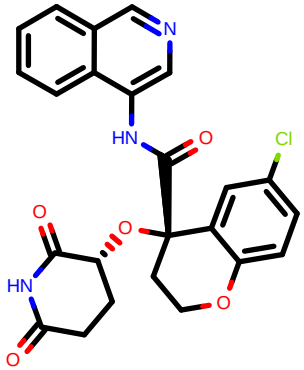
CID:	EN300-159953_1_1
SMILES:	CN([C@@H]1CCN2CCOC1C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN9977
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.41

EN300-91905_4_1



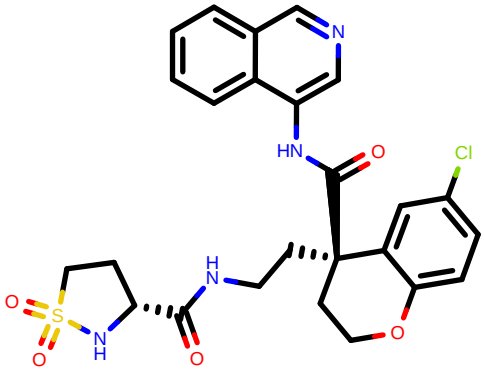
CID:	EN300-91905_4_1
SMILES:	C[C@@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN10219
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.30

EN300-120920_1_1



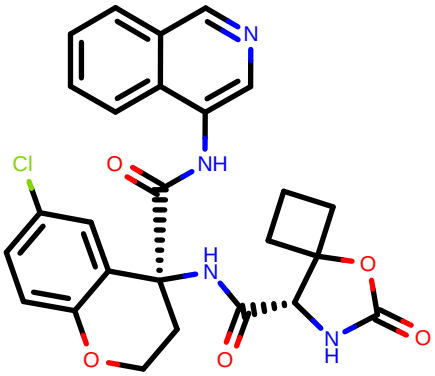
CID:	EN300-120920_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5CCC(=O)NC5=O
RUN:	RUN2401
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.25

EN300-45049_3_2



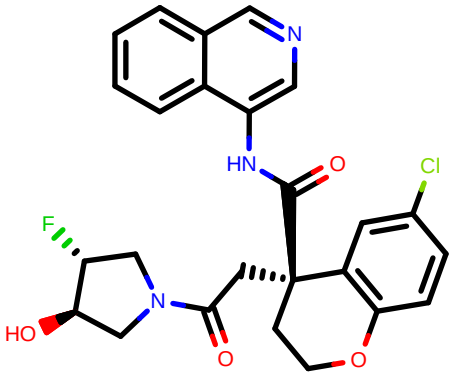
CID:	EN300-45049_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCS(=O)(=O)N5
RUN:	RUN11280
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.28

EN300-7432415_1_1



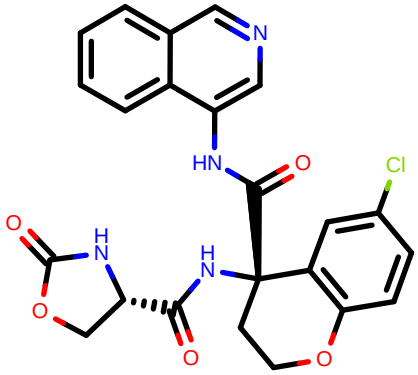
CID:	EN300-7432415_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5C6(CCC6)OC(=O)N5
RUN:	RUN6116
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.25

EN300-317085_1_1



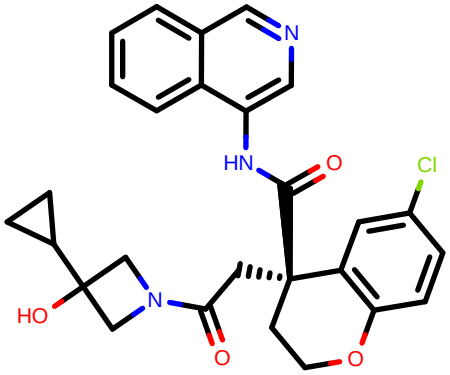
CID:	EN300-317085_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]([C@@H](C5)F)O
RUN:	RUN5626
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.22

EN300-126389_1_1



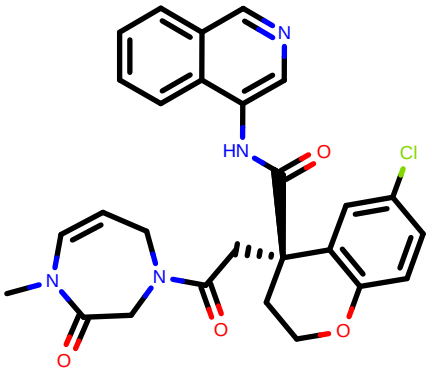
CID:	EN300-126389_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5COC(=O)N5
RUN:	RUN3034
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.23

EN300-126127_1_1



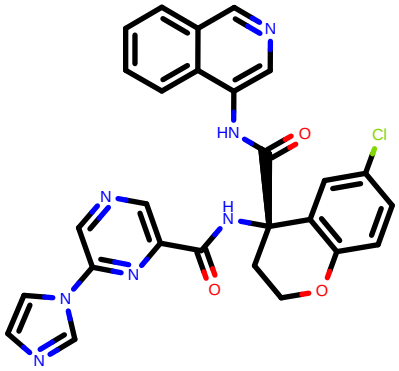
CID:	EN300-126127_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C6CC6)O
RUN:	RUN4279
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.30

EN300-160143_1_1



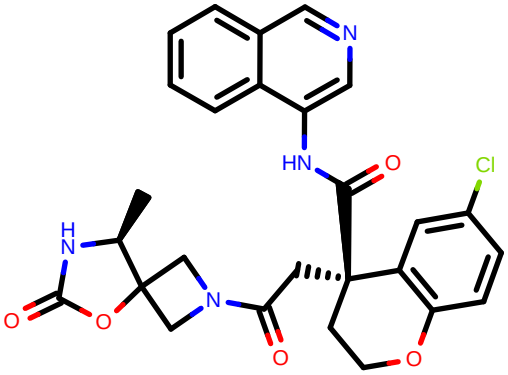
CID:	EN300-160143_1_1
SMILES:	CN1CCCN(CC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9900
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.23

EN300-2666482_1_1



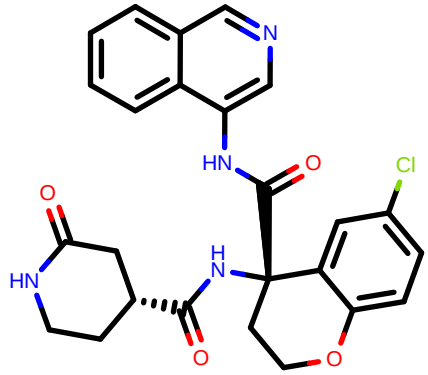
CID:	EN300-2666482_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cncc(n5)n6ccnc6
RUN:	RUN8646
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.25

EN300-6486763_1_2



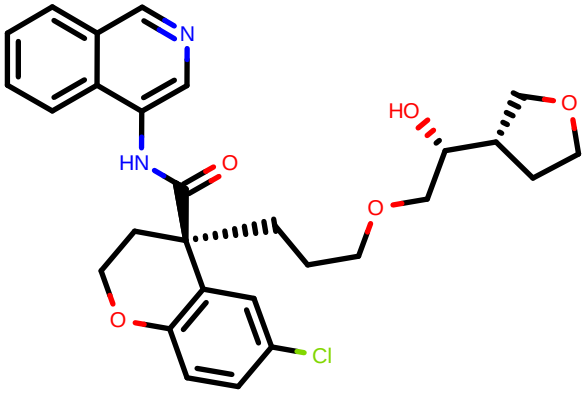
CID:	EN300-6486763_1_2
SMILES:	C[C@H]1C2(CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)OC(=O)N1
RUN:	RUN574
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.27

EN300-107493_1_1



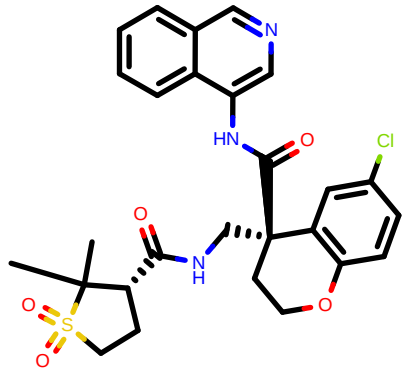
CID:	EN300-107493_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCNC(=O)C5
RUN:	RUN3741
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.23

EN300-1911992_4_3



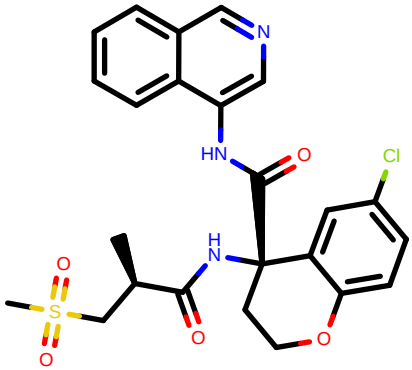
CID:	EN300-1911992_4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]([C@H]5CCOC5)O
RUN:	RUN675
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.44

EN300-2007564_2_1



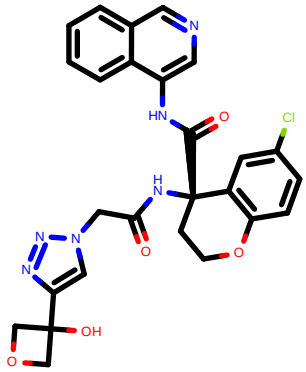
CID:	EN300-2007564_2_1
SMILES:	CC1([C@@H](CCS1(=O)=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN5461
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.35

EN300-97699_1_2



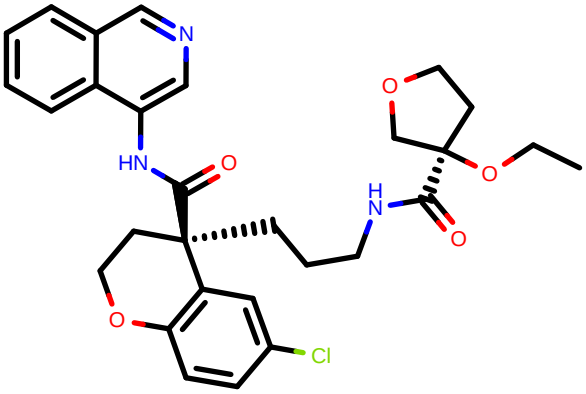
CID:	EN300-97699_1_2
SMILES:	C[C@H](CS(=O)(=O)C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4129
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.38

EN300-7445540_1_1



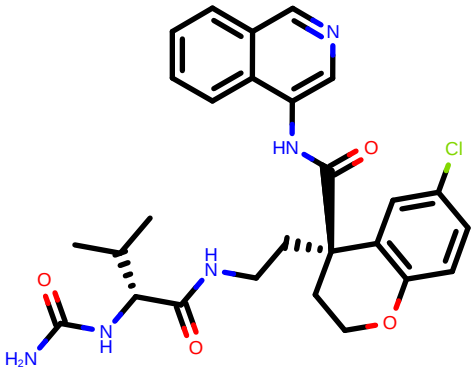
CID:	EN300-7445540_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(nn5)C6(COC6)O
RUN:	RUN8258
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.30

EN300-259694_4_1



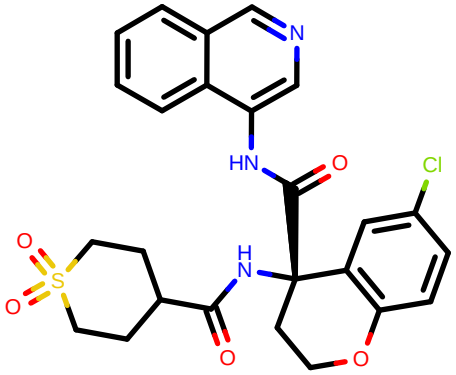
CID:	EN300-259694_4_1
SMILES:	CCO[C@@]1(CCOC1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10140
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.47

EN300-2972220_3_1



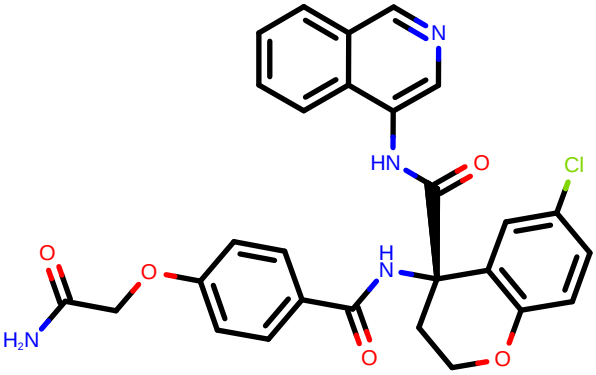
CID:	EN300-2972220_3_1
SMILES:	CC(C)[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN1362
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.31

EN300-75807_1_1



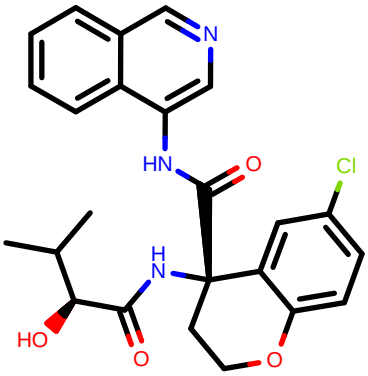
CID:	EN300-75807_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CCS(=O)(=O)CC5
RUN:	RUN6080
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.23

EN300-14949_1_1



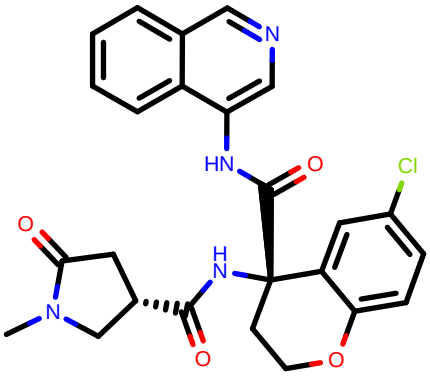
CID:	EN300-14949_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(cc5)OCC(=O)N
RUN:	RUN9068
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.24

EN300-199359_1_1



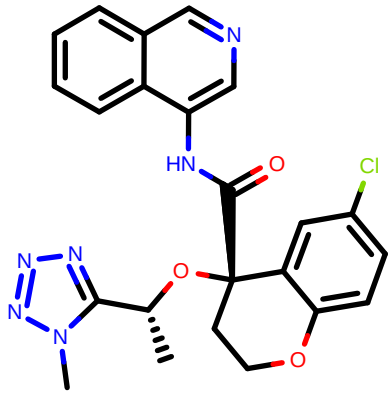
CID:	EN300-199359_1_1
SMILES:	CC(C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3670
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.30

EN300-33601_1_2



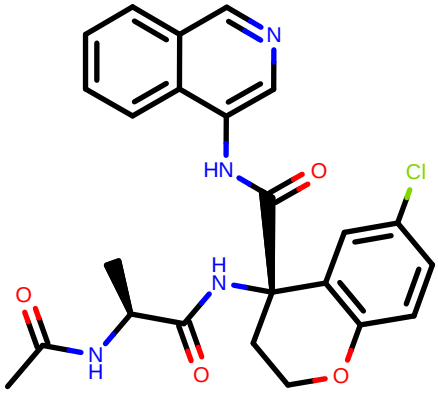
CID:	EN300-33601_1_2
SMILES:	CN1C[C@H](CC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5624
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.29

EN300-173006_1_2



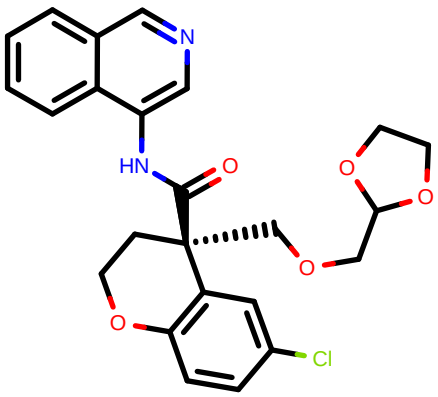
CID:	EN300-173006_1_2
SMILES:	C[C@H](c1nnnn1C)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1823
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.26

EN300-18569_1_1



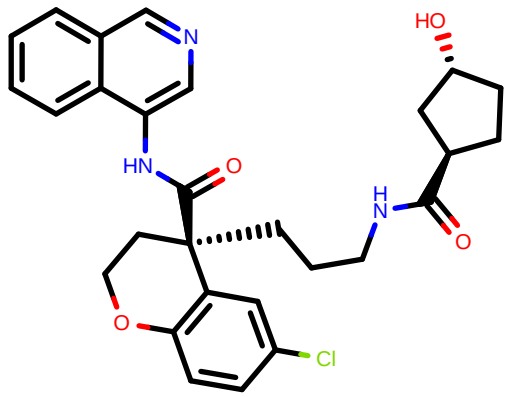
CID:	EN300-18569_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN4769
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.24

EN300-77092_2_1



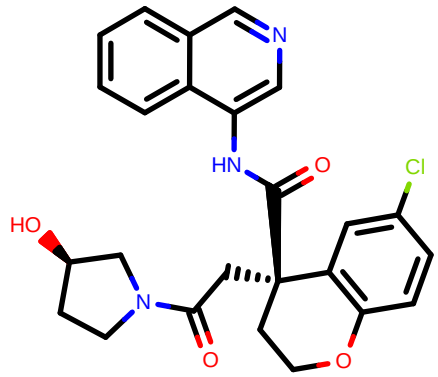
CID:	EN300-77092_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5OCCO5
RUN:	RUN1382
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.22

EN300-321597_4_1



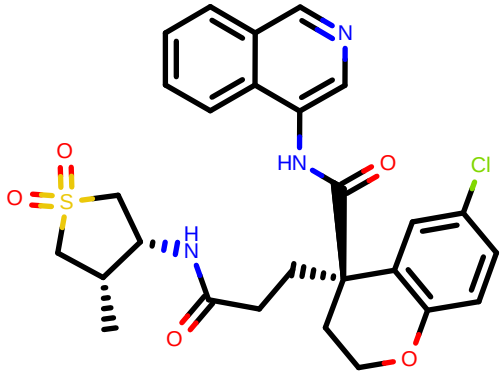
CID:	EN300-321597_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CC[C@H](C5)O
RUN:	RUN9212
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.38

EN300-295515_1_2



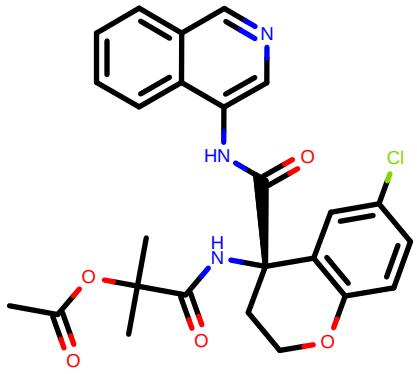
CID:	EN300-295515_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)O
RUN:	RUN5187
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.30

EN300-371704_2_1



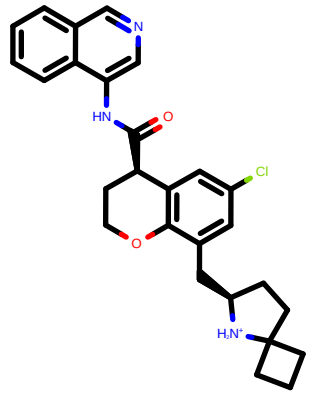
CID:	EN300-371704_2_1
SMILES:	C[C@@H]1CS(=O)(=O)C[C@@H]1NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7353
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.33

EN300-155589_1_1



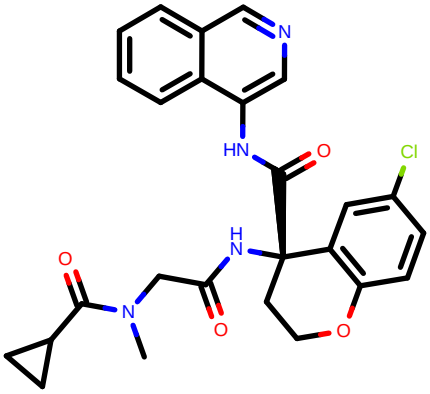
CID:	EN300-155589_1_1
SMILES:	CC(=O)OC(C)(C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3654
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.30

DAR-DIA-23e5a6a0-6_2



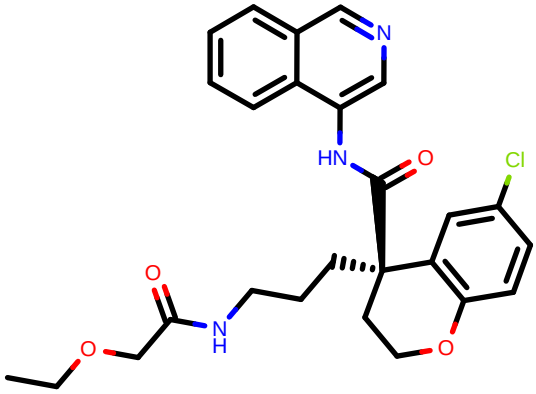
CID:	DAR-DIA-23e5a6a0-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CCC6(N5)CCC6)Cl
RUN:	RUN133
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.30

EN300-31146_1_1



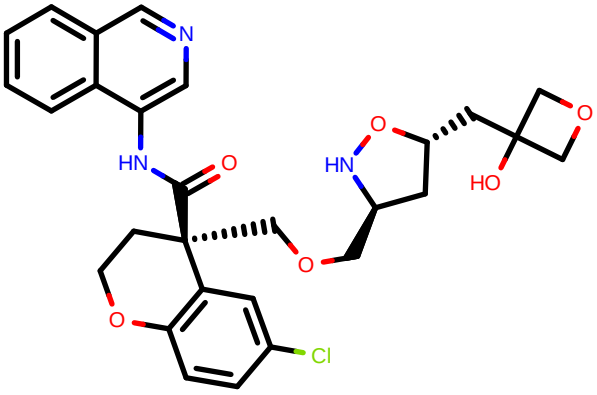
CID:	EN300-31146_1_1
SMILES:	CN(CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)C5CC5
RUN:	RUN4517
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.37

EN300-21303_4_1



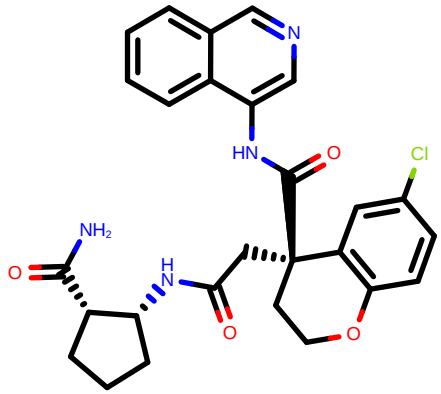
CID:	EN300-21303_4_1
SMILES:	CCOCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9061
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.37

EN300-7457160_2_1



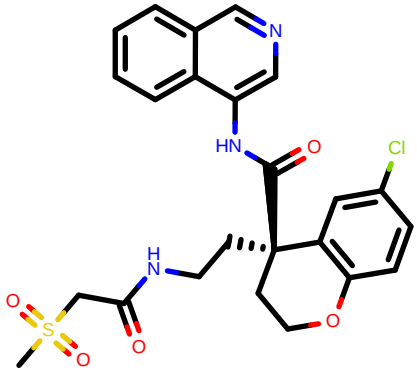
CID:	EN300-7457160_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5=NO[C@@H](C5)CC6(COC6)O
RUN:	RUN2603
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.34

EN300-257573_1_1



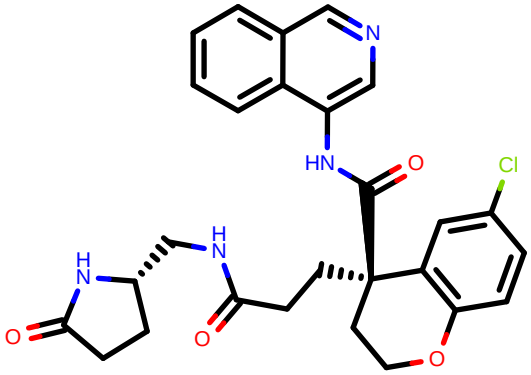
CID:	EN300-257573_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCC[C@@H]5C(=O)N
RUN:	RUN11134
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.32

EN300-53677_3_1



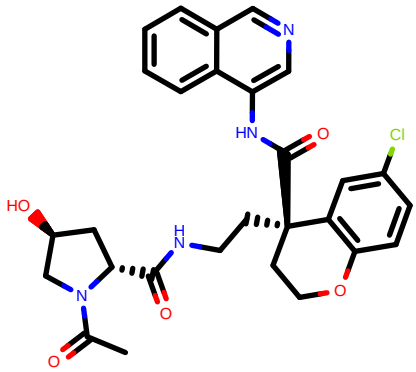
CID:	EN300-53677_3_1
SMILES:	CS(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9494
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.29

EN300-75030_2_1



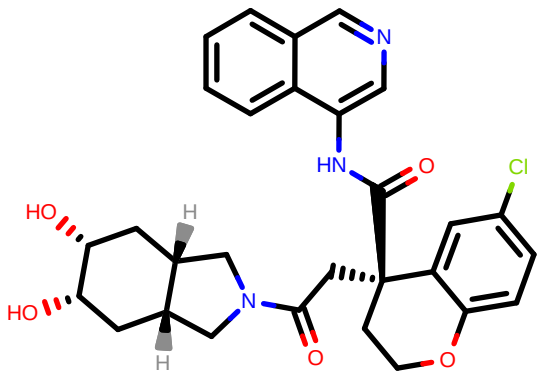
CID:	EN300-75030_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H]5CCC(=O)N5
RUN:	RUN6961
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.30

EN300-158274_3_1



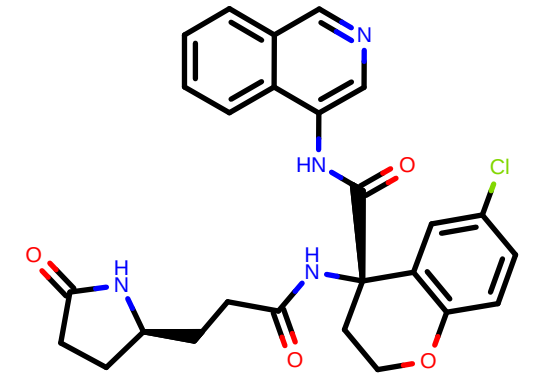
CID:	EN300-158274_3_1
SMILES:	CC(=O)N1C[C@H](C[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6537
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.37

EN300-7355477_1_1



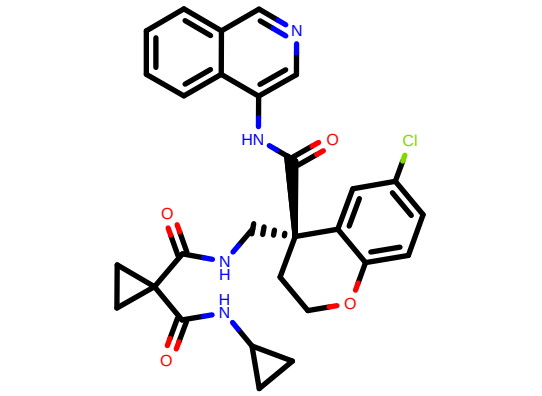
CID:	EN300-7355477_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@H]([C@H](C[C@H]6C5)O)O
RUN:	RUN7816
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.27

EN300-104592_1_2



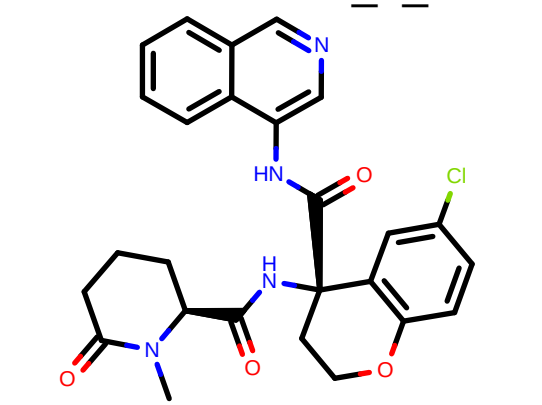
CID:	EN300-104592_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H]5CCC(=O)N5
RUN:	RUN378
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.29

EN300-61636_2_1



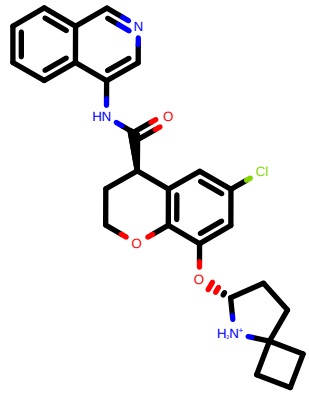
CID:	EN300-61636_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)C(=O)NC6CC6
RUN:	RUN4998
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.45

EN300-325738_1_1



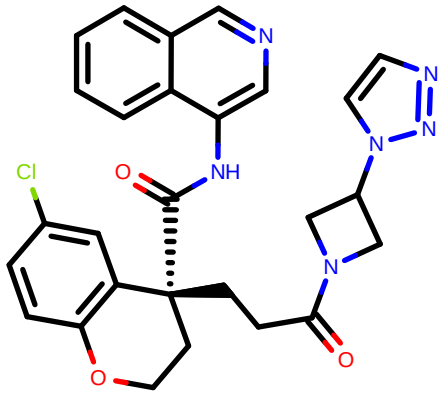
CID:	EN300-325738_1_1
SMILES:	CN1[C@@H](CCCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6778
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.28

DAR-DIA-23e5a6a0-1_1



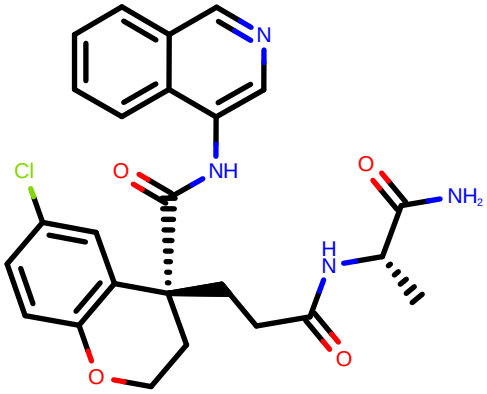
CID:	DAR-DIA-23e5a6a0-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CCC6(N5)CCC6)Cl
RUN:	RUN225
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.36

EN300-367405_2_1



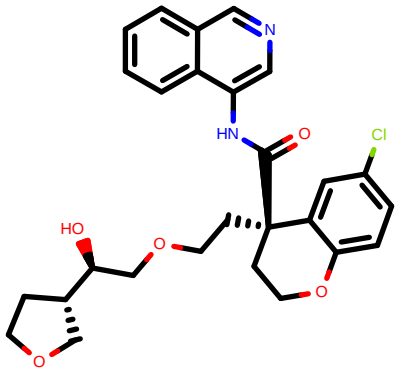
CID:	EN300-367405_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)n6ccnn6
RUN:	RUN1914
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.28

EN300-23648_2_1



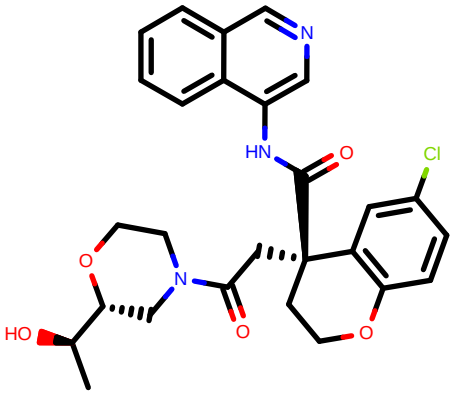
CID:	EN300-23648_2_1
SMILES:	C[C@@H](C(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1794
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.27

EN300-1911992_3_3



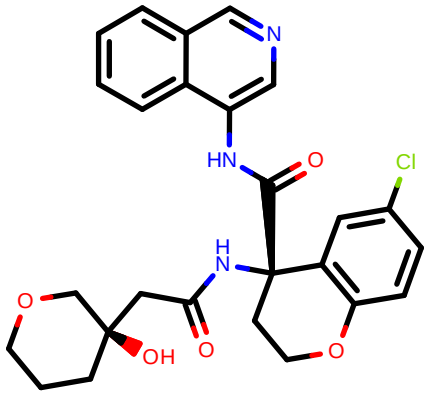
CID:	EN300-1911992_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H][[C@H]5CCOC5)O
RUN:	RUN695
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.35

EN300-1708637_1_2



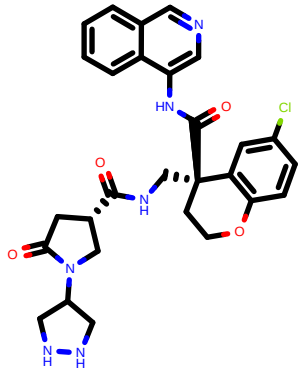
CID:	EN300-1708637_1_2
SMILES:	C[C@H]([C@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10386
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.33

EN300-1071940_1_1



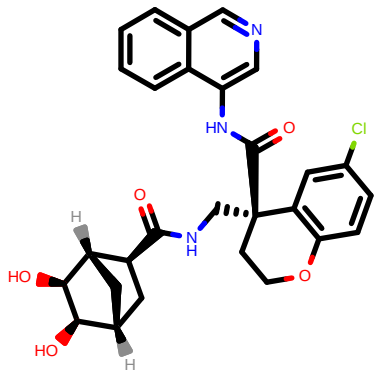
CID:	EN300-1071940_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@]5(CCCOC5)O
RUN:	RUN1013
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.28

EN300-99064_2_2



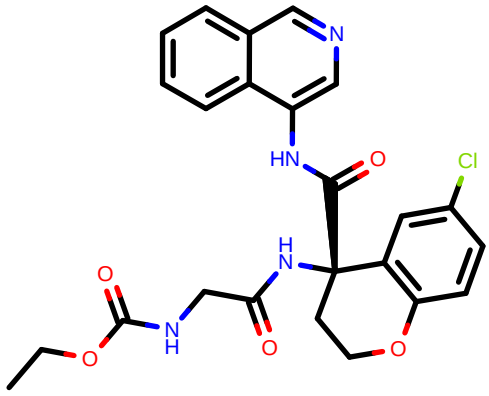
CID:	EN300-99064_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC(=O)N(C5)c6c[nH]nc6
RUN:	RUN4082
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.36

EN300-6744028_2_2



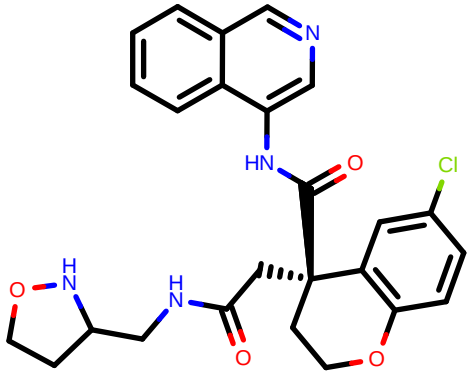
CID:	EN300-6744028_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC6CC5[C@@H][C@@H]6O)O
RUN:	RUN8043
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.28

EN300-36390_1_1



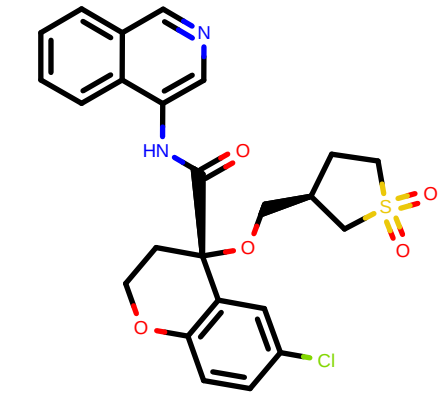
CID:	EN300-36390_1_1
SMILES:	CCOC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3162
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.24

EN300-1720418_1_1



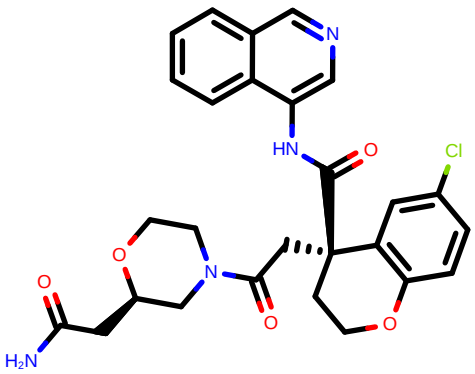
CID:	EN300-1720418_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5=NOCC5
RUN:	RUN9610
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.20

EN300-1448603_1_2



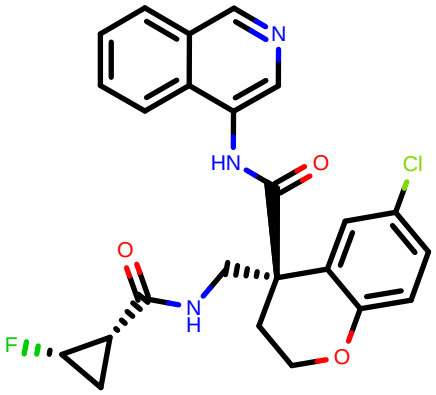
CID:	EN300-1448603_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCS(=O)(=O)C5
RUN:	RUN2366
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.27

EN300-321558_1_1



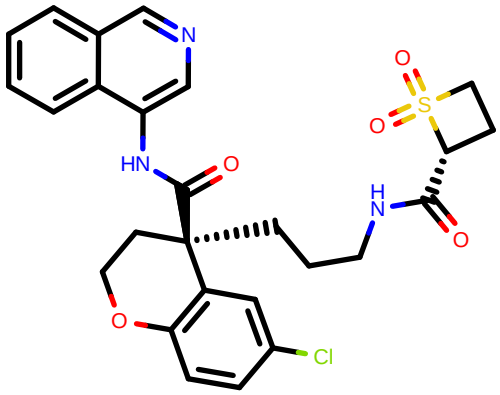
CID:	EN300-321558_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)CC(=O)N
RUN:	RUN8652
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.41

EN300-97300_2_1



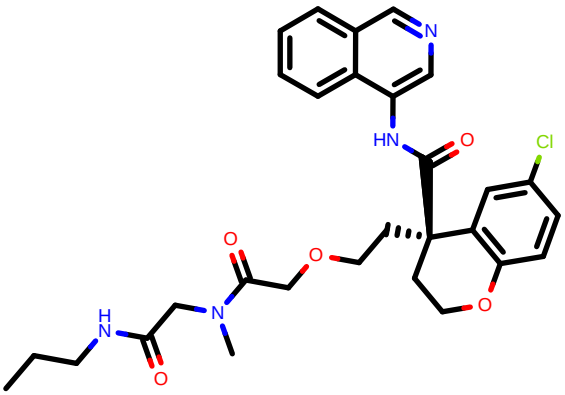
CID:	EN300-97300_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@@H]5F
RUN:	RUN3882
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.22

EN300-1387104_4_2



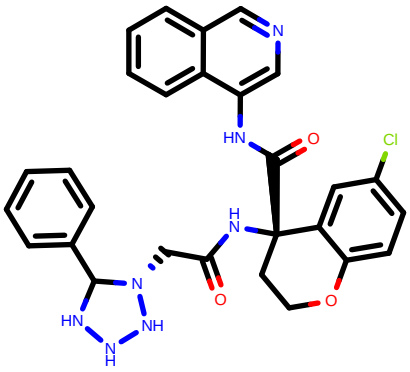
CID:	EN300-1387104_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCS5(=O)=O
RUN:	RUN8041
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.46

EN300-12204_3_1



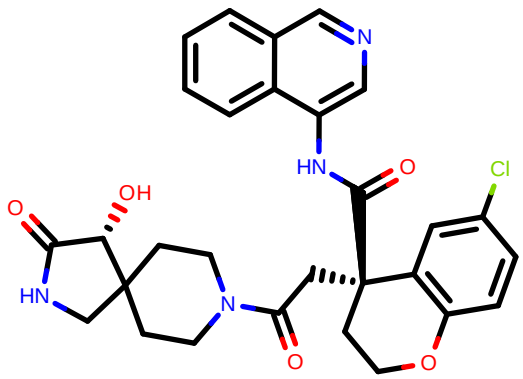
CID:	EN300-12204_3_1
SMILES:	CCCNC(=O)CN(C)C(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1987
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.41

EN300-702735_1_1



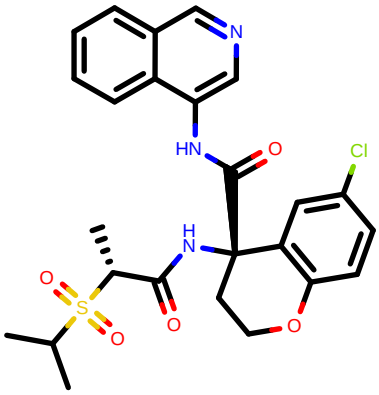
CID:	EN300-702735_1_1
SMILES:	c1ccc(cc1)c2nnnn2CC(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN6447
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.32

EN300-6478434_1_1



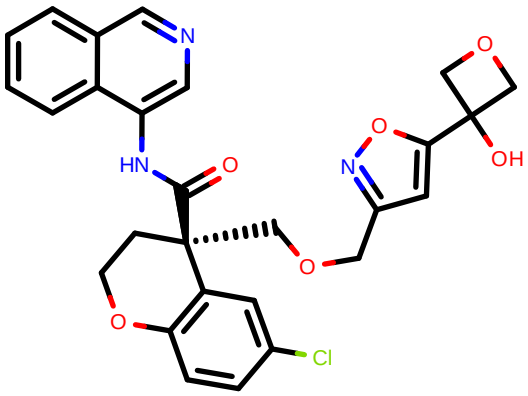
CID:	EN300-6478434_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC6(CC5)CNC(=O)[C@@H]6O
RUN:	RUN5051
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.37

EN300-40947_1_2



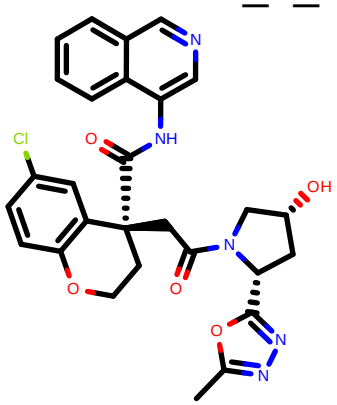
CID:	EN300-40947_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C(C)C
RUN:	RUN2108
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.26

EN300-7457159_2_1



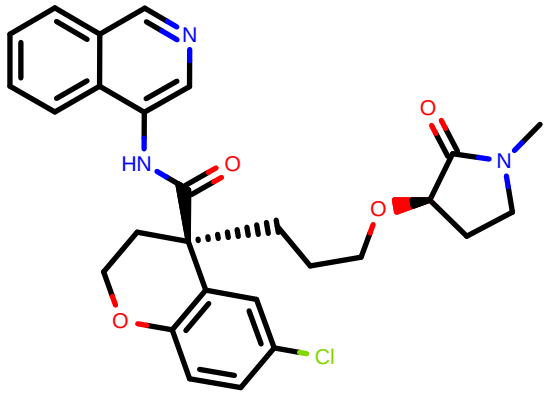
CID:	EN300-7457159_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5cc(on5)C6(COC6)O
RUN:	RUN2553
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.31

EN300-158207_1_1



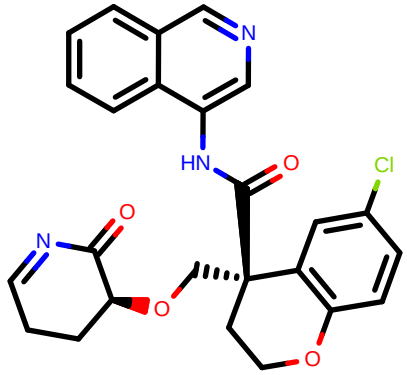
CID:	EN300-158207_1_1
SMILES:	Cc1nnc(o1)[C@H]2C[C@H](CN2C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)O
RUN:	RUN10672
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.43

EN300-98648_4_2



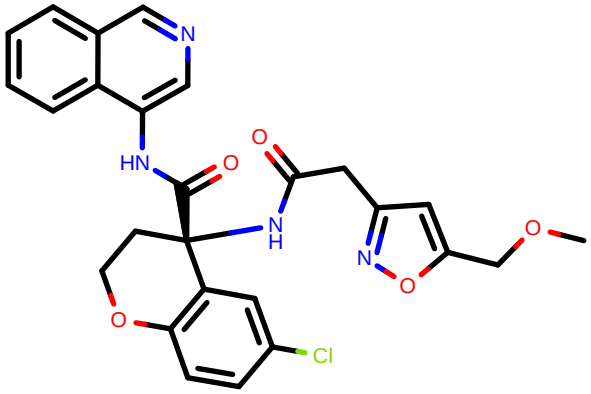
CID:	EN300-98648_4_2
SMILES:	CN1CC[C@H](C1=O)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1686
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.26

EN300-107267_2_2



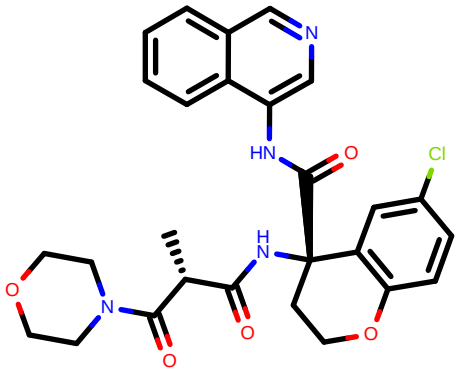
CID:	EN300-107267_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCCNC5=O
RUN:	RUN966
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.24

EN300-6477475_1_1



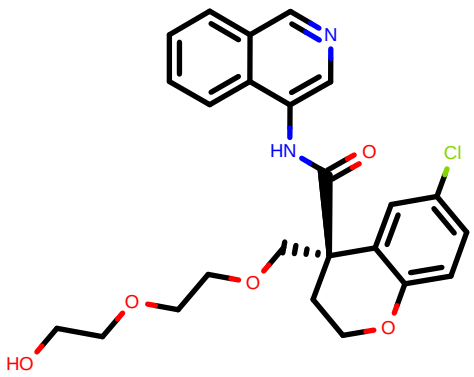
CID:	EN300-6477475_1_1
SMILES:	COCc1cc(no1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6954
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.26

EN300-2855057_1_2



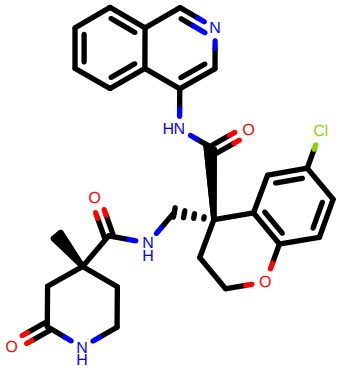
CID:	EN300-2855057_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)N5CCOCC5
RUN:	RUN7834
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.38

EN300-52467_2_1



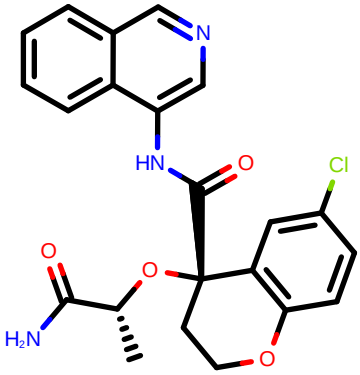
CID:	EN300-52467_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCOCCO
RUN:	RUN1573
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.33

EN300-315854_2_2



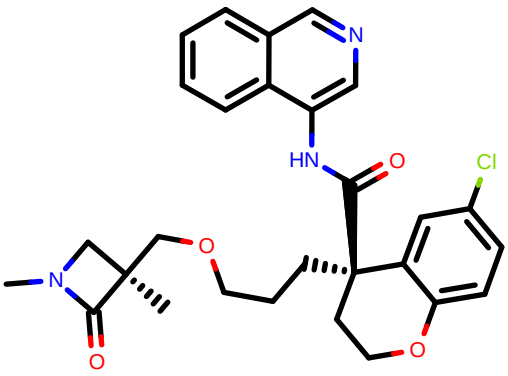
CID:	EN300-315854_2_2
SMILES:	C[C@]1(CCNC(=O)C1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4598
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.22

EN300-17381_1_2



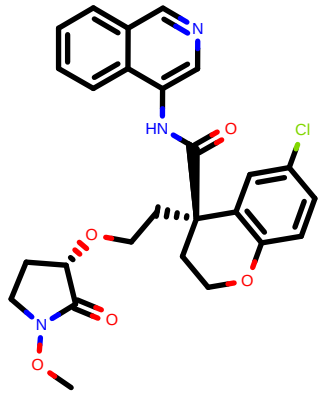
CID:	EN300-17381_1_2
SMILES:	C[C@H](C(=O)N)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN825
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.19

EN300-1273362_4_2



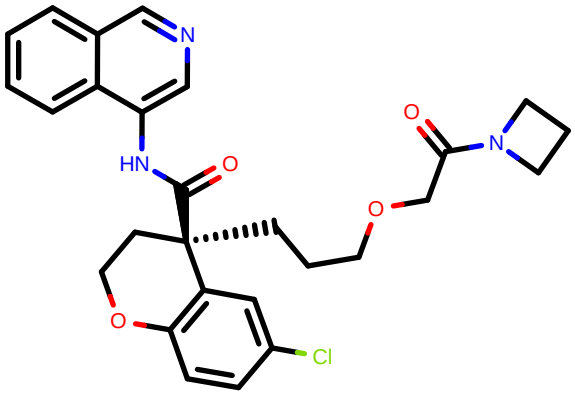
CID:	EN300-1273362_4_2
SMILES:	C[C@]1(CN(C1=O)C)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1998
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.39

EN300-302058_3_1



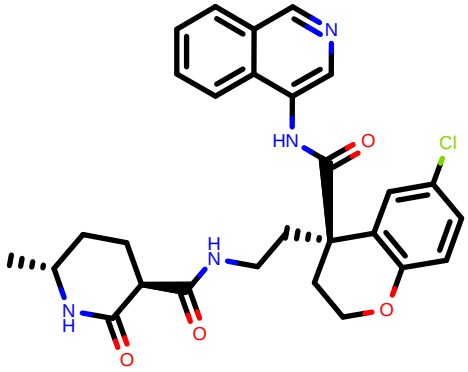
CID:	EN300-302058_3_1
SMILES:	CON1CC[C@@H](C1=O)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1707
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.27

EN300-11195_4_1



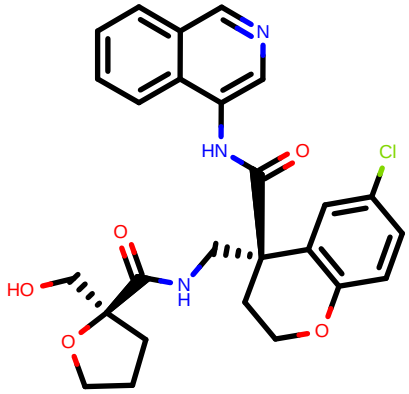
CID:	EN300-11195_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)N5CCC5
RUN:	RUN1255
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.28

EN300-6505003_3_3



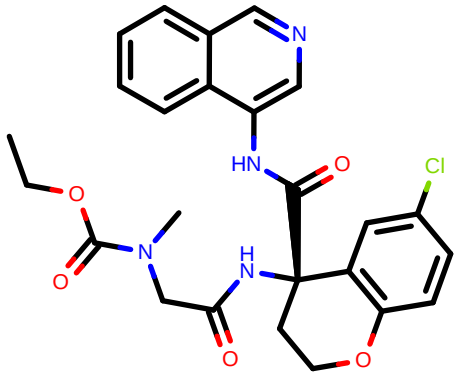
CID:	EN300-6505003_3_3
SMILES:	C[C@@H]1CC[C@H](C(=O)N1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9842
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.39

EN300-1425677_2_2



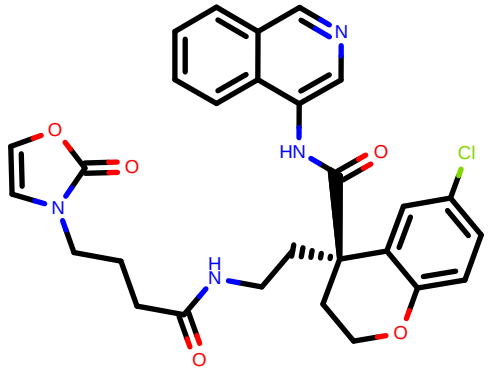
CID:	EN300-1425677_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCCO5)CO
RUN:	RUN3527
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.33

EN300-39101_1_1



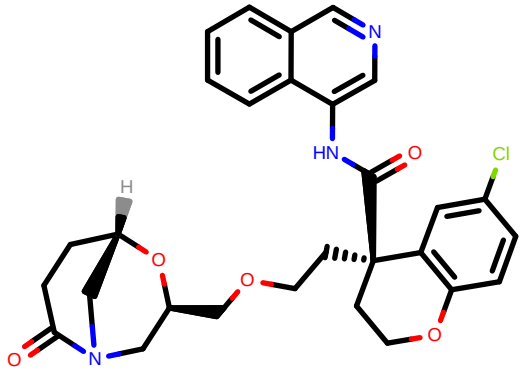
CID:	EN300-39101_1_1
SMILES:	CCOC(=O)N(C)CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3394
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.26

EN300-45182_3_1



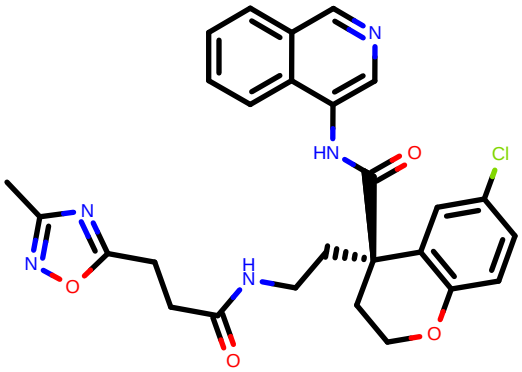
CID:	EN300-45182_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCN5CCOC5=O
RUN:	RUN10986
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.35

EN300-2008102_3_2



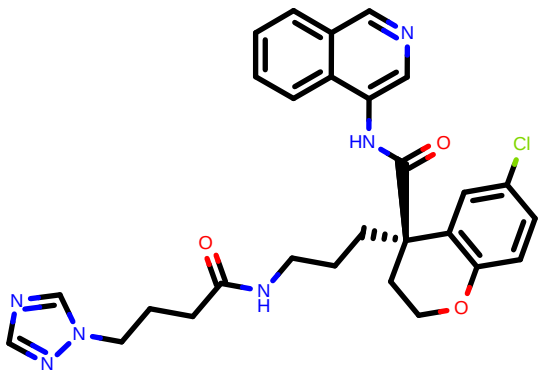
CID:	EN300-2008102_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5CN6CC(O5)CCC6=O
RUN:	RUN2321
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.34

EN300-27268_3_1



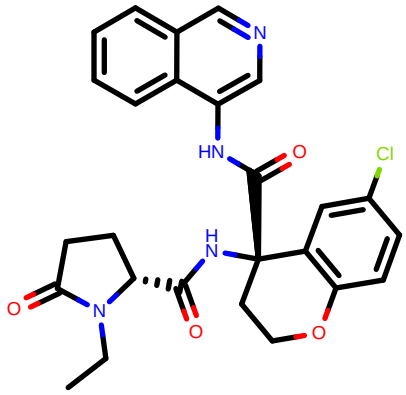
CID:	EN300-27268_3_1
SMILES:	Cc1nc(on1)CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7408
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.26

EN300-316216_4_1



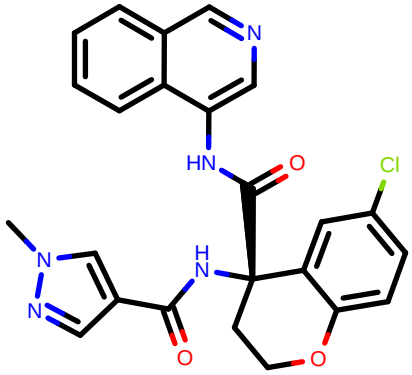
CID:	EN300-316216_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCCn5cncn5
RUN:	RUN11117
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.35

EN300-718785_1_2



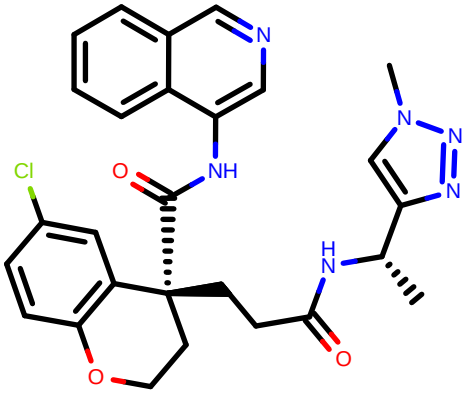
CID:	EN300-718785_1_2
SMILES:	CCN1[C@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3781
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.23

EN300-14395_1_1



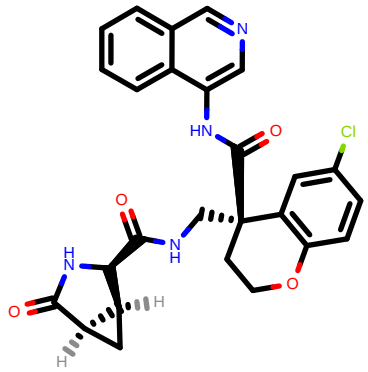
CID:	EN300-14395_1_1
SMILES:	Cn1cc(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3130
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.24

EN300-393300_2_1



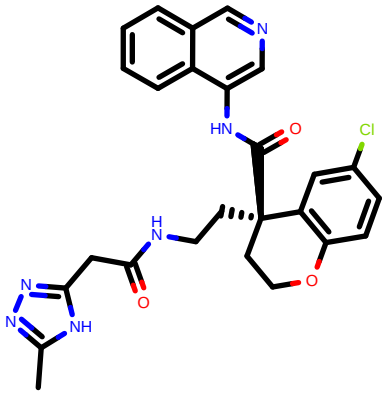
CID:	EN300-393300_2_1
SMILES:	C[C@@H](c1cn(nn1)C)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6119
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.26

EN300-6766359_2_1



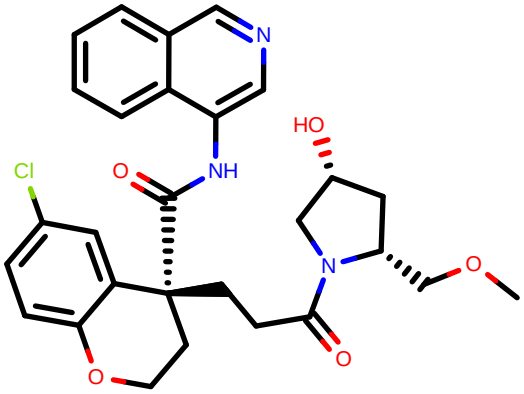
CID:	EN300-6766359_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5[C@H]6C[C@H]6C(=O)N5
RUN:	RUN4966
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.27

EN300-119126_3_1



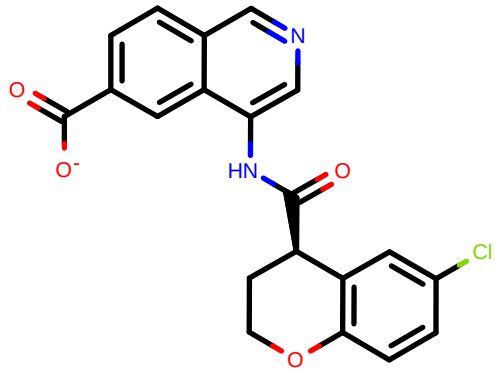
CID:	EN300-119126_3_1
SMILES:	Cc1[nH]c(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8740
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.43

EN300-252961_2_4



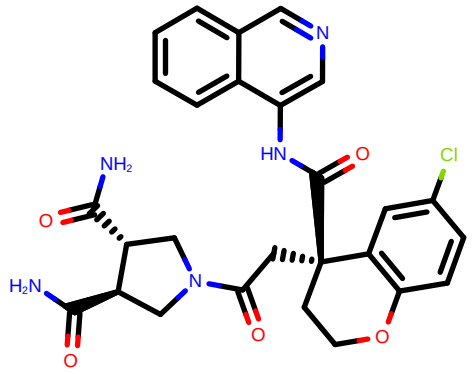
CID:	EN300-252961_2_4
SMILES:	COC[C@H]1C[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1706
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.33

MAK-UNK-8be7dca9-7_1



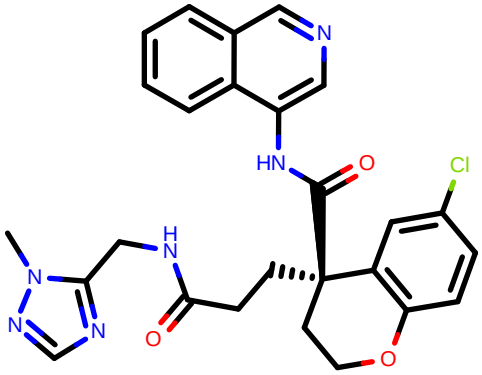
CID:	MAK-UNK-8be7dca9-7_1
SMILES:	c1cc2cncc(c2cc1C(=O)O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN29
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.08

EN300-7444316_1_1



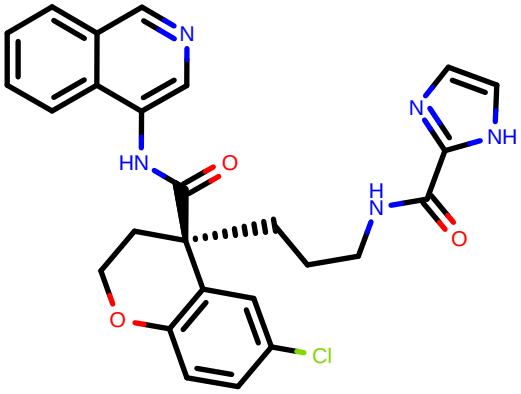
CID:	EN300-7444316_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H][C@@H](C5)C(=O)N)C(=O)N
RUN:	RUN1402
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.38

EN300-124063_2_1



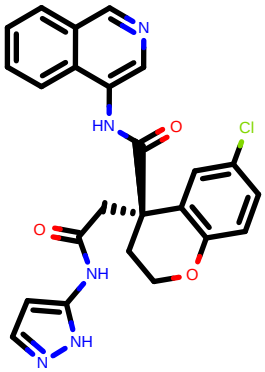
CID:	EN300-124063_2_1
SMILES:	Cn1c(ncn1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5771
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.33

EN300-315836_4_1



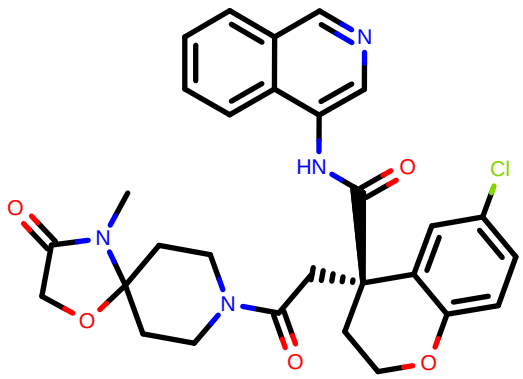
CID:	EN300-315836_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5[nH]ccn5
RUN:	RUN9685
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.32

JAG-UCB-706446eb-6_1



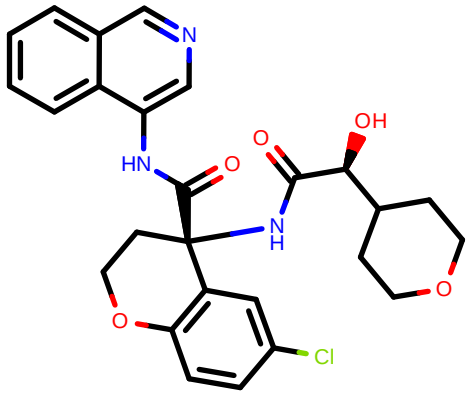
CID:	JAG-UCB-706446eb-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ccn[nH]5
RUN:	RUN272
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.23

EN300-6479892_1_1



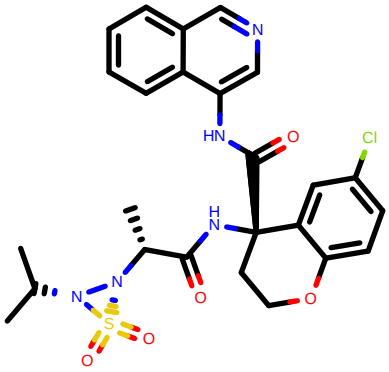
CID:	EN300-6479892_1_1
SMILES:	CN1C(=O)COC12CCN(CC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7008
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.30

EN300-6792206_1_1



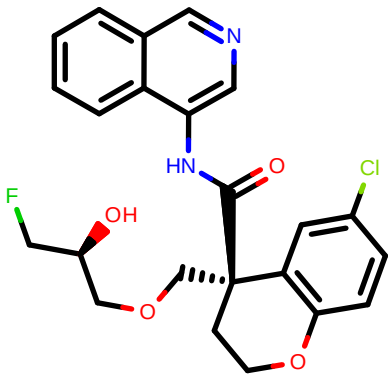
CID:	EN300-6792206_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5CCOCC5)O
RUN:	RUN6192
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.29

EN300-151268_1_2



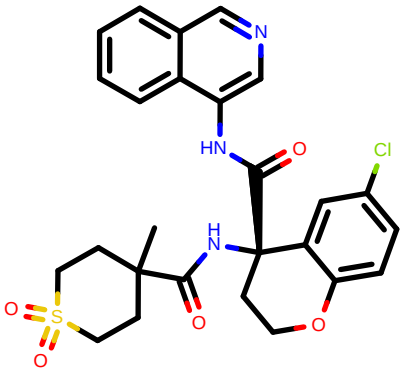
CID:	EN300-151268_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)NC(C)C
RUN:	RUN3102
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.66

EN300-1968342_2_1



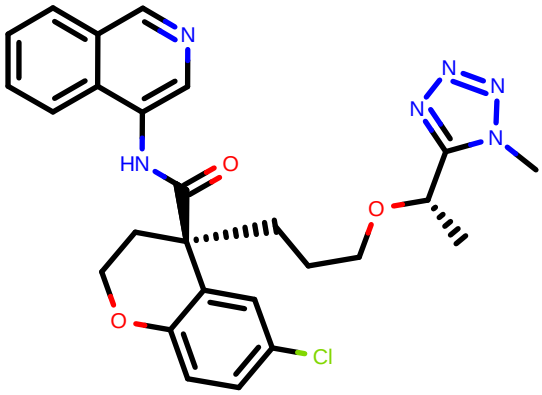
CID:	EN300-1968342_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H](CF)O
RUN:	RUN491
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.29

EN300-188585_1_1



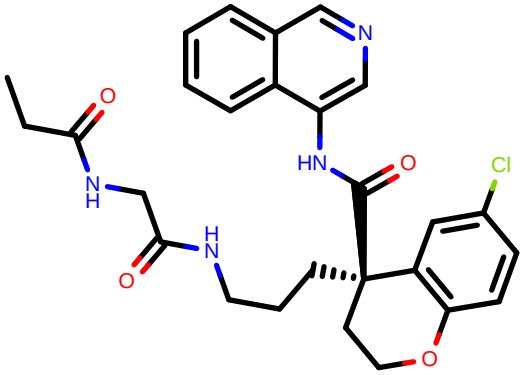
CID:	EN300-188585_1_1
SMILES:	CC1(CCS(=O)(=O)CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7286
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.30

EN300-173006_4_1



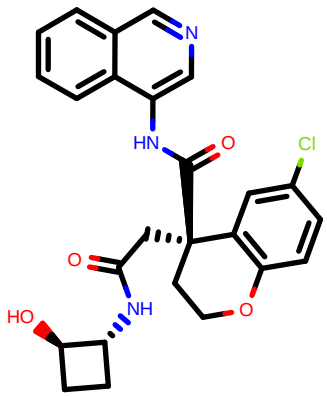
CID:	EN300-173006_4_1
SMILES:	C[C@@H](c1nnnn1C)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1838
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.36

EN300-31099_4_1



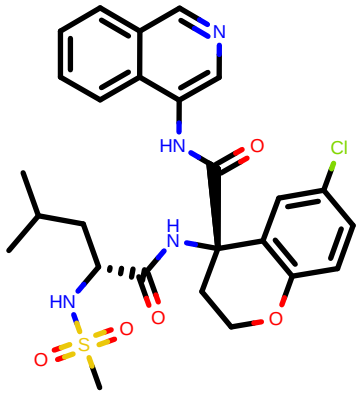
CID:	EN300-31099_4_1
SMILES:	CCC(=O)NCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10595
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.38

EN300-129424_1_3



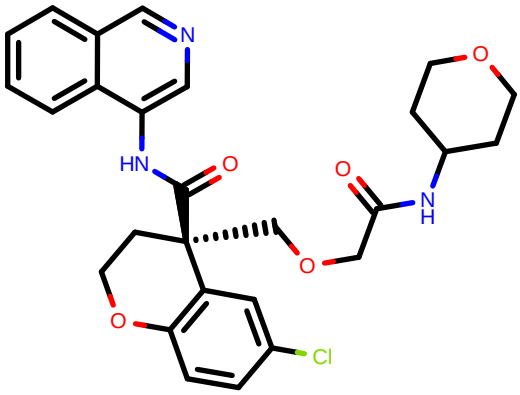
CID:	EN300-129424_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@H]5O
RUN:	RUN10340
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.26

EN300-11835_1_2



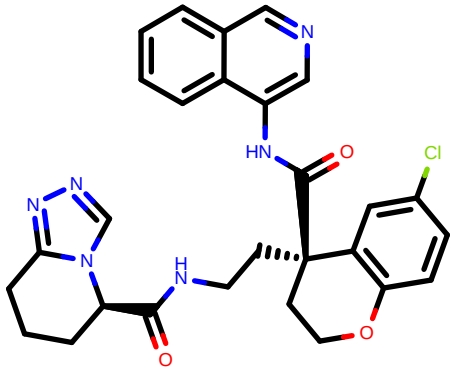
CID:	EN300-11835_1_2
SMILES:	CC(C)C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN5724
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.51

EN300-67573_2_1



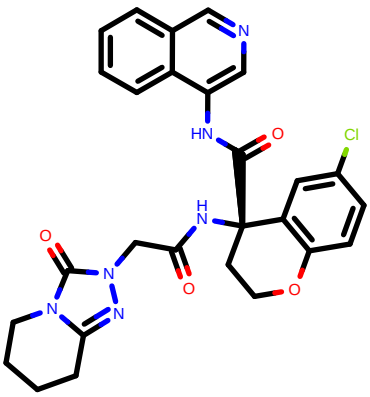
CID:	EN300-67573_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)NC5CCOCC5
RUN:	RUN626
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.29

EN300-6478631_3_2



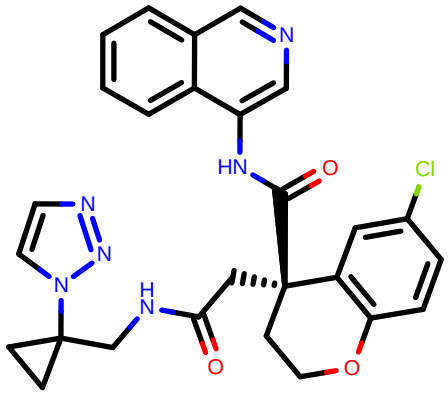
CID:	EN300-6478631_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCc6n5cnn6
RUN:	RUN9114
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.35

EN300-263346_1_1



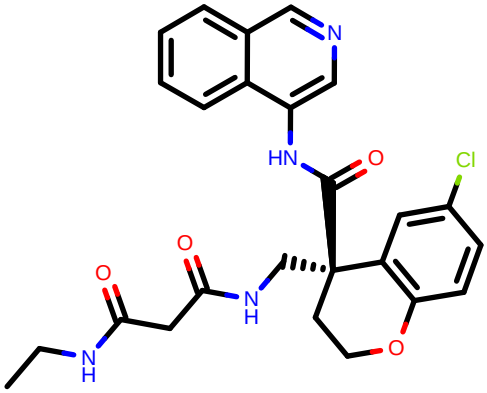
CID:	EN300-263346_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5c(=O)n6c(n5)CCCC6
RUN:	RUN7902
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.39

EN300-1721883_1_1



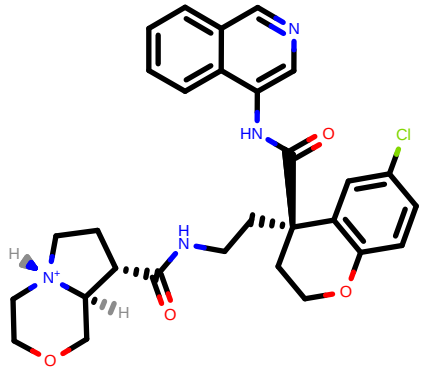
CID:	EN300-1721883_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CC5)n6ccnn6
RUN:	RUN9850
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.31

EN300-129455_2_1



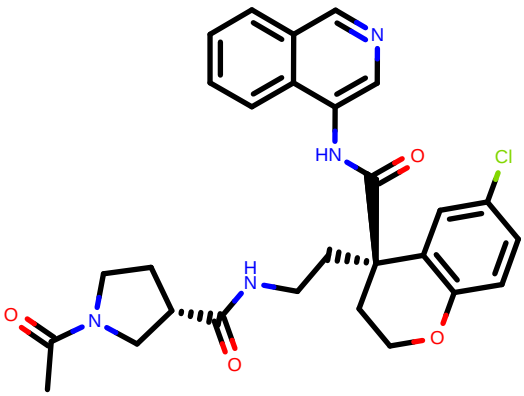
CID:	EN300-129455_2_1
SMILES:	CCNC(=O)CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1608
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.29

EN300-1588613_3_2



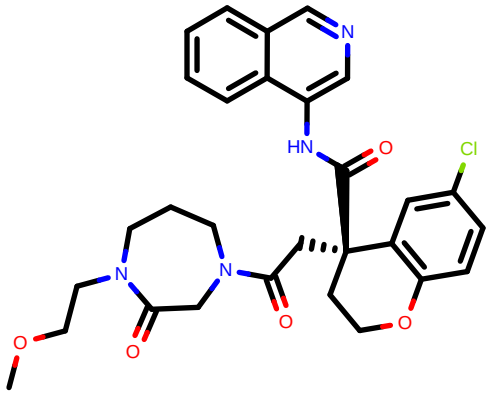
CID:	EN300-1588613_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCN6[C@@H]5COCC6
RUN:	RUN7248
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.44

EN300-100180_3_1



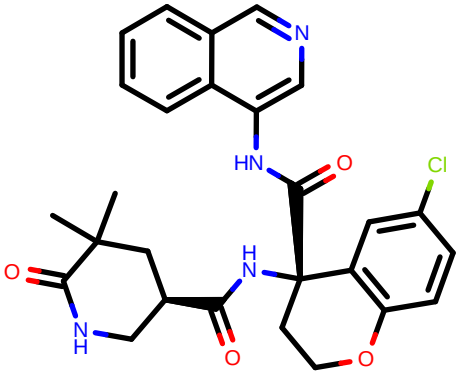
CID:	EN300-100180_3_1
SMILES:	CC(=O)N1CC[C@@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6106
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.42

EN300-154168_1_1



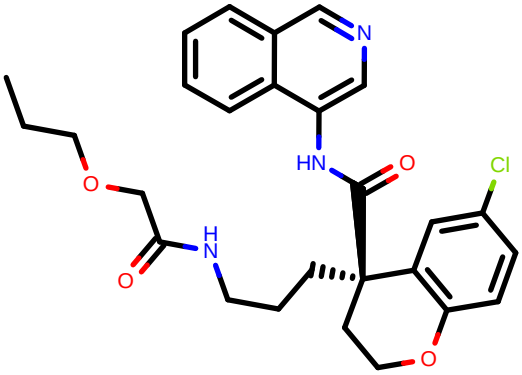
CID:	EN300-154168_1_1
SMILES:	COCCN1CCCN(CC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9378
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.26

EN300-7351945_1_2



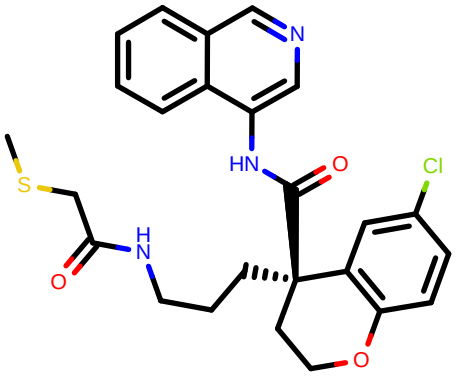
CID:	EN300-7351945_1_2
SMILES:	CC1(C[C@H](CNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN7506
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.26

EN300-44821_4_1



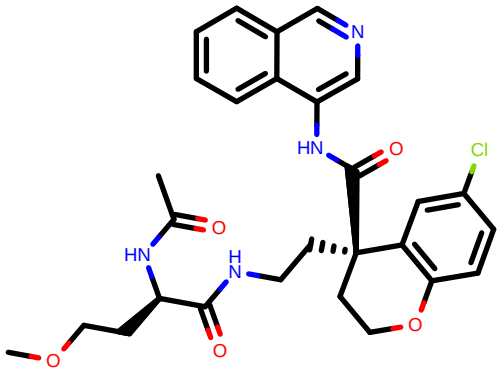
CID:	EN300-44821_4_1
SMILES:	C=CCOCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8797
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.35

EN300-07879_4_1



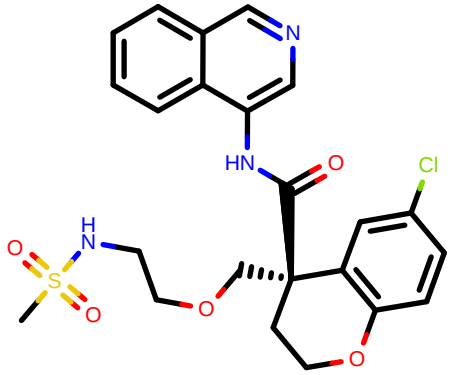
CID:	EN300-07879_4_1
SMILES:	CSCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8801
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.32

EN300-62074_3_2



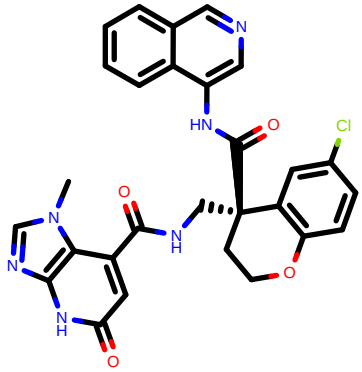
CID:	EN300-62074_3_2
SMILES:	CC(=O)N[C@H](CCOC)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9704
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.36

EN300-1238839_2_1



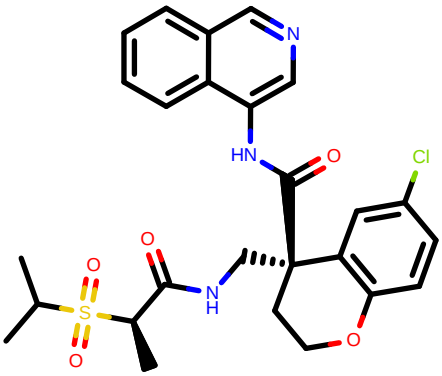
CID:	EN300-1238839_2_1
SMILES:	CS(=O)(=O)NCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN275
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.32

EN300-219802_2_1



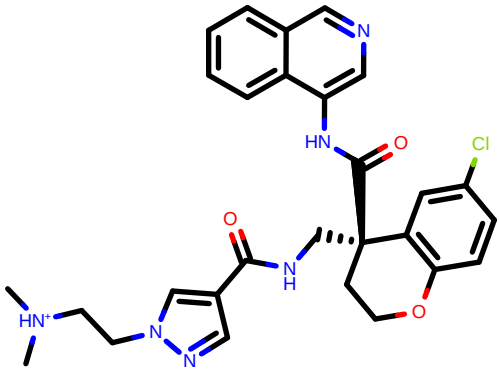
CID:	EN300-219802_2_1
SMILES:	Cn1cnc2c1c(cc(=O)[nH]2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8655
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.34

EN300-40947_2_2



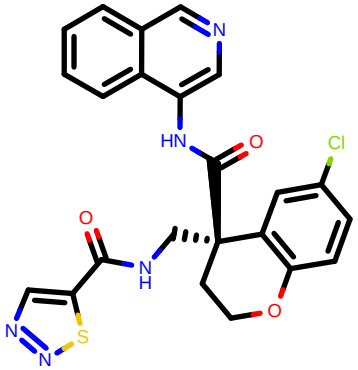
CID:	EN300-40947_2_2
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C(C)C
RUN:	RUN3339
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.37

EN300-255086_2_1



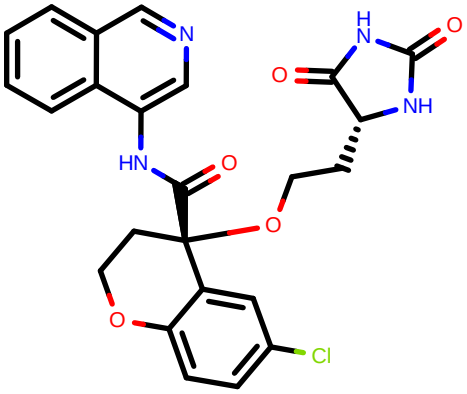
CID:	EN300-255086_2_1
SMILES:	CN(C)CCn1cc(cn1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7279
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.29

EN300-42269_2_1



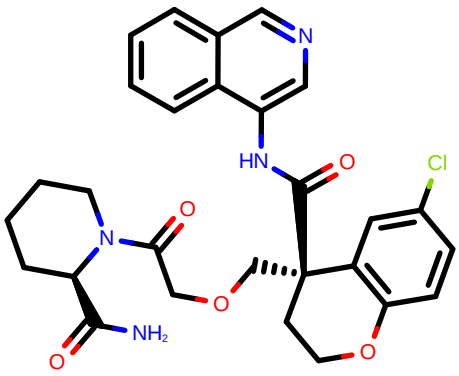
CID:	EN300-42269_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnns5
RUN:	RUN7007
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.26

EN300-6498856_1_1



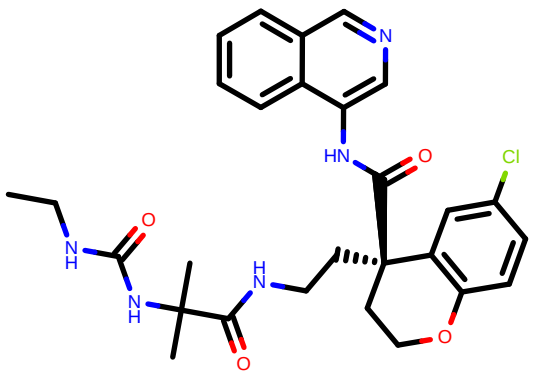
CID:	EN300-6498856_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[C@@H]5C(=O)NC(=O)N5
RUN:	RUN1999
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.27

EN300-22879_2_1



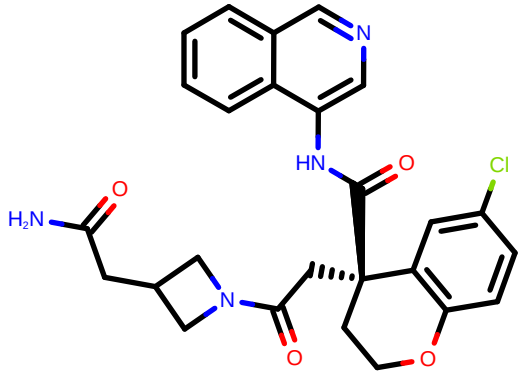
CID:	EN300-22879_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCCC[C@@H]5C(=O)N
RUN:	RUN752
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.37

EN300-76382_3_1



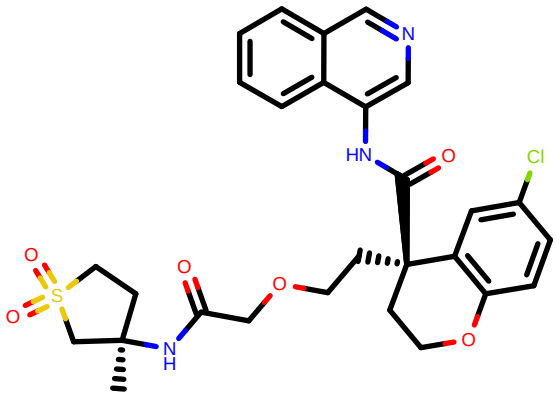
CID:	EN300-76382_3_1
SMILES:	CCNC(=O)NC(C)(C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6241
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.46

EN300-194172_1_1



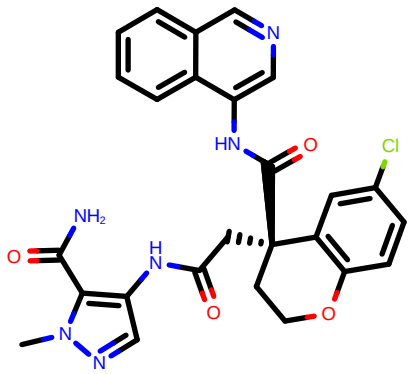
CID:	EN300-194172_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CC(=O)N
RUN:	RUN3320
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.29

EN300-10414_3_2



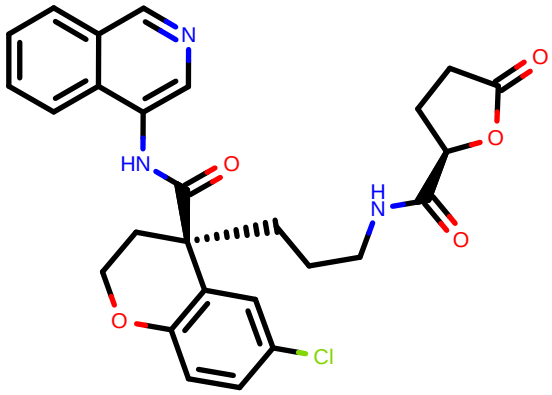
CID:	EN300-10414_3_2
SMILES:	C[C@]1(CCS(=O)(=O)C1)NC(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN988
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.48

EN300-110134_1_1



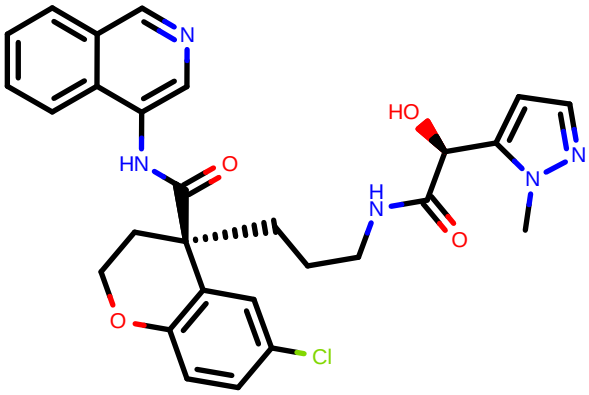
CID:	EN300-110134_1_1
SMILES:	Cn1c(c(cn1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN11194
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.28

EN300-332606_4_1



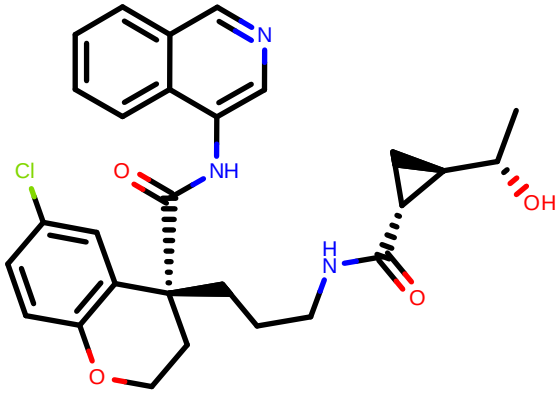
CID:	EN300-332606_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCC(=O)O5
RUN:	RUN9709
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.31

EN300-6473273_4_1



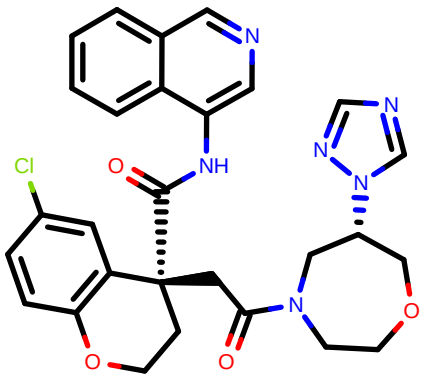
CID:	EN300-6473273_4_1
SMILES:	Cn1c(ccn1)[C@@H](C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10064
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.33

EN300-6729572_4_5



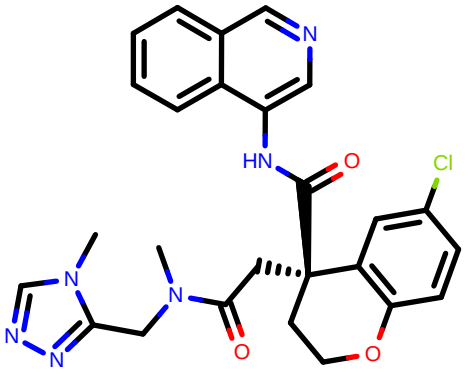
CID:	EN300-6729572_4_5
SMILES:	C[C@@H]([C@@H]1C[C@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10211
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.32

EN300-6504498_1_2



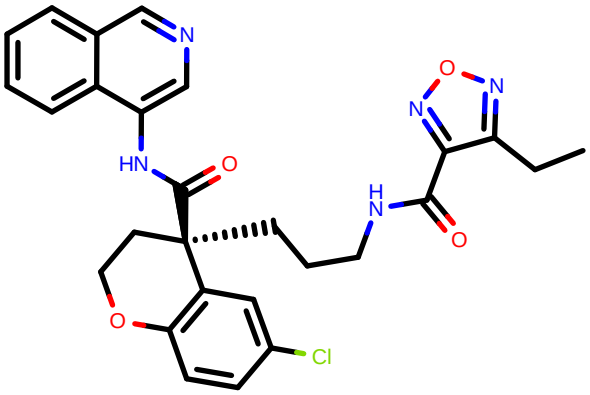
CID:	EN300-6504498_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)n6cncn6
RUN:	RUN6090
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.34

EN300-212365_1_1



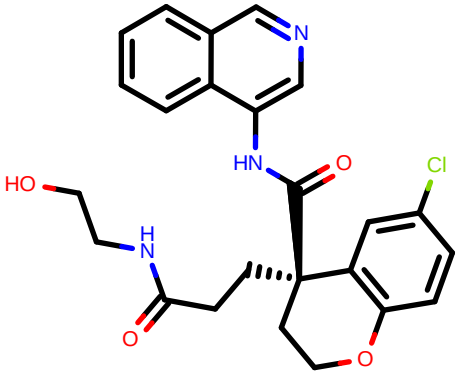
CID:	EN300-212365_1_1
SMILES:	Cn1cnnc1CN(C)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11206
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.30

EN300-1723498_4_1



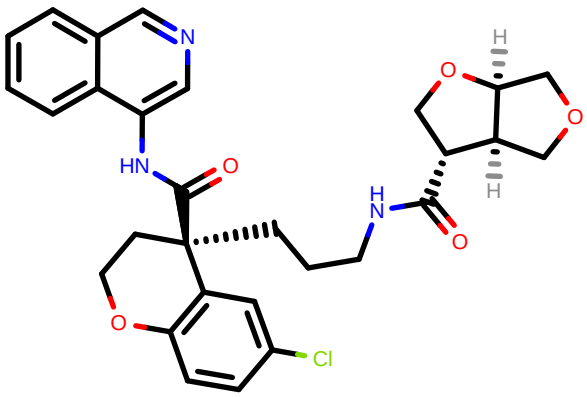
CID:	EN300-1723498_4_1
SMILES:	CCc1c(non1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10739
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.39

EN300-19392_2_1



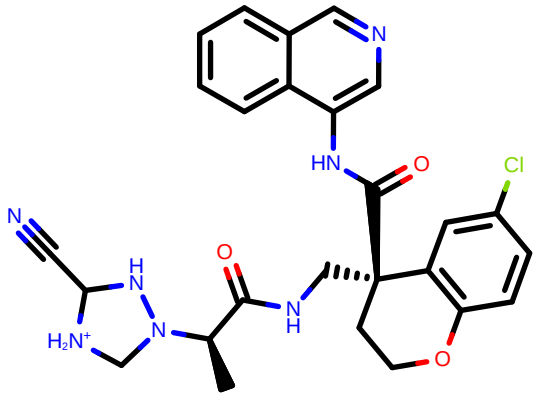
CID:	EN300-19392_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCO
RUN:	RUN2749
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.28

EN300-6482296_4_5



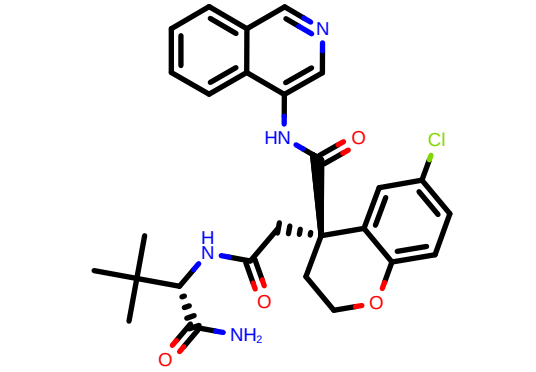
CID:	EN300-6482296_4_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CO[C@@H]6[C@H]5COC6
RUN:	RUN9525
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.48

EN300-198515_2_2



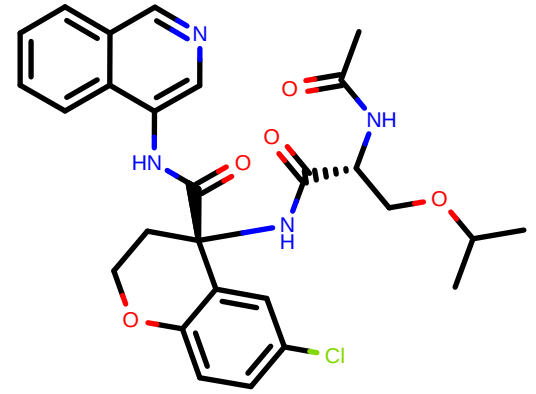
CID:	EN300-198515_2_2
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnc(n5)C#N
RUN:	RUN2160
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.26

EN300-96001_1_1



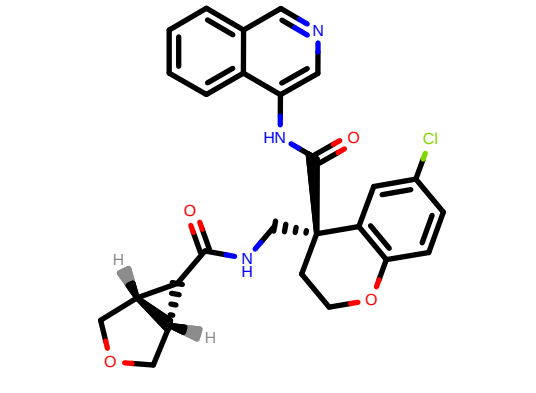
CID:	EN300-96001_1_1
SMILES:	CC(C)(C)[C@@H](C(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8928
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.26

EN300-1299691_1_2



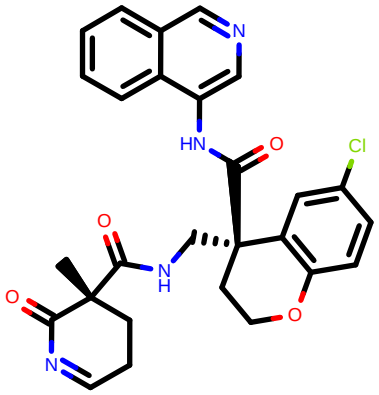
CID:	EN300-1299691_1_2
SMILES:	CC(C)OC[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN4965
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.31

EN300-257945_2_1



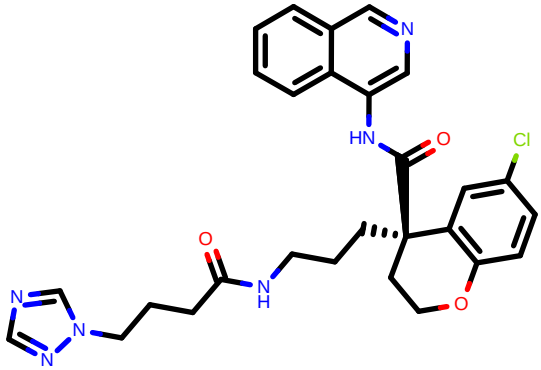
CID:	EN300-257945_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5[C@H]6[C@@H]5COC6
RUN:	RUN6791
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.25

EN300-178876_2_2



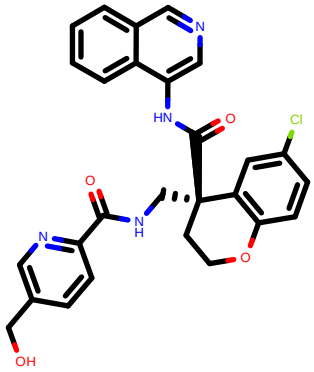
CID:	EN300-178876_2_2
SMILES:	C[C@]1(CCCNC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4650
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.41

EN300-316216_4_1



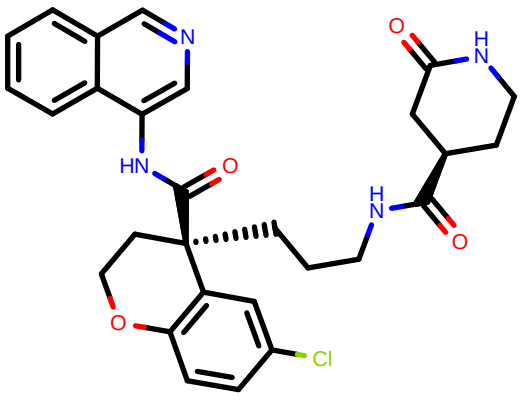
CID:	EN300-316216_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCCn5cncn5
RUN:	RUN11119
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.35

EN300-1270299_2_1



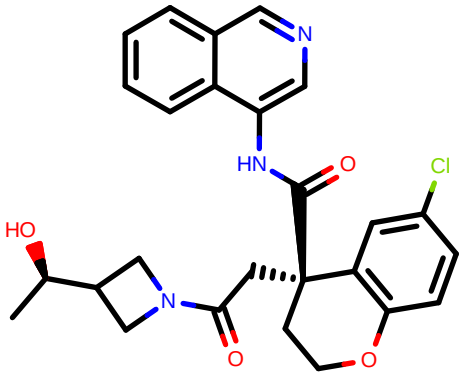
CID:	EN300-1270299_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cn5)CO
RUN:	RUN8263
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.26

EN300-107493_4_1



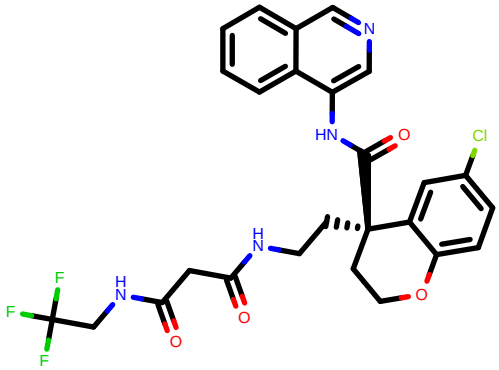
CID:	EN300-107493_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCNC(=O)C5
RUN:	RUN10807
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.31

EN300-365791_1_1



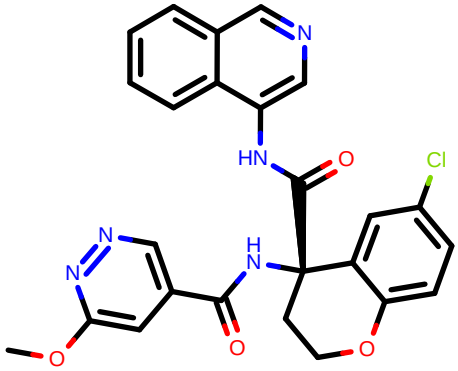
CID:	EN300-365791_1_1
SMILES:	C[C@H](C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2932
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.26

EN300-128715_3_1



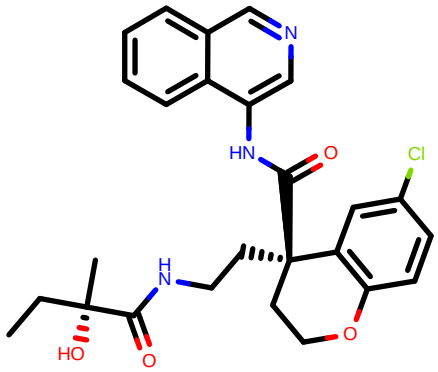
CID:	EN300-128715_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC(=O)NCC(F)(F)F
RUN:	RUN7876
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.33

EN300-252260_1_1



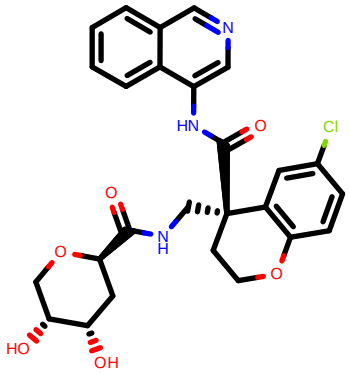
CID:	EN300-252260_1_1
SMILES:	COc1cc(cnn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5364
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.28

EN300-248888_3_2



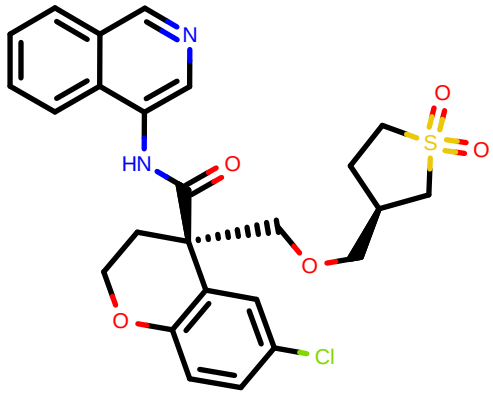
CID:	EN300-248888_3_2
SMILES:	C[C@](C=C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN678
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.38

EN300-7352736_2_1



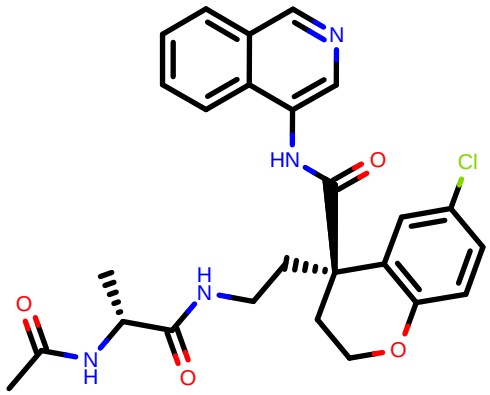
CID:	EN300-7352736_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5C[C@@H]([C@@H](CO5)O)O
RUN:	RUN5106
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.27

EN300-1448603_2_2



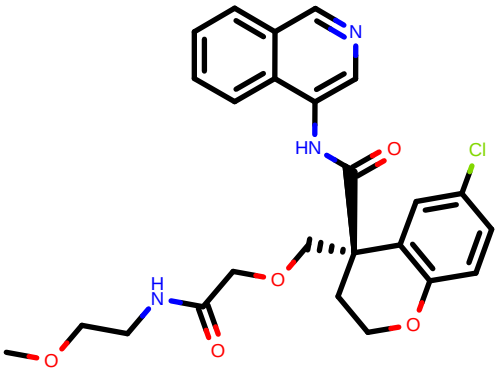
CID:	EN300-1448603_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCS(=O)(=O)C5
RUN:	RUN2532
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.29

EN300-18569_3_2



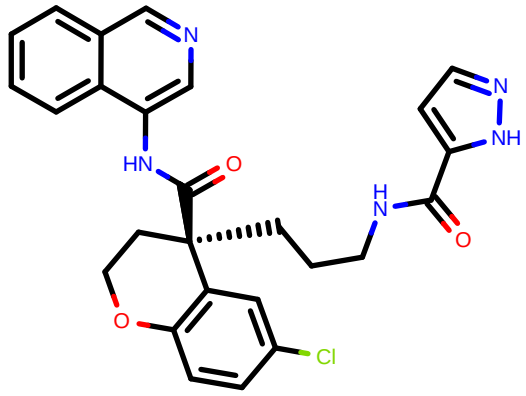
CID:	EN300-18569_3_2
SMILES:	C[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN8548
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.28

EN300-02015_2_1



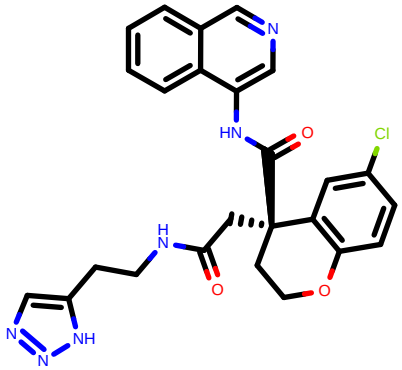
CID:	EN300-02015_2_1
SMILES:	COCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN395
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.36

EN300-37077_4_1



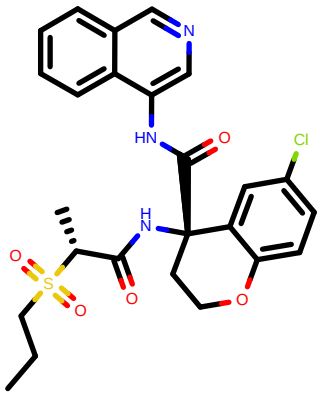
CID:	EN300-37077_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5ccn[nH]5
RUN:	RUN9046
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.25

EN300-1178209_1_1



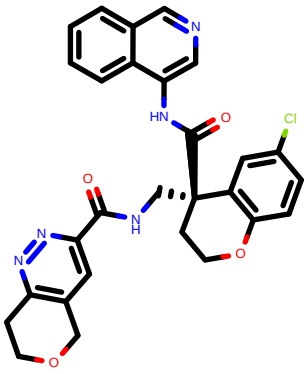
CID:	EN300-1178209_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCc5c[nH]nn5
RUN:	RUN4455
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.33

EN300-52768_1_2



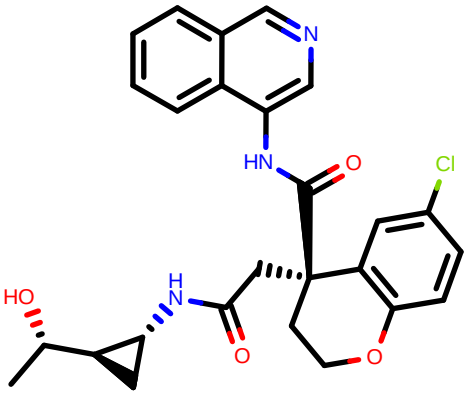
CID:	EN300-52768_1_2
SMILES:	CCCS(=O)(=O)[C@H](C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1772
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.37

EN300-7456641_2_1



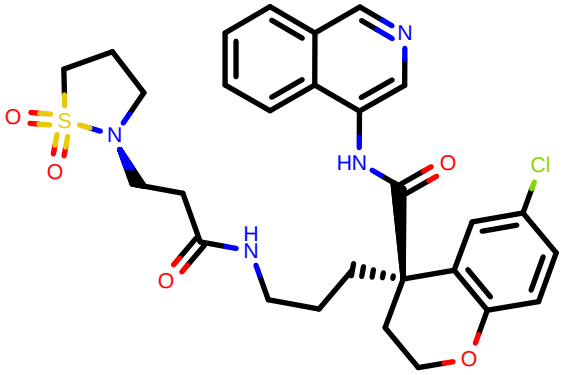
CID:	EN300-7456641_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6c(nn5)CCOC6
RUN:	RUN8251
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.31

EN300-7463275_1_1



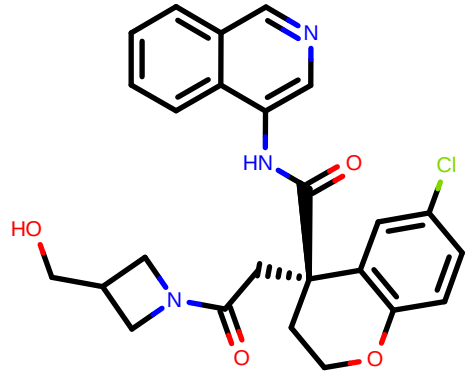
CID:	EN300-7463275_1_1
SMILES:	C[C@@H]([C@@H]1C[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10047
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.28

EN300-44873_4_1



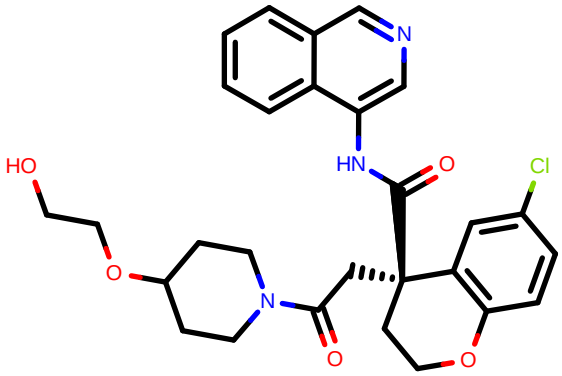
CID:	EN300-44873_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCN5CCCS5(=O)=O
RUN:	RUN11149
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.64

EN300-7370063_1_1



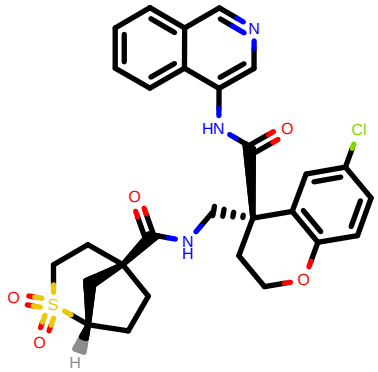
CID:	EN300-7370063_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)CO
RUN:	RUN2718
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.22

EN300-104088_1_1



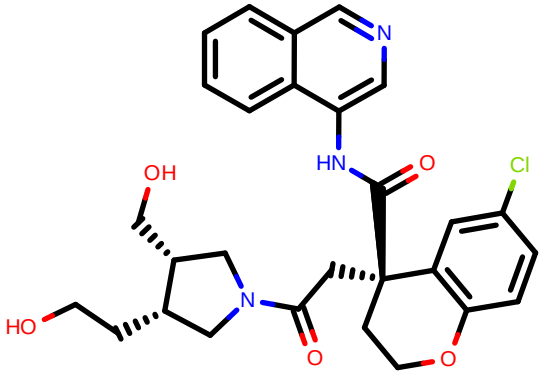
CID:	EN300-104088_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)OCCO
RUN:	RUN6337
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.36

EN300-6503702_2_1



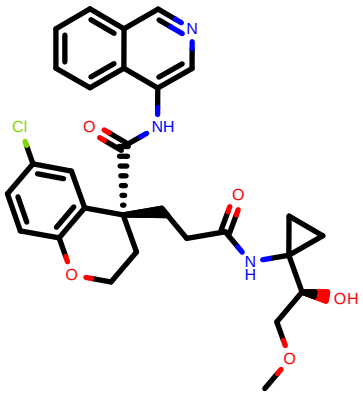
CID:	EN300-6503702_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CCC(C5)S(=O)(=O)CC6
RUN:	RUN7775
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.32

EN300-1425608_1_1



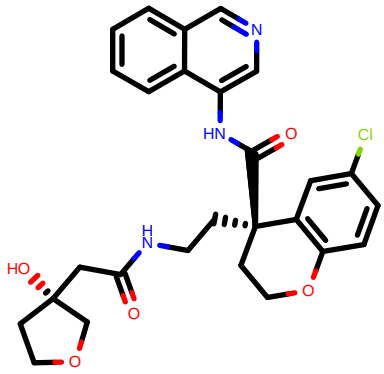
CID:	EN300-1425608_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H](C5)CO)CCO
RUN:	RUN375
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.29

EN300-1709202_2_1



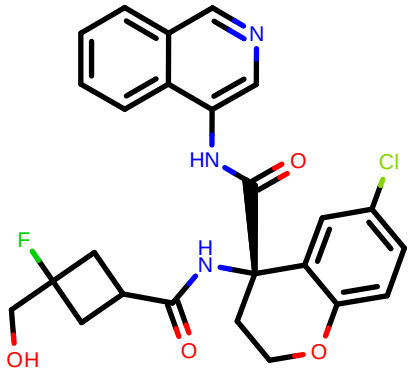
CID:	EN300-1709202_2_1
SMILES:	COC[C@@H](C1(CC1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4996
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.48

EN300-360157_3_1



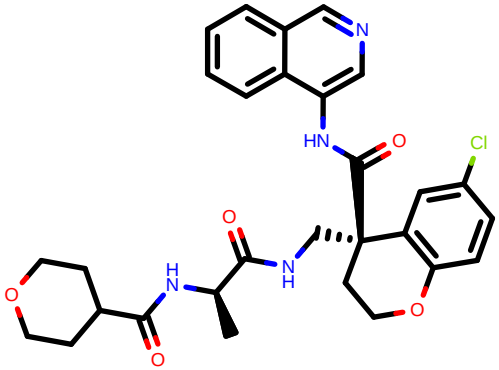
CID:	EN300-360157_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5(CCOC5)O
RUN:	RUN10009
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.32

EN300-6746890_1_1



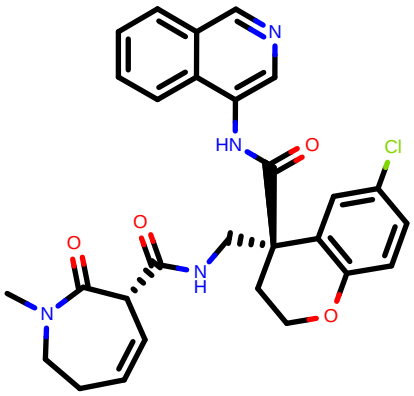
CID:	EN300-6746890_1_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@H]5C[C@@](C5)(F)CO)cc1
RUN:	RUN1596
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.27

EN300-73102_2_2



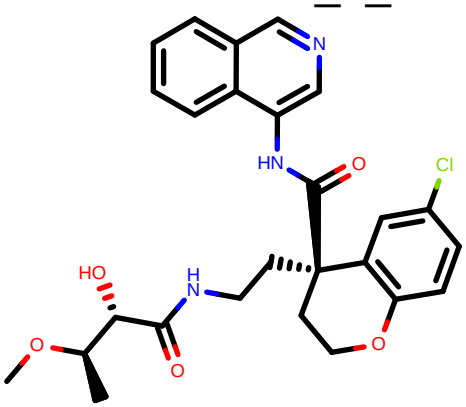
CID:	EN300-73102_2_2
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCOCC5
RUN:	RUN1768
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.45

EN300-304695_2_2



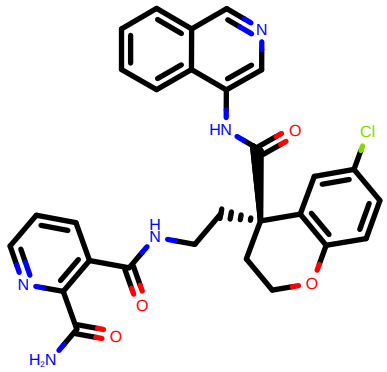
CID:	EN300-304695_2_2
SMILES:	CN1CCCC[C@H](C1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7435
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.43

EN300-220194_3_2



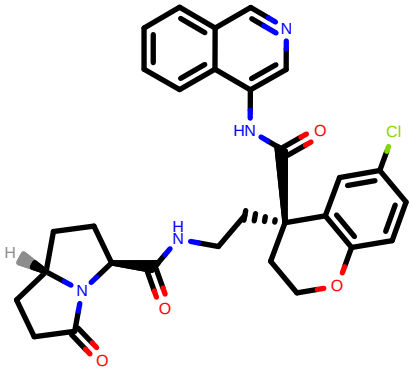
CID:	EN300-220194_3_2
SMILES:	C[C@H]([C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN1889
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.40

EN300-135530_3_1



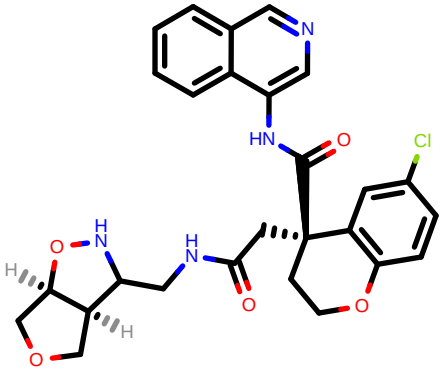
CID:	EN300-135530_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cccnc5C(=O)N
RUN:	RUN11056
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.35

EN300-6479181_3_1



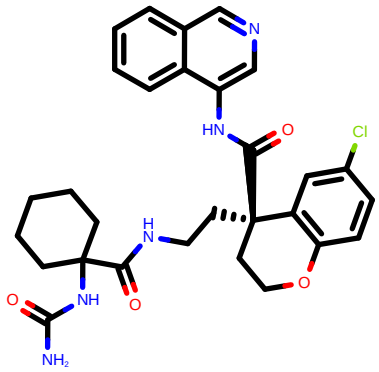
CID:	EN300-6479181_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@@H]6N5C(=O)CC6
RUN:	RUN6928
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.33

EN300-7435581_1_1



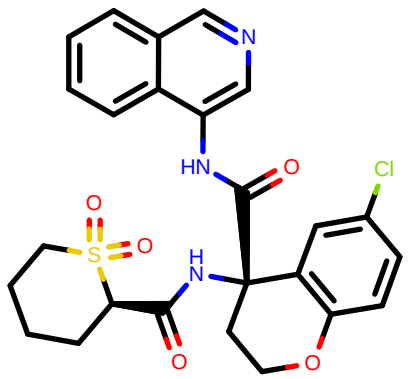
CID:	EN300-7435581_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5=NO[C@H]6[C@@H]5COC6
RUN:	RUN10968
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.26

EN300-78368_3_1



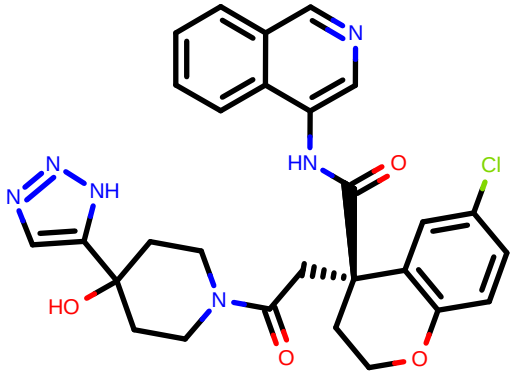
CID:	EN300-78368_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCCCC5)NC(=O)N
RUN:	RUN10514
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.37

EN300-107435_1_2



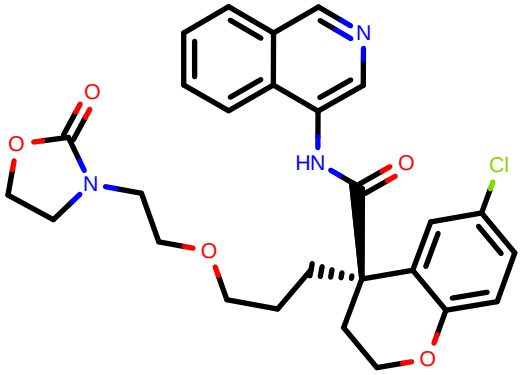
CID:	EN300-107435_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCCCS5(=O)=O
RUN:	RUN4217
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.25

EN300-1588753_1_1



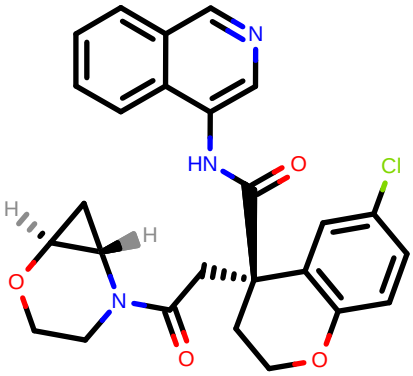
CID:	EN300-1588753_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)(c6cnn[nH]6)O
RUN:	RUN9340
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.37

EN300-370967_4_1



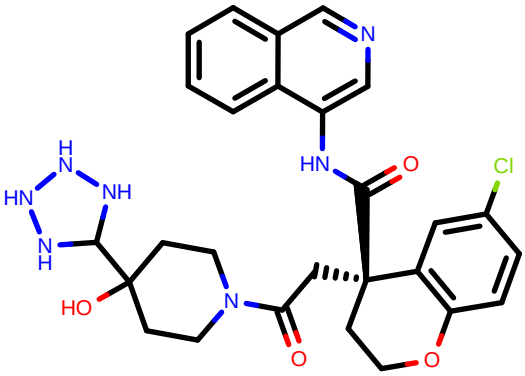
CID:	EN300-370967_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCN5CCOC5=O
RUN:	RUN1814
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.36

EN300-91609_1_1



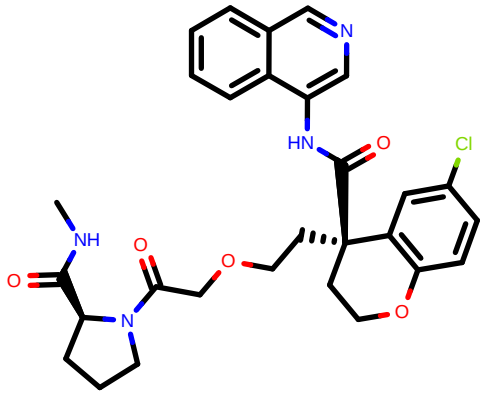
CID:	EN300-91609_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H]6[C@@H]5C6
RUN:	RUN3676
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.25

EN300-196160_1_1



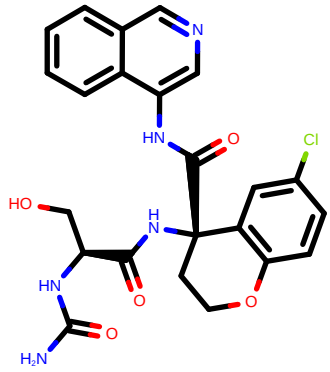
CID:	EN300-196160_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)(c6[nH]nnn6)O
RUN:	RUN10964
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.30

EN300-48902_3_1



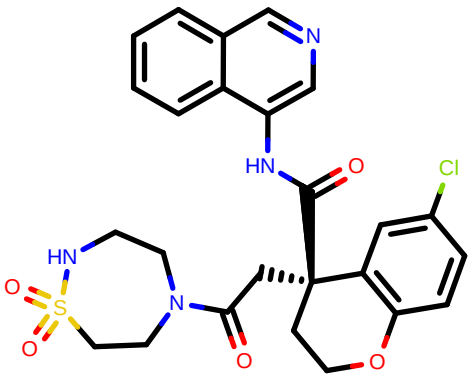
CID:	EN300-48902_3_1
SMILES:	CNC(=O)[C@@H]1CCCN1C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2279
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.34

EN300-10170_1_2



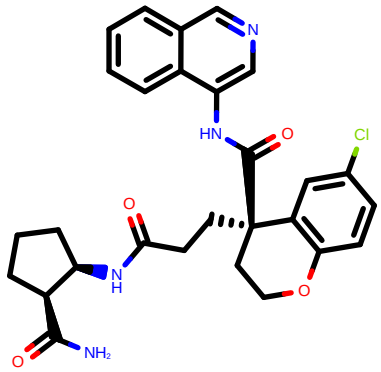
CID:	EN300-10170_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](CO)NC(=O)N
RUN:	RUN4265
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.23

EN300-6489145_1_1



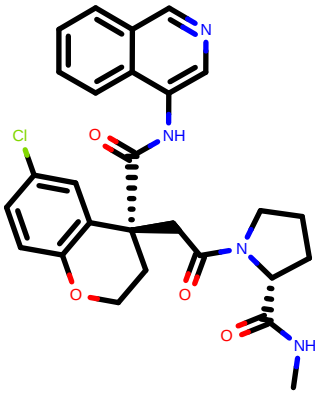
CID:	EN300-6489145_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNS(=O)(=O)CC5
RUN:	RUN3332
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.32

EN300-90531_2_1



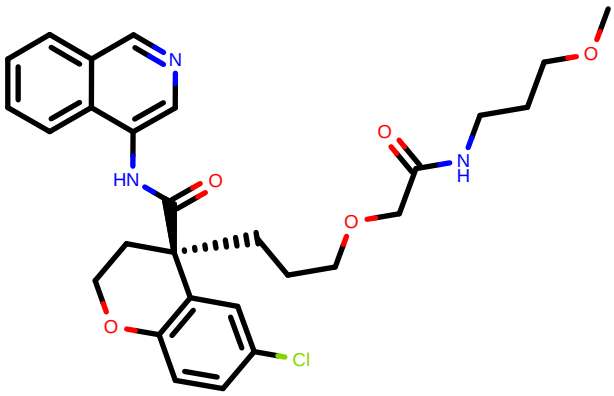
CID:	EN300-90531_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCC[C@@H]5C(=O)N
RUN:	RUN5491
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.31

EN300-6492197_1_1



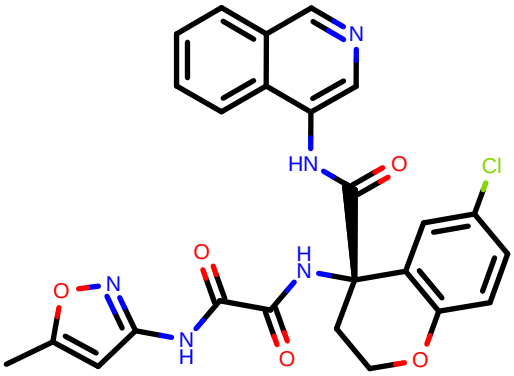
CID:	EN300-6492197_1_1
SMILES:	CNC(=O)[C@H]1CCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4431
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.24

EN300-04492_4_1



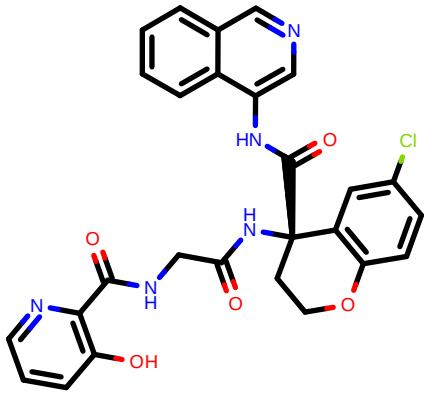
CID:	EN300-04492_4_1
SMILES:	COCCCNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1710
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.36

EN300-36938_1_1



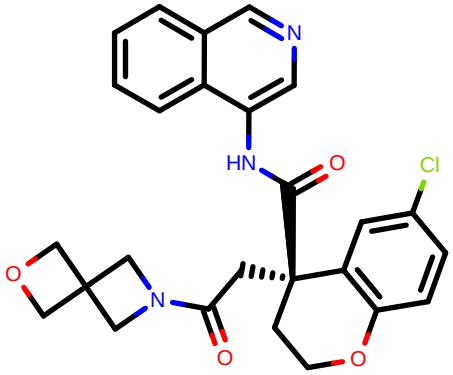
CID:	EN300-36938_1_1
SMILES:	Cc1cc(no1)NC(=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8870
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.26

EN300-115421_1_1



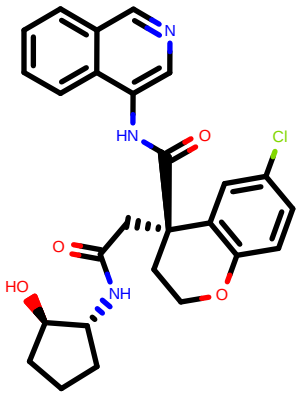
CID:	EN300-115421_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5c(cccn5)O
RUN:	RUN6763
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.35

EN300-81038_1_1



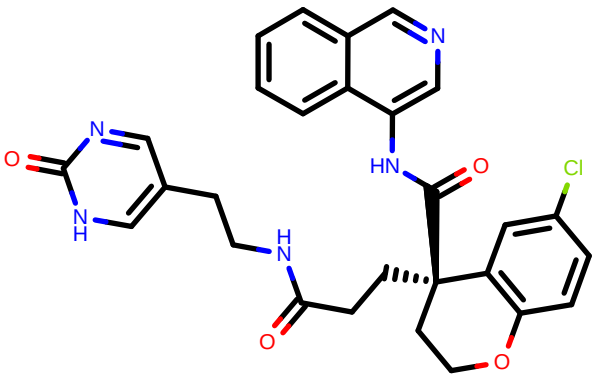
CID:	EN300-81038_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)COC6
RUN:	RUN7476
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.25

EN300-60314_1_1



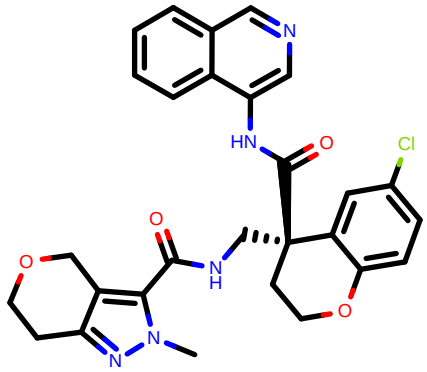
CID:	EN300-60314_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCC[C@H]5O
RUN:	RUN8696
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.27

EN300-343433_2_1



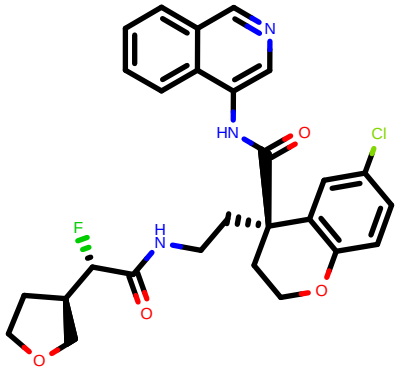
CID:	EN300-343433_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCc5c[nH]c(=O)nc5
RUN:	RUN6666
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.28

EN300-6481960_2_1



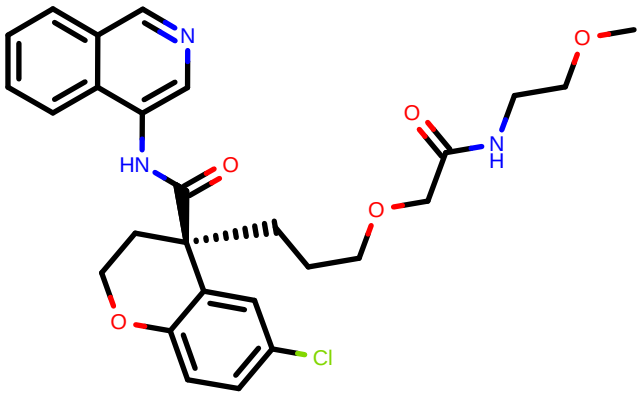
CID:	EN300-6481960_2_1
SMILES:	Cn1c(c2c(n1)CCOC2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8087
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.47

EN300-783124_3_2



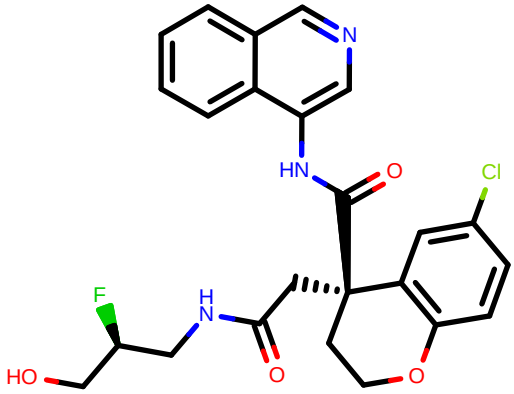
CID:	EN300-783124_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]([C@@H]5CCOC5)F
RUN:	RUN6932
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.25

EN300-02015_4_1



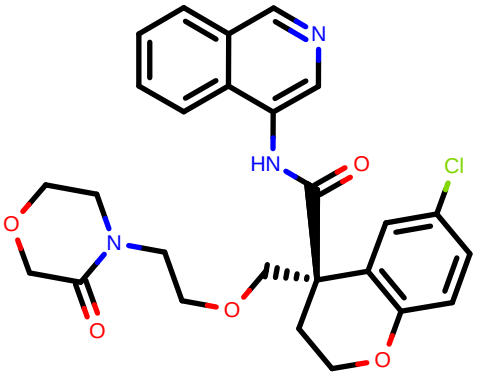
CID:	EN300-02015_4_1
SMILES:	COCCNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1646
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.39

EN300-7353973_1_1



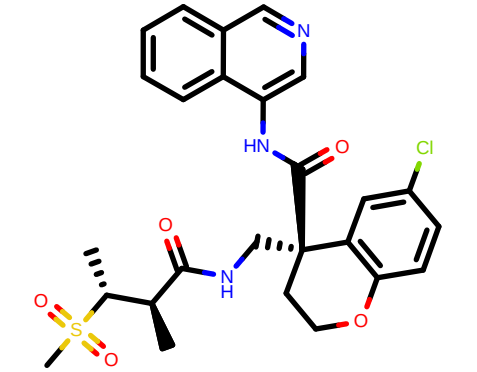
CID:	EN300-7353973_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H](CO)F
RUN:	RUN5067
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.28

EN300-219330_2_1



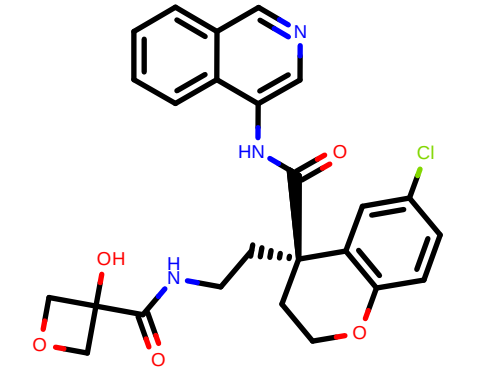
CID:	EN300-219330_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCN5CCOCC5=O
RUN:	RUN499
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.29

EN300-182725_2_1



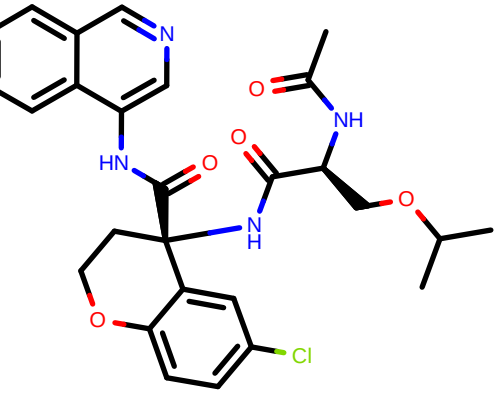
CID:	EN300-182725_2_1
SMILES:	C[C@@H]([C@@H](C)S(=O)(=O)C)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1664
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.28

EN300-101443_3_1



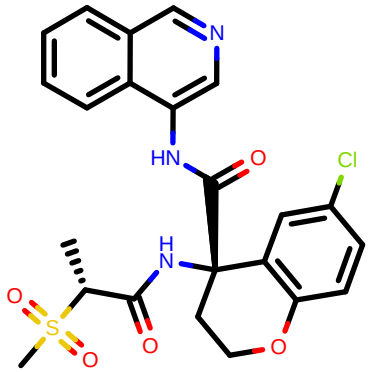
CID:	EN300-101443_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(COC5)O
RUN:	RUN6273
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.20

EN300-1299691_1_1



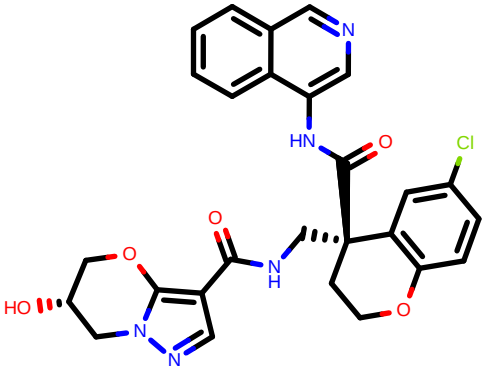
CID:	EN300-1299691_1_1
SMILES:	CC(C)OC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN5284
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.28

EN300-39405_1_2



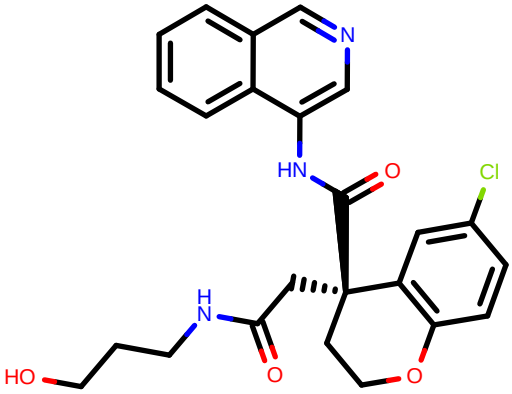
CID:	EN300-39405_1_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN2068
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.26

EN300-6497444_2_2



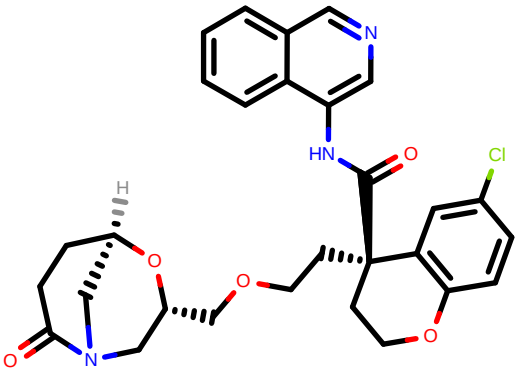
CID:	EN300-6497444_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnn6c5OC[C@H](C6)O
RUN:	RUN8031
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.31

EN300-16772_1_1



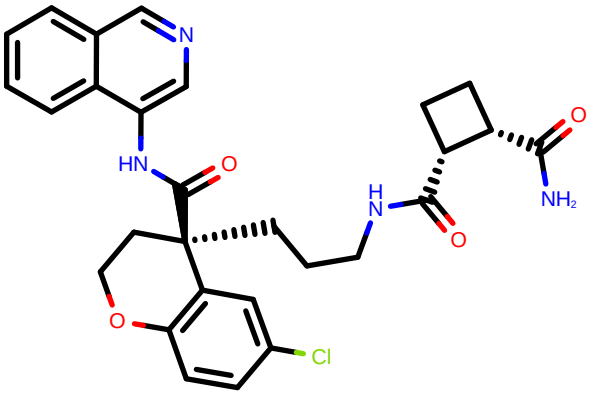
CID:	EN300-16772_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCCO
RUN:	RUN9219
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.25

EN300-2008102_3_1



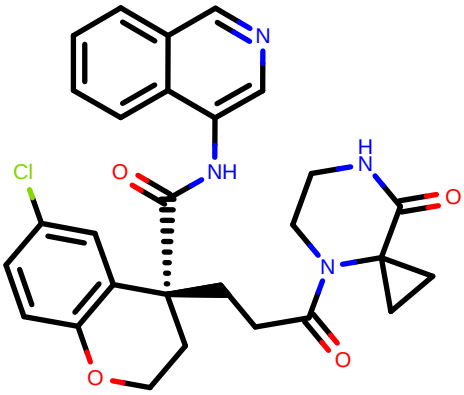
CID:	EN300-2008102_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5CN6CC(O5)CCC6=O
RUN:	RUN2412
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.34

EN300-217107_4_1



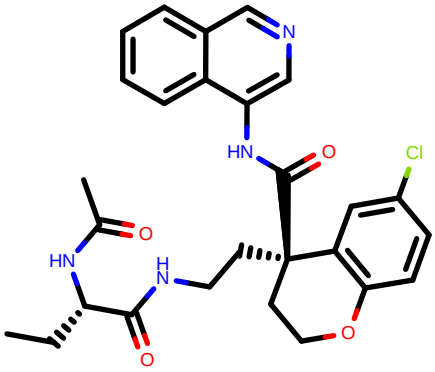
CID:	EN300-217107_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CC[C@@H]5C(=O)N
RUN:	RUN10203
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.32

EN300-1067786_2_1



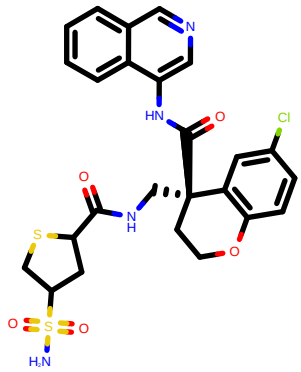
CID:	EN300-1067786_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCNC(=O)C56CC6
RUN:	RUN3960
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.27

EN300-332601_3_1



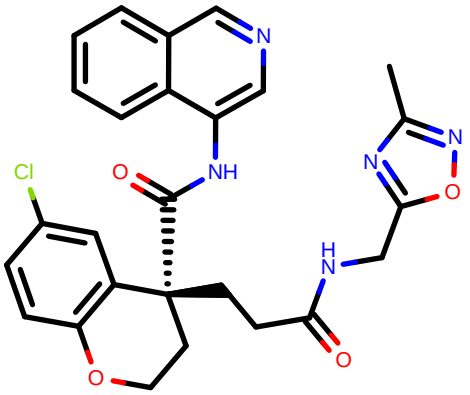
CID:	EN300-332601_3_1
SMILES:	CC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C
RUN:	RUN858
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.30

EN300-98099_2_1



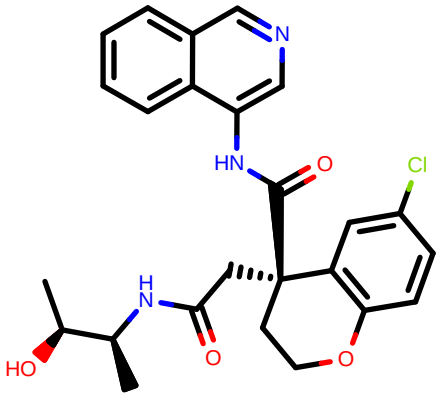
CID:	EN300-98099_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc(cs5)S(=O)(=O)N
RUN:	RUN7903
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.31

EN300-50657_2_1



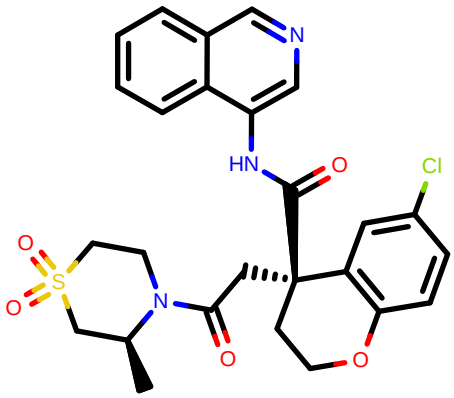
CID:	EN300-50657_2_1
SMILES:	Cc1nc(on1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4340
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.25

EN300-72272_1_3



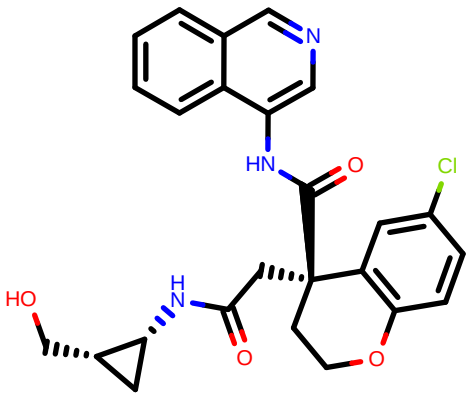
CID:	EN300-72272_1_3
SMILES:	C[C@@H]([C@H](C)O)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9848
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.25

EN300-171215_1_2



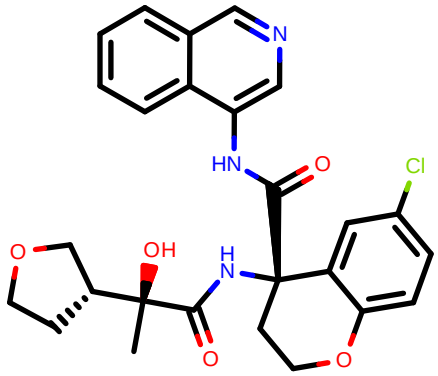
CID:	EN300-171215_1_2
SMILES:	C[C@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4099
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.31

EN300-399072_1_1



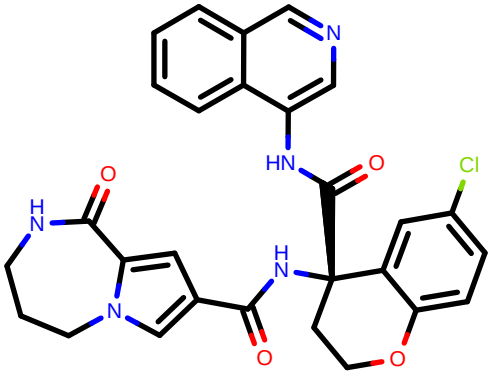
CID:	EN300-399072_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]5CO
RUN:	RUN10902
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.28

EN300-217494_1_2



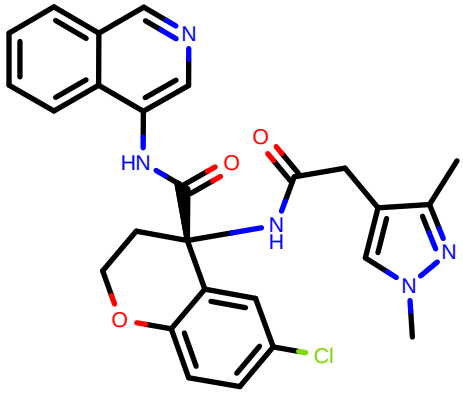
CID:	EN300-217494_1_2
SMILES:	C[C@]([C@@H]1CCOC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4189
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.26

EN300-7431365_1_1



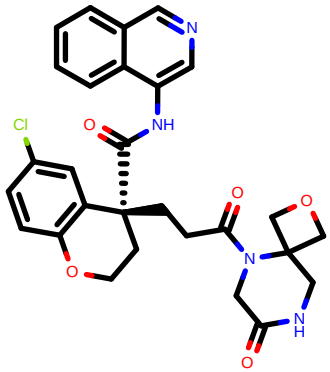
CID:	EN300-7431365_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(c5)CCCNC6=O
RUN:	RUN9050
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.32

EN300-245061_1_1



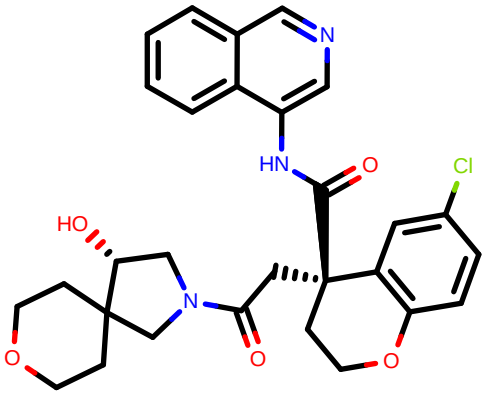
CID:	EN300-245061_1_1
SMILES:	Cc1c(cn(n1)C)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5304
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.27

EN300-366278_2_1



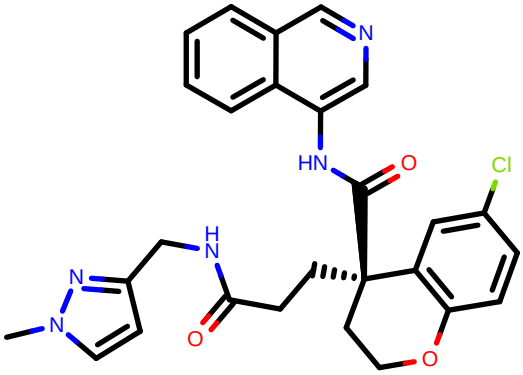
CID:	EN300-366278_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(=O)NCC56COC6
RUN:	RUN4428
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.24

EN300-7435482_1_2



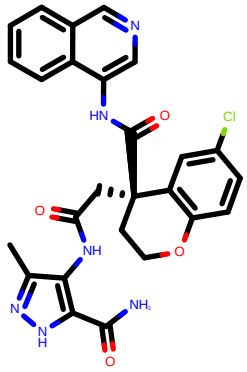
CID:	EN300-7435482_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C6(C5)CCOCC6)O
RUN:	RUN7784
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.30

EN300-122847_2_1



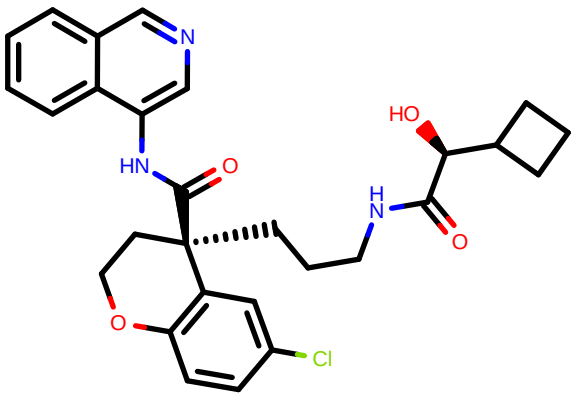
CID:	EN300-122847_2_1
SMILES:	Cn1ccc(n1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5575
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.23

EN300-67302_1_1



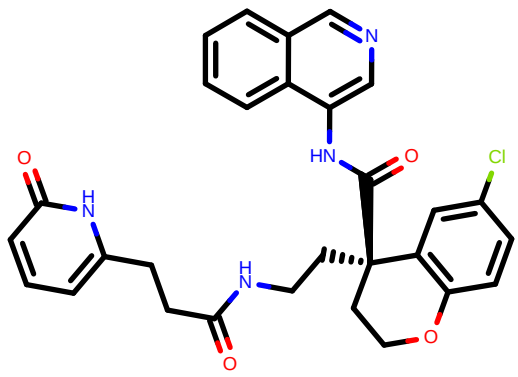
CID:	EN300-67302_1_1
SMILES:	Cc1c(c(n[nH]1)C(=O)N)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9912
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.29

EN300-249764_4_2



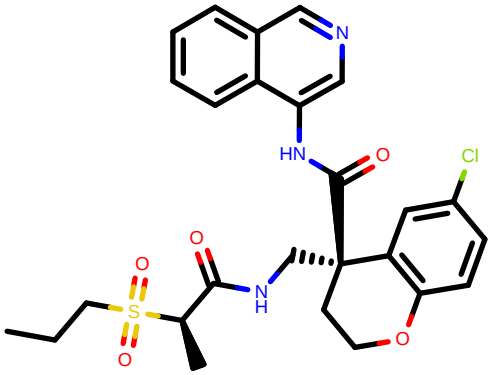
CID:	EN300-249764_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H](C5CCC5)O
RUN:	RUN9935
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.32

EN300-6491697_3_1



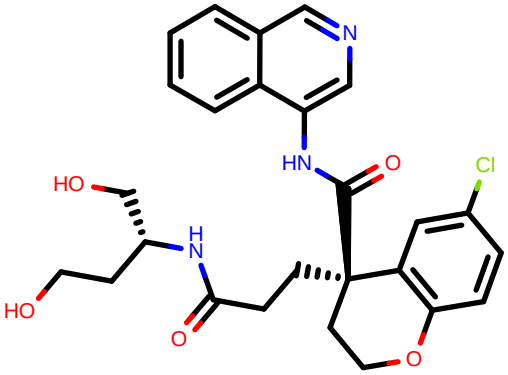
CID:	EN300-6491697_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCc5cccc(=O)[nH]5
RUN:	RUN3979
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.30

EN300-52768_2_2



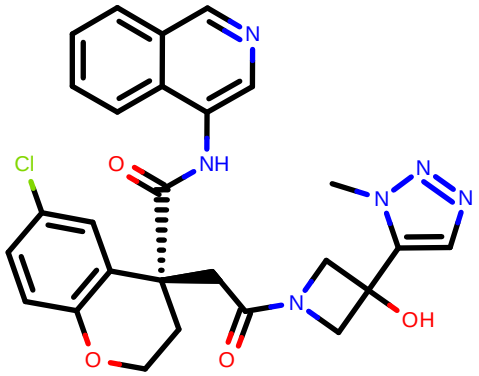
CID:	EN300-52768_2_2
SMILES:	CCCS(=O)(=O)[C@H](C)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3227
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.59

EN300-195743_2_1



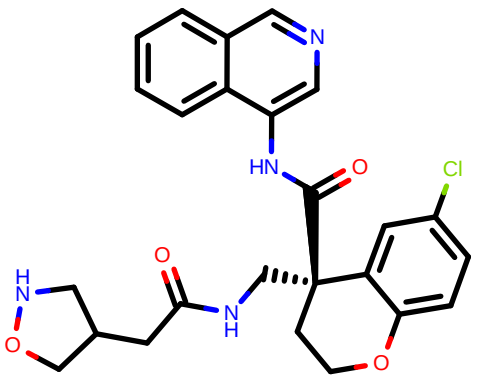
CID:	EN300-195743_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H](CCO)CO
RUN:	RUN10381
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.28

EN300-367351_1_1



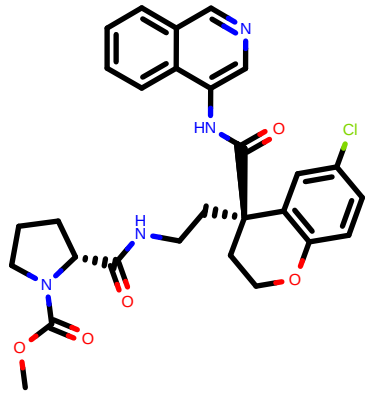
CID:	EN300-367351_1_1
SMILES:	Cn1c(cnn1)C2(CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)O
RUN:	RUN6481
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.31

EN300-315963_2_1



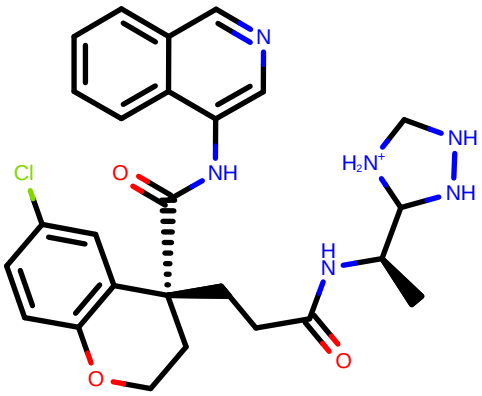
CID:	EN300-315963_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5cnoc5
RUN:	RUN4806
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.23

EN300-66845_3_1



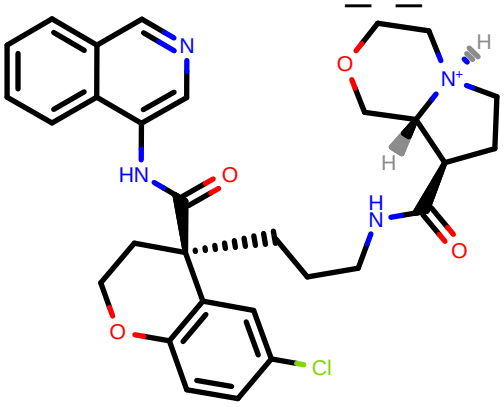
CID:	EN300-66845_3_1
SMILES:	COC(=O)N1CCC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6046
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.32

EN300-123834_2_2



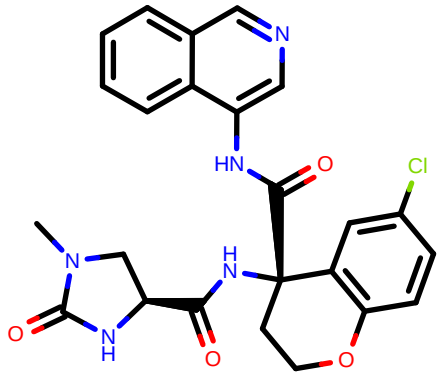
CID:	EN300-123834_2_2
SMILES:	C[C@H](c1[nH]cnn1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2002
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.26

EN300-1588613_4_3



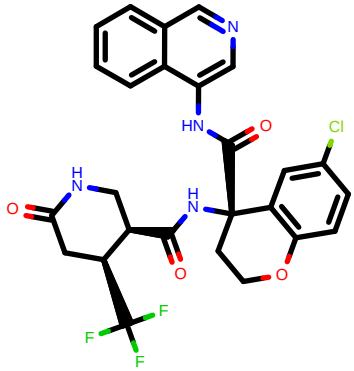
CID:	EN300-1588613_4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCN6[C@H]5COCC6
RUN:	RUN10649
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.42

EN300-255795_1_2



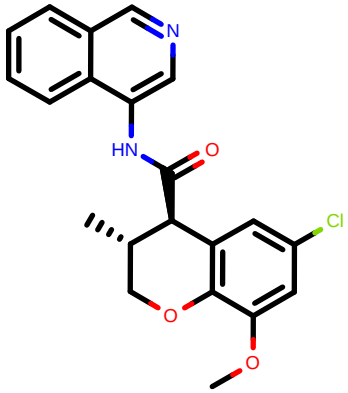
CID:	EN300-255795_1_2
SMILES:	CN1C[C@H](NC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4125
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.23

EN300-208959_1_1



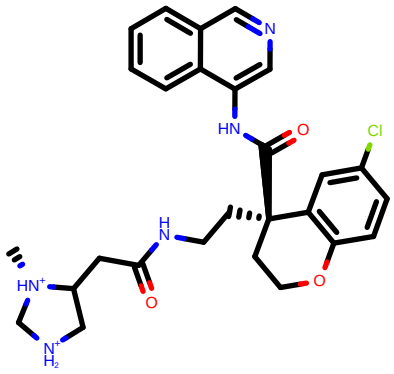
CID:	EN300-208959_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CNC(=O)C[C@@H]5C(F)(F)F
RUN:	RUN6802
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.31

DAR-DIA-0d514e7d-1_1



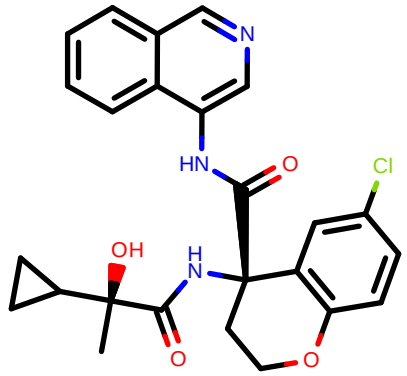
CID:	DAR-DIA-0d514e7d-1_1
SMILES:	C[C@H]1COc2c(cc(cc2OC)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4
RUN:	RUN79
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.11

EN300-152418_3_1



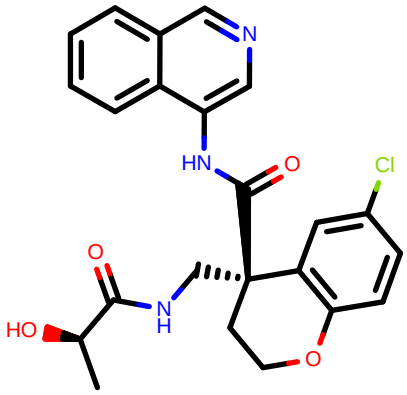
CID:	EN300-152418_3_1
SMILES:	Cn1cncc1CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1170
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.29

EN300-118760_1_2



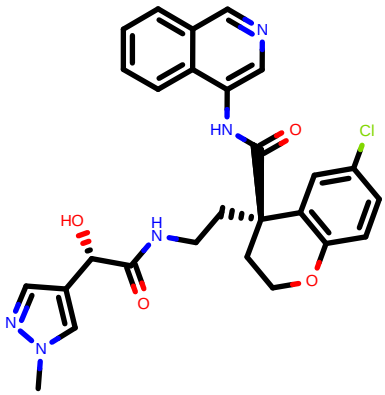
CID:	EN300-118760_1_2
SMILES:	C[C@](C1CC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3610
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.31

EN300-19542_2_2



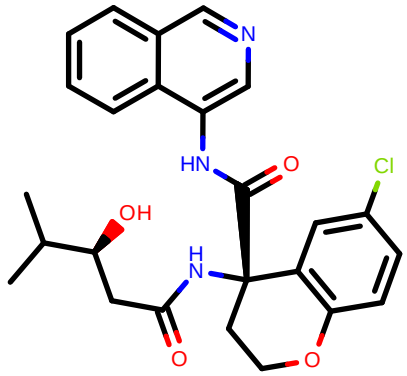
CID:	EN300-19542_2_2
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2040
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.23

EN300-198540_3_1



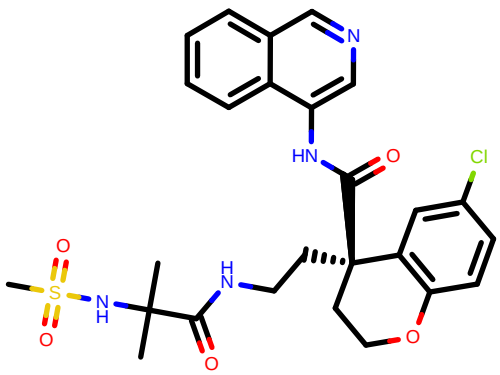
CID:	EN300-198540_3_1
SMILES:	Cn1cc(cn1)[C@@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5083
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.37

EN300-155498_1_1



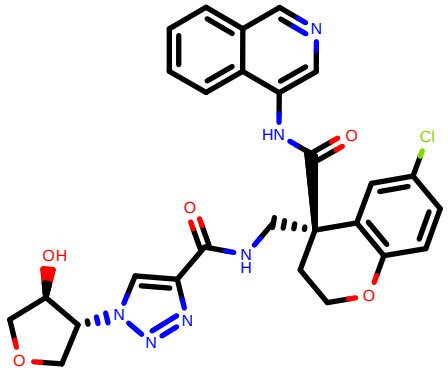
CID:	EN300-155498_1_1
SMILES:	CC(=C)[C@H](CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN442
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.27

EN300-85849_3_1



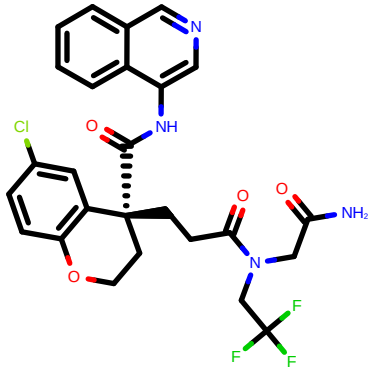
CID:	EN300-85849_3_1
SMILES:	CC(C)(C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN2808
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.31

EN300-637424_2_1



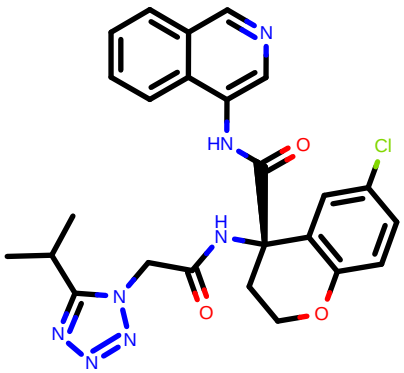
CID:	EN300-637424_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)[C@@H]6COC[C@H]6O
RUN:	RUN7183
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.36

EN300-138676_2_1



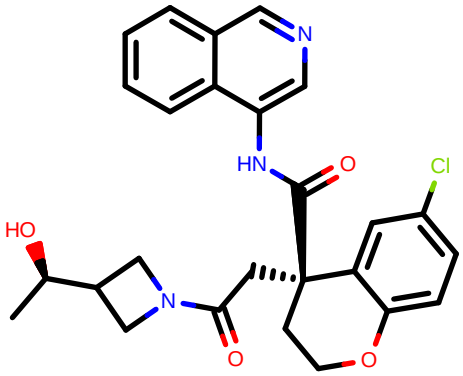
CID:	EN300-138676_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N(CC(=O)N)CC(F)(F)F
RUN:	RUN9919
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.23

EN300-96933_1_1



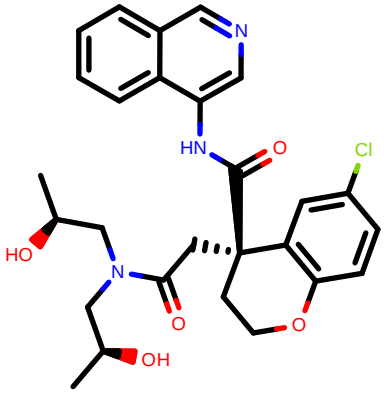
CID:	EN300-96933_1_1
SMILES:	CC(C)c1nnnn1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3913
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.25

EN300-301721_1_2



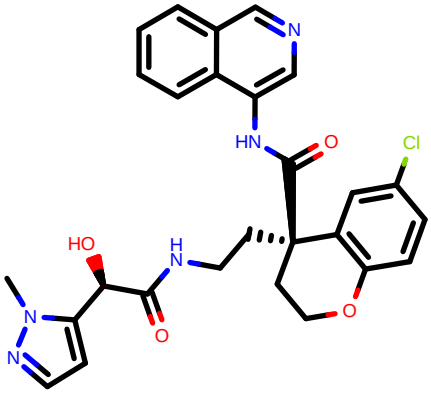
CID:	EN300-301721_1_2
SMILES:	C[C@H](C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2936
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.25

EN300-722418_1_3



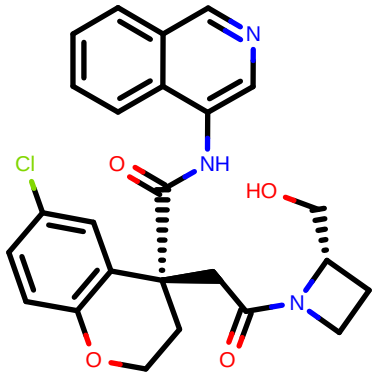
CID:	EN300-722418_1_3
SMILES:	C[C@@H](CN(C[C@H](C)O)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN7536
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.43

EN300-6473273_3_2



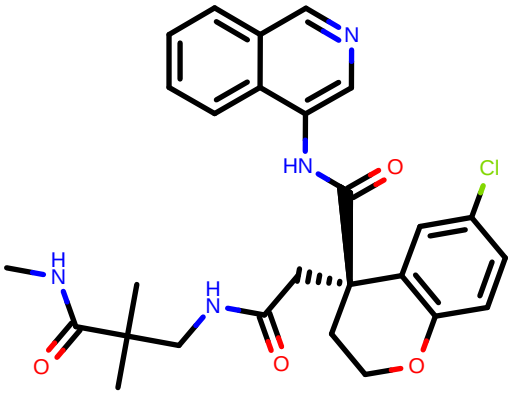
CID:	EN300-6473273_3_2
SMILES:	Cn1c(ccn1)[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1106
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.38

EN300-154332_1_2



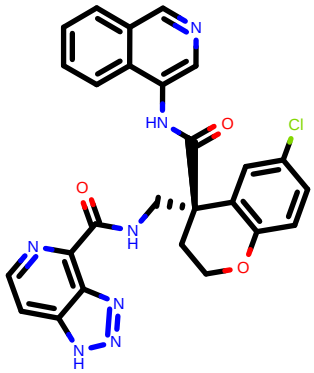
CID:	EN300-154332_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5CO
RUN:	RUN4631
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.31

EN300-114112_1_1



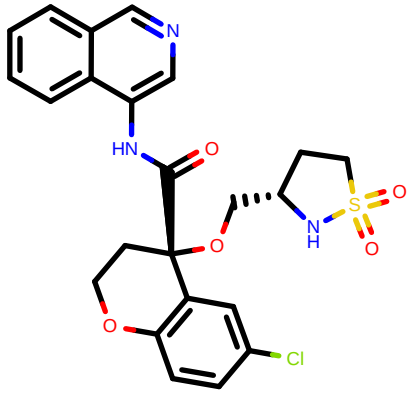
CID:	EN300-114112_1_1
SMILES:	CC(C)(CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)NC
RUN:	RUN9183
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.27

EN300-7426383_2_1



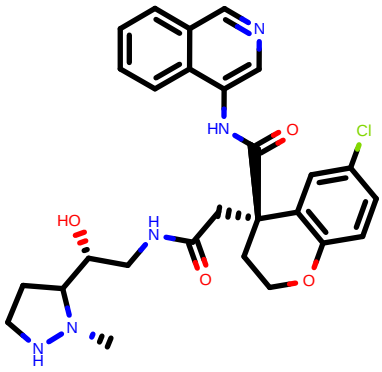
CID:	EN300-7426383_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c6c(ccn5)[nH]nn6
RUN:	RUN7711
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.31

EN300-1699871_1_1



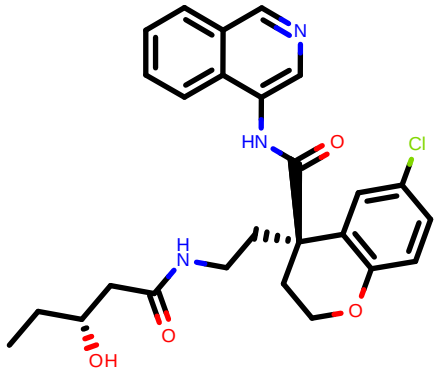
CID:	EN300-1699871_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCS(=O)(=O)N5
RUN:	RUN2464
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.25

EN300-716082_1_1



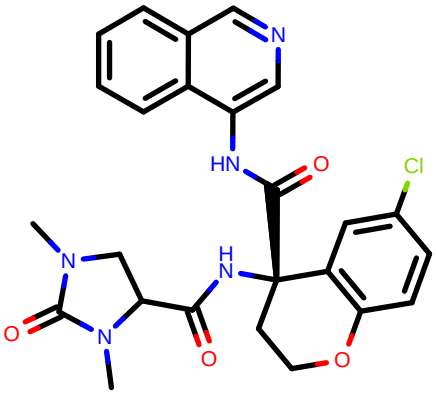
CID:	EN300-716082_1_1
SMILES:	Cn1c(ccn1)[C@@H](CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5722
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.33

EN300-224741_3_2



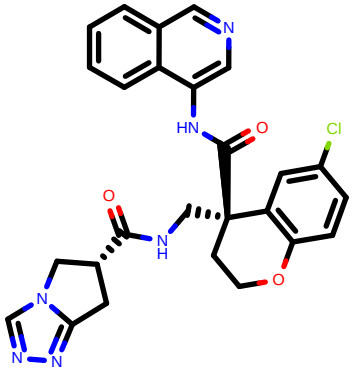
CID:	EN300-224741_3_2
SMILES:	CC[C@H](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5598
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.28

EN300-312618_1_1



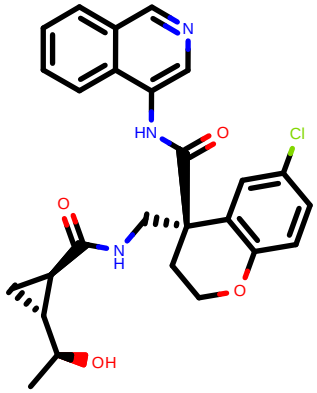
CID:	EN300-312618_1_1
SMILES:	Cn1cc(n(c1=O)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6910
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.24

EN300-6745453_2_1



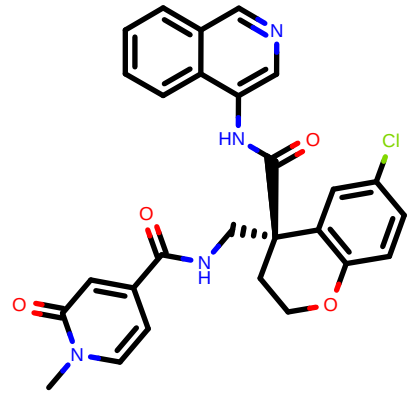
CID:	EN300-6745453_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5Cc6nncn6C5
RUN:	RUN5713
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.32

EN300-6729572_2_5



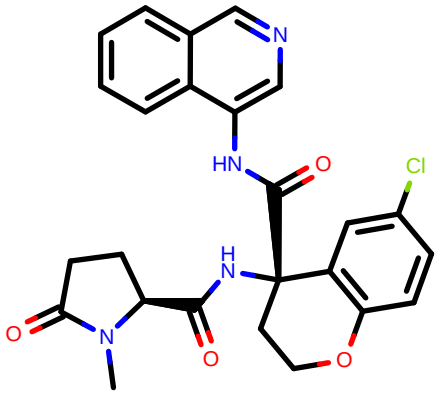
CID:	EN300-6729572_2_5
SMILES:	C[C@@H]([C@@H]1C[C@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5885
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.26

EN300-30480_2_1



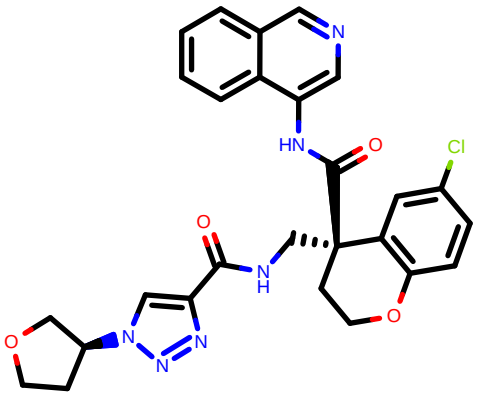
CID:	EN300-30480_2_1
SMILES:	Cn1ccc(cc1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8215
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.28

EN300-130825_1_1



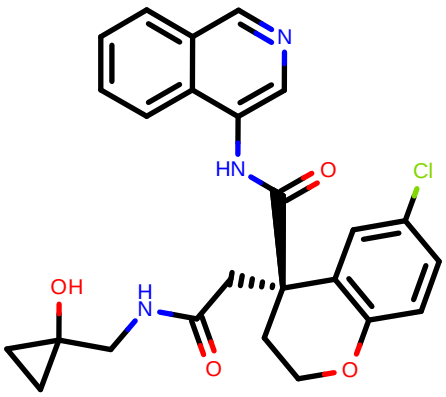
CID:	EN300-130825_1_1
SMILES:	CN1[C@@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3502
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.25

EN300-151461_2_2



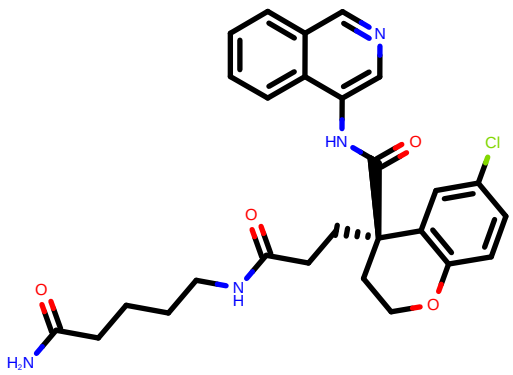
CID:	EN300-151461_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)[C@H]6CCOC6
RUN:	RUN7027
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.31

EN300-1644703_1_1



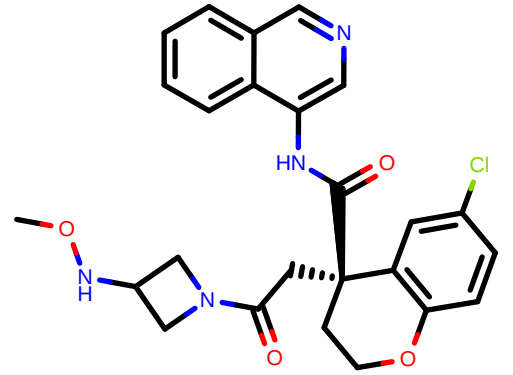
CID:	EN300-1644703_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CC5)O
RUN:	RUN10154
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.33

EN300-125143_2_1



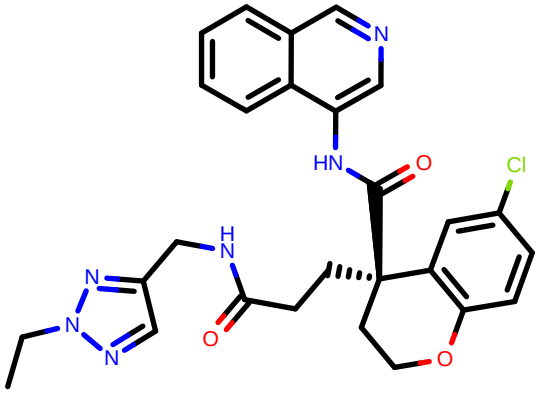
CID:	EN300-125143_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCCCC(=O)N
RUN:	RUN9759
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.30

EN300-6745214_1_1



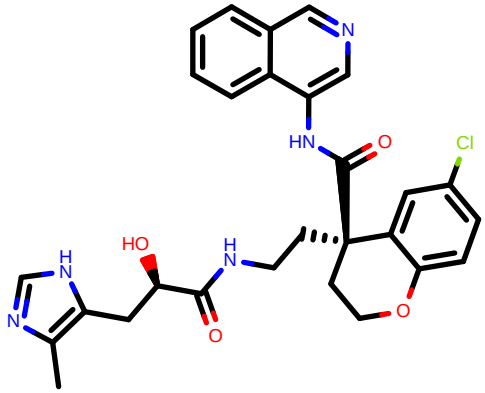
CID:	EN300-6745214_1_1
SMILES:	CON=C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7416
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.22

EN300-226486_2_1



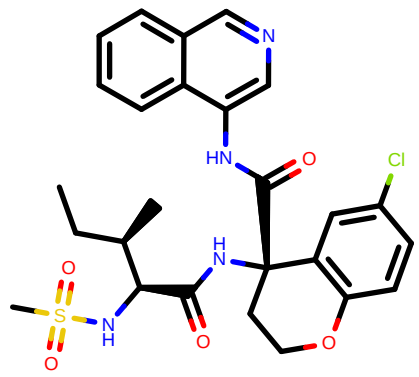
CID:	EN300-226486_2_1
SMILES:	CCn1ncc(n1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10999
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.24

EN300-7494324_3_2



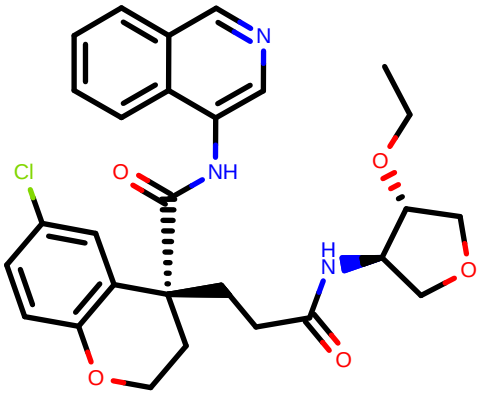
CID:	EN300-7494324_3_2
SMILES:	Cc1c(nc[nH]1)C[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN8512
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.35

EN300-76541_1_1



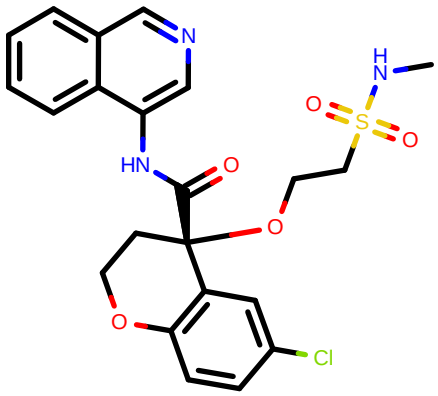
CID:	EN300-76541_1_1
SMILES:	CC[C@@H](C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN5556
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.44

EN300-248374_2_1



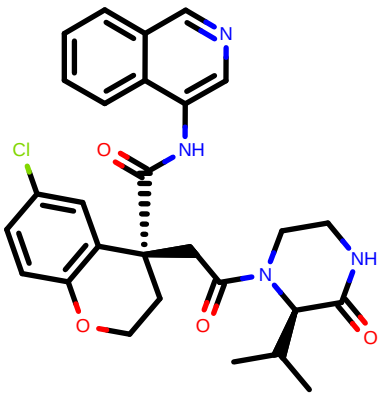
CID:	EN300-248374_2_1
SMILES:	CCO[C@@H]1COC[C@H]1NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5995
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.28

EN300-6482967_1_1



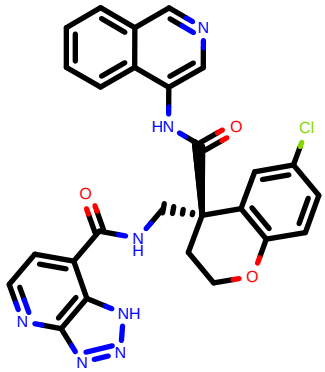
CID:	EN300-6482967_1_1
SMILES:	CNS(=O)(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1599
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.26

EN300-67791_1_1



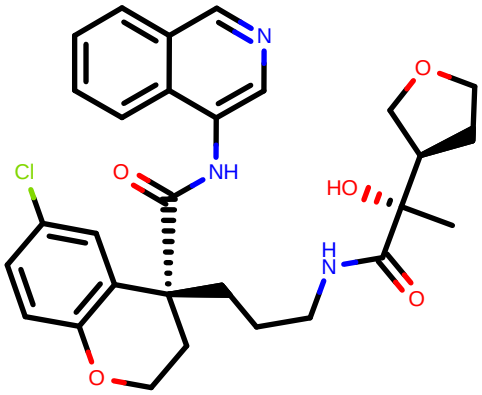
CID:	EN300-67791_1_1
SMILES:	CC(C)[C@@H]1C(=O)NCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5267
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.33

EN300-188377_2_1



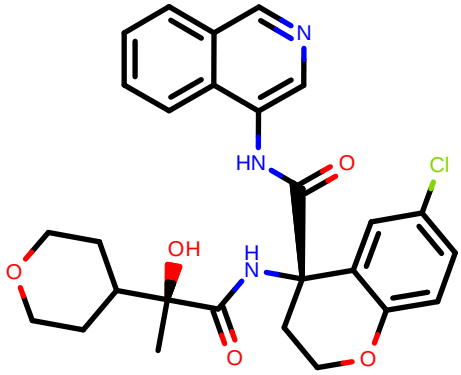
CID:	EN300-188377_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccnc6c5[nH]nn6
RUN:	RUN8543
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.30

EN300-217494_4_2



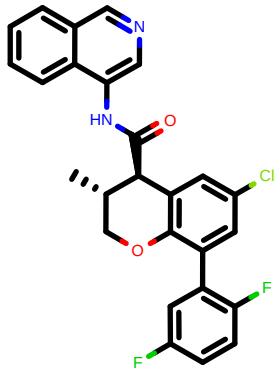
CID:	EN300-217494_4_2
SMILES:	C[C@][[C@@H]1CCOC1)(C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10541
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.28

EN300-217499_1_2



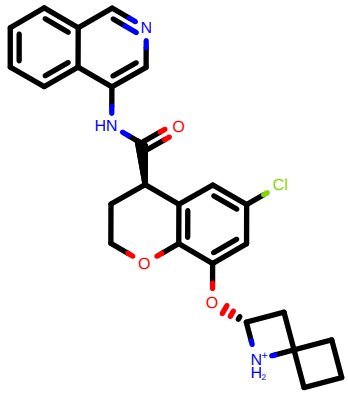
CID:	EN300-217499_1_2
SMILES:	C[C@](C1CCOCC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7210
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.29

DAR-DIA-0d514e7d-15_1



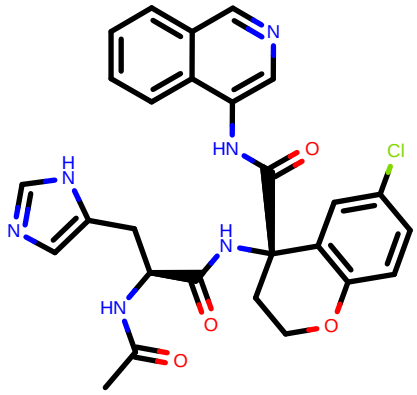
CID:	DAR-DIA-0d514e7d-15_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5cc(ccc5F)F
RUN:	RUN263
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.22

DAR-DIA-23e5a6a0-2_1



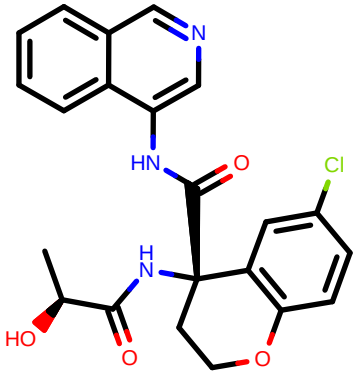
CID:	DAR-DIA-23e5a6a0-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6(N5)CCC6)Cl
RUN:	RUN81
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.36

EN300-196320_1_1



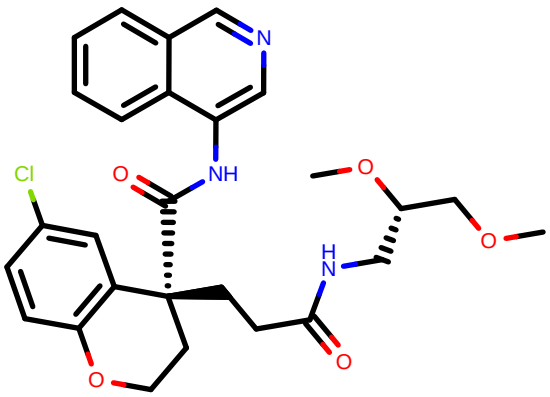
CID:	EN300-196320_1_1
SMILES:	CC(=O)N[C@@H](Cc1cnc[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5452
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.31

EN300-91905_1_1



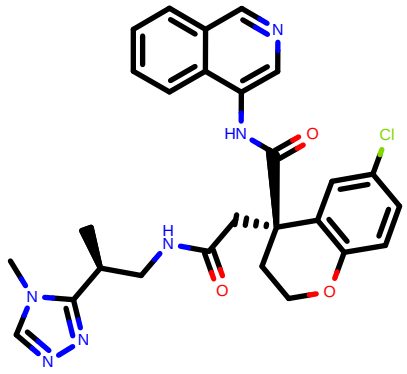
CID:	EN300-91905_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1221
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.20

EN300-129710_2_2



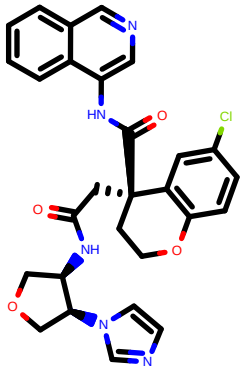
CID:	EN300-129710_2_2
SMILES:	COC[C@H](CNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN11007
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.29

EN300-170715_1_1



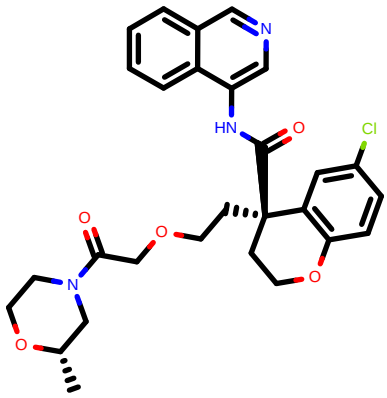
CID:	EN300-170715_1_1
SMILES:	C[C@@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)c5nncn5C
RUN:	RUN8412
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.42

EN300-6736890_1_1



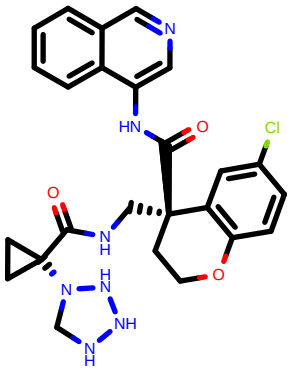
CID:	EN300-6736890_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5n6ccnc6
RUN:	RUN9945
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.29

EN300-25572_3_2



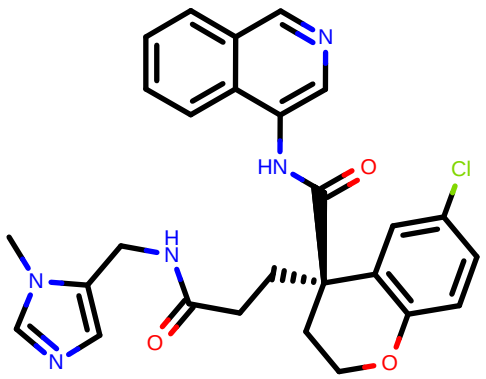
CID:	EN300-25572_3_2
SMILES:	C[C@H]1CN(CCO1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN592
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.35

EN300-263085_2_1



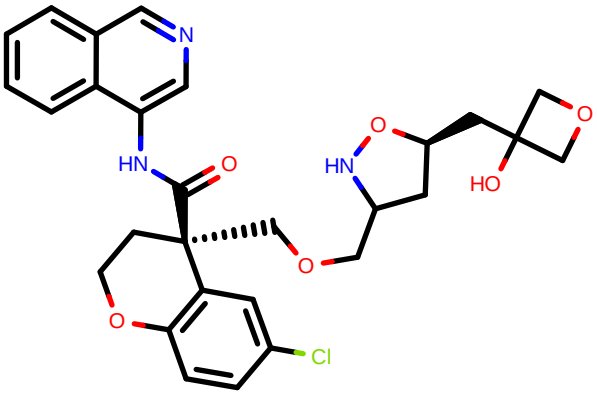
CID:	EN300-263085_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)n6cnnn6
RUN:	RUN5765
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.28

EN300-216594_2_1



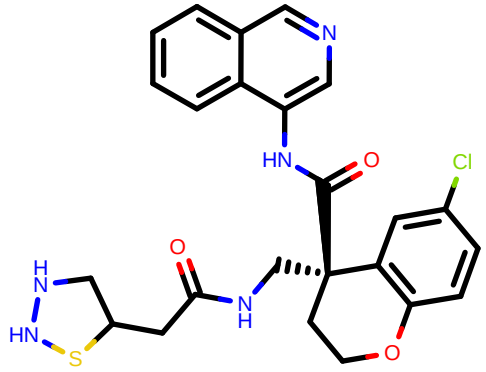
CID:	EN300-216594_2_1
SMILES:	Cn1cncc1CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6869
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.28

EN300-7457160_2_2



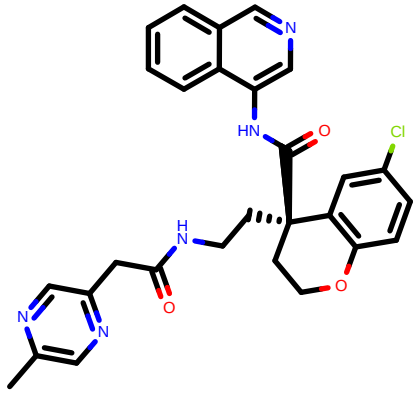
CID:	EN300-7457160_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC5=NO[C@H](C5)CC6(COC6)O
RUN:	RUN2674
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.36

EN300-260152_2_1



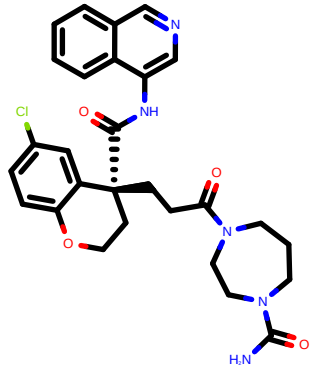
CID:	EN300-260152_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5cnns5
RUN:	RUN3151
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.25

EN300-1709295_3_1



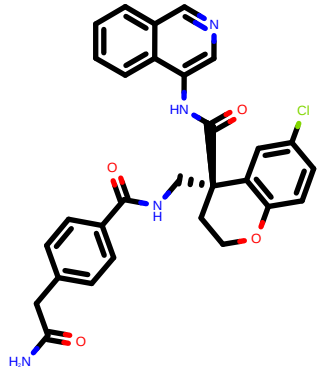
CID:	EN300-1709295_3_1
SMILES:	Cc1cnc(cn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10334
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.44

EN300-65063_2_1



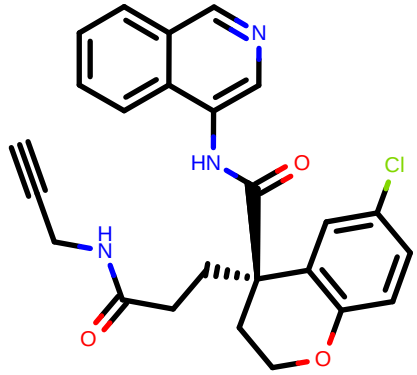
CID:	EN300-65063_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCN(CC5)C(=O)N
RUN:	RUN7901
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.36

EN300-2924757_2_1



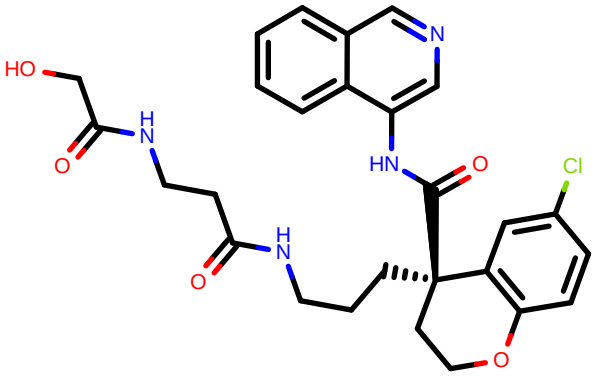
CID:	EN300-2924757_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cc5)CC(=O)N
RUN:	RUN8547
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.25

EN300-21409_2_1



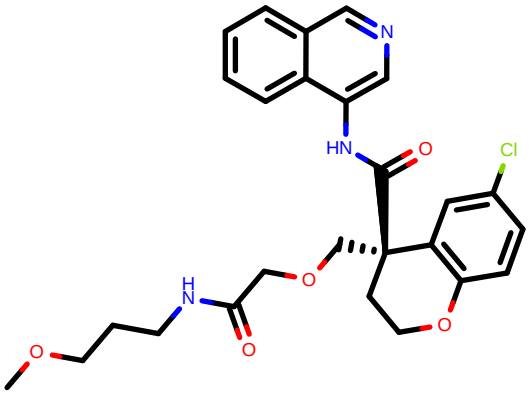
CID:	EN300-21409_2_1
SMILES:	C#CCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5627
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.25

EN300-383904_4_1



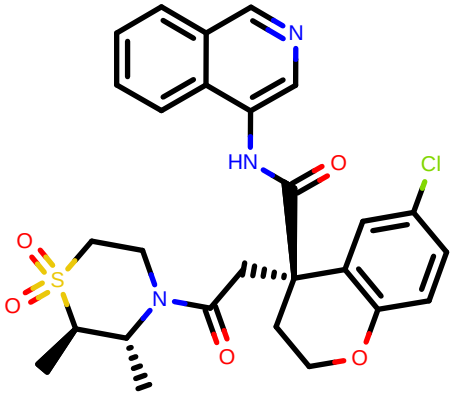
CID:	EN300-383904_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCNC(=O)CO
RUN:	RUN9511
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.33

EN300-04492_2_1



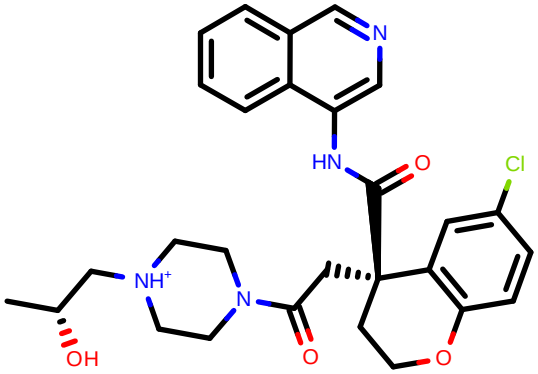
CID:	EN300-04492_2_1
SMILES:	COCCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1398
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.36

EN300-80940_1_3



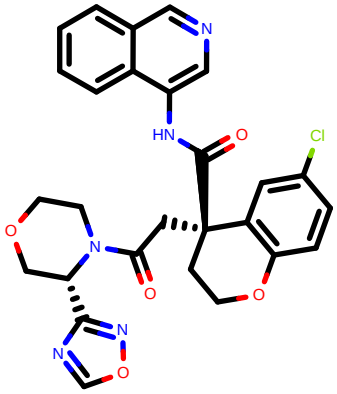
CID:	EN300-80940_1_3
SMILES:	C[C@@H]1[C@H](S(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN9784
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.30

EN300-154229_1_1



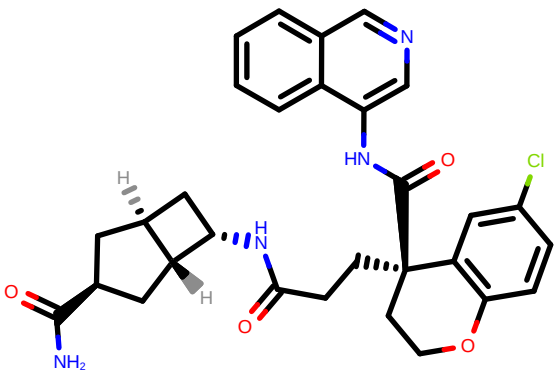
CID:	EN300-154229_1_1
SMILES:	C[C@H](CN1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2660
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.39

EN300-122849_1_2



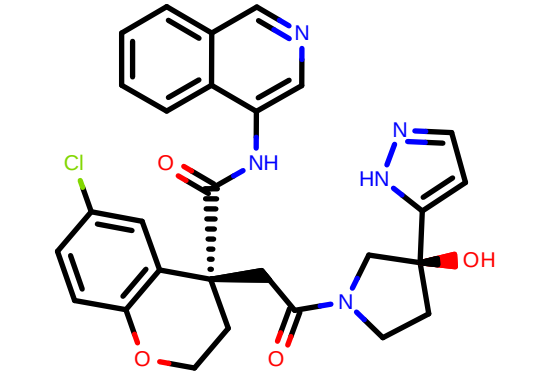
CID:	EN300-122849_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5c6ncon6
RUN:	RUN4963
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.32

EN300-1268016_2_16



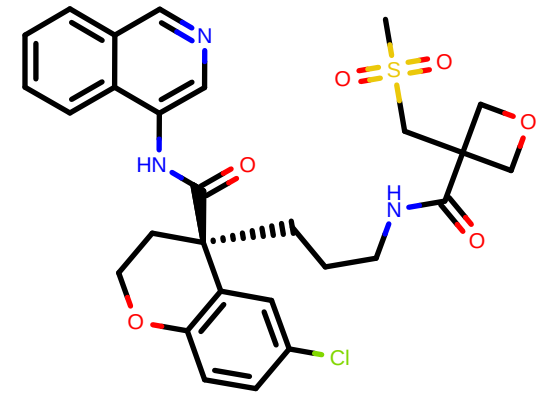
CID:	EN300-1268016_2_16
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5C[C@H]6[C@H]5C[C@H](C6)C(=O)N
RUN:	RUN4572
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.26

EN300-1609922_1_2



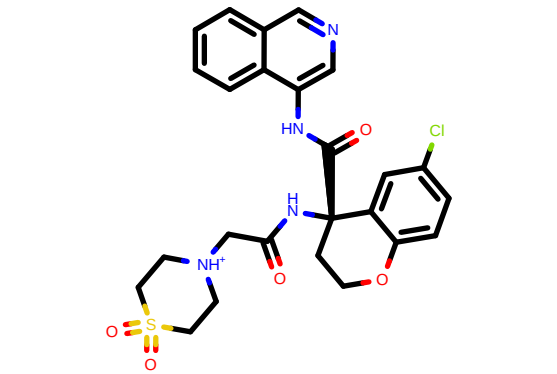
CID:	EN300-1609922_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@](C5)(c6ccn[nH]6)O
RUN:	RUN10430
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.37

EN300-262204_4_1



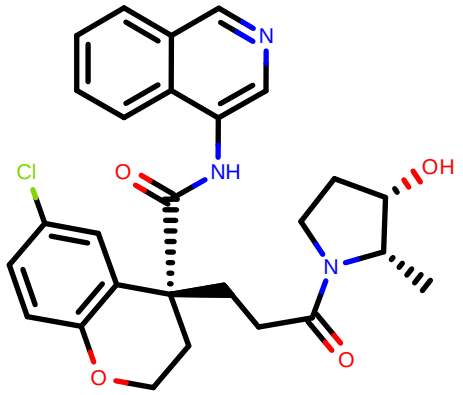
CID:	EN300-262204_4_1
SMILES:	CS(=O)(=O)CC1(COC1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9703
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.34

EN300-39305_1_1



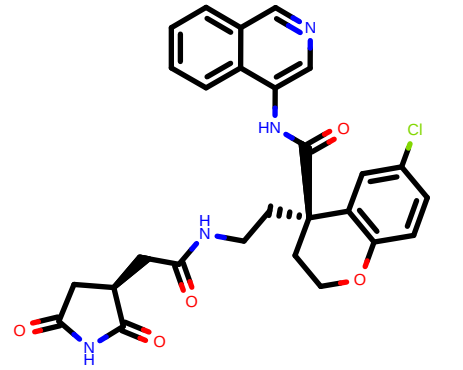
CID:	EN300-39305_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCS(=O)(=O)CC5
RUN:	RUN6303
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.31

EN300-2008120_2_1



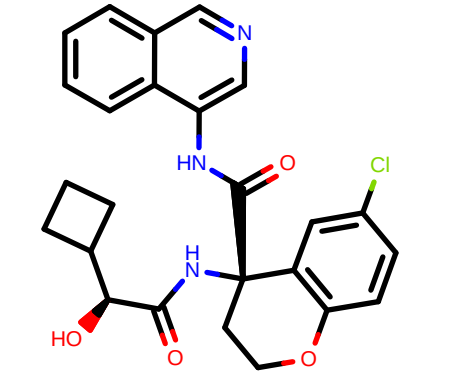
CID:	EN300-2008120_2_1
SMILES:	C[C@H]1[C@H](CCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN1107
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.23

EN300-227055_3_1



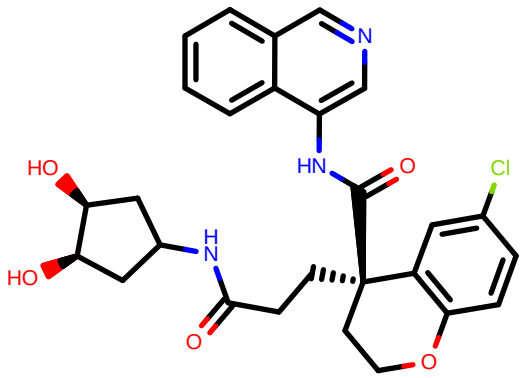
CID:	EN300-227055_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@H]5CC(=O)NC5=O
RUN:	RUN9910
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.30

EN300-249764_1_2



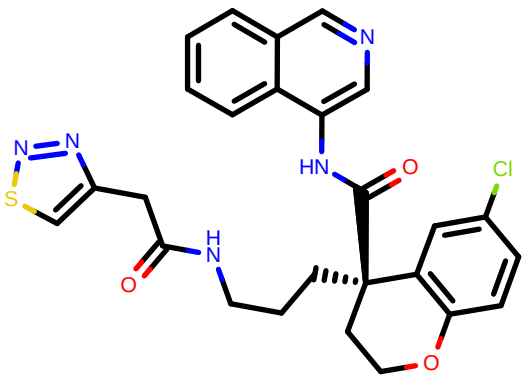
CID:	EN300-249764_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5CCC5)O
RUN:	RUN949
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.22

EN300-392656_2_1



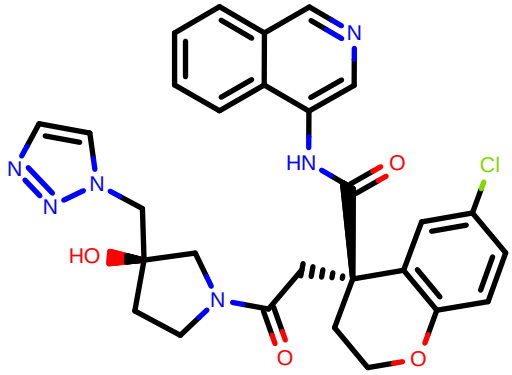
CID:	EN300-392656_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5C[C@H]([C@H](C5)O)O
RUN:	RUN3049
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.32

EN300-300519_4_1



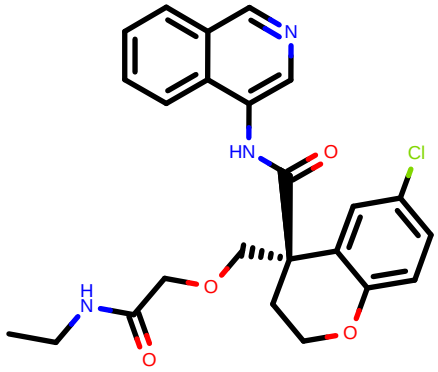
CID:	EN300-300519_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)Cc5csnn5
RUN:	RUN11229
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.26

EN300-269627_1_1



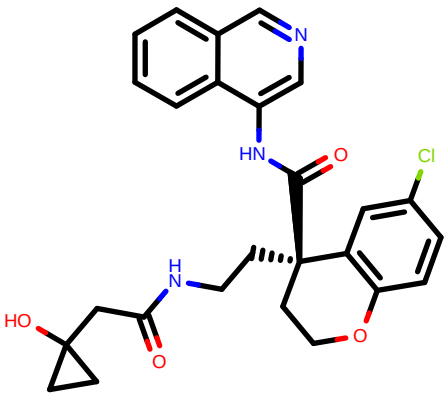
CID:	EN300-269627_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(Cn6ccnn6)O
RUN:	RUN9446
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.37

EN300-7003350_2_1



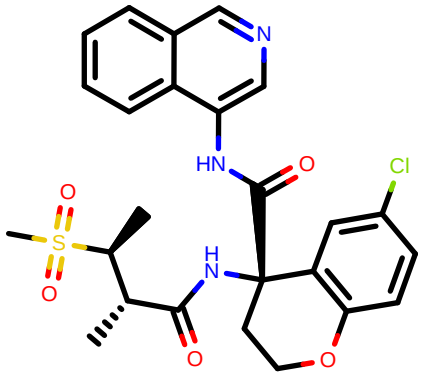
CID:	EN300-7003350_2_1
SMILES:	CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN942
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.20

EN300-207873_3_1



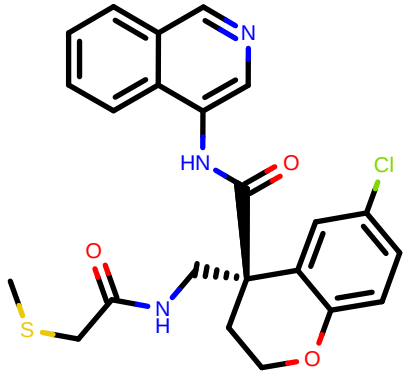
CID:	EN300-207873_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC5(CC5)O
RUN:	RUN6182
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.28

EN300-182725_1_4



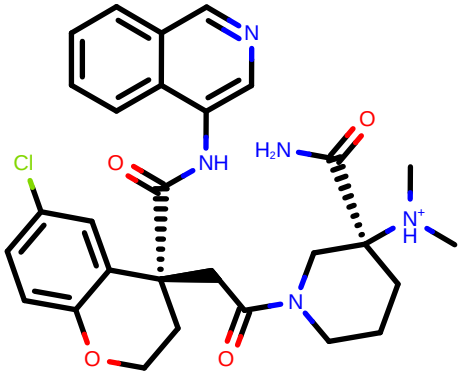
CID:	EN300-182725_1_4
SMILES:	C[C@H]([C@H](C)S(=O)(=O)C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3290
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.32

EN300-07879_2_1



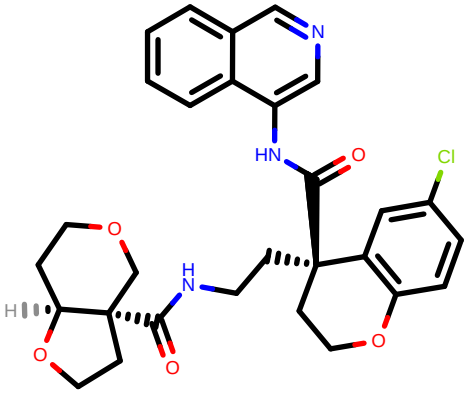
CID:	EN300-07879_2_1
SMILES:	CSCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3902
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.24

EN300-7433071_1_2



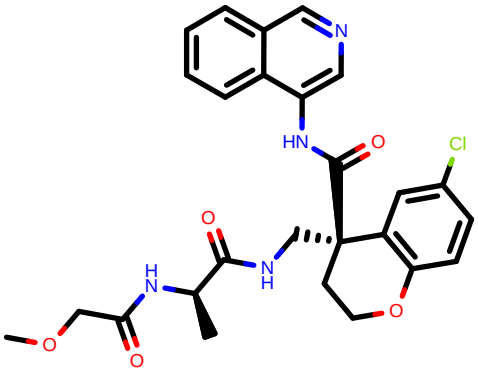
CID:	EN300-7433071_1_2
SMILES:	CN(C)[C@]1(CCCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN471
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.47

EN300-341337_3_4



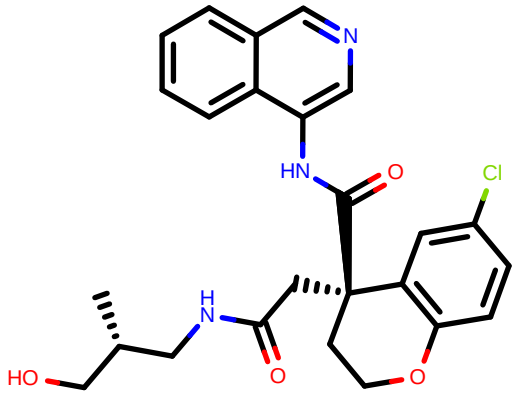
CID:	EN300-341337_3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56CCO[C@H]5CCOC6
RUN:	RUN3020
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.34

EN300-31183_2_2



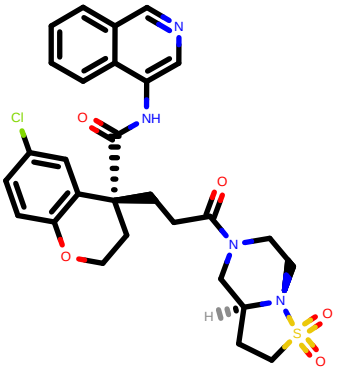
CID:	EN300-31183_2_2
SMILES:	C[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)COC
RUN:	RUN5134
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.32

EN300-53656_1_2



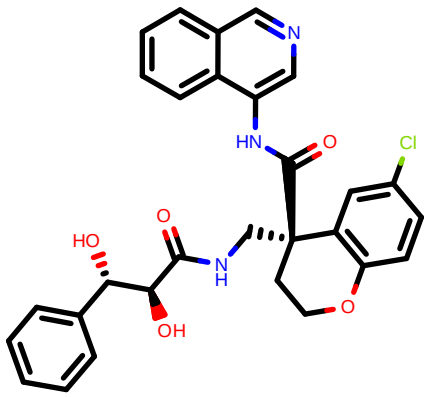
CID:	EN300-53656_1_2
SMILES:	C[C@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)CO
RUN:	RUN5235
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.31

EN300-1091496_2_2



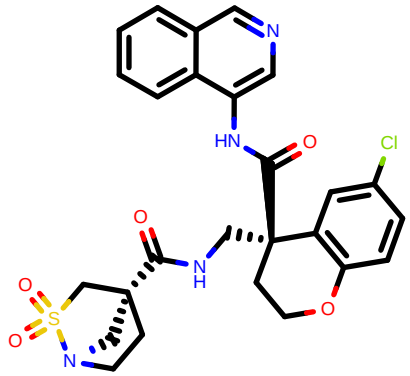
CID:	EN300-1091496_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCN6[C@H](C5)CCS6(=O)=O
RUN:	RUN8217
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.30

EN300-2923949_2_1



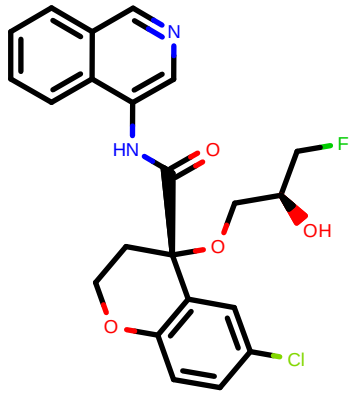
CID:	EN300-2923949_2_1
SMILES:	c1ccc(cc1)[C@@H]([C@@H](C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)O
RUN:	RUN4402
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.32

EN300-7432022_2_1



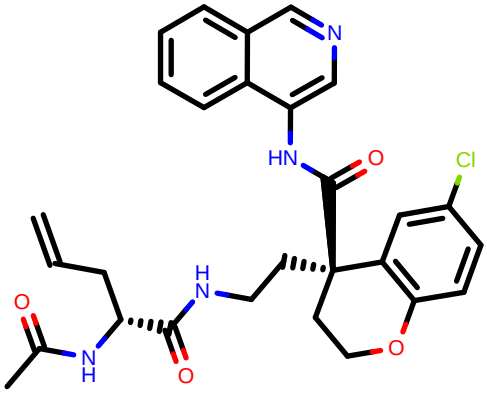
CID:	EN300-7432022_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C56CCN(C5)S(=O)(=O)C6
RUN:	RUN7031
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.35

EN300-1968342_1_1



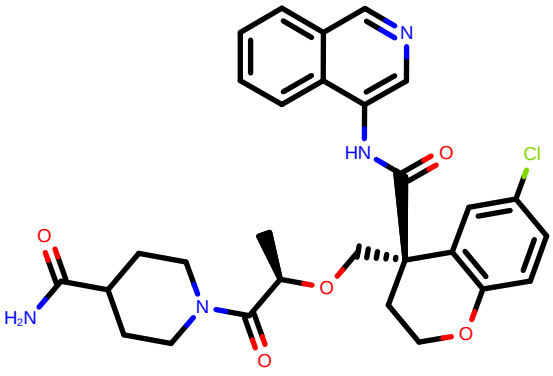
CID:	EN300-1968342_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](CF)O
RUN:	RUN1951
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.32

EN300-43047_3_2



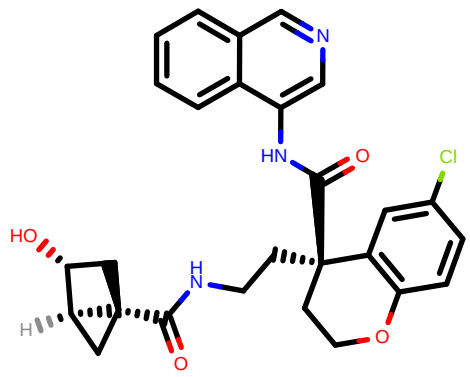
CID:	EN300-43047_3_2
SMILES:	CC(=O)N[C@H](CC=C)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN11276
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.28

EN300-28113_2_2



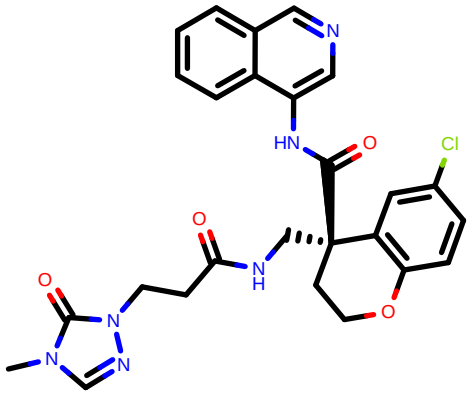
CID:	EN300-28113_2_2
SMILES:	C[C@H](C(=O)N1CCC(CC1)C(=O)N)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1661
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.30

EN300-6493972_3_1



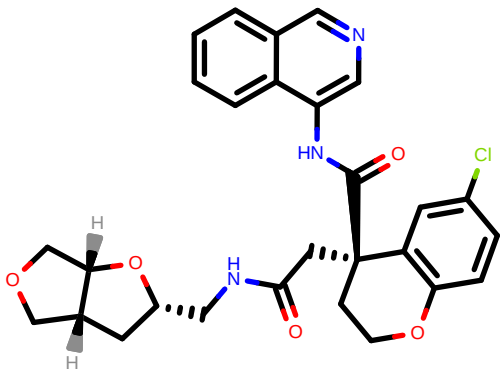
CID:	EN300-6493972_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56C[C@H]5[C@@H](C6)O
RUN:	RUN8164
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.35

EN300-223491_2_1



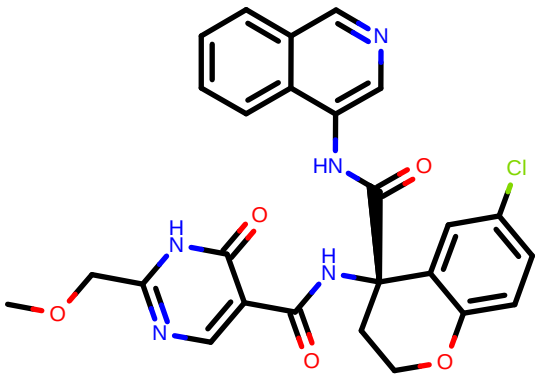
CID:	EN300-223491_2_1
SMILES:	Cn1cnn(c1=O)CCC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN454
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.25

EN300-657222_1_1



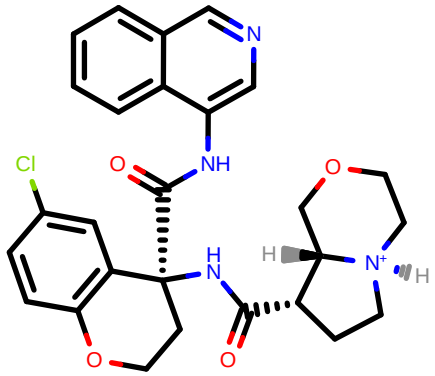
CID:	EN300-657222_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5C[C@@H]6COC[C@@H]6O5
RUN:	RUN7004
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.29

EN300-685492_1_1



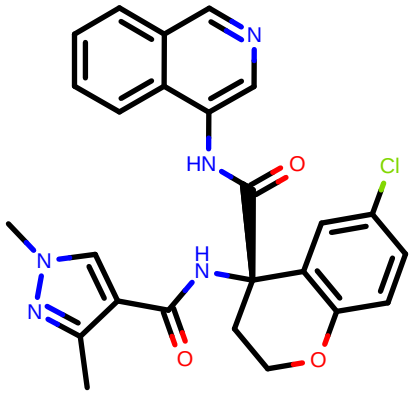
CID:	EN300-685492_1_1
SMILES:	COCc1[nH]c(=O)c(cn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8951
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.34

EN300-1588613_1_4



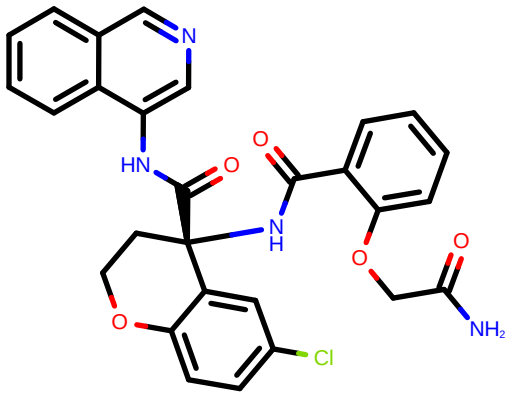
CID:	EN300-1588613_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CCN6[C@H]5COCC6
RUN:	RUN4681
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.38

EN300-76584_1_1



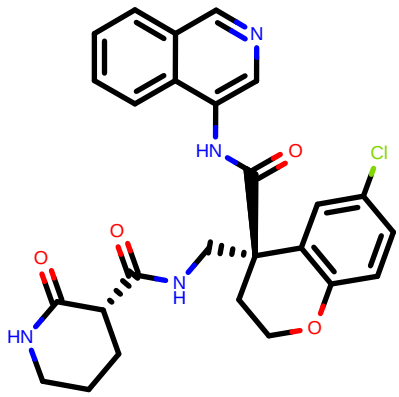
CID:	EN300-76584_1_1
SMILES:	Cc1c(cn(n1)C)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6204
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.25

EN300-15368_1_1



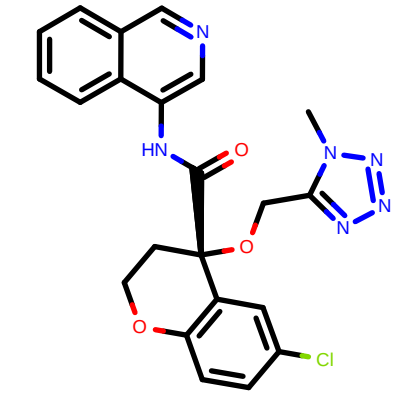
CID:	EN300-15368_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccccc5OCC(=O)N
RUN:	RUN4613
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.33

EN300-82616_2_1



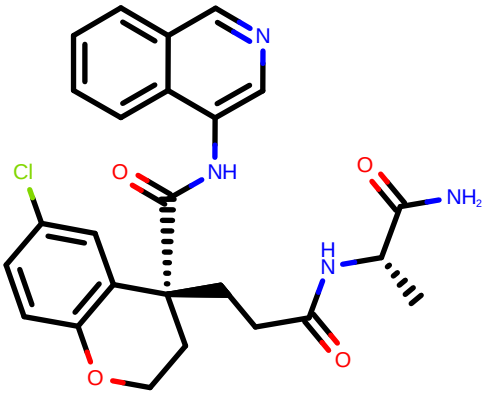
CID:	EN300-82616_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCCNC5=O
RUN:	RUN6831
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.32

EN300-62574_1_1



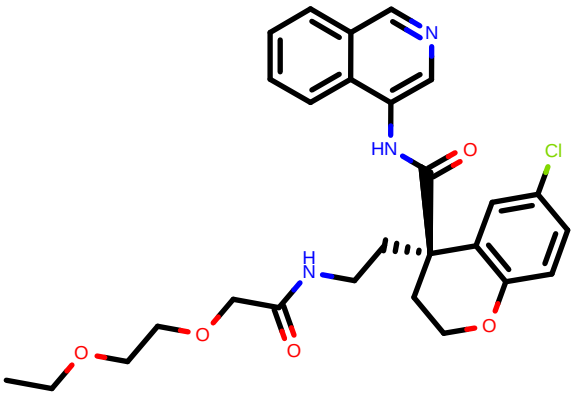
CID:	EN300-62574_1_1
SMILES:	Cn1c(nnn1)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1240
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.24

EN300-23648_2_1



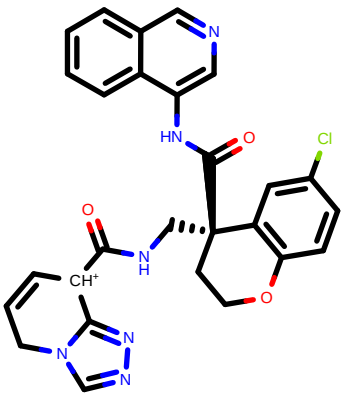
CID:	EN300-23648_2_1
SMILES:	C[C@@H](C(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1810
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.24

EN300-54304_3_1



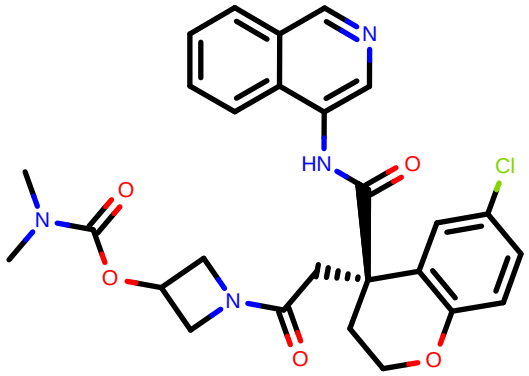
CID:	EN300-54304_3_1
SMILES:	CCOCCOCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10428
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.31

EN300-1726153_2_1



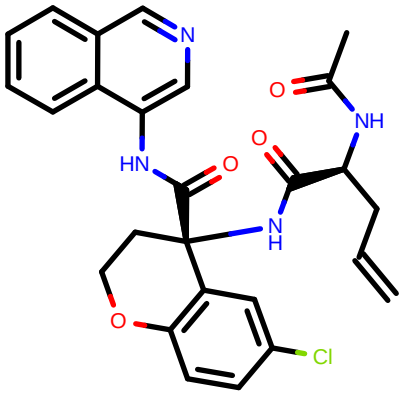
CID:	EN300-1726153_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cccn6c5nnc6
RUN:	RUN8079
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.26

EN300-1272529_1_1



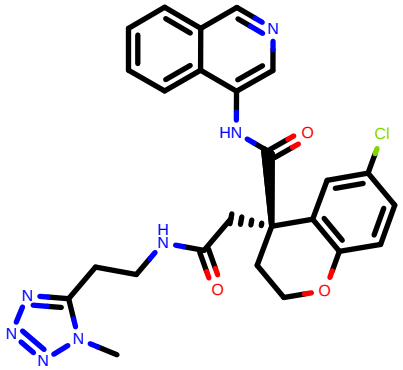
CID:	EN300-1272529_1_1
SMILES:	CN(C)C(=O)OC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10324
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.28

EN300-43047_1_1



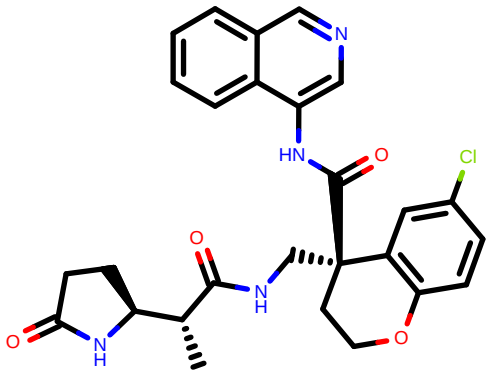
CID:	EN300-43047_1_1
SMILES:	CC(=O)N[C@@H](CC=C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4809
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.23

EN300-124904_1_1



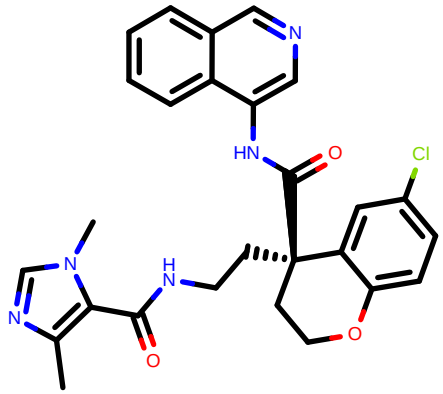
CID:	EN300-124904_1_1
SMILES:	Cn1c(nnn1)CCNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10374
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.30

EN300-249421_2_2



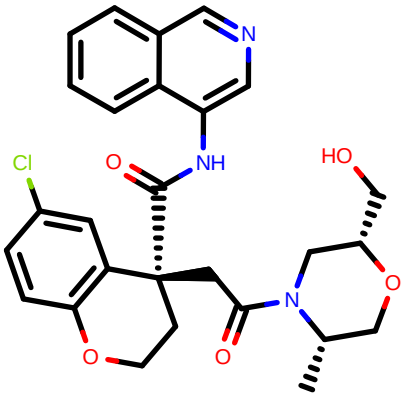
CID:	EN300-249421_2_2
SMILES:	C[C@H]([C@@H]1CCC(=O)N1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3367
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.36

EN300-6498351_3_1



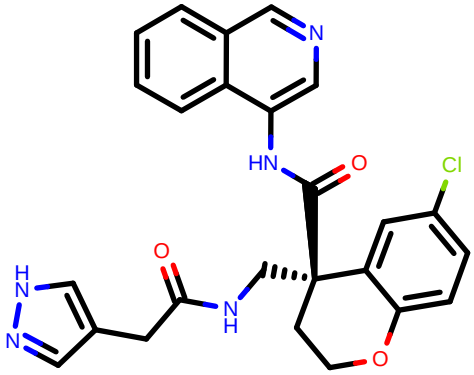
CID:	EN300-6498351_3_1
SMILES:	Cc1c(n(cn1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10135
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.41

EN300-109920_1_4



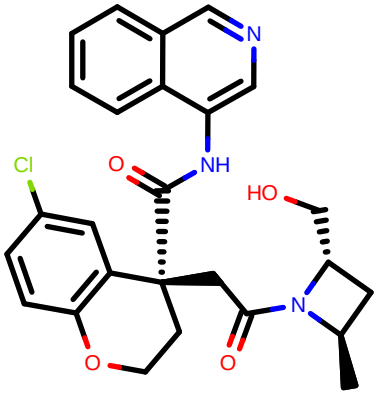
CID:	EN300-109920_1_4
SMILES:	C[C@H]1CO[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN5111
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.36

EN300-1589101_2_1



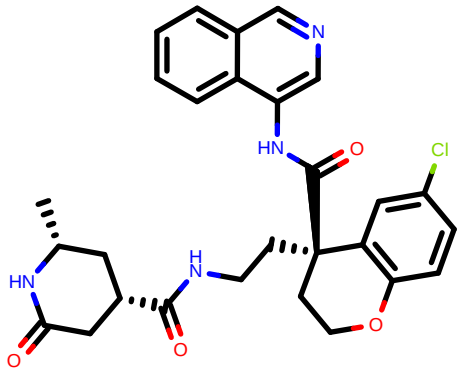
CID:	EN300-1589101_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5c[nH]nc5
RUN:	RUN5485
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.28

EN300-1709410_1_3



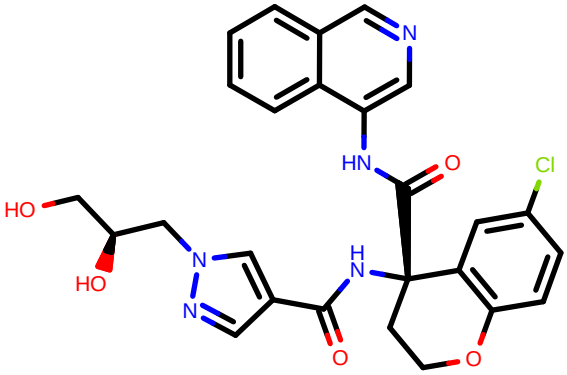
CID:	EN300-1709410_1_3
SMILES:	C[C@@H]1C[C@H](N1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)CO
RUN:	RUN10602
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.31

EN300-7435400_3_1



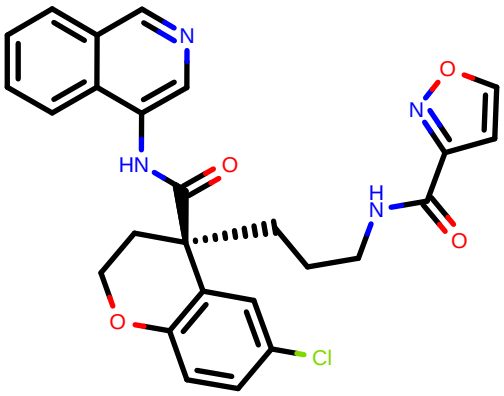
CID:	EN300-7435400_3_1
SMILES:	C[C@@H]1C[C@@H](CC(=O)N1)C(=O)NCC[C@]2(COOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11300
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.29

EN300-246178_1_2



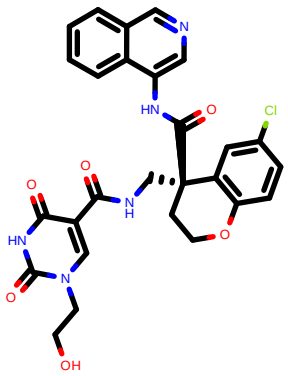
CID:	EN300-246178_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnn(c5)C[C@H](CO)O
RUN:	RUN5600
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.38

EN300-22245_4_1



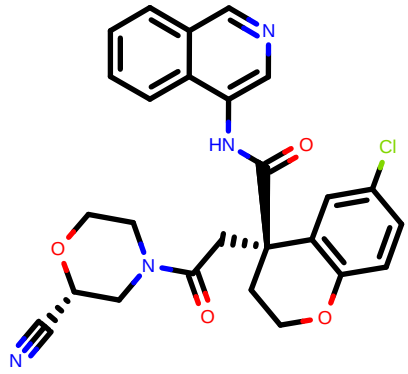
CID:	EN300-22245_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5ccon5
RUN:	RUN8953
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.31

EN300-101291_2_1



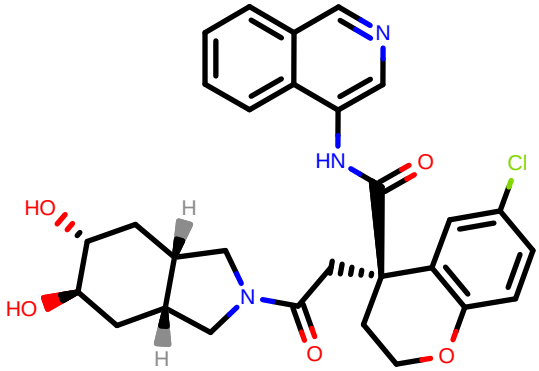
CID:	EN300-101291_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(c(=O)[nH]c5=O)CCO
RUN:	RUN7859
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.42

EN300-70489_1_2



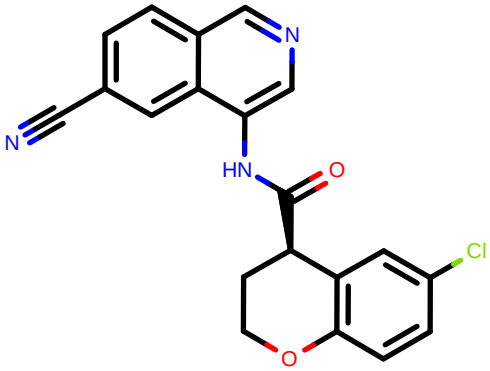
CID:	EN300-70489_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@H](C5)C#N
RUN:	RUN9983
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.24

EN300-7355477_1_3



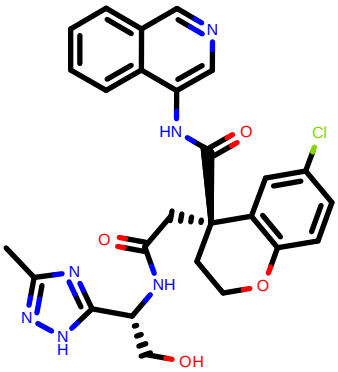
CID:	EN300-7355477_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6C[C@H][C@@H](C[C@H]6C5)O)O
RUN:	RUN3052
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.45

BEN-DND-c852c98b-1_1



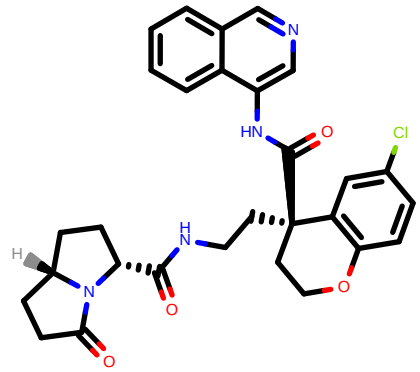
CID:	BEN-DND-c852c98b-1_1
SMILES:	c1cc2cncc(c2cc1C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN25
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.04

EN300-1699797_1_1



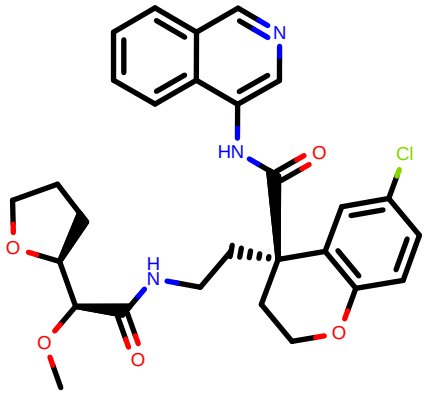
CID:	EN300-1699797_1_1
SMILES:	Cc1[nH]c(nn1)[C@@H](CO)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9516
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.33

EN300-6479181_3_2



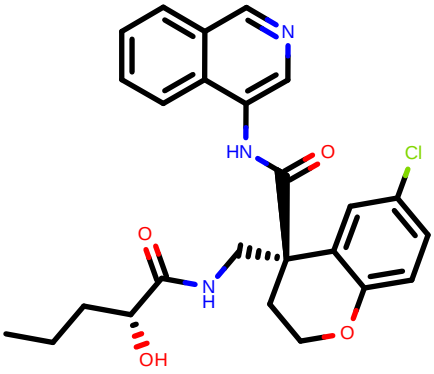
CID:	EN300-6479181_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC[C@@H]6N5C(=O)CC6
RUN:	RUN4723
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.28

EN300-6277108_3_1



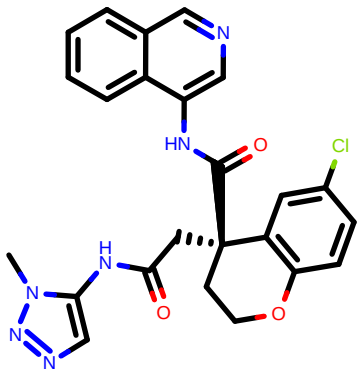
CID:	EN300-6277108_3_1
SMILES:	CO[C@@H]([C@@H]1CCCO1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5850
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.36

EN300-300217_2_3



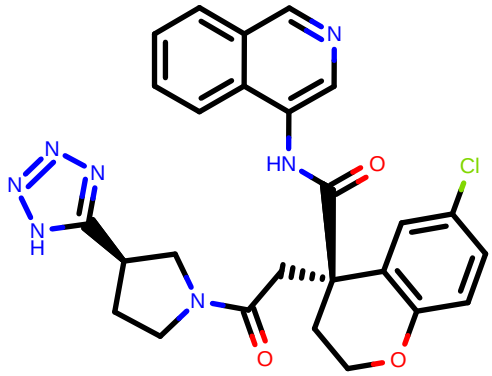
CID:	EN300-300217_2_3
SMILES:	C/C=C\[C@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4022
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.26

EN300-199290_1_1



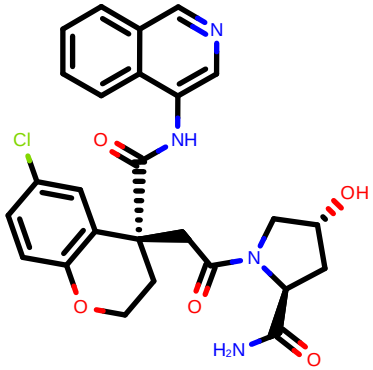
CID:	EN300-199290_1_1
SMILES:	Cn1c(cnn1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9334
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.26

EN300-366852_1_2



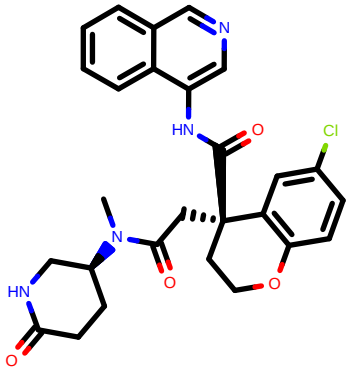
CID:	EN300-366852_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H](C5)c6[nH]nnn6
RUN:	RUN7012
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.37

EN300-07752_1_3



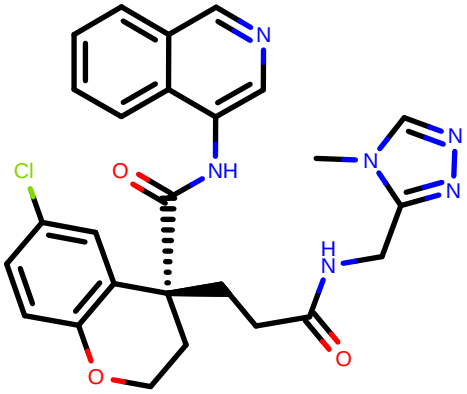
CID:	EN300-07752_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@H]5C(=O)N)O
RUN:	RUN11126
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.33

EN300-1253092_1_2



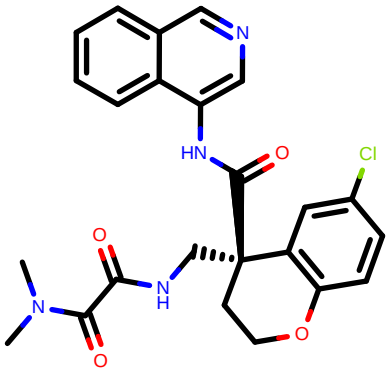
CID:	EN300-1253092_1_2
SMILES:	CN([C@H]1CCC(=O)NC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9221
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.28

EN300-30859_2_1



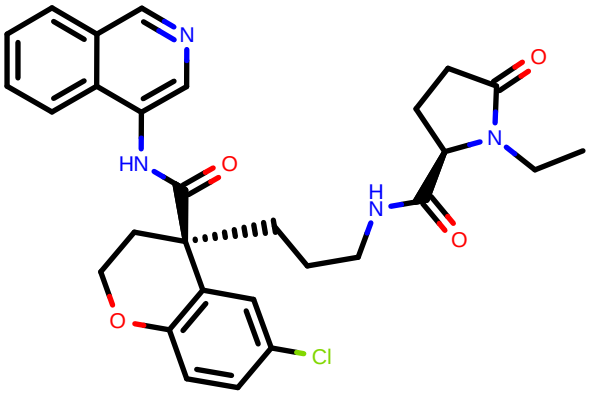
CID:	EN300-30859_2_1
SMILES:	Cn1cnnc1CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5743
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.24

EN300-118647_2_1



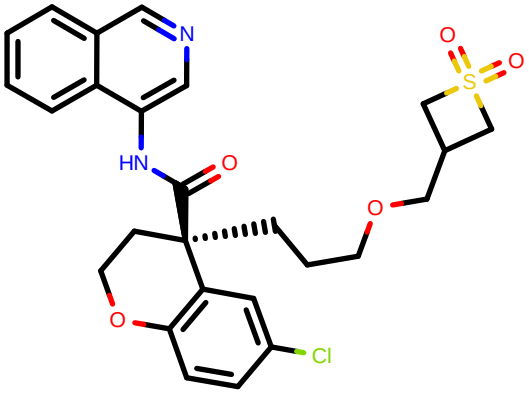
CID:	EN300-118647_2_1
SMILES:	CN(C)C(=O)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4690
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.28

EN300-718785_4_2



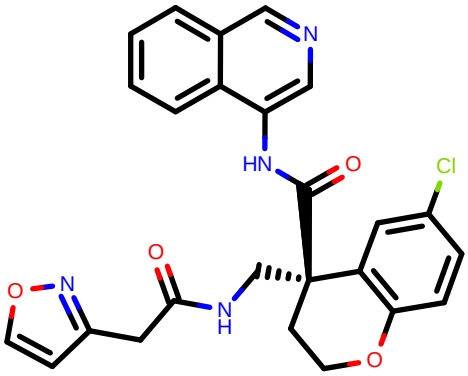
CID:	EN300-718785_4_2
SMILES:	CCN1[C@H](CCC1=O)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10275
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.32

EN300-5638430_4_1



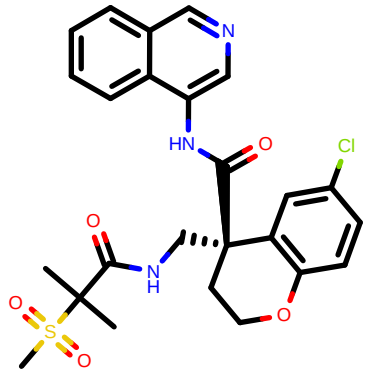
CID:	EN300-5638430_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC5CS(=O)(=O)C5
RUN:	RUN816
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.41

EN300-82037_2_1



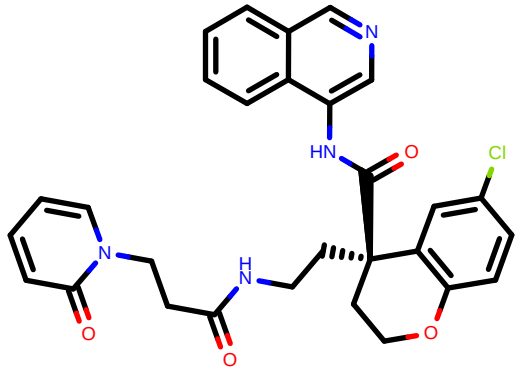
CID:	EN300-82037_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5ccon5
RUN:	RUN3659
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.28

EN300-76205_2_1



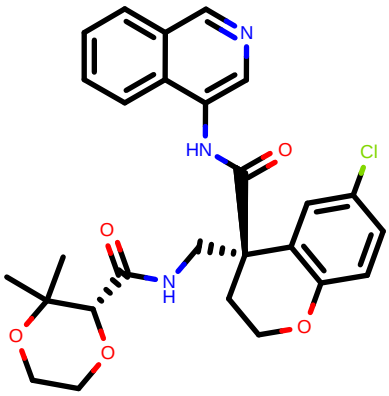
CID:	EN300-76205_2_1
SMILES:	CC(C)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN2507
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.33

EN300-36622_3_1



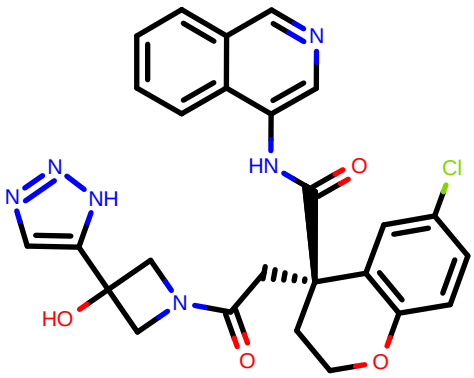
CID:	EN300-36622_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCn5ccccc5=O
RUN:	RUN10740
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.36

EN300-1601684_2_1



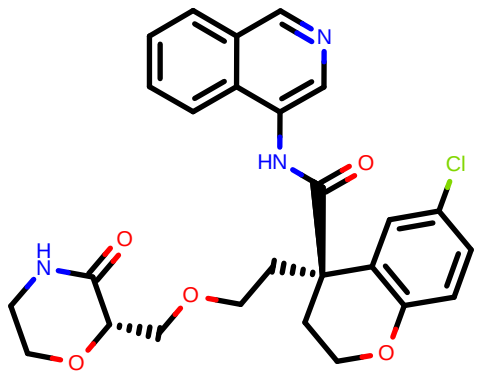
CID:	EN300-1601684_2_1
SMILES:	CC1([C@@H](OCCO1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2732
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.48

EN300-384234_1_1



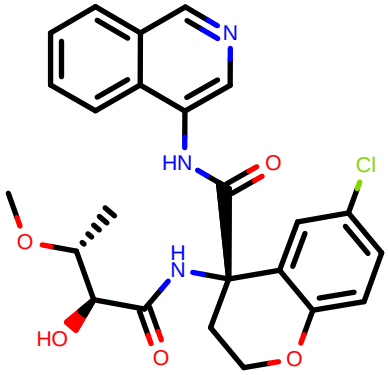
CID:	EN300-384234_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(c6cnn[nH]6)O
RUN:	RUN3452
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.30

EN300-1706036_3_2



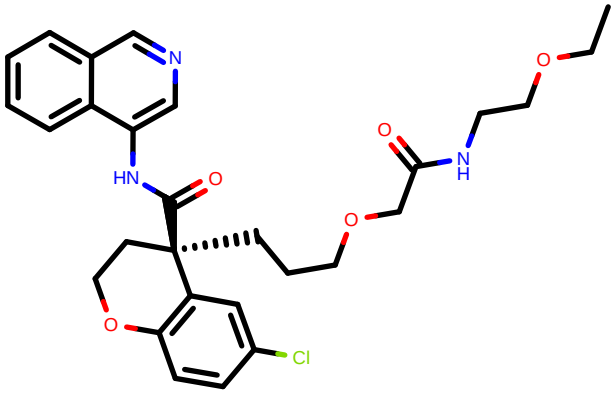
CID:	EN300-1706036_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@H]5C(=O)NCCO5
RUN:	RUN1835
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.26

EN300-220194_1_2



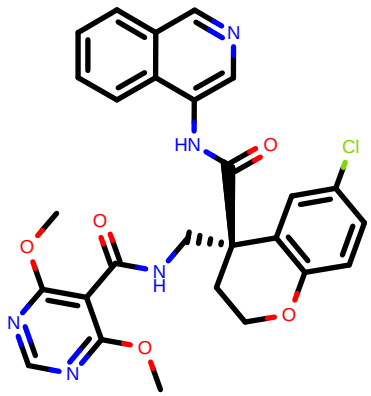
CID:	EN300-220194_1_2
SMILES:	C[C@H]([C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O)OC
RUN:	RUN4369
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.28

EN300-103187_4_1



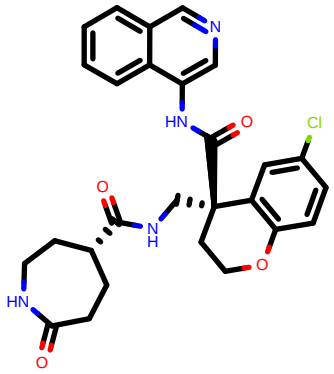
CID:	EN300-103187_4_1
SMILES:	CCOCCNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1718
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.40

EN300-70431_2_1



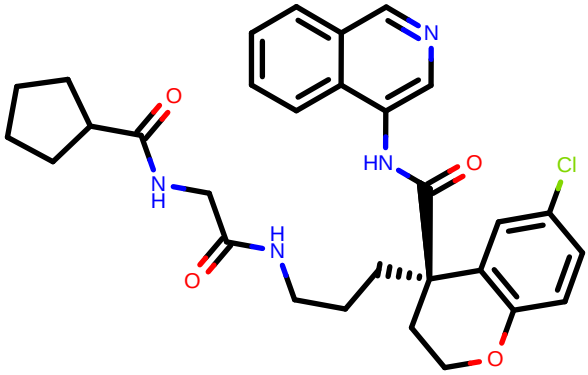
CID:	EN300-70431_2_1
SMILES:	COc1c(c(ncn1)OC)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8055
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.37

EN300-152337_2_1



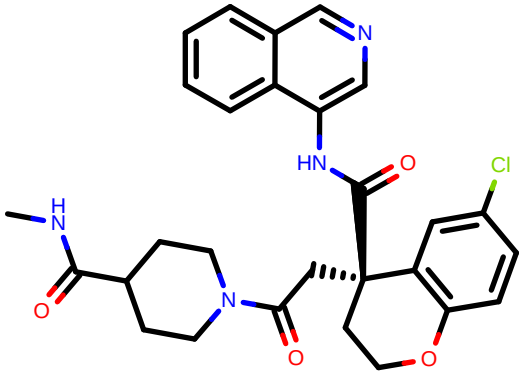
CID:	EN300-152337_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCC(=O)NCC5
RUN:	RUN2777
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.34

EN300-36845_4_1



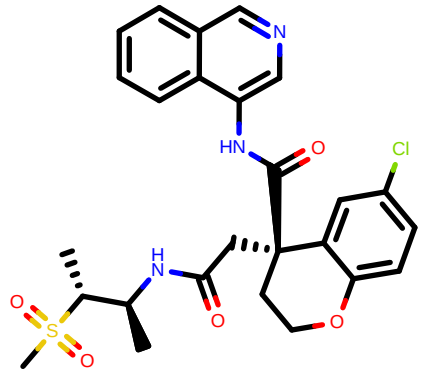
CID:	EN300-36845_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CNC(=O)C5CCCC5
RUN:	RUN11073
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.44

EN300-24653_1_1



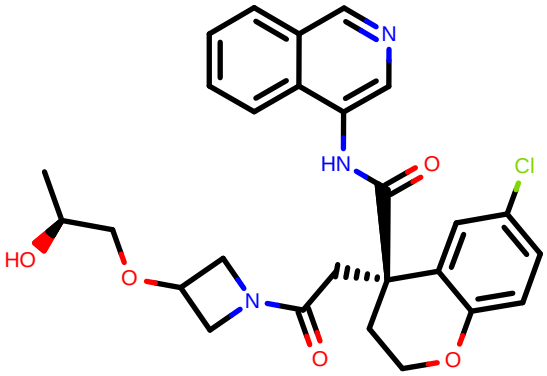
CID:	EN300-24653_1_1
SMILES:	CNC(=O)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9991
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.35

EN300-83434_1_1



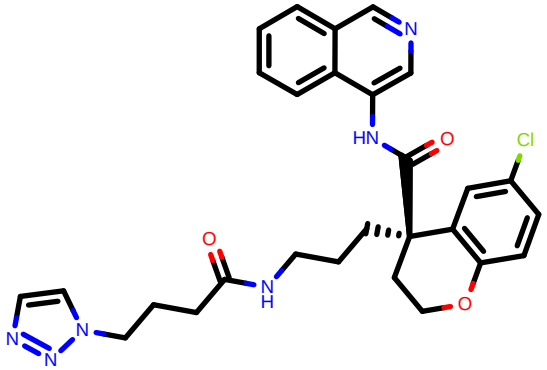
CID:	EN300-83434_1_1
SMILES:	C[C@@H]([C@@H](C)S(=O)(=O)C)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10568
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.29

EN300-6498888_1_1



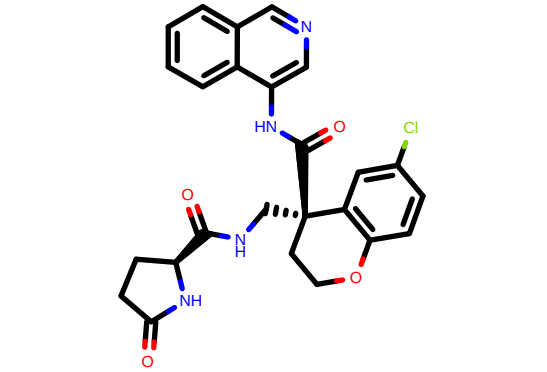
CID:	EN300-6498888_1_1
SMILES:	C[C@@H](COC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6992
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.41

EN300-124301_4_1



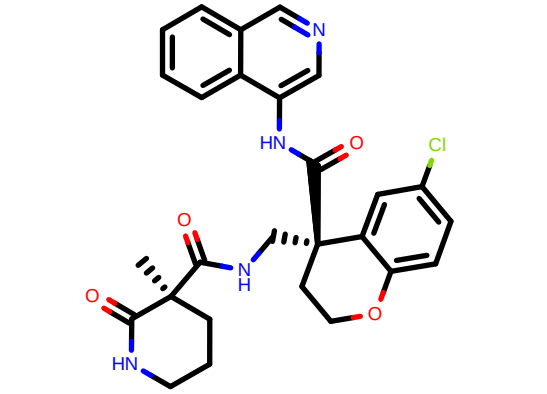
CID:	EN300-124301_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCCn5ccnn5
RUN:	RUN10907
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.33

EN300-72896_2_1



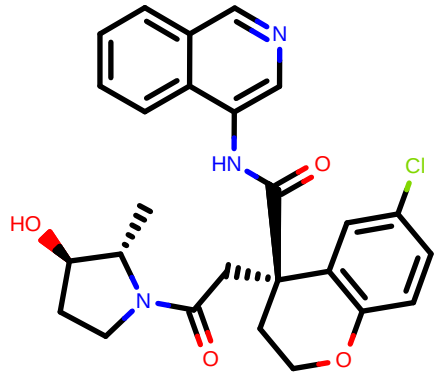
CID:	EN300-72896_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCC(=O)N5
RUN:	RUN4202
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.21

EN300-178876_2_1



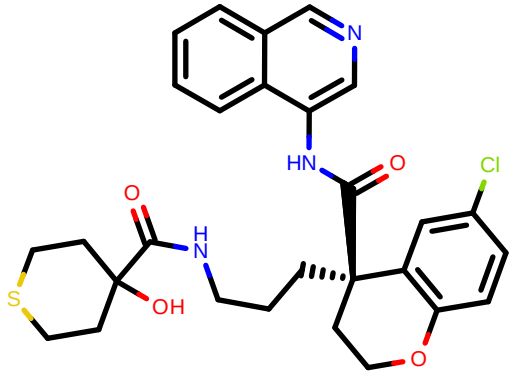
CID:	EN300-178876_2_1
SMILES:	C[C@@]1(CCCNC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5206
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.39

EN300-245036_1_1



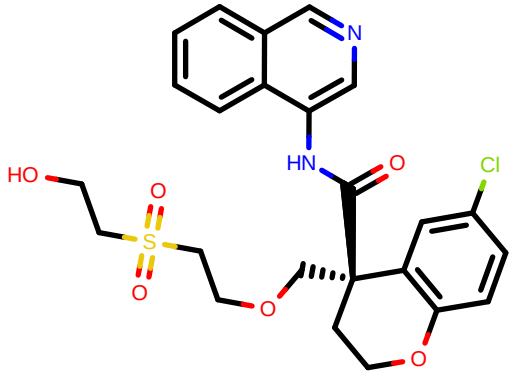
CID:	EN300-245036_1_1
SMILES:	C[C@H]1[C@@H](CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10079
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.28

EN300-122340_4_1



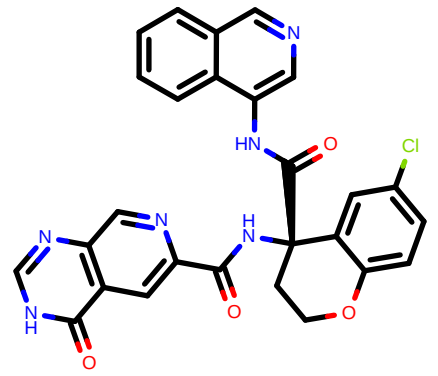
CID:	EN300-122340_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C5(CCSCC5)O
RUN:	RUN9883
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.39

EN300-7463171_2_1



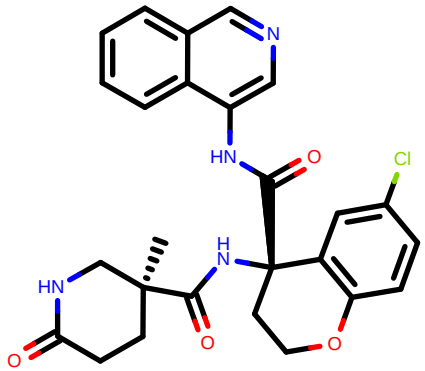
CID:	EN300-7463171_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCS(=O)(=O)CCO
RUN:	RUN1358
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.56

EN300-151756_1_1



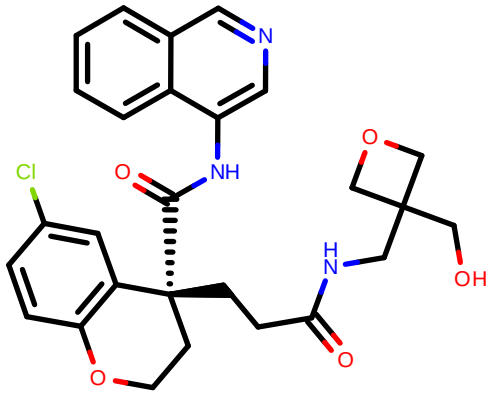
CID:	EN300-151756_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(cn5)nc[nH]c6=O
RUN:	RUN8996
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.25

EN300-195924_1_1



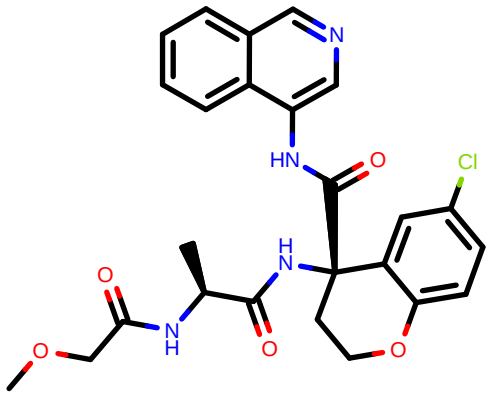
CID:	EN300-195924_1_1
SMILES:	C[C@@]1(CCC(=O)NC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5404
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.25

EN300-105482_2_1



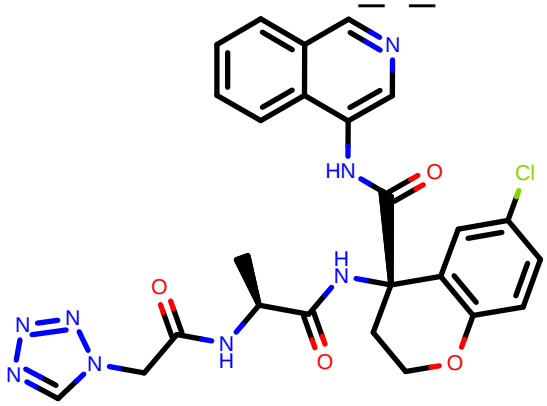
CID:	EN300-105482_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5(COC5)CO
RUN:	RUN5899
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.26

EN300-31183_1_1



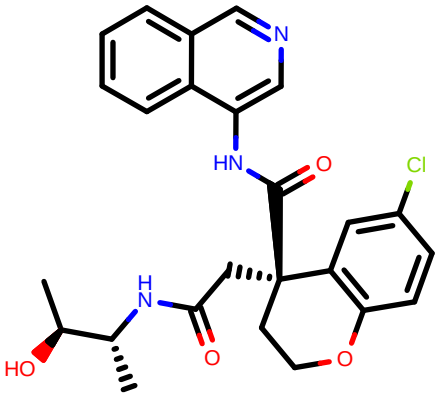
CID:	EN300-31183_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)COC
RUN:	RUN4901
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.32

EN300-651177_1_1



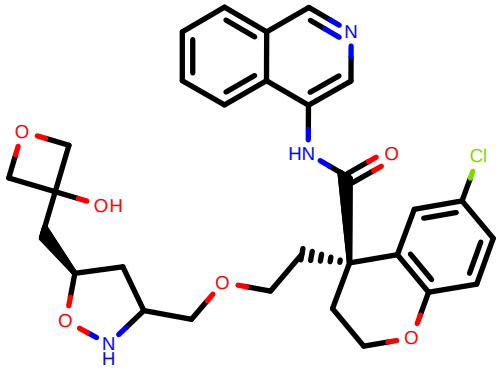
CID:	EN300-651177_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)Cn5cnnn5
RUN:	RUN7170
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.36

EN300-72272_1_4



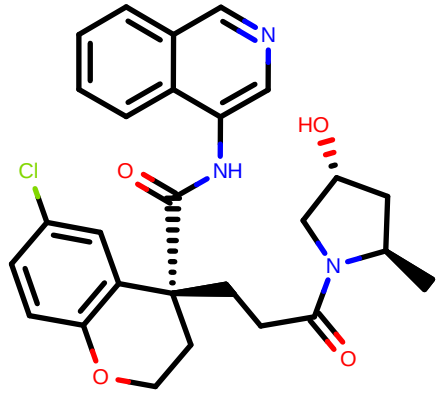
CID:	EN300-72272_1_4
SMILES:	C[C@H]([C@H](C)O)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9564
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.24

EN300-7457160_3_2



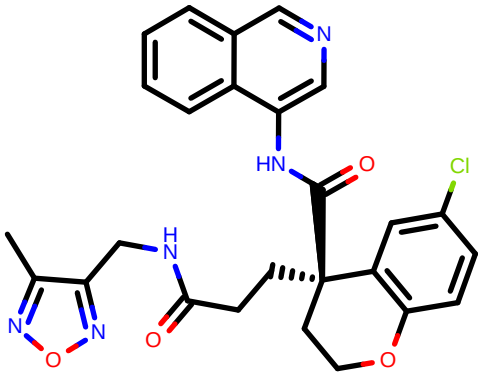
CID:	EN300-7457160_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC5=NO[C@H](C5)CC6(COC6)O
RUN:	RUN2517
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.35

EN300-173562_2_3



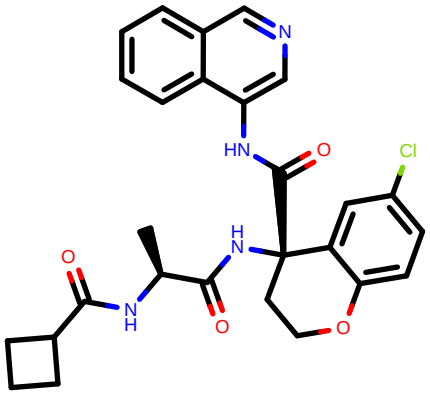
CID:	EN300-173562_2_3
SMILES:	C[C@@H]1C[C@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2299
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.29

EN300-79538_2_1



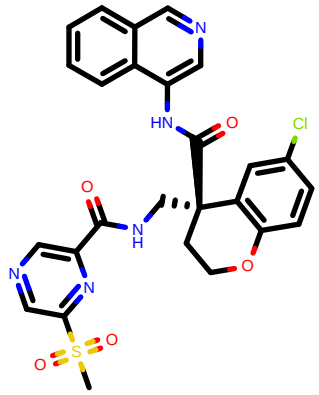
CID:	EN300-79538_2_1
SMILES:	Cc1c(non1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3249
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.26

EN300-66082_1_1



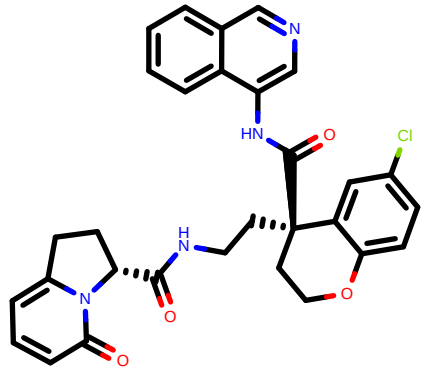
CID:	EN300-66082_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCC5
RUN:	RUN7978
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.38

EN300-206646_2_1



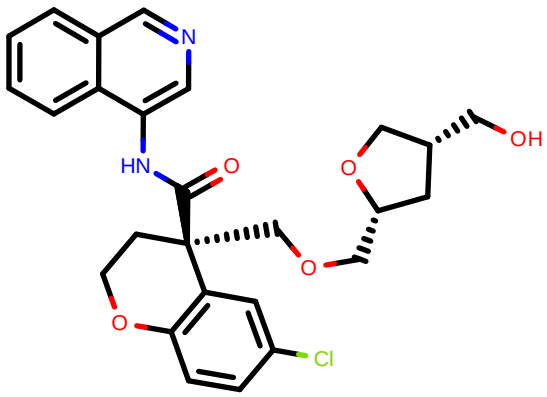
CID:	EN300-206646_2_1
SMILES:	CS(=O)(=O)c1cncc(n1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7159
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.35

EN300-332002_3_2



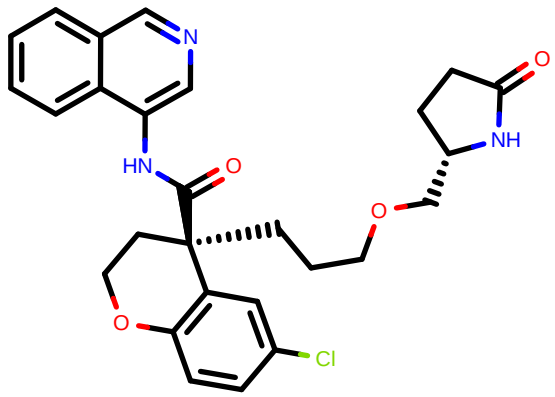
CID:	EN300-332002_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCc6n5c(=O)ccc6
RUN:	RUN10512
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.36

EN300-6494158_2_4



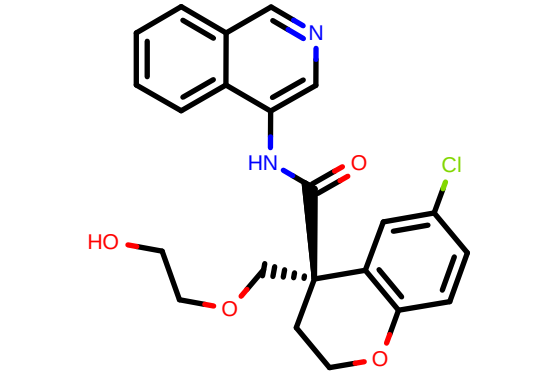
CID:	EN300-6494158_2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5C[C@H](CO5)CO
RUN:	RUN1821
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.33

EN300-264301_4_1



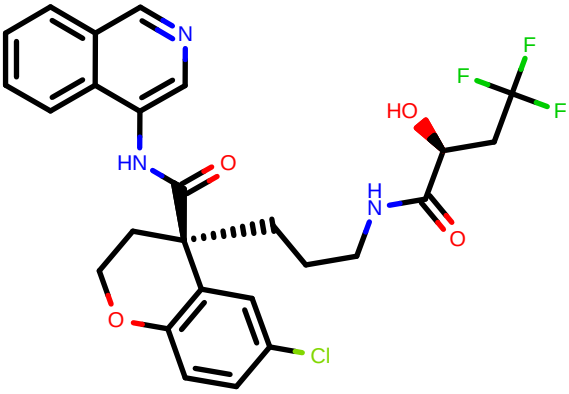
CID:	EN300-264301_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H]5CCC(=O)N5
RUN:	RUN1463
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.35

EN300-21258_2_1



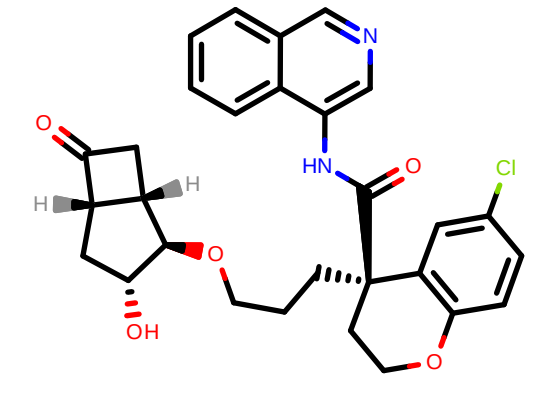
CID:	EN300-21258_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCO
RUN:	RUN783
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.18

EN300-1932013_4_2



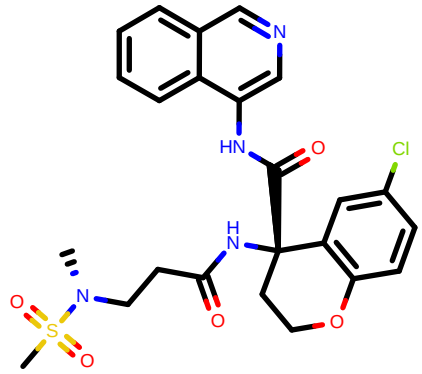
CID:	EN300-1932013_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H](CC(F)(F)F)O
RUN:	RUN10267
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.39

EN300-6481287_4_1



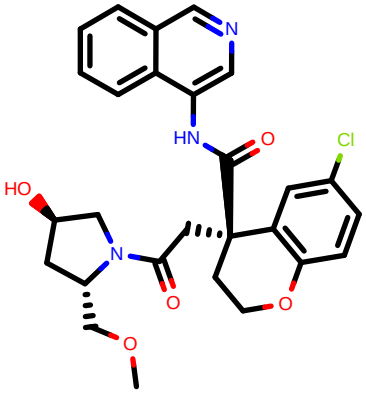
CID:	EN300-6481287_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@H]5[C@@H](C[C@H]6[C@@H]5CC6=O)O
RUN:	RUN2238
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.33

EN300-132523_1_1



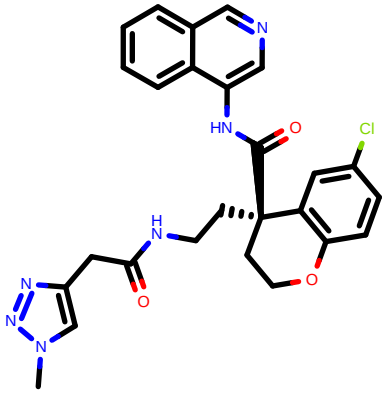
CID:	EN300-132523_1_1
SMILES:	CN(CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN625
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.34

EN300-252961_1_3



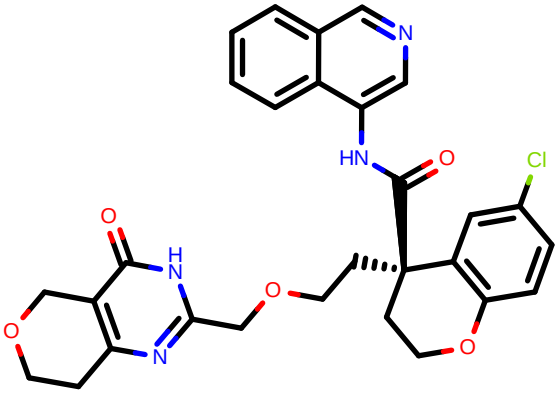
CID:	EN300-252961_1_3
SMILES:	COC[C@@H]1C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10818
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.36

EN300-1073264_3_1



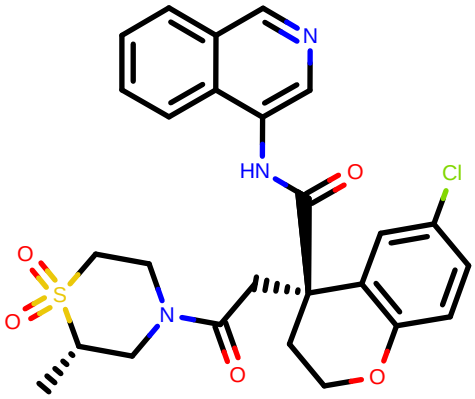
CID:	EN300-1073264_3_1
SMILES:	Cn1cc(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4859
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.30

EN300-343103_3_1



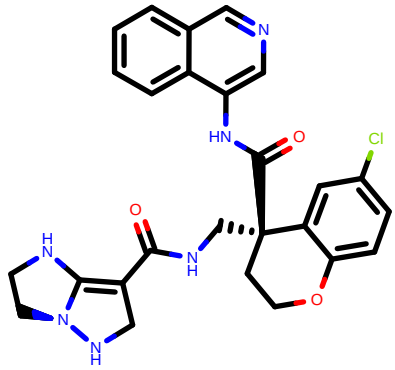
CID:	EN300-343103_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCc5[nH]c(=O)c6c(n5)CCOC6
RUN:	RUN1779
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.36

EN300-331704_1_1



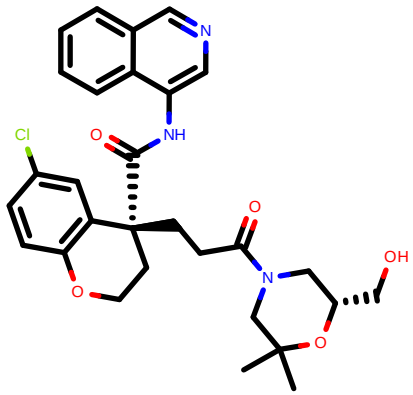
CID:	EN300-331704_1_1
SMILES:	C[C@H]1CN(CCS1(=O)=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3284
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.29

EN300-135238_2_1



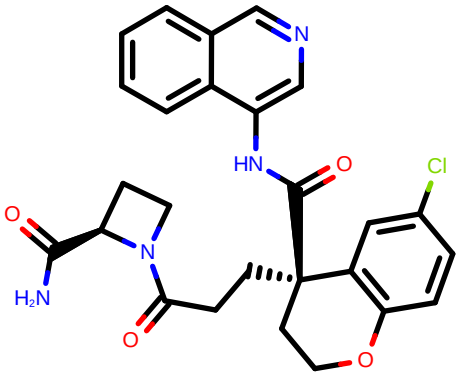
CID:	EN300-135238_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnn6c5[nH]cc6
RUN:	RUN7867
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.25

EN300-7412943_2_1



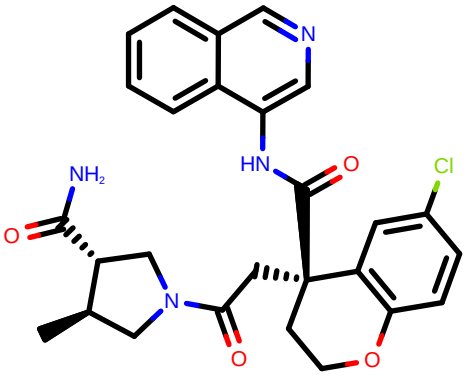
CID:	EN300-7412943_2_1
SMILES:	CC1(CN(C[C@@H](O1)CO)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN8941
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.40

EN300-862094_2_1



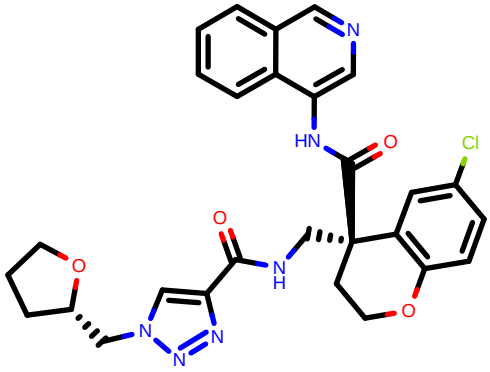
CID:	EN300-862094_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H]5C(=O)N
RUN:	RUN5443
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.27

EN300-244842_1_1



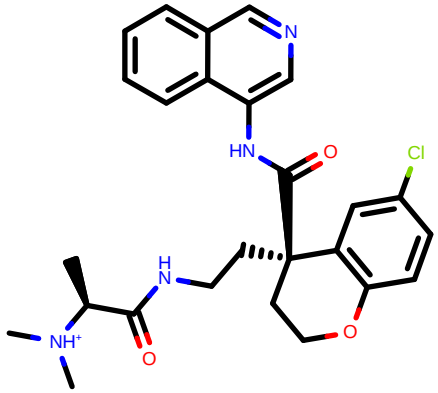
CID:	EN300-244842_1_1
SMILES:	C[C@@H]1CN(C[C@H]1C(=O)N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2594
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.30

EN300-368758_2_1



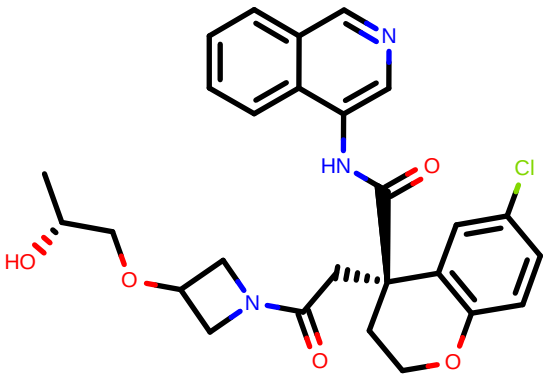
CID:	EN300-368758_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn(nn5)C[C@@H]6CCCO6
RUN:	RUN6516
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.30

EN300-306495_3_1



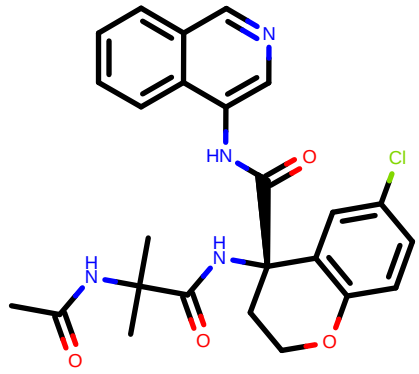
CID:	EN300-306495_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C)C
RUN:	RUN287
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.34

EN300-6498888_1_2



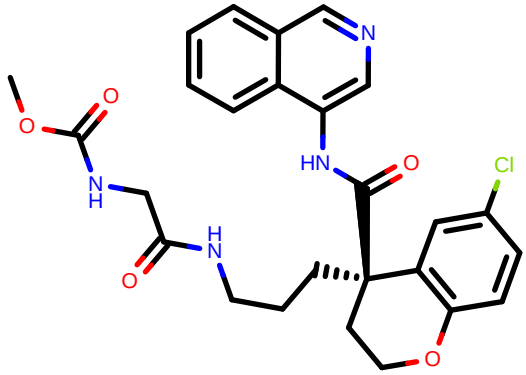
CID:	EN300-6498888_1_2
SMILES:	C[C@H](COC1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4611
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.32

EN300-65414_1_1



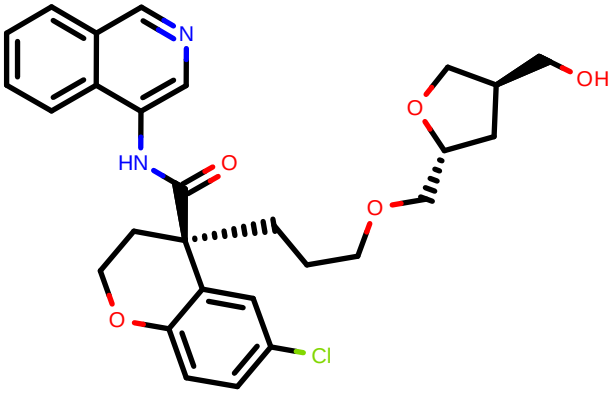
CID:	EN300-65414_1_1
SMILES:	CC(=O)NC(C)(C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5820
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.29

EN300-50009_4_1



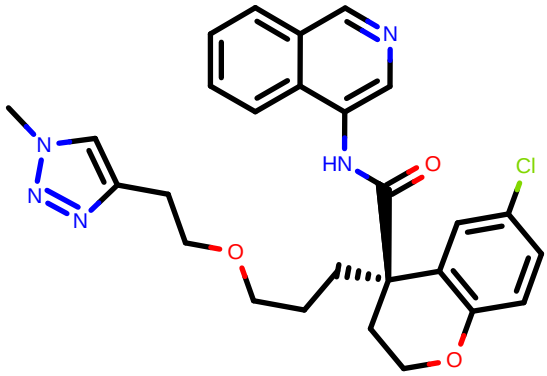
CID:	EN300-50009_4_1
SMILES:	COC(=O)NCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10691
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.25

EN300-6494158_4_2



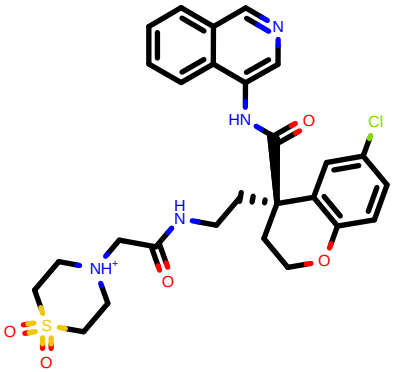
CID:	EN300-6494158_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5C[C@@H](CO5)CO
RUN:	RUN571
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.31

EN300-1600786_4_1



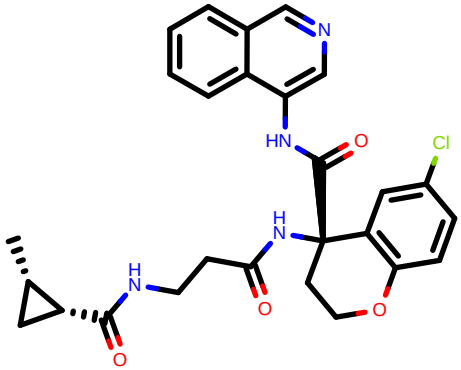
CID:	EN300-1600786_4_1
SMILES:	Cn1cc(nn1)CCOCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1910
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.36

EN300-39305_3_1



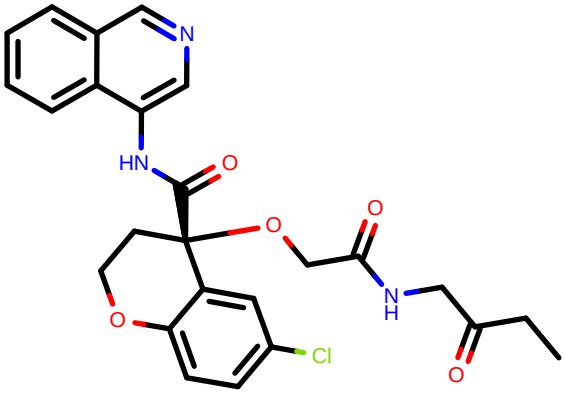
CID:	EN300-39305_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CN5CCS(=O)(=O)CC5
RUN:	RUN5139
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.37

EN300-36851_1_4



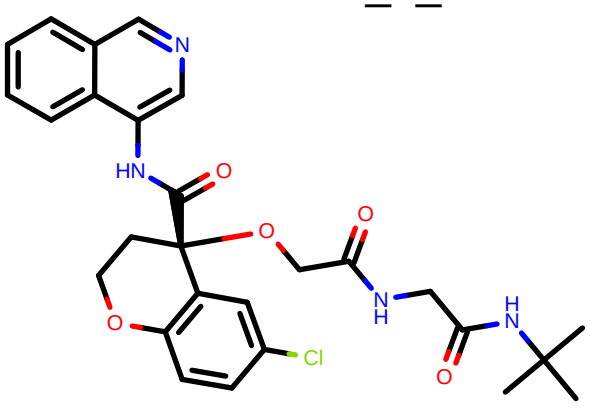
CID:	EN300-36851_1_4
SMILES:	C[C@H]1C[C@H]1C(=O)NCCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN837
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.37

EN300-132624_1_1



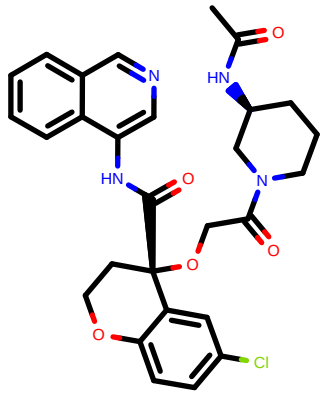
CID:	EN300-132624_1_1
SMILES:	CCC(=O)CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1735
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.29

EN300-48760_1_1



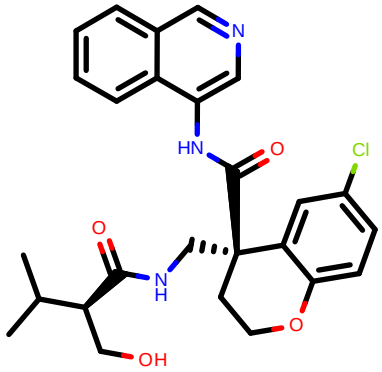
CID:	EN300-48760_1_1
SMILES:	CC(C)(C)NC(=O)CNC(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2023
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.34

EN300-48886_1_2



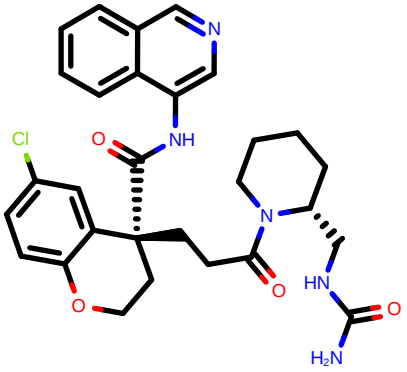
CID:	EN300-48886_1_2
SMILES:	CC(=O)N[C@H]1CCCN(C1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1416
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.34

EN300-153257_2_2



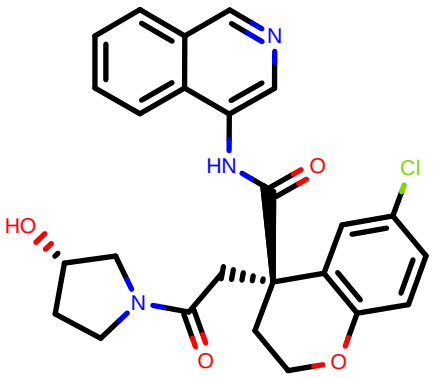
CID:	EN300-153257_2_2
SMILES:	CC(C)[C@H](CO)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3127
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.29

EN300-62166_2_1



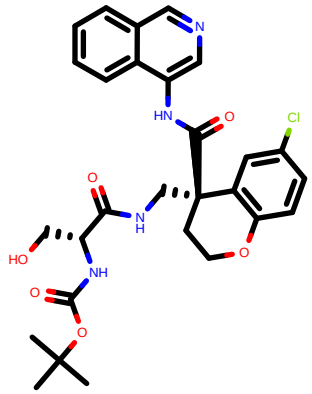
CID:	EN300-62166_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCC[C@@H]5CNC(=O)N
RUN:	RUN7373
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.35

EN300-295515_1_1



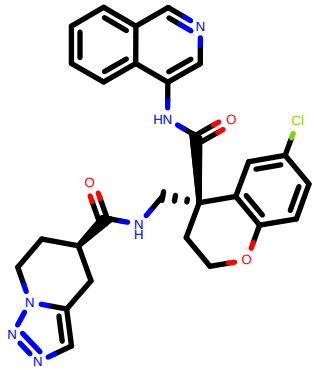
CID:	EN300-295515_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)O
RUN:	RUN5762
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.27

EN300-72109_2_2



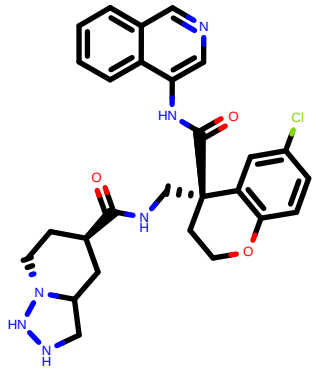
CID:	EN300-72109_2_2
SMILES:	CC(C)(C)OC(=O)N[C@H](CO)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2088
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.38

EN300-7430501_2_1



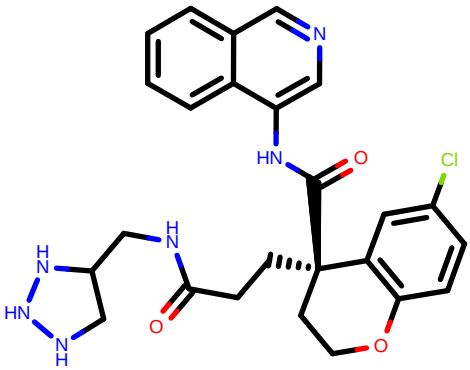
CID:	EN300-7430501_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCn6c(cnn6)C5
RUN:	RUN6608
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.27

EN300-7430501_2_1



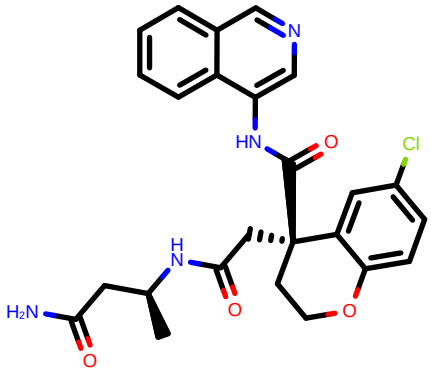
CID:	EN300-7430501_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCn6c(cnn6)C5
RUN:	RUN6612
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.34

EN300-98429_2_1



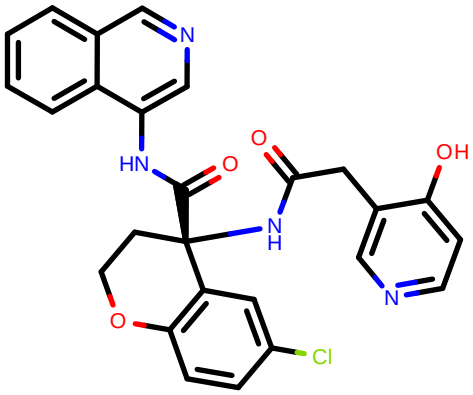
CID:	EN300-98429_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5c[nH]nn5
RUN:	RUN3133
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.31

EN300-84785_1_1



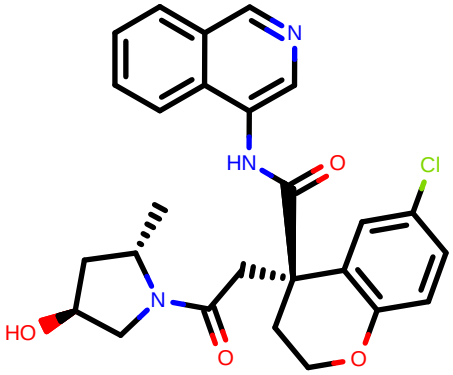
CID:	EN300-84785_1_1
SMILES:	C[C@@H](CC(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6757
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.24

EN300-205486_1_1



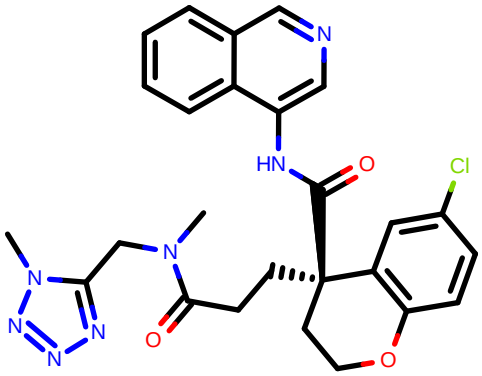
CID:	EN300-205486_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnccc5O
RUN:	RUN1724
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.35

EN300-173562_1_2



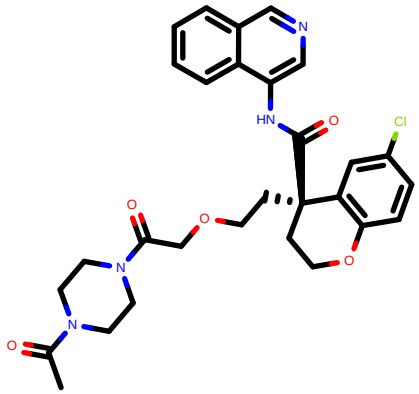
CID:	EN300-173562_1_2
SMILES:	C[C@H]1C[C@@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7684
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.30

EN300-148515_2_1



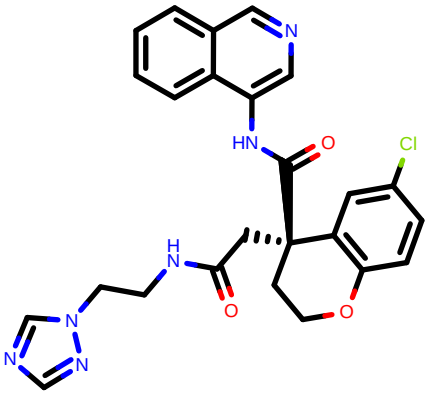
CID:	EN300-148515_2_1
SMILES:	Cn1c(nnn1)CN(C)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7029
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.30

EN300-1724771_3_1



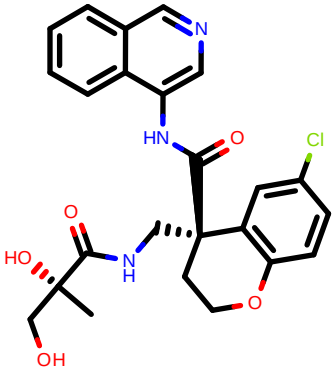
CID:	EN300-1724771_3_1
SMILES:	CC(=O)N1CCN(CC1)C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1595
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.32

EN300-69553_1_1



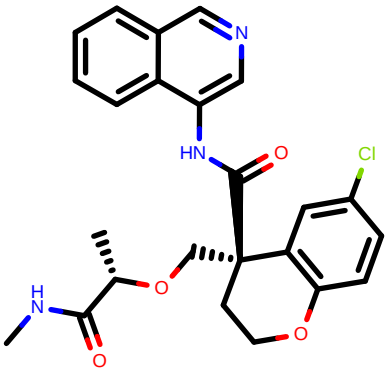
CID:	EN300-69553_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCn5cncn5
RUN:	RUN5007
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.27

EN300-89418_2_1



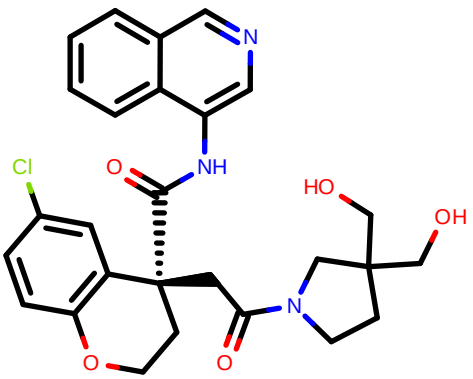
CID:	EN300-89418_2_1
SMILES:	C[C@@](CO)(C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4534
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.39

EN300-211482_2_1



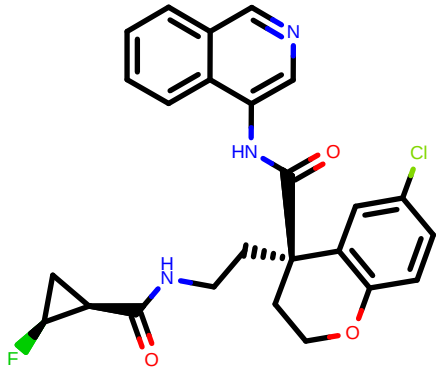
CID:	EN300-211482_2_1
SMILES:	C[C@@H](C(=O)NC)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1326
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.22

EN300-306144_1_1



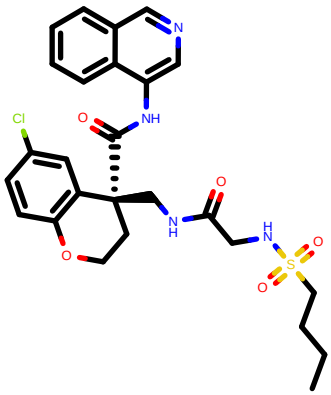
CID:	EN300-306144_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(C5)(CO)CO
RUN:	RUN2753
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.27

EN300-97300_3_1



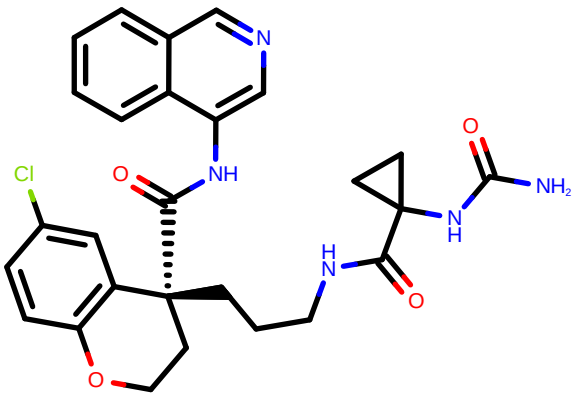
CID:	EN300-97300_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5C[C@@H]5F
RUN:	RUN3831
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.19

EN300-117756_2_1



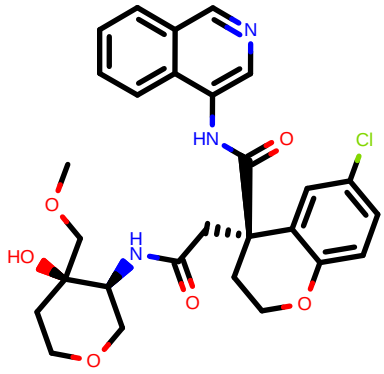
CID:	EN300-117756_2_1
SMILES:	CCCCS(=O)(=O)NCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5329
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.37

EN300-123614_4_1



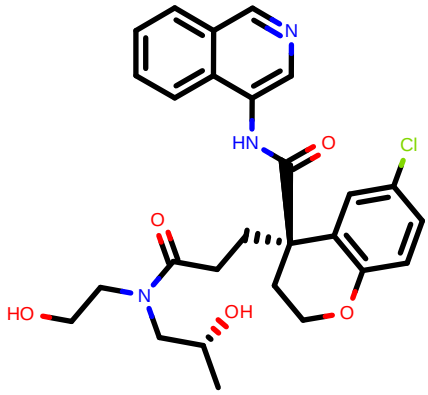
CID:	EN300-123614_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C5(CC5)NC(=O)N
RUN:	RUN10607
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.36

EN300-1178014_1_2



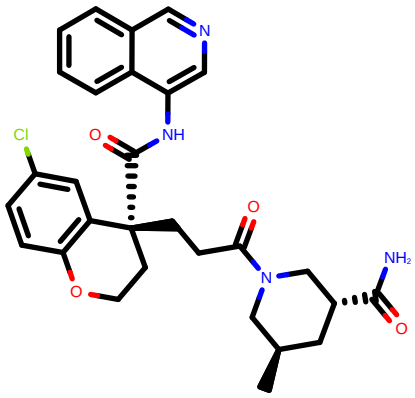
CID:	EN300-1178014_1_2
SMILES:	COC[C@]1(CCOC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10560
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.54

EN300-214038_2_2



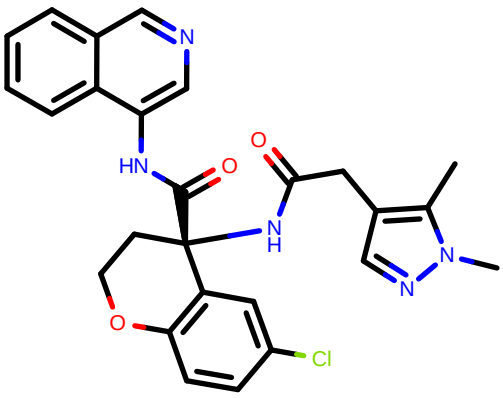
CID:	EN300-214038_2_2
SMILES:	C[C@H](CN(CCO)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN9103
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.33

EN300-1724086_2_3



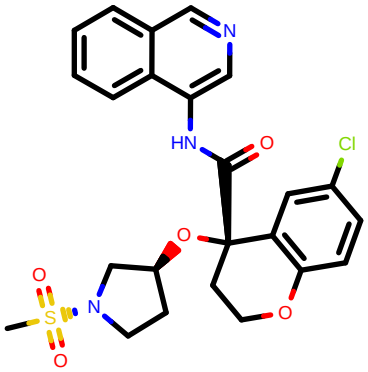
CID:	EN300-1724086_2_3
SMILES:	C[C@@H]1C[C@H](CN(C1)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN8373
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.39

EN300-219437_1_1



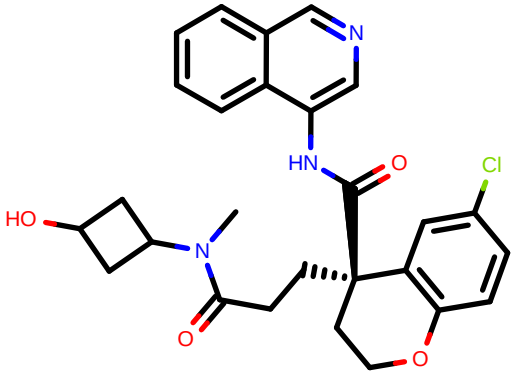
CID:	EN300-219437_1_1
SMILES:	Cc1c(cnn1C)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1852
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.32

EN300-301690_1_1



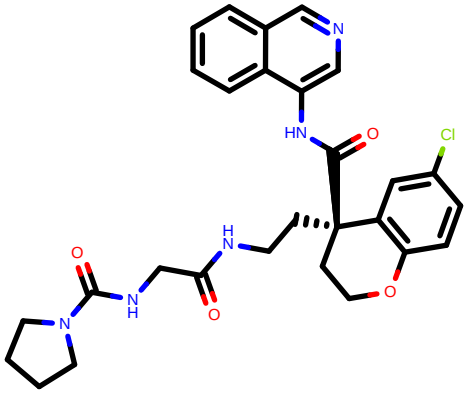
CID:	EN300-301690_1_1
SMILES:	CS(=O)(=O)N1CC[C@@H](C1)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2634
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.34

EN300-97697_2_1



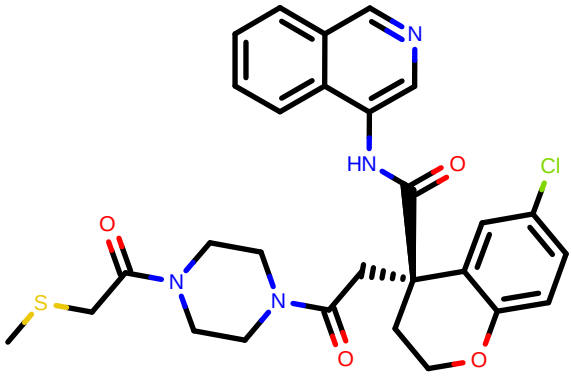
CID:	EN300-97697_2_1
SMILES:	CN(C1CC(C1)O)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3501
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.26

EN300-383906_3_1



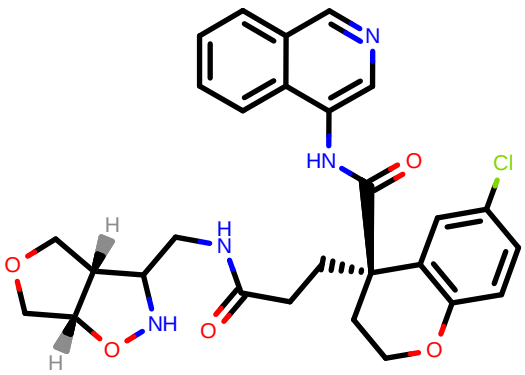
CID:	EN300-383906_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CNC(=O)N5CCCC5
RUN:	RUN6385
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.33

EN300-7443667_1_1



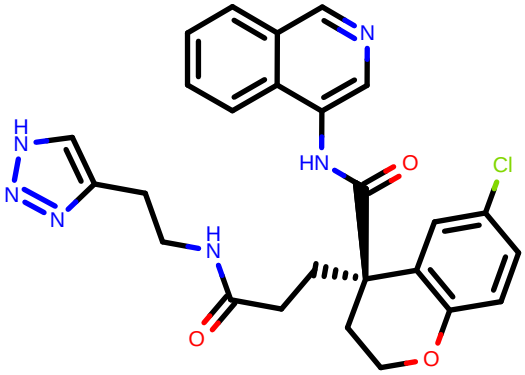
CID:	EN300-7443667_1_1
SMILES:	CSCC(=O)N1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9724
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.38

EN300-7435581_2_1



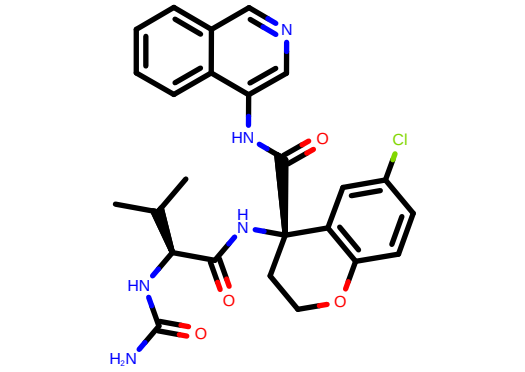
CID:	EN300-7435581_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5=NO[C@H]6[C@@H]5COC6
RUN:	RUN7861
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.31

EN300-1178209_2_1



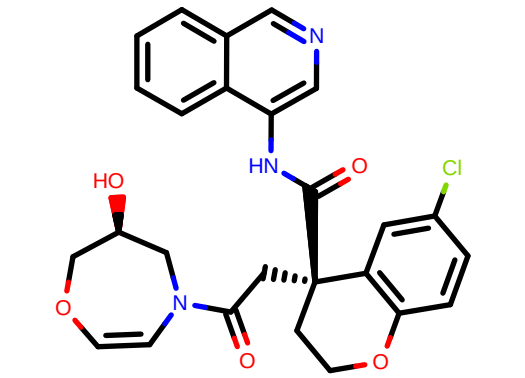
CID:	EN300-1178209_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCc5c[nH]nn5
RUN:	RUN5020
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.28

EN300-87528_1_1



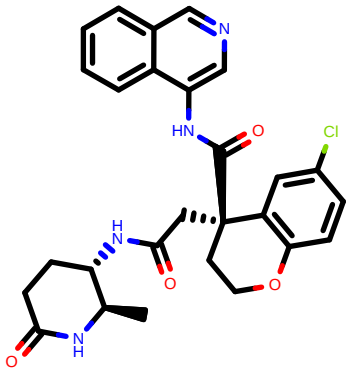
CID:	EN300-87528_1_1
SMILES:	CC(C)[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN6603
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.33

EN300-233951_1_2



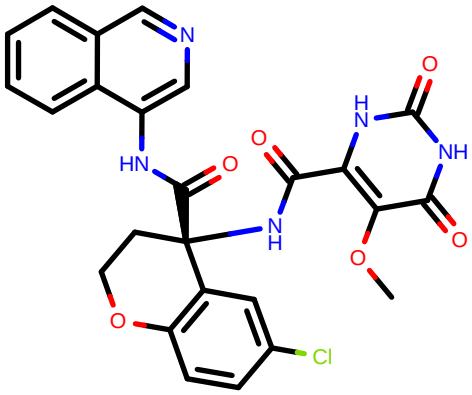
CID:	EN300-233951_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H](C5)O
RUN:	RUN1969
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.35

EN300-199449_1_3



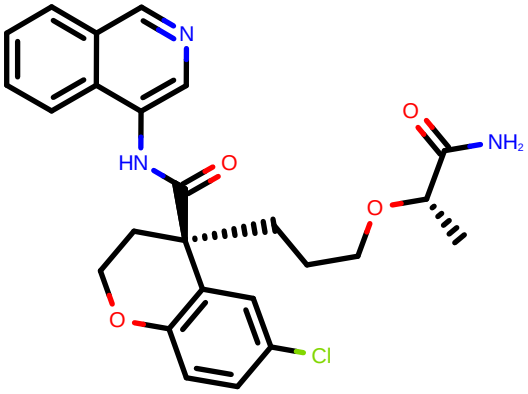
CID:	EN300-199449_1_3
SMILES:	C[C@@H]1[C@H](CCC(=O)N1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8324
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.27

EN300-160498_1_1



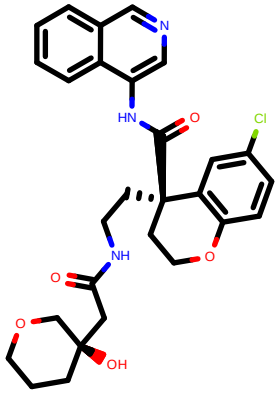
CID:	EN300-160498_1_1
SMILES:	COc1c([nH]c(=O)[nH]c1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8446
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.27

EN300-17381_4_1



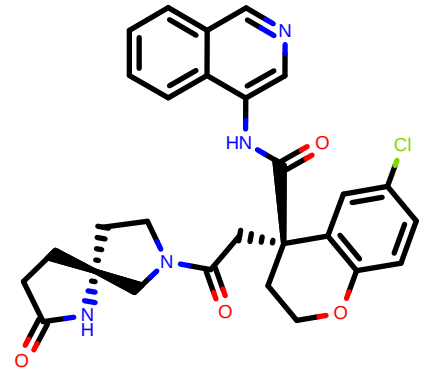
CID:	EN300-17381_4_1
SMILES:	C[C@@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1087
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.34

EN300-1071940_3_1



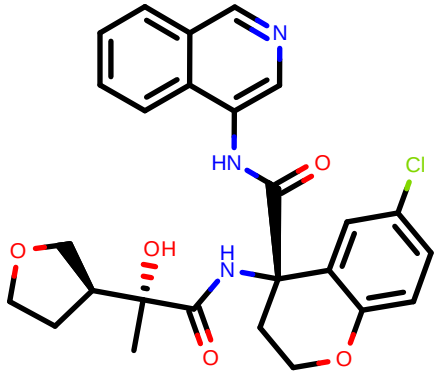
CID:	EN300-1071940_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C[C@@]5(CCCOC5)O
RUN:	RUN9177
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.25

EN300-1718424_1_1



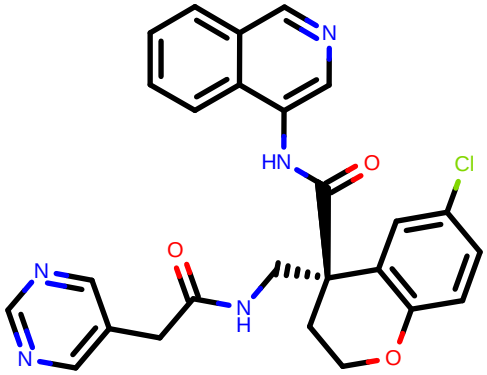
CID:	EN300-1718424_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC6(C5)CCC(=O)N6
RUN:	RUN6601
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.33

EN300-217494_1_3



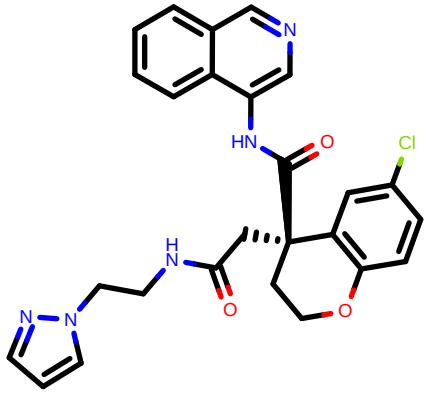
CID:	EN300-217494_1_3
SMILES:	C[C@@]([C@H]1CCOC1)(C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2092
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.25

EN300-185751_2_1



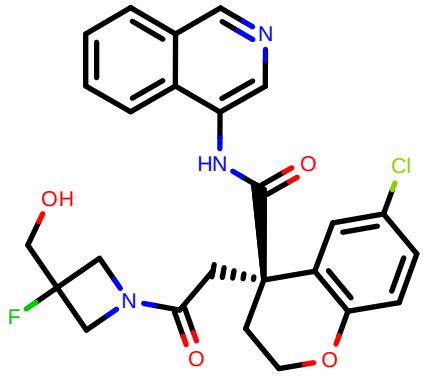
CID:	EN300-185751_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cc5cncnc5
RUN:	RUN6077
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.25

EN300-50194_1_1



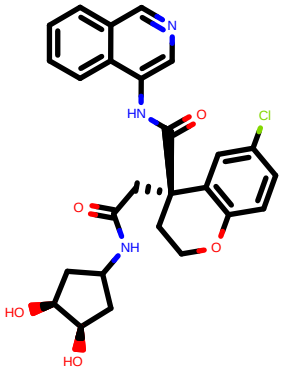
CID:	EN300-50194_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCn5cccn5
RUN:	RUN6725
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.28

EN300-204507_1_1



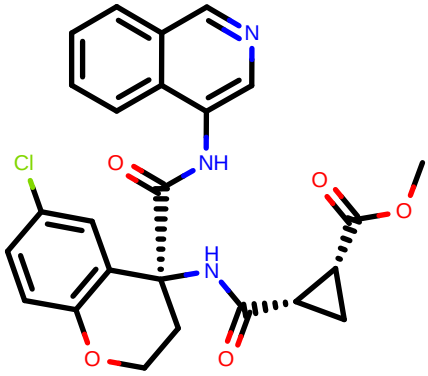
CID:	EN300-204507_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(CO)F
RUN:	RUN3903
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.33

EN300-392640_1_1



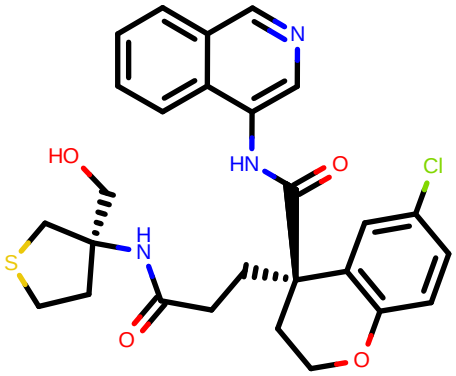
CID:	EN300-392640_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]([C@H](C5)O)O
RUN:	RUN9374
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.36

EN300-66764_1_1



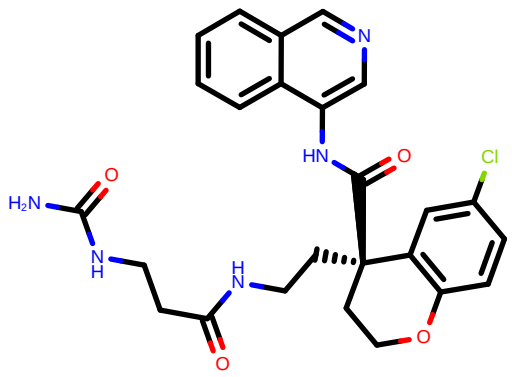
CID:	EN300-66764_1_1
SMILES:	COC(=O)[C@@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3753
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.28

EN300-1260794_2_2



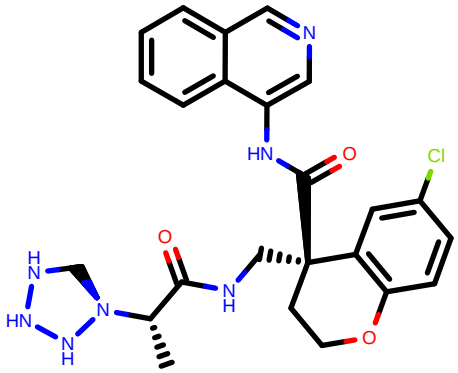
CID:	EN300-1260794_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@]5(CCSC5)CO
RUN:	RUN3669
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.38

EN300-10729_3_1



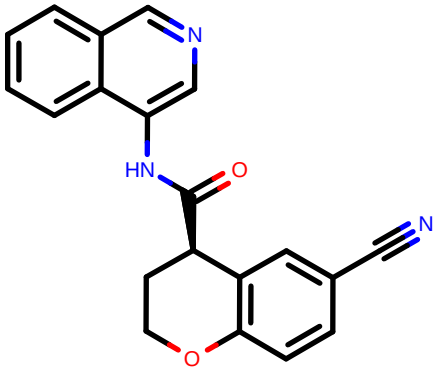
CID:	EN300-10729_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCNC(=O)N
RUN:	RUN6162
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.33

EN300-191915_2_1



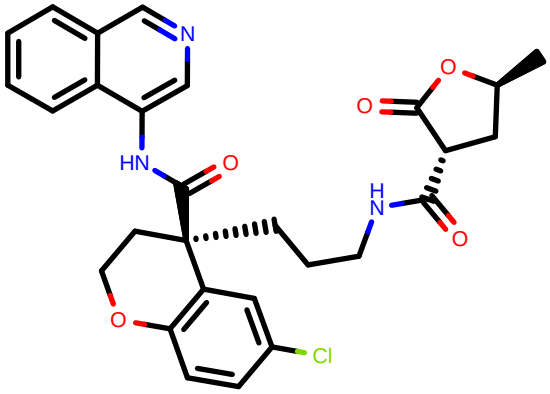
CID:	EN300-191915_2_1
SMILES:	C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5cnnn5
RUN:	RUN2787
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.29

DAR-DIA-6a508060-3_1



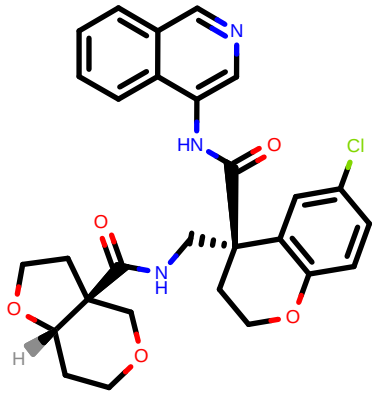
CID:	DAR-DIA-6a508060-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C#N
RUN:	RUN26
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.06

EN300-7444533_4_2



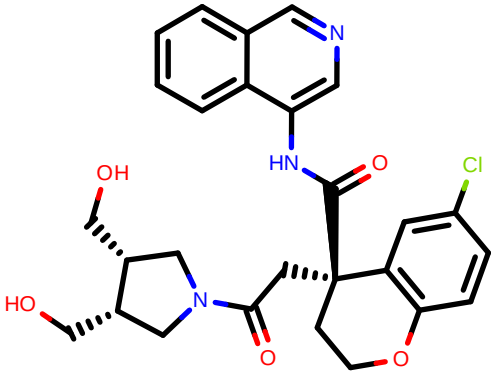
CID:	EN300-7444533_4_2
SMILES:	C[C@H]1C[C@@H](C(=O)O1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8721
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.36

EN300-341337_2_4



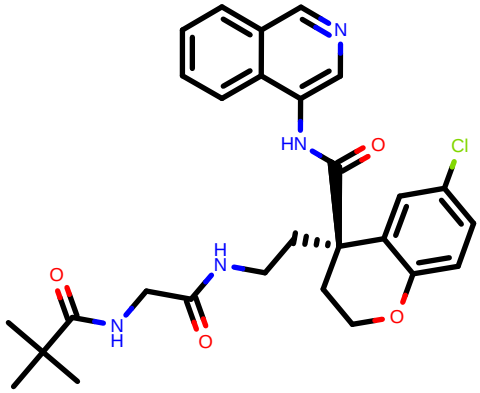
CID:	EN300-341337_2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]56CCO[C@H]5CCOC6
RUN:	RUN5421
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.39

EN300-333677_1_1



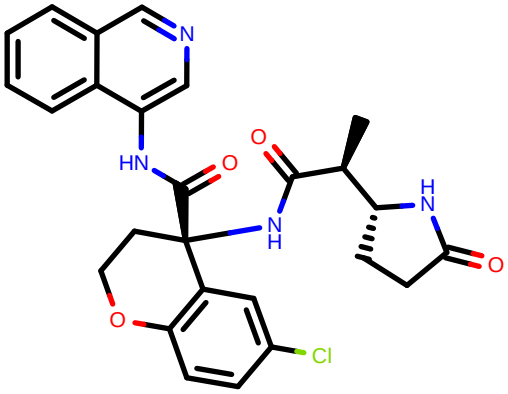
CID:	EN300-333677_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@@H](C5)CO)CO
RUN:	RUN550
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.35

EN300-12247_3_1



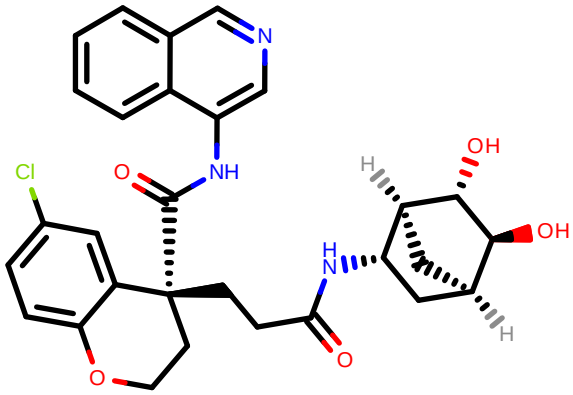
CID:	EN300-12247_3_1
SMILES:	CC(C)(C)C(=O)NCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9538
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.26

EN300-249421_1_3



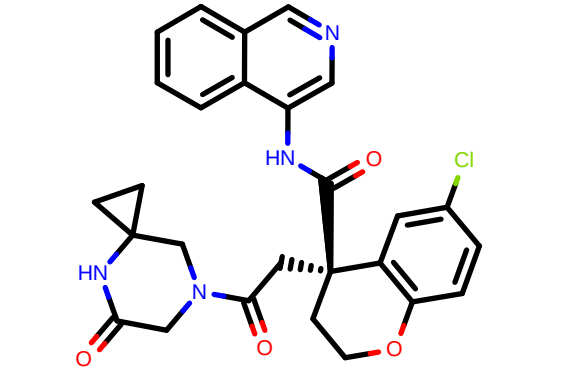
CID:	EN300-249421_1_3
SMILES:	C[C@@H]([C@H]1CCC(=O)N1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2846
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.33

EN300-6763291_2_6



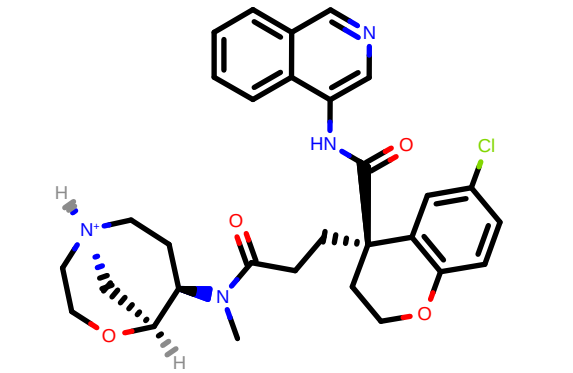
CID:	EN300-6763291_2_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CC6CC5[C@@H]([C@H]6O)O
RUN:	RUN9905
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.31

EN300-6472573_1_1



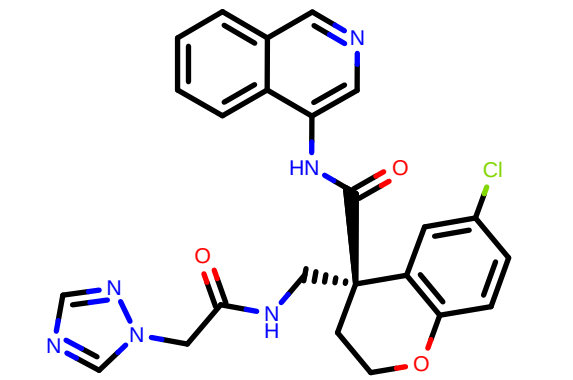
CID:	EN300-6472573_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(=O)NC6(C5)CC6
RUN:	RUN5994
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.32

EN300-159953_2_1



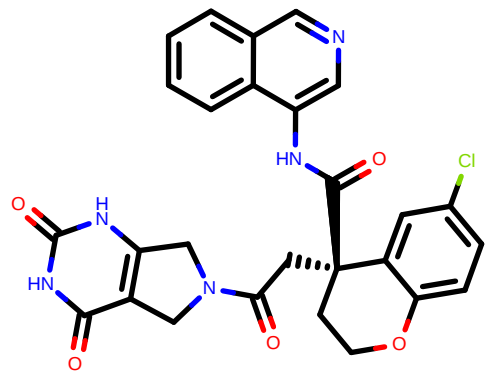
CID:	EN300-159953_2_1
SMILES:	CN([C@@H]1CCN2CCOC1C2)C(=O)CC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8269
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.42

EN300-06654_2_1



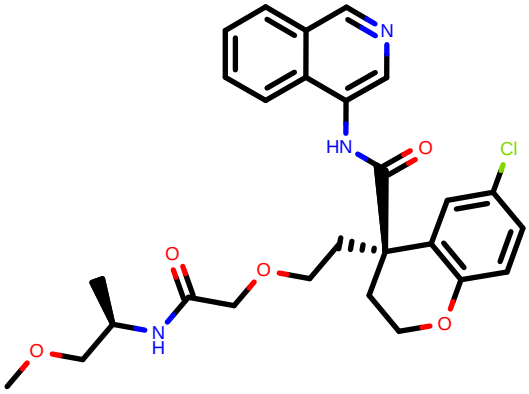
CID:	EN300-06654_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cncn5
RUN:	RUN4830
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.32

EN300-6746727_1_1



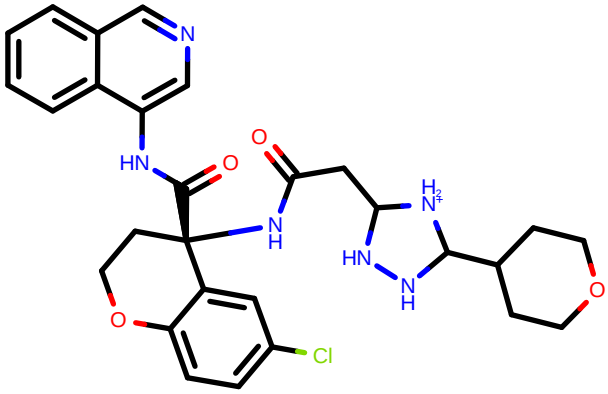
CID:	EN300-6746727_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cc6c([nH]c(=O)[nH]c6=O)C5
RUN:	RUN11062
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.28

EN300-02067_3_2



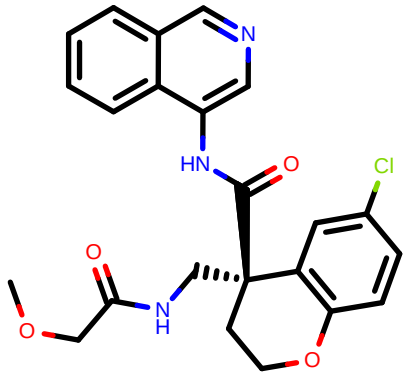
CID:	EN300-02067_3_2
SMILES:	C[C@H](COC)NC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN711
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.32

EN300-385132_1_1



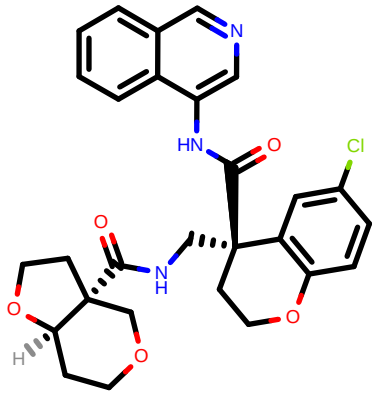
CID:	EN300-385132_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5[nH]c(nn5)C6CCOCC6
RUN:	RUN5816
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.30

EN300-20233_2_1



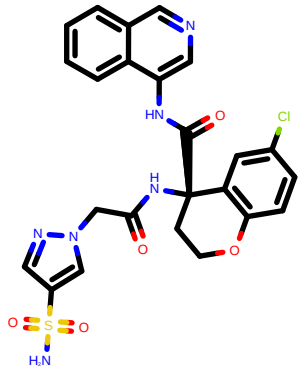
CID:	EN300-20233_2_1
SMILES:	COCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3894
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.20

EN300-341337_2_1



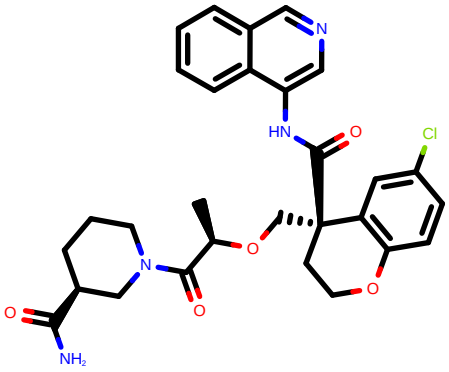
CID:	EN300-341337_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]56CCO[C@@H]5CCOC6
RUN:	RUN5429
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.38

EN300-60514_1_1



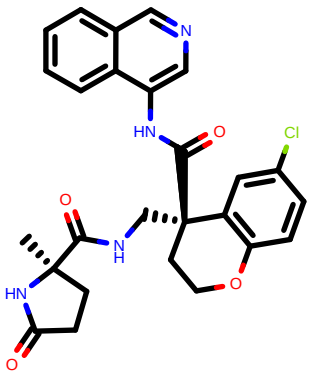
CID:	EN300-60514_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(cn5)S(=O)(=O)N
RUN:	RUN7846
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.40

EN300-28177_2_2



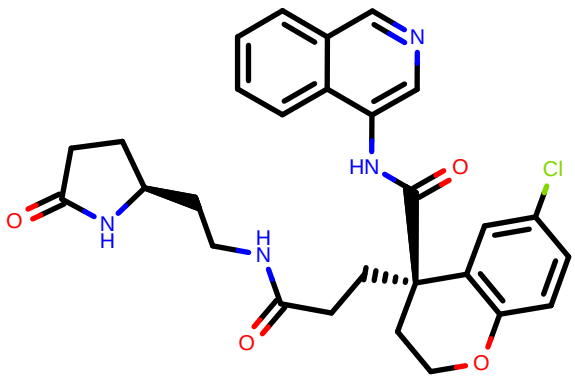
CID:	EN300-28177_2_2
SMILES:	C[C@H](C(=O)N1CCC[C@@H](C1)C(=O)N)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1302
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.41

EN300-177118_2_1



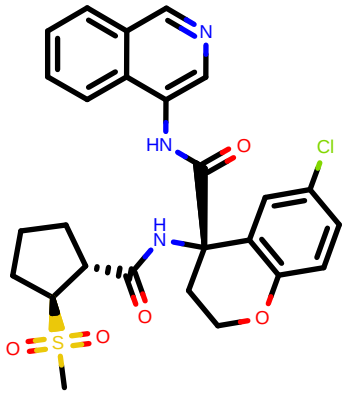
CID:	EN300-177118_2_1
SMILES:	C[C@@]1(CCC(=O)N1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4814
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.24

EN300-205779_2_1



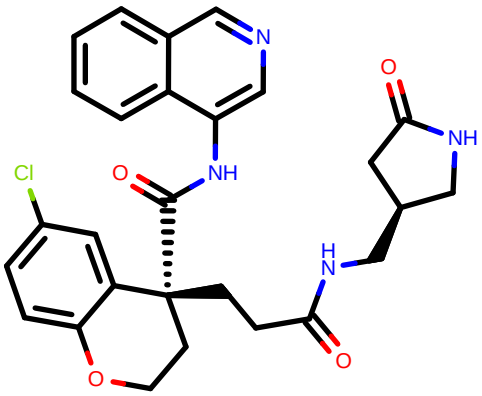
CID:	EN300-205779_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC[C@@H]5CCC(=O)N5
RUN:	RUN11329
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.31

EN300-1387145_1_2



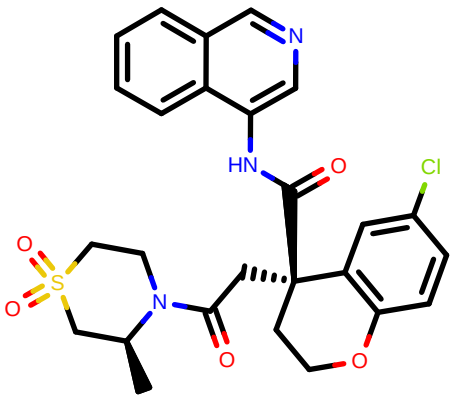
CID:	EN300-1387145_1_2
SMILES:	CS(=O)(=O)[C@H]1CCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4393
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.80

EN300-238405_2_2



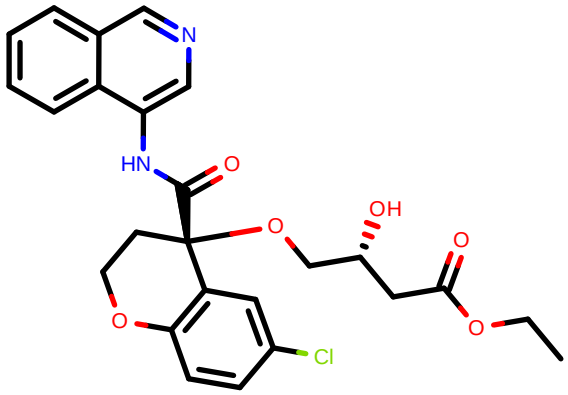
CID:	EN300-238405_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@H]5CC(=O)NC5
RUN:	RUN4640
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.26

EN300-171215_1_2



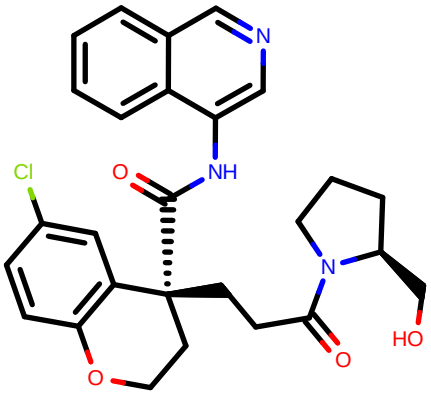
CID:	EN300-171215_1_2
SMILES:	C[C@H]1CS(=O)(=O)CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4103
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.45

EN300-82539_1_2



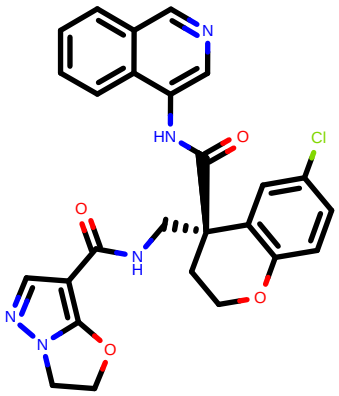
CID:	EN300-82539_1_2
SMILES:	CCOC(=O)C[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN952
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.38

EN300-70033_2_1



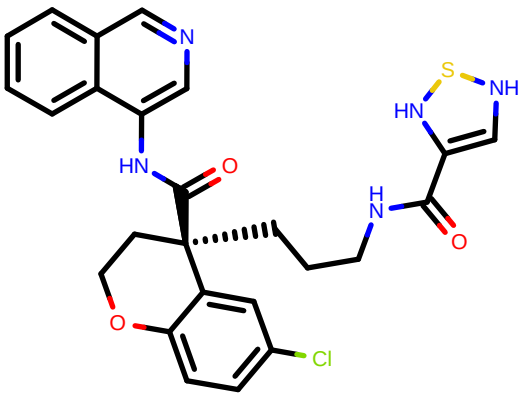
CID:	EN300-70033_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@H]5CO
RUN:	RUN1882
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.27

EN300-303519_2_1



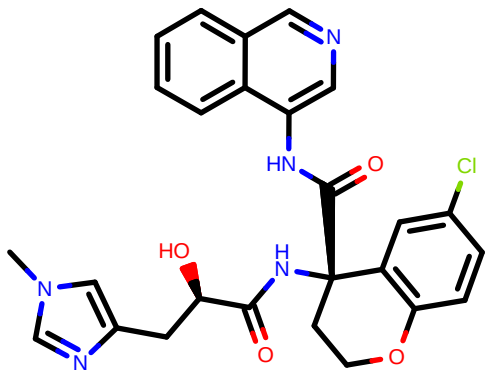
CID:	EN300-303519_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnn6c5OCC6
RUN:	RUN6752
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.23

EN300-42270_4_1



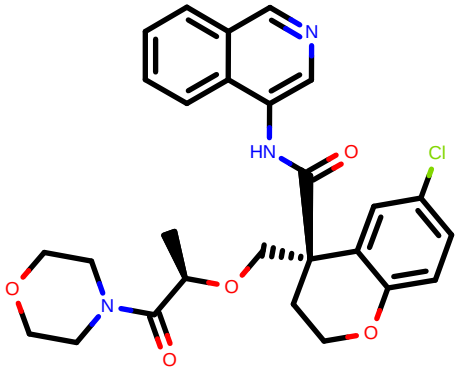
CID:	EN300-42270_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cnsn5
RUN:	RUN9543
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.24

EN300-1725538_1_2



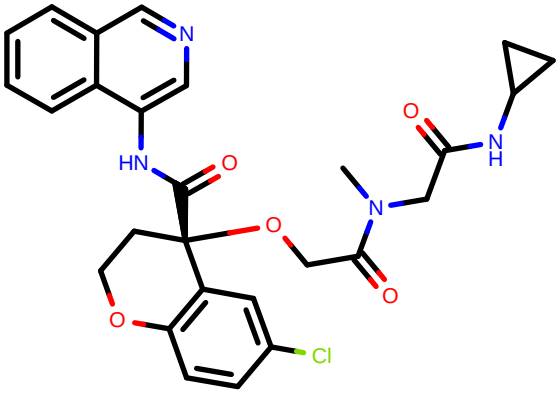
CID:	EN300-1725538_1_2
SMILES:	Cn1cc(nc1)C[C@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4477
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.30

EN300-05754_2_2



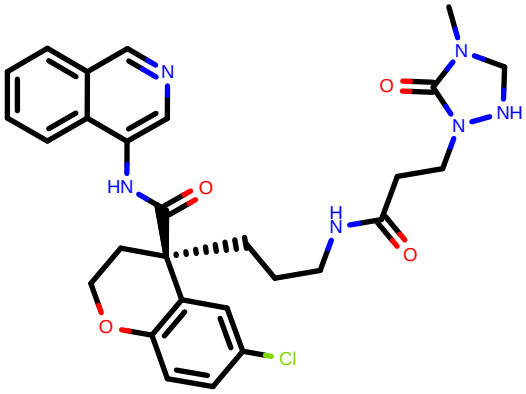
CID:	EN300-05754_2_2
SMILES:	C[C@H](C(=O)N1CCOCC1)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1757
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.34

EN300-13668_1_1



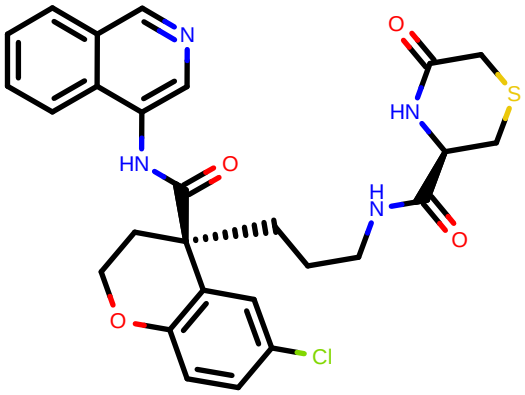
CID:	EN300-13668_1_1
SMILES:	CN(CC(=O)NC1CC1)C(=O)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2352
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.35

EN300-223491_4_1



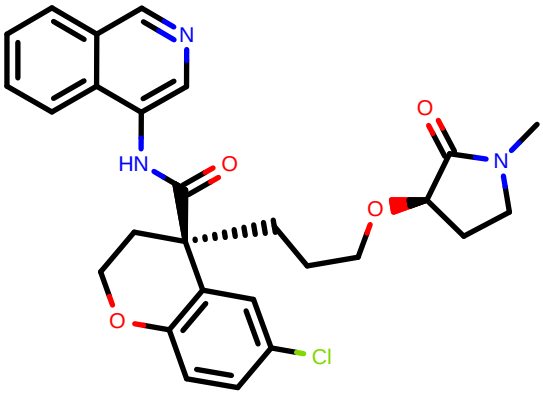
CID:	EN300-223491_4_1
SMILES:	Cn1cnn(c1=O)CCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10371
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.42

EN300-657320_4_1



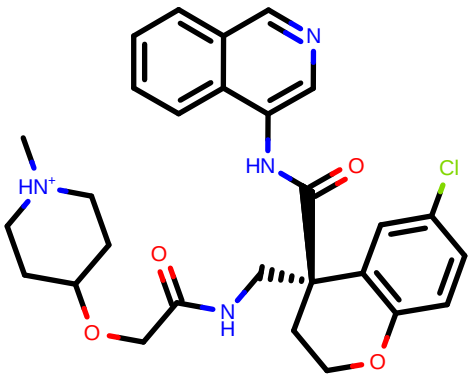
CID:	EN300-657320_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CSCC(=O)N5
RUN:	RUN9909
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.36

EN300-98648_4_2



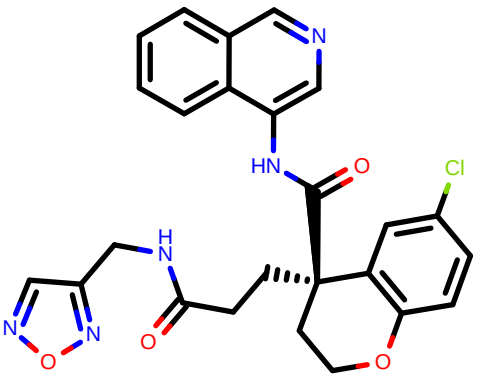
CID:	EN300-98648_4_2
SMILES:	CN1CC[C@H](C1=O)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1678
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.27

EN300-237224_2_1



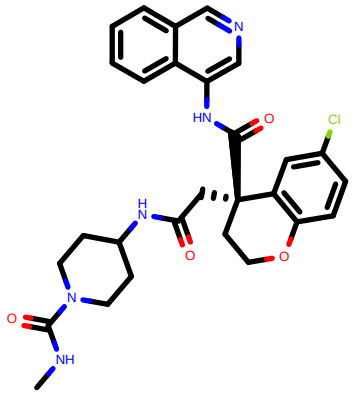
CID:	EN300-237224_2_1
SMILES:	CN1CCC(CC1)OCC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2919
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.29

EN300-1068239_2_1



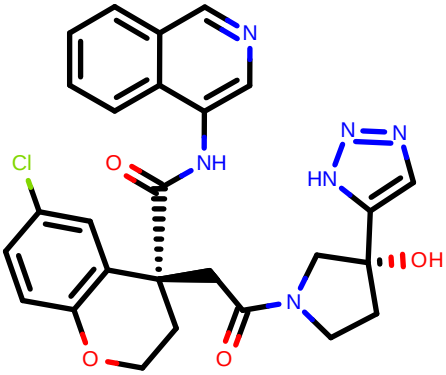
CID:	EN300-1068239_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cnon5
RUN:	RUN3988
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.27

EN300-6764450_1_1



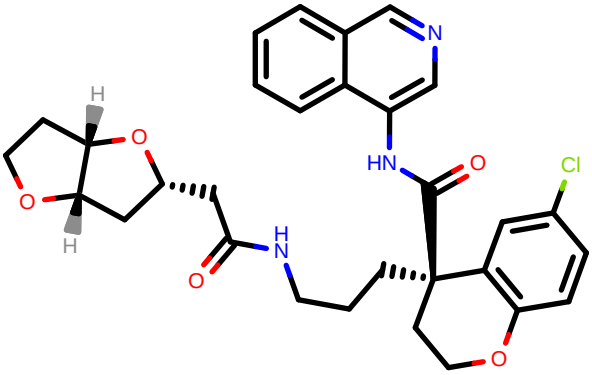
CID:	EN300-6764450_1_1
SMILES:	CNC(=O)N1CCC(CC1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10848
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.26

EN300-221122_1_1



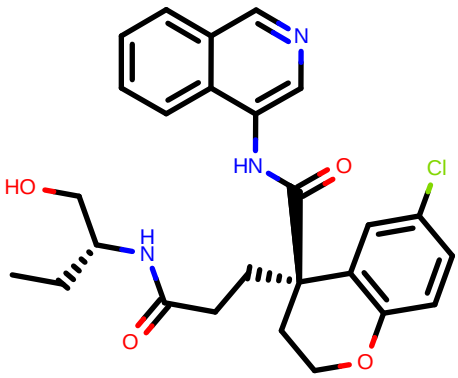
CID:	EN300-221122_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(c6cnn[nH]6)O
RUN:	RUN10408
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.44

EN300-7355519_4_3



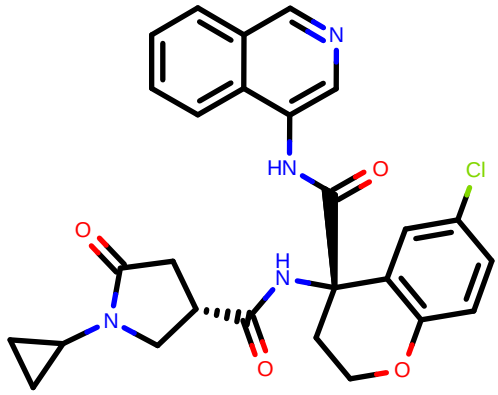
CID:	EN300-7355519_4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C[C@@H]5C[C@H]6[C@@H](O5)CCO6
RUN:	RUN11147
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.45

EN300-307658_2_1



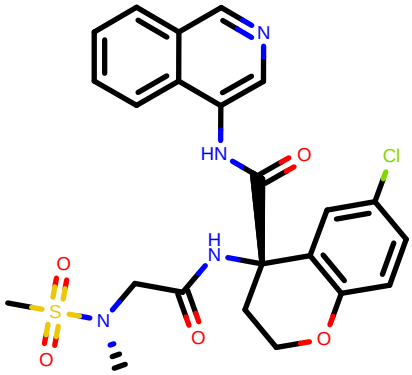
CID:	EN300-307658_2_1
SMILES:	C=C[C@H](CO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4960
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.27

EN300-12440_1_2



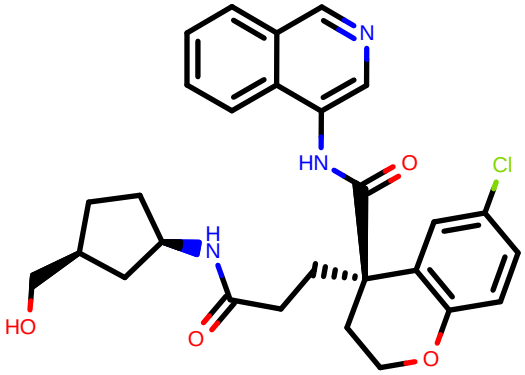
CID:	EN300-12440_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N(C5)C6CC6
RUN:	RUN7326
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.32

EN300-35642_1_1



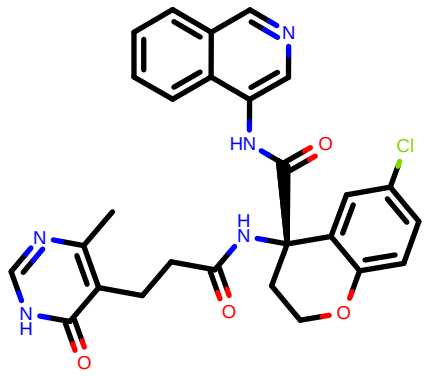
CID:	EN300-35642_1_1
SMILES:	CN(CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN1533
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.43

EN300-93474_2_1



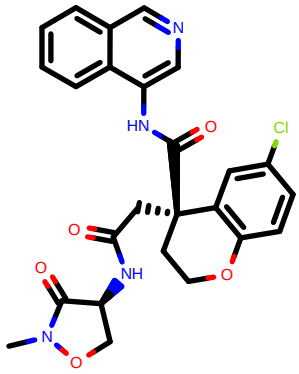
CID:	EN300-93474_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5C[C@H](C=C5)CO
RUN:	RUN2271
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.24

EN300-33553_1_1



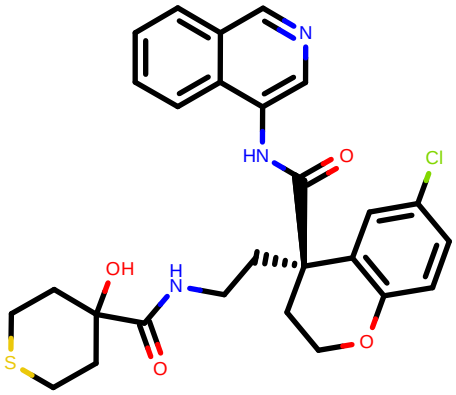
CID:	EN300-33553_1_1
SMILES:	Cc1c(c(=O)[nH]cn1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN362
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.26

EN300-7543383_1_2



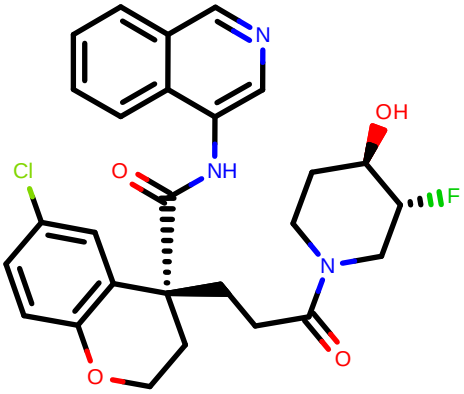
CID:	EN300-7543383_1_2
SMILES:	CN1C(=O)[C@H](CO1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10826
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.21

EN300-122340_3_1



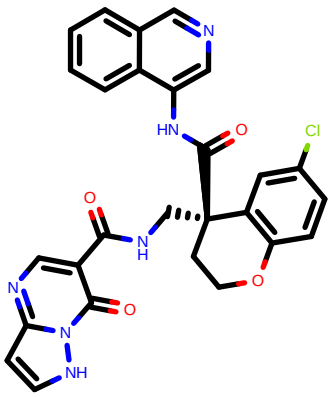
CID:	EN300-122340_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5(CCSCC5)O
RUN:	RUN5043
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.48

EN300-741926_2_2



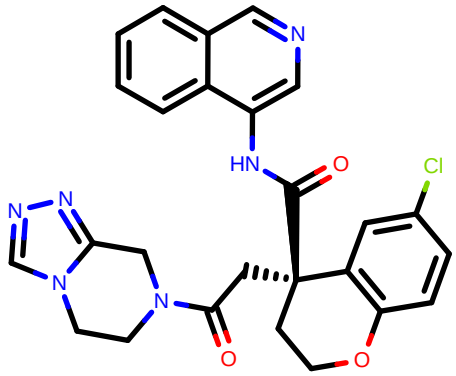
CID:	EN300-741926_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@H]([C@@H](C5)F)O
RUN:	RUN8045
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.26

EN300-220228_2_1



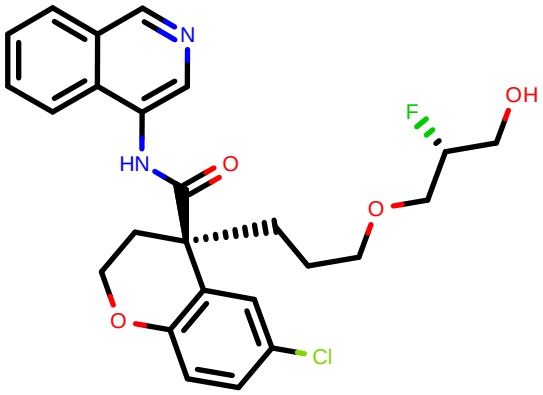
CID:	EN300-220228_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnc6ccnn6c5O
RUN:	RUN8119
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.33

EN300-71125_1_1



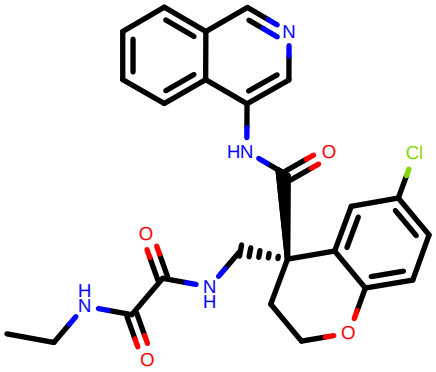
CID:	EN300-71125_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCn6cnnc6C5
RUN:	RUN2563
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.26

EN300-1600517_4_1



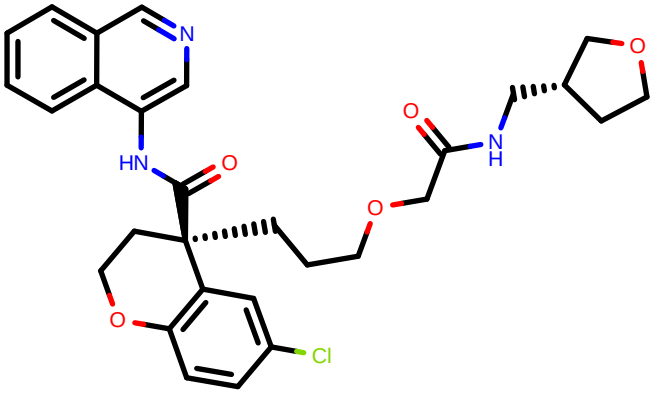
CID:	EN300-1600517_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H](CO)F
RUN:	RUN706
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.40

EN300-1262608_2_1



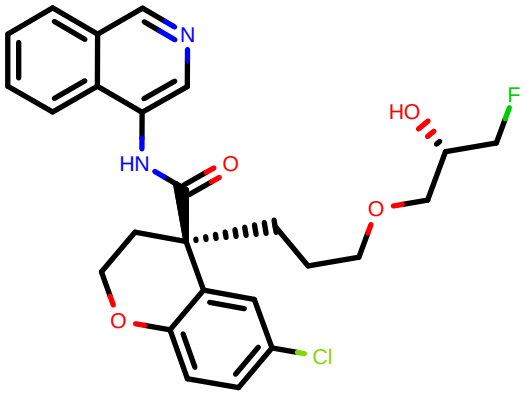
CID:	EN300-1262608_2_1
SMILES:	CCNC(=O)C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6280
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.26

EN300-46832_4_2



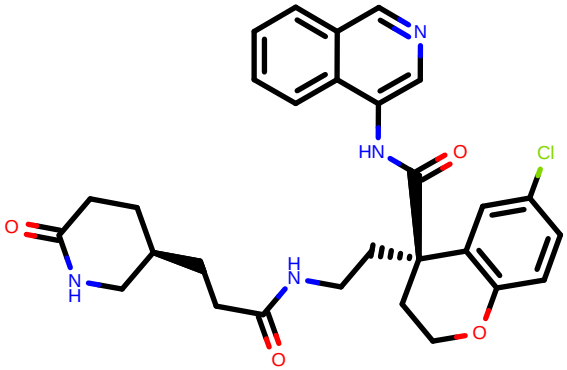
CID:	EN300-46832_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)NC[C@H]5CCOC5
RUN:	RUN1870
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.34

EN300-1968342_4_1



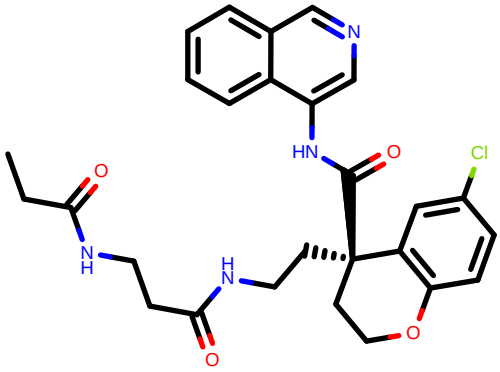
CID:	EN300-1968342_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H](CF)O
RUN:	RUN412
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.40

EN300-1215738_3_1



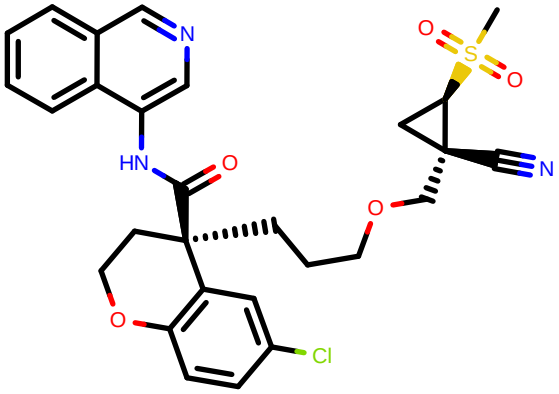
CID:	EN300-1215738_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[C@@H]5CCC(=O)NC5
RUN:	RUN9486
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.41

EN300-31186_3_1



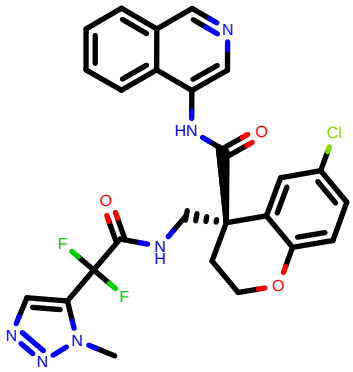
CID:	EN300-31186_3_1
SMILES:	CCC(=O)NCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10354
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.31

EN300-633533_4_1



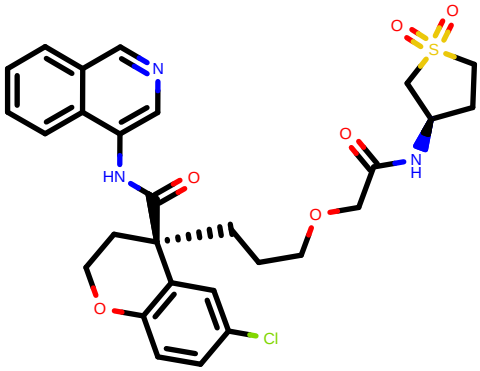
CID:	EN300-633533_4_1
SMILES:	CS(=O)(=O)[C@@H]1C[C@]1(COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)C#N
RUN:	RUN1383
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.40

EN300-1726073_2_1



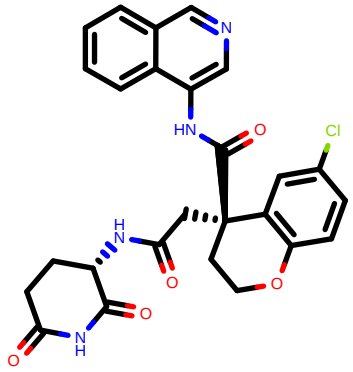
CID:	EN300-1726073_2_1
SMILES:	Cn1c(cnn1)C(C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)(F)F
RUN:	RUN5921
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.28

EN300-05512_4_1



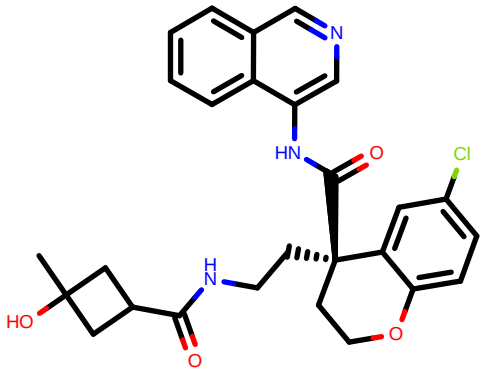
CID:	EN300-05512_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)N[C@@H]5CCS(=O)(=O)C5
RUN:	RUN2174
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.45

EN300-113633_1_2



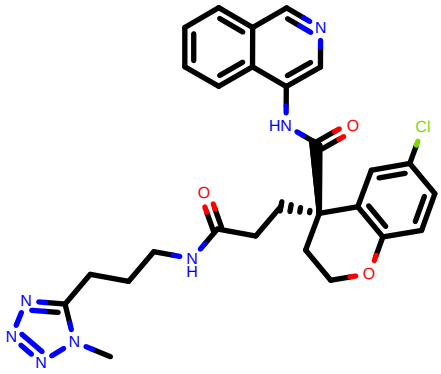
CID:	EN300-113633_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCC(=O)NC5=O
RUN:	RUN9828
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.28

EN300-247343_3_1



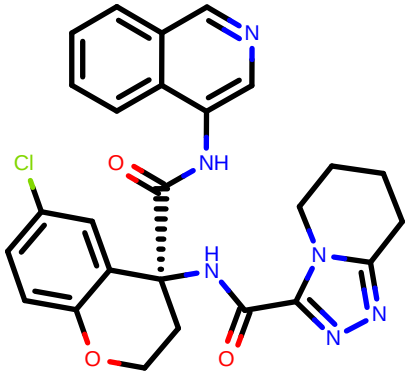
CID:	EN300-247343_3_1
SMILES:	CC1(CC(C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN8140
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.28

EN300-370182_2_1



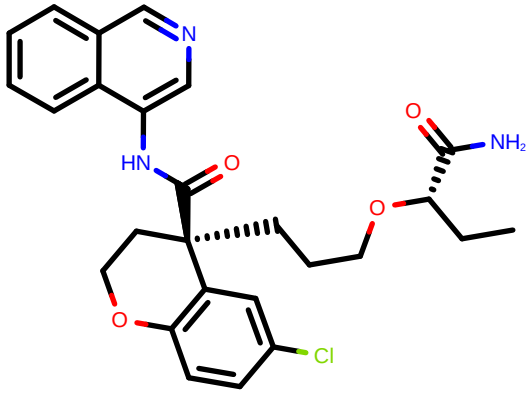
CID:	EN300-370182_2_1
SMILES:	Cn1c(nnn1)CCCNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11279
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.24

EN300-6746631_1_1



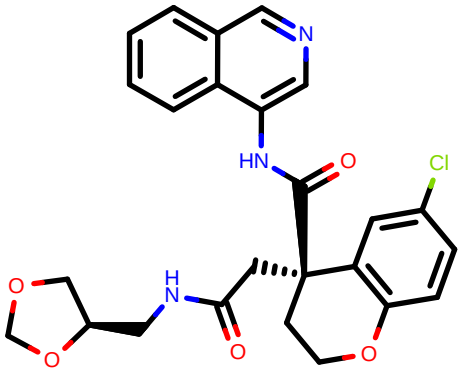
CID:	EN300-6746631_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5nnc6n5CCCC6
RUN:	RUN6176
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.31

EN300-65839_4_1



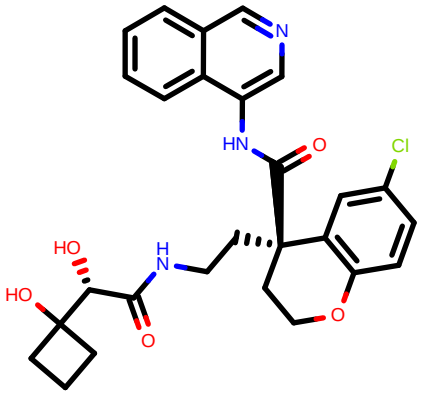
CID:	EN300-65839_4_1
SMILES:	CC[C@@H](C(=O)N)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN808
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.40

EN300-253187_1_1



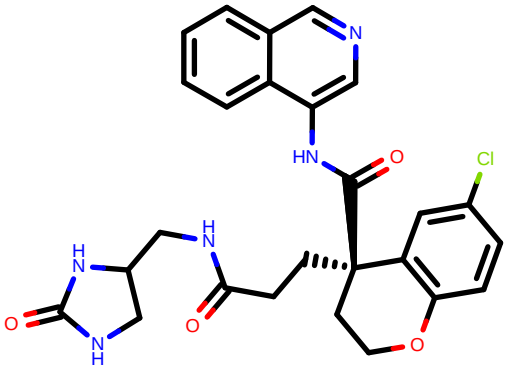
CID:	EN300-253187_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5COCO5
RUN:	RUN9354
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.30

EN300-1073320_3_2



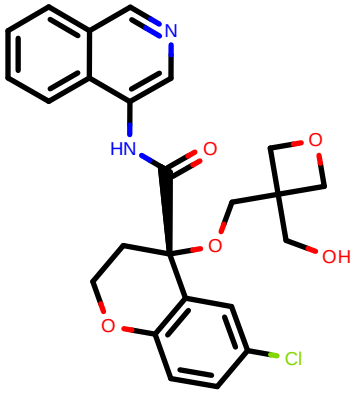
CID:	EN300-1073320_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H](C5(CCC5)O)O
RUN:	RUN2840
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.32

EN300-260603_2_1



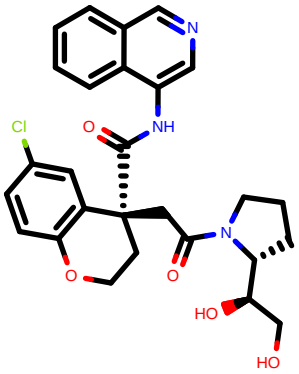
CID:	EN300-260603_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5c[nH]c(=O)[nH]5
RUN:	RUN5100
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.31

EN300-102347_1_1



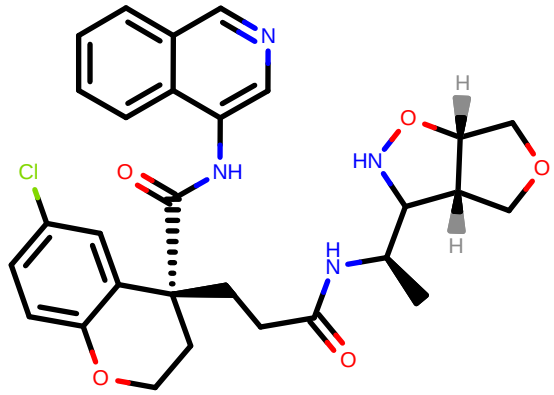
CID:	EN300-102347_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5(COC5)CO
RUN:	RUN2103
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.21

EN300-7459540_1_1



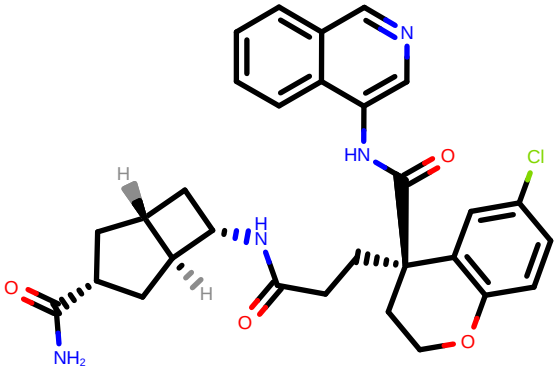
CID:	EN300-7459540_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5[C@@H](CO)O
RUN:	RUN2129
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.52

EN300-7438575_2_2



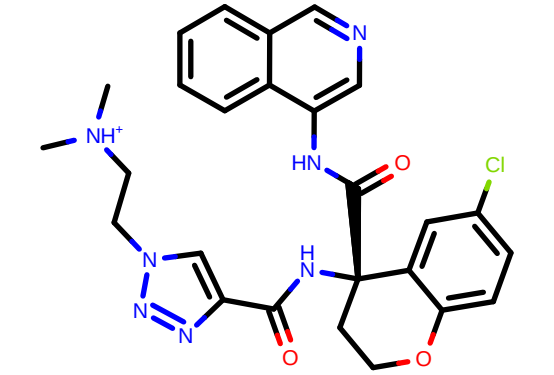
CID:	EN300-7438575_2_2
SMILES:	C[C@H](C1=NO[C@H]2[C@@H]1COC2)NC(=O)CC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7269
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.30

EN300-1268016_2_2



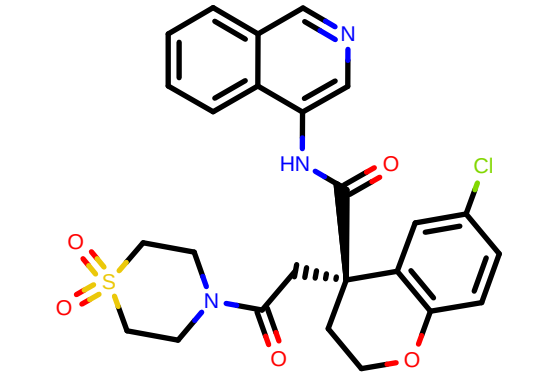
CID:	EN300-1268016_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5C[C@@H]6[C@@H]5C[C@@H](C6)C(=O)N
RUN:	RUN8866
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.35

EN300-7543132_1_1



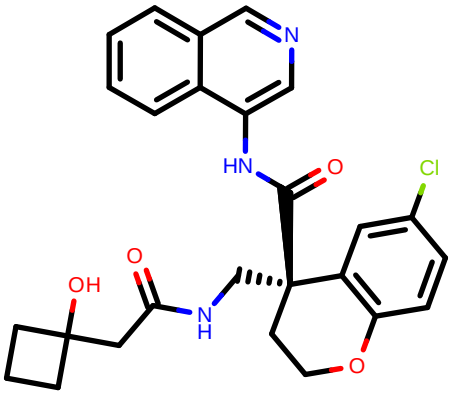
CID:	EN300-7543132_1_1
SMILES:	CN(C)CCn1cc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8954
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.33

EN300-67050_1_1



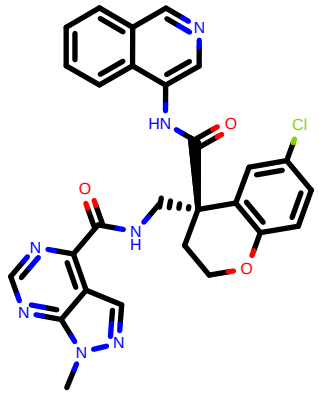
CID:	EN300-67050_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)CC5
RUN:	RUN3056
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.32

EN300-246423_2_1



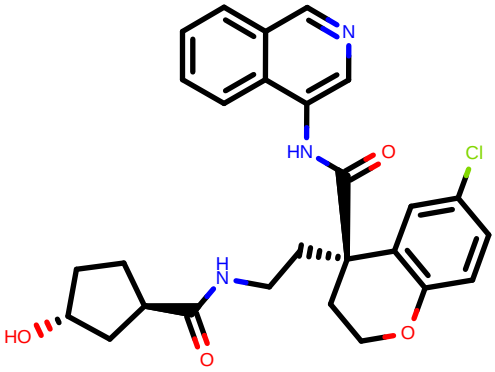
CID:	EN300-246423_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CC5(CCC5)O
RUN:	RUN3675
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.31

EN300-313438_2_1



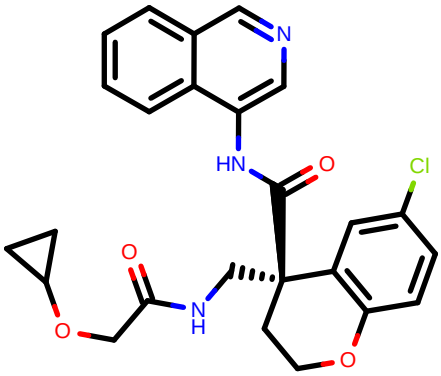
CID:	EN300-313438_2_1
SMILES:	Cn1c2c(cn1)c(ncn2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8247
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.26

EN300-321597_3_1



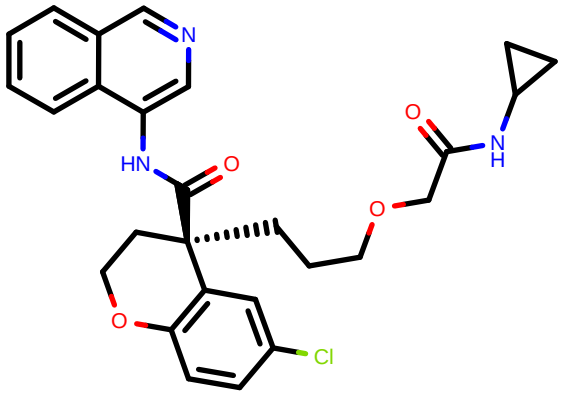
CID:	EN300-321597_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CC[C@H](C5)O
RUN:	RUN8500
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.35

EN300-378373_2_1



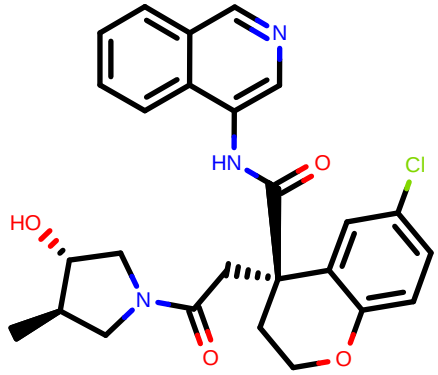
CID:	EN300-378373_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)COC5CC5
RUN:	RUN3603
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.23

EN300-1253178_4_1



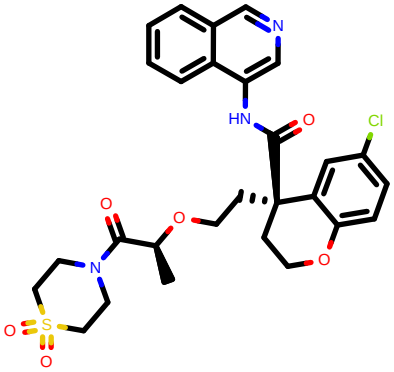
CID:	EN300-1253178_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)NC5CC5
RUN:	RUN1423
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.35

EN300-6497226_1_1



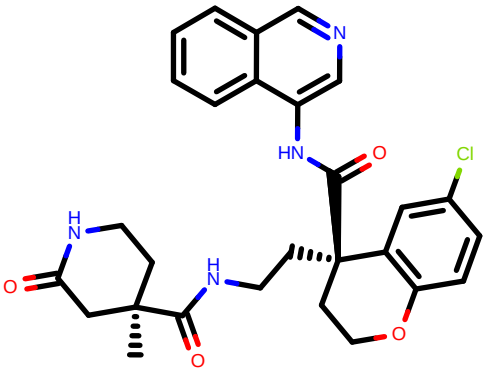
CID:	EN300-6497226_1_1
SMILES:	C[C@@H]1CN(C[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4731
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.28

EN300-1265949_3_1



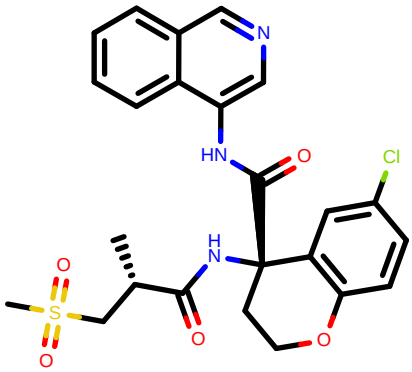
CID:	EN300-1265949_3_1
SMILES:	C[C@@H](C(=O)N1CCS(=O)(=O)CC1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1188
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.36

EN300-315854_3_2



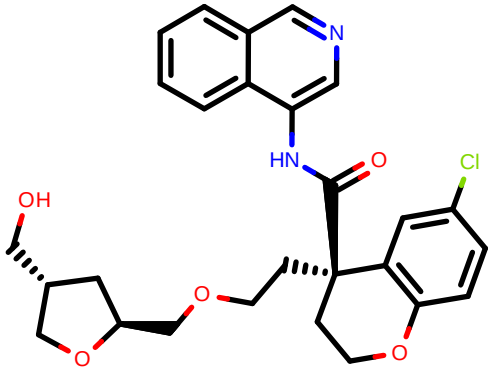
CID:	EN300-315854_3_2
SMILES:	C[C@]1(CCNC(=O)C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2145
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.41

EN300-97699_1_1



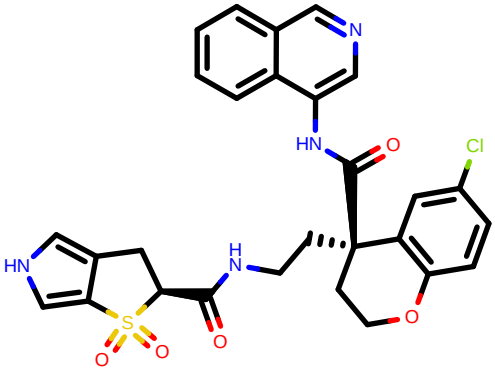
CID:	EN300-97699_1_1
SMILES:	C[C@@H](CS(=O)(=O)C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3674
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.34

EN300-6494158_3_3



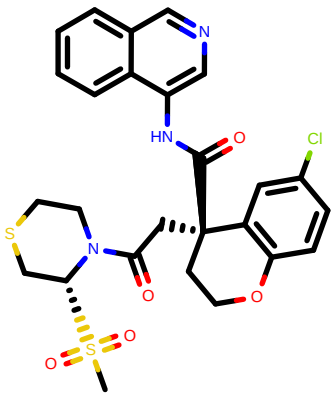
CID:	EN300-6494158_3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOC[C@@H]5C[C@H](CO5)CO
RUN:	RUN505
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.33

EN300-7445396_3_1



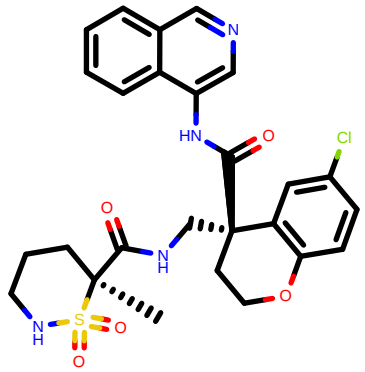
CID:	EN300-7445396_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5Cc6c[nH]cc6SS(=O)=O
RUN:	RUN10330
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.36

EN300-83827_1_1



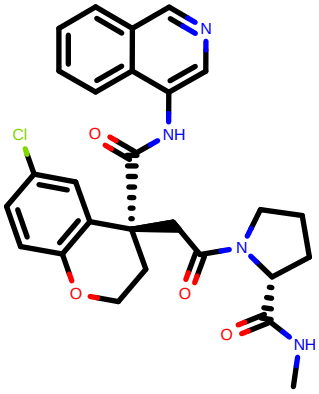
CID:	EN300-83827_1_1
SMILES:	CS(=O)(=O)[C@@H]1CSCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5746
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.34

EN300-1709315_2_2



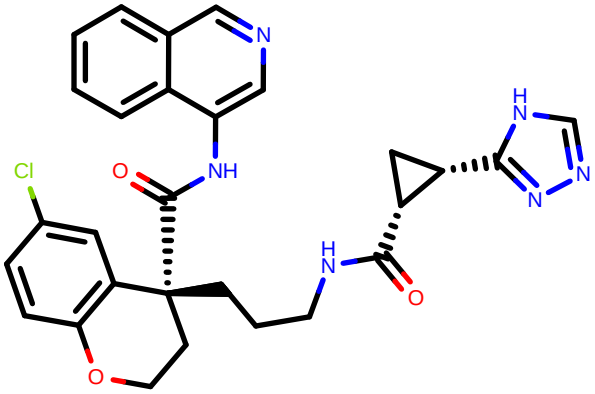
CID:	EN300-1709315_2_2
SMILES:	C[C@]1(CCCNS1(=O)=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3359
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.34

EN300-55355_1_2



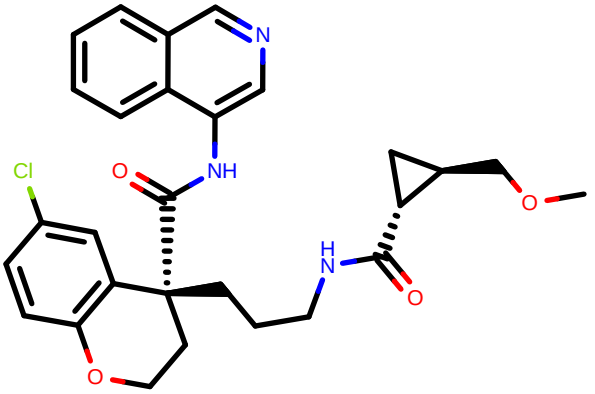
CID:	EN300-55355_1_2
SMILES:	CNC(=O)[C@H]1CCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4435
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.31

EN300-6477724_4_1



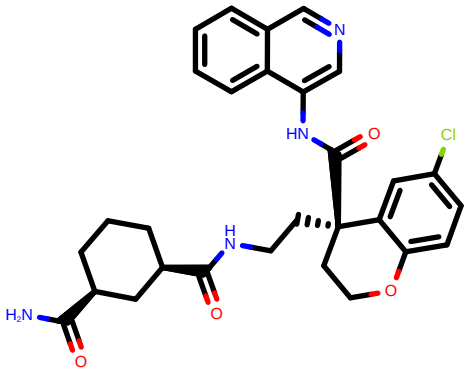
CID:	EN300-6477724_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5C[C@@H]5c6[nH]cnn6
RUN:	RUN9245
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.40

EN300-705386_4_1



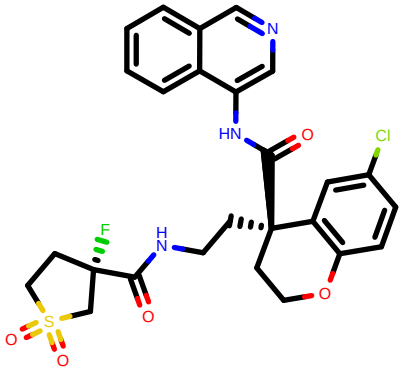
CID:	EN300-705386_4_1
SMILES:	COC[C@@H]1C[C@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9629
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.35

EN300-90142_3_1



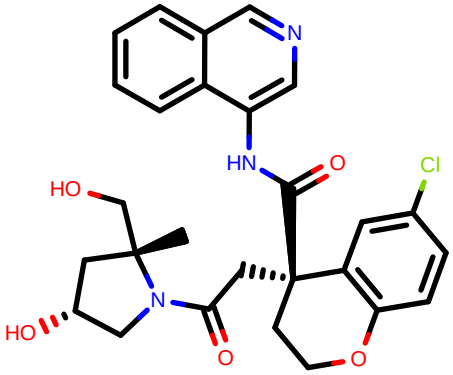
CID:	EN300-90142_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@H]5CCC[C@@H](C5)C(=O)N
RUN:	RUN10776
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.31

EN300-311920_3_1



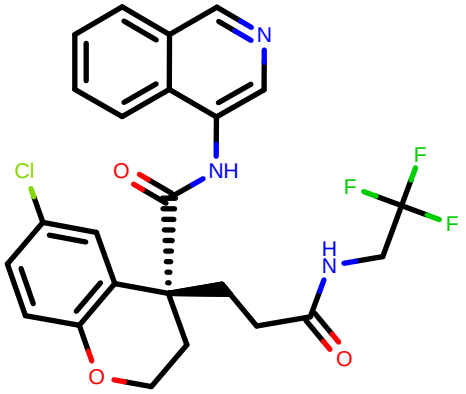
CID:	EN300-311920_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCNC(=O)[C@@]5(CCS(=O)(=O)C5)F
RUN:	RUN10448
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.26

EN300-307336_1_3



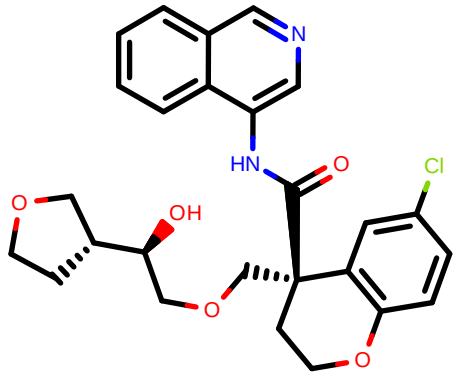
CID:	EN300-307336_1_3
SMILES:	C[C@@]1(C[C@H](CN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O)CO
RUN:	RUN6226
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.37

JAG-UCB-706446eb-1_1



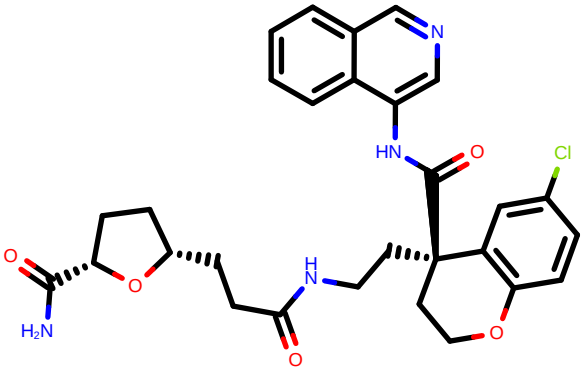
CID:	JAG-UCB-706446eb-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)NCC(F)(F)F
RUN:	RUN267
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.24

EN300-1911992_2_1



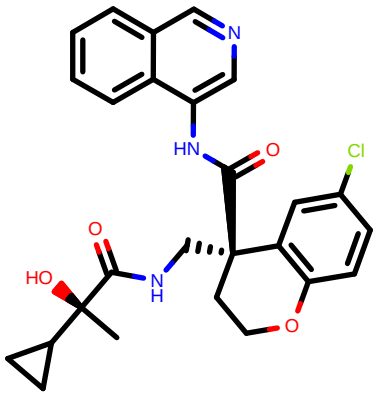
CID:	EN300-1911992_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]([C@@H]5CCOC5)O
RUN:	RUN1294
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.38

EN300-364992_3_1



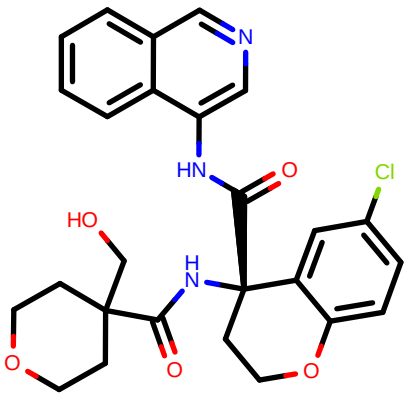
CID:	EN300-364992_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC[C@H]5CC[C@H](O5)C(=O)N
RUN:	RUN10232
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.40

EN300-118760_2_2



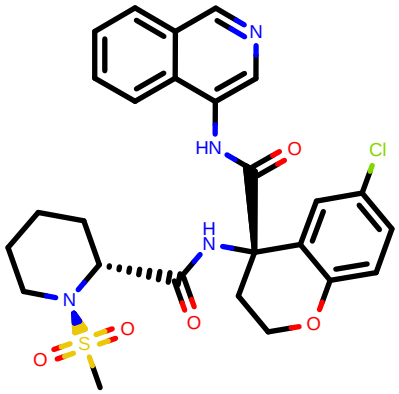
CID:	EN300-118760_2_2
SMILES:	C[C@](C1CC1)(C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3383
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.36

EN300-244909_1_1



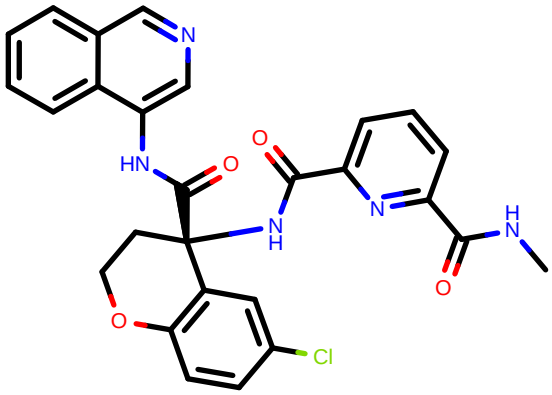
CID:	EN300-244909_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(CCOCC5)CO
RUN:	RUN5025
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.26

EN300-24014_1_1



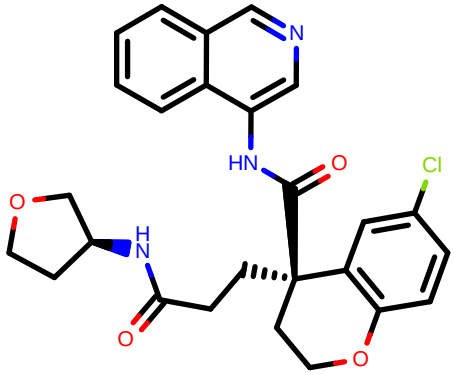
CID:	EN300-24014_1_1
SMILES:	CS(=O)(=O)N1CCCC[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4529
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.26

EN300-104891_1_1



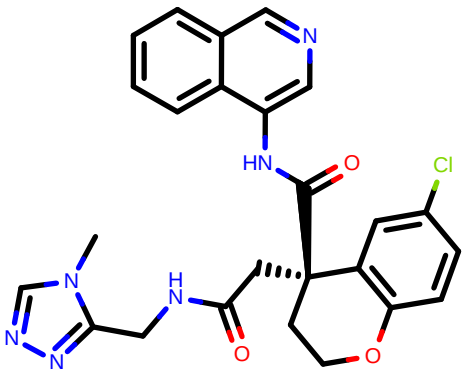
CID:	EN300-104891_1_1
SMILES:	CNC(=O)c1cccc(n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3773
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.28

EN300-171752_2_2



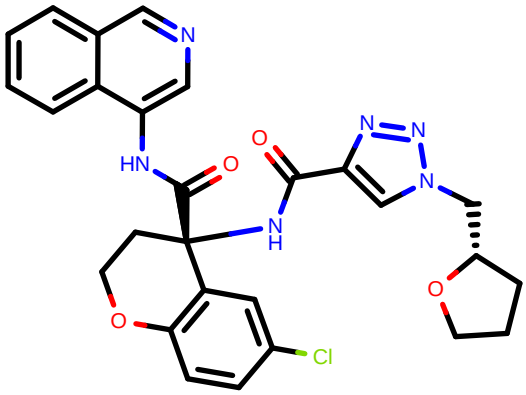
CID:	EN300-171752_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCOC5
RUN:	RUN5463
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.30

EN300-30859_1_1



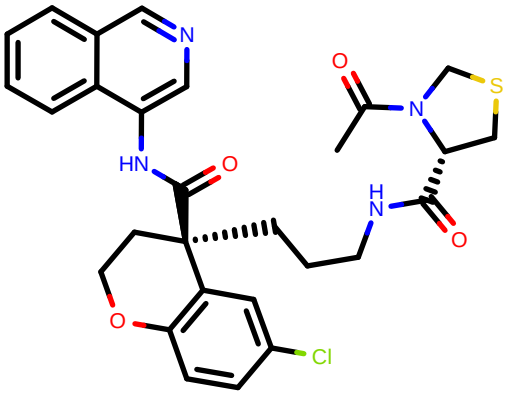
CID:	EN300-30859_1_1
SMILES:	Cn1cnnc1CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11228
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.25

EN300-368758_1_1



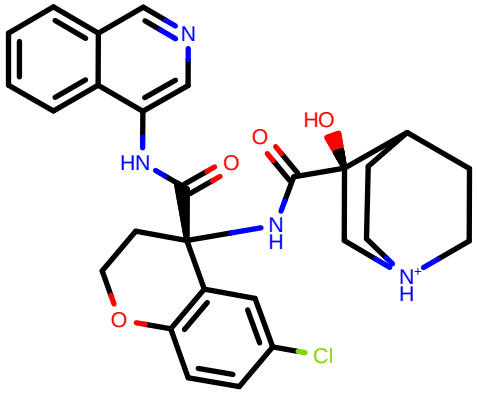
CID:	EN300-368758_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@H]6CCCO6
RUN:	RUN7786
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.30

EN300-56202_4_1



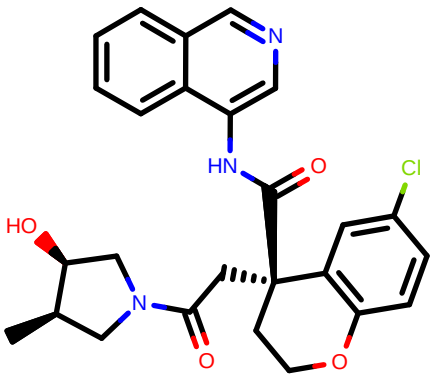
CID:	EN300-56202_4_1
SMILES:	CC(=O)N1CSC[C@@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10052
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.43

EN300-7442191_1_2



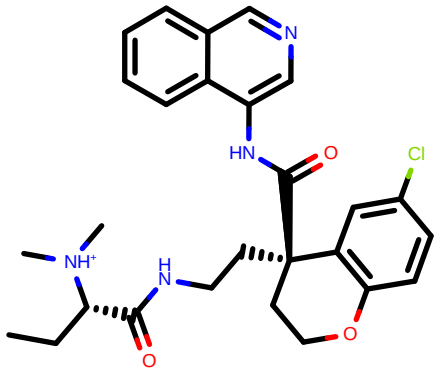
CID:	EN300-7442191_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@]5(CN6CCC5CC6)O
RUN:	RUN6623
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.44

EN300-124052_1_1



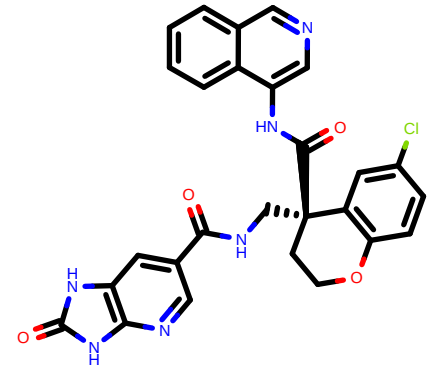
CID:	EN300-124052_1_1
SMILES:	C[C@@H]1CN(C[C@@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3216
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.30

EN300-110012_3_1



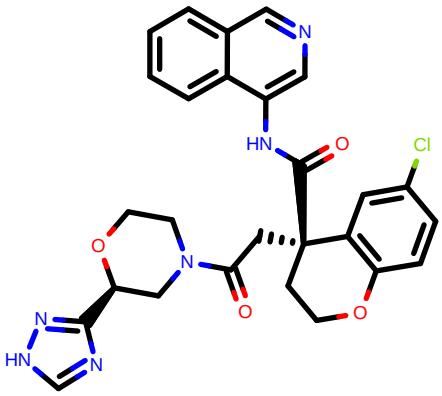
CID:	EN300-110012_3_1
SMILES:	CC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)N(C)C
RUN:	RUN582
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.29

EN300-214552_2_1



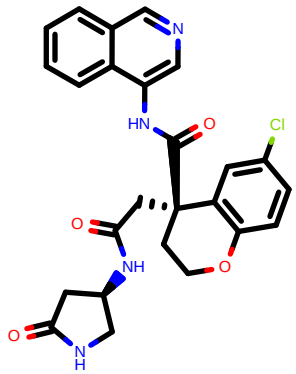
CID:	EN300-214552_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6c([nH]c(=O)[nH]6)nc5
RUN:	RUN8619
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.25

EN300-1709213_1_1



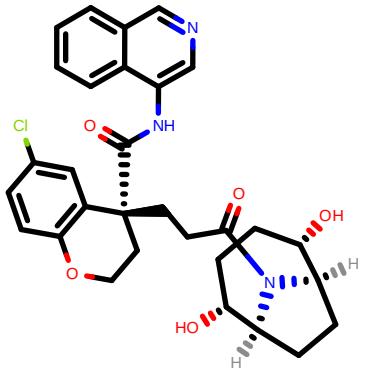
CID:	EN300-1709213_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)c6[nH]cnn6
RUN:	RUN4215
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.28

EN300-127487_1_1



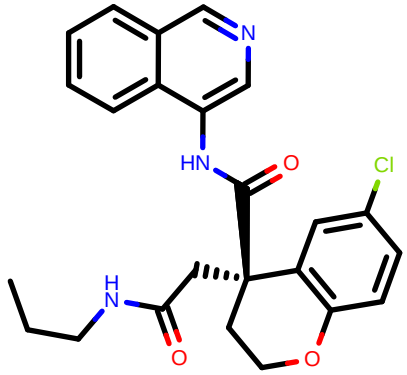
CID:	EN300-127487_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC(=O)NC5
RUN:	RUN10722
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.31

EN300-6738887_2_1



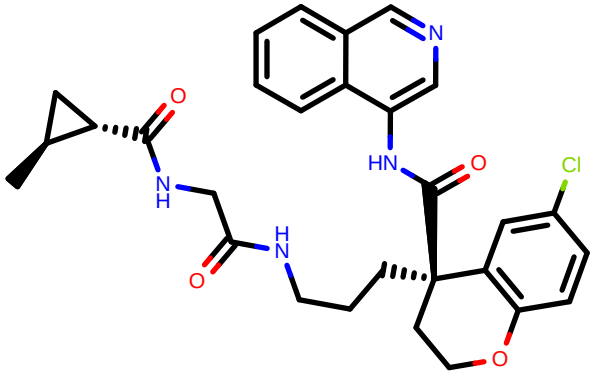
CID:	EN300-6738887_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C6CCC5[C@H](CC[C@H]6O)O
RUN:	RUN6770
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.31

EN300-21409_1_1



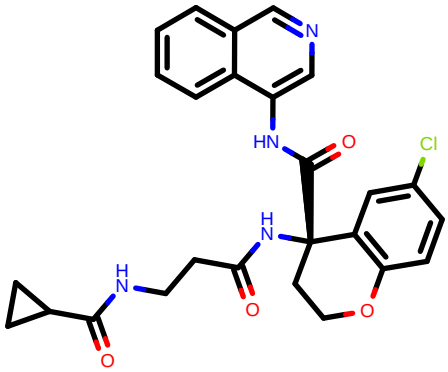
CID:	EN300-21409_1_1
SMILES:	C#CCNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10936
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.20

EN300-30768_4_2



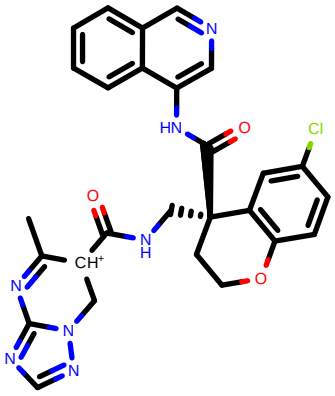
CID:	EN300-30768_4_2
SMILES:	C[C@H]1C[C@@H]1C(=O)NCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10971
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.33

EN300-31147_1_1



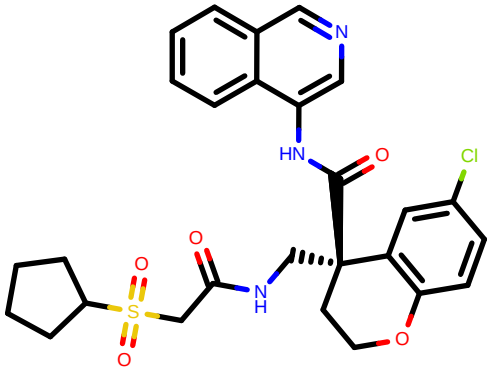
CID:	EN300-31147_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCNC(=O)C5CC5
RUN:	RUN2228
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.25

EN300-1602334_2_1



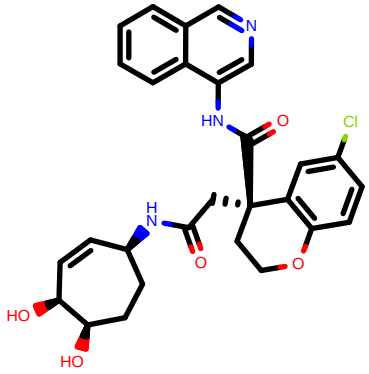
CID:	EN300-1602334_2_1
SMILES:	Cc1c(cn2c(n1)ncn2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8507
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.36

EN300-42154_2_1



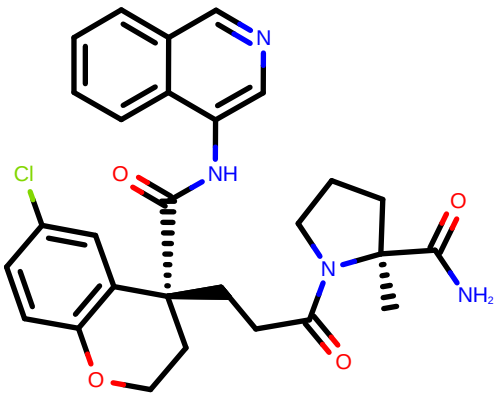
CID:	EN300-42154_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS(=O)(=O)C5CCCC5
RUN:	RUN1017
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.36

EN300-386200_1_1



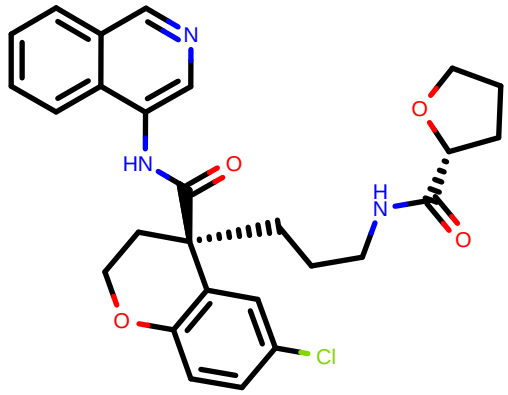
CID:	EN300-386200_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC[C@H]([C@H](CC5)O)O
RUN:	RUN6984
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.27

EN300-1697763_2_1



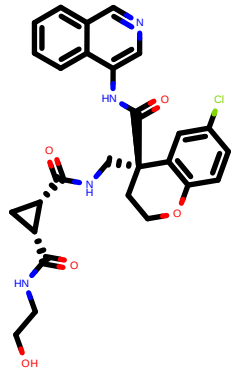
CID:	EN300-1697763_2_1
SMILES:	C[C@]1(CCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN2764
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.31

EN300-21009_4_2



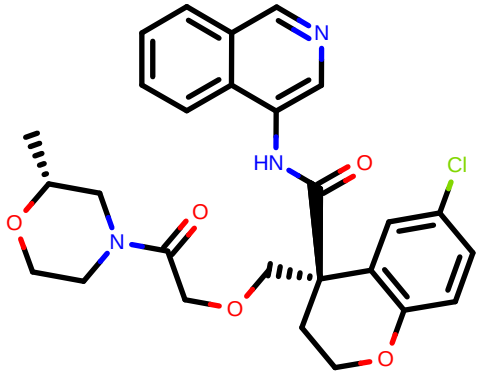
CID:	EN300-21009_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCCO5
RUN:	RUN11299
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.34

EN300-6335413_2_1



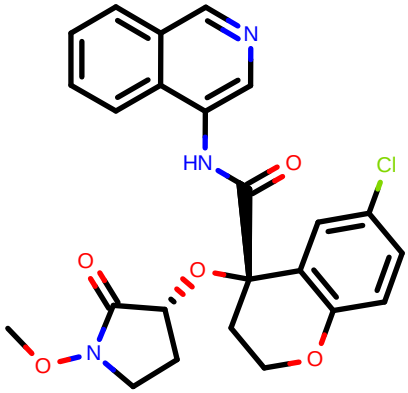
CID:	EN300-6335413_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5C[C@H]5C(=O)NCCO
RUN:	RUN478
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.39

EN300-25572_2_1



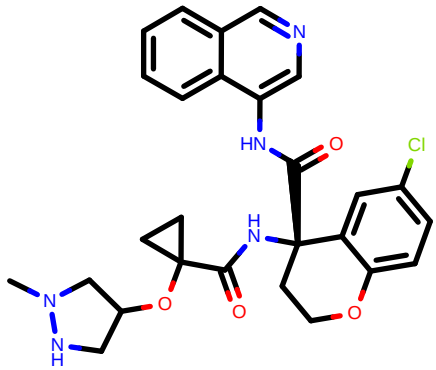
CID:	EN300-25572_2_1
SMILES:	C[C@@H]1CN(CCO1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN419
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.29

EN300-302058_1_2



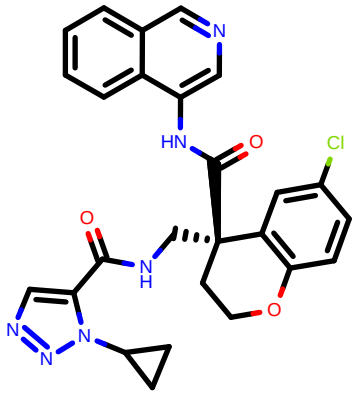
CID:	EN300-302058_1_2
SMILES:	CON1CC[C@H](C1=O)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2261
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.27

EN300-7352812_1_1



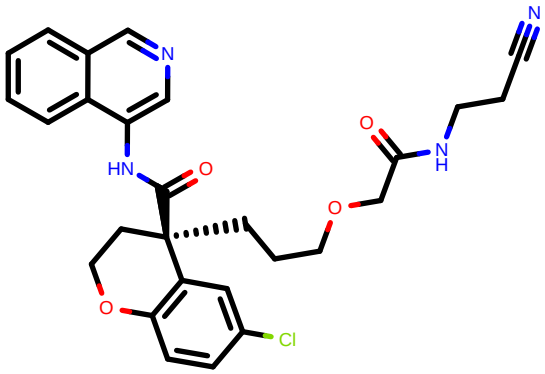
CID:	EN300-7352812_1_1
SMILES:	Cn1cc(cn1)OC2(CC2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN5732
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.33

EN300-1718675_2_1



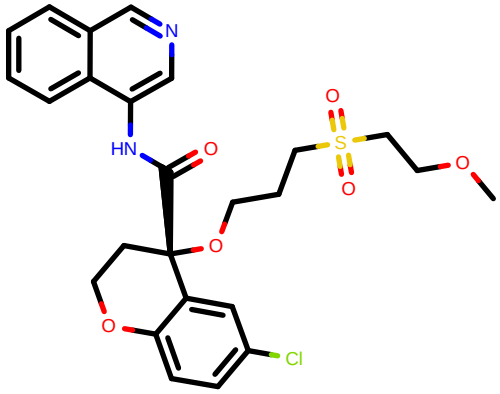
CID:	EN300-1718675_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnnn5C6CC6
RUN:	RUN7215
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.40

EN300-10895_4_1



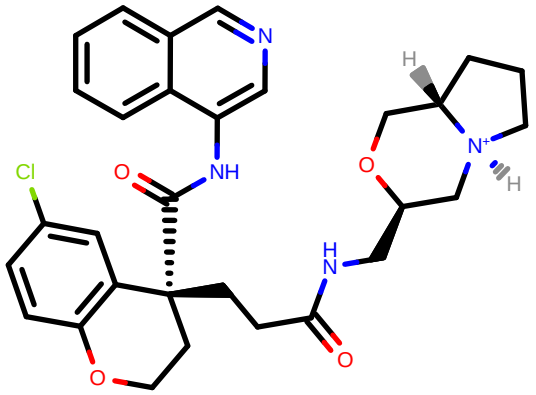
CID:	EN300-10895_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)NCCC#N
RUN:	RUN1766
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.35

EN300-62857_1_1



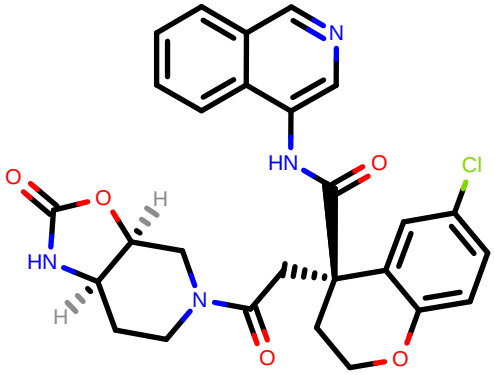
CID:	EN300-62857_1_1
SMILES:	COCCS(=O)(=O)CCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1296
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.51

EN300-60049_2_3



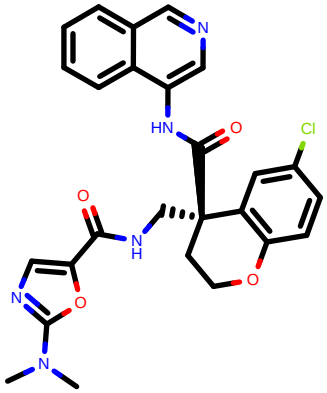
CID:	EN300-60049_2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@@H]5CN6CCC[C@H]6CO5
RUN:	RUN7333
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.34

EN300-6739162_1_1



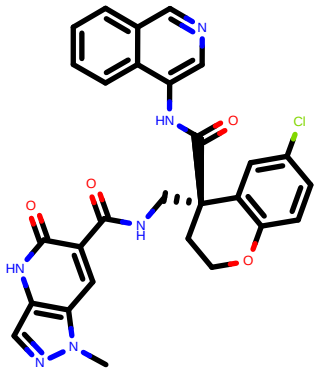
CID:	EN300-6739162_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6[C@H](C5)OC(=O)N6
RUN:	RUN9396
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.39

EN300-137243_2_1



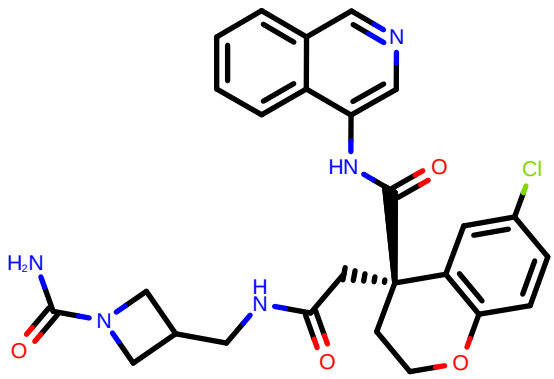
CID:	EN300-137243_2_1
SMILES:	CN(C)c1ncc(o1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7803
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.32

EN300-805037_2_1



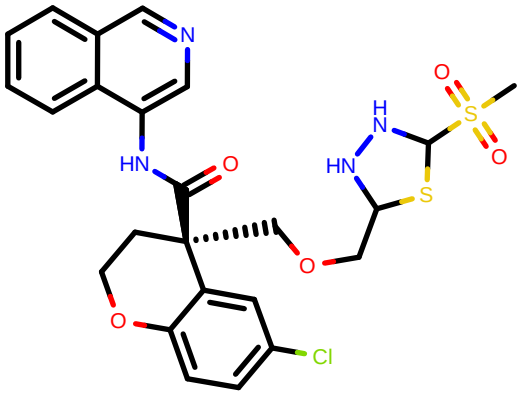
CID:	EN300-805037_2_1
SMILES:	Cn1c2cc(c(=O)[nH]c2cn1)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8495
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.32

EN300-7431964_1_1



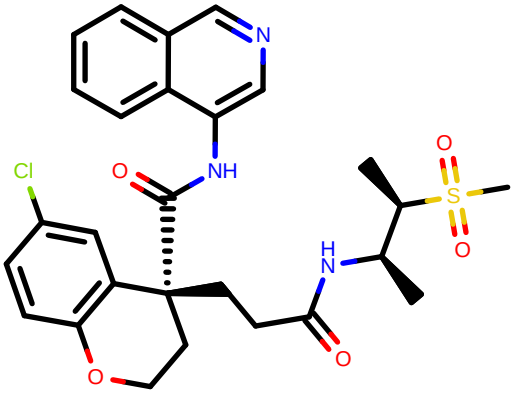
CID:	EN300-7431964_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5CN(C5)C(=O)N
RUN:	RUN2824
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.31

EN300-160080_2_1



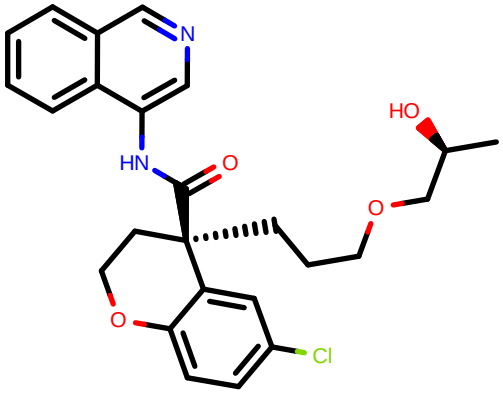
CID:	EN300-160080_2_1
SMILES:	CS(=O)(=O)c1nnc(s1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2585
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.33

EN300-83434_2_2



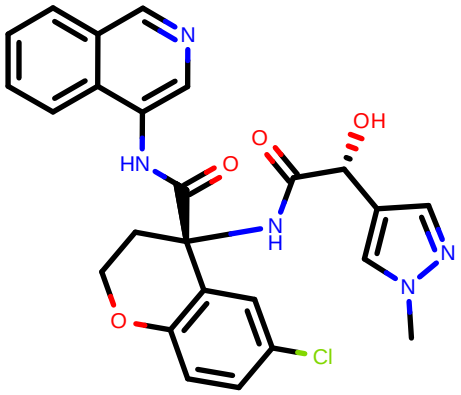
CID:	EN300-83434_2_2
SMILES:	C[C@H]([C@@H](C)S(=O)(=O)C)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN6837
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.32

EN300-185378_4_1



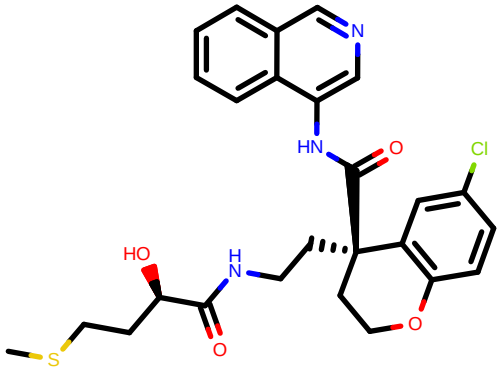
CID:	EN300-185378_4_1
SMILES:	C[C@@H](COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN595
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.36

EN300-198540_1_2



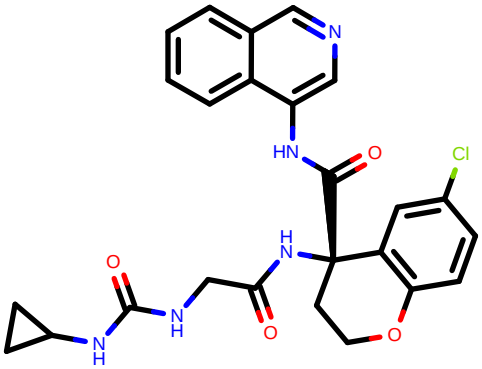
CID:	EN300-198540_1_2
SMILES:	Cn1cc(cn1)[C@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN6168
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.29

EN300-103144_3_2



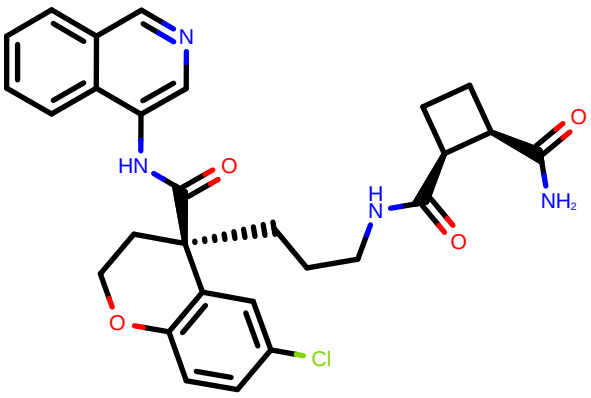
CID:	EN300-103144_3_2
SMILES:	CSCC[C@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN6501
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.38

EN300-42591_1_1



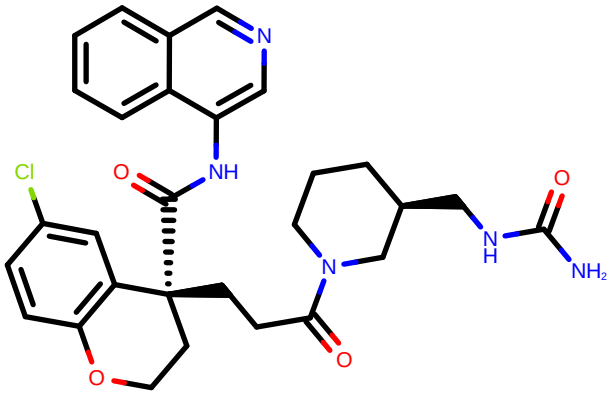
CID:	EN300-42591_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)NC5CC5
RUN:	RUN1964
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.25

EN300-217107_4_4



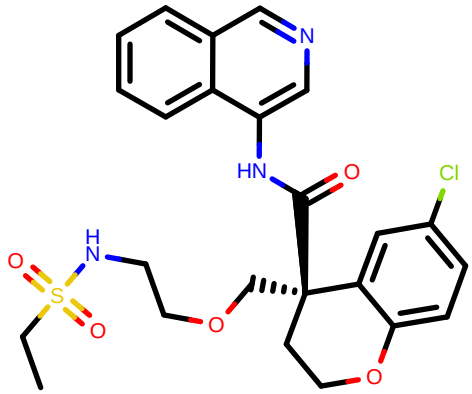
CID:	EN300-217107_4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CC[C@H]5C(=O)N
RUN:	RUN9455
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.26

EN300-42195_2_2



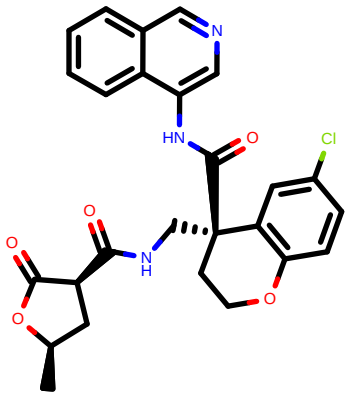
CID:	EN300-42195_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@H](C5)CNC(=O)N
RUN:	RUN9585
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.31

EN300-73582_2_1



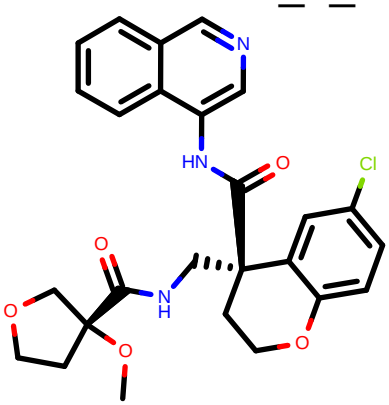
CID:	EN300-73582_2_1
SMILES:	CCS(=O)(=O)NCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1110
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.34

EN300-7444533_2_1



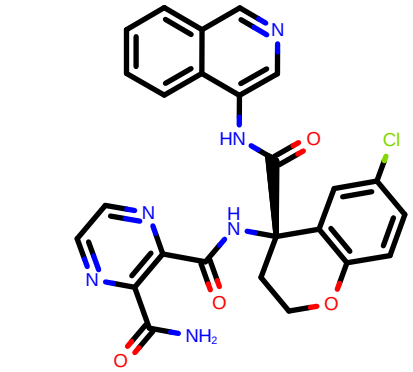
CID:	EN300-7444533_2_1
SMILES:	C[C@@H]1C[C@@H](C(=O)O1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5242
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.33

EN300-174668_2_1



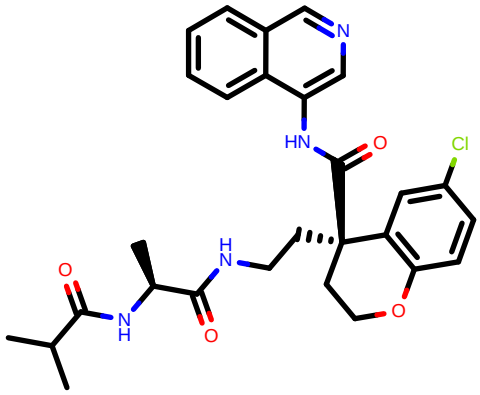
CID:	EN300-174668_2_1
SMILES:	CO[C@@]1(CCOC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3439
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.52

EN300-21200_1_1



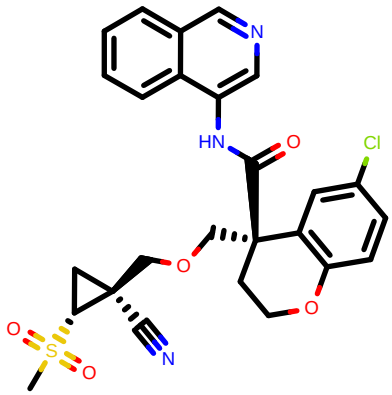
CID:	EN300-21200_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5c(nccn5)C(=O)N
RUN:	RUN7390
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.21

EN300-31184_3_1



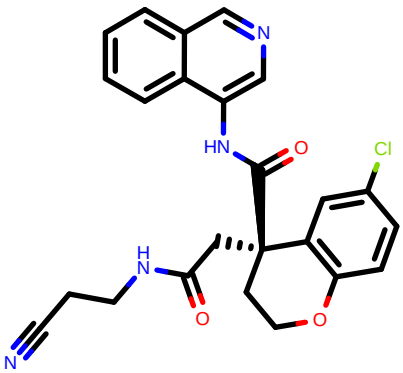
CID:	EN300-31184_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C(C)C
RUN:	RUN5103
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.34

EN300-633533_2_1



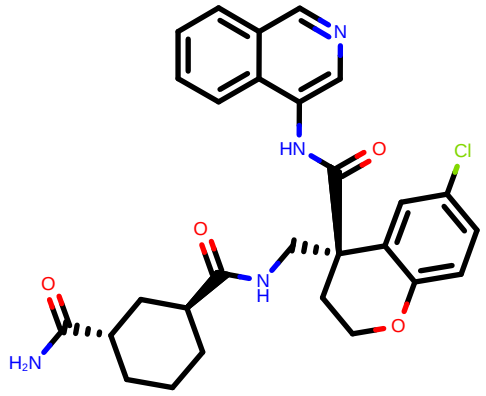
CID:	EN300-633533_2_1
SMILES:	CS(=O)(=O)[C@@H]1C[C@]1(COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C#N
RUN:	RUN2463
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.35

EN300-183001_1_1



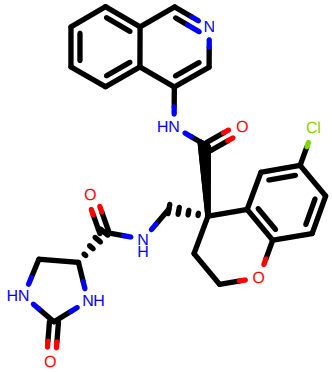
CID:	EN300-183001_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCC#N
RUN:	RUN10490
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.21

EN300-90142_2_2



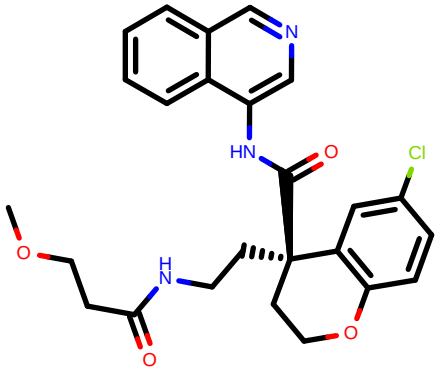
CID:	EN300-90142_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCC[C@@H](C5)C(=O)N
RUN:	RUN3271
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.29

EN300-222145_2_1



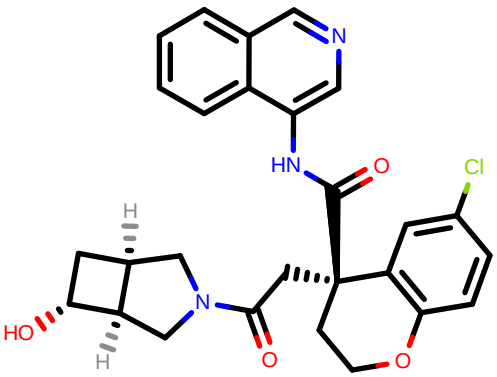
CID:	EN300-222145_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CNC(=O)N5
RUN:	RUN4342
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.22

EN300-64536_3_1



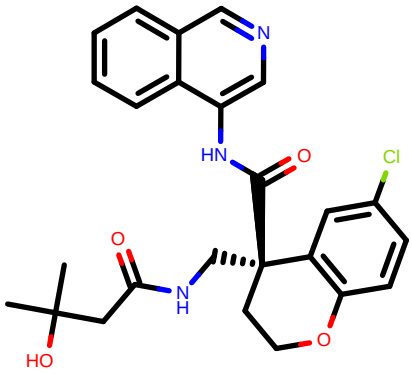
CID:	EN300-64536_3_1
SMILES:	COCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10694
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.26

EN300-305294_1_3



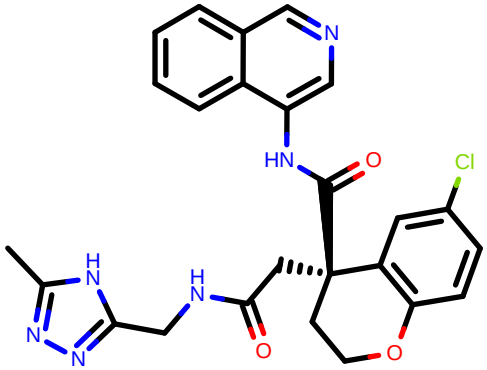
CID:	EN300-305294_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@@H][C@@H]6C5)O
RUN:	RUN5406
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.23

EN300-117931_2_1



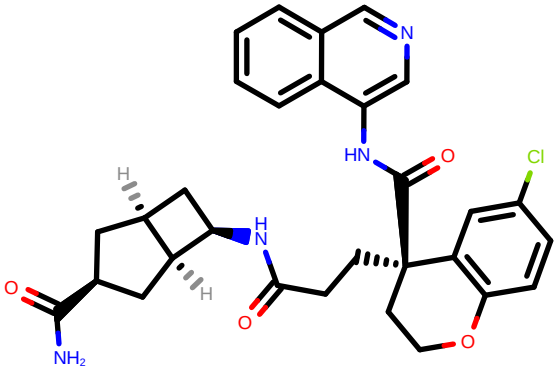
CID:	EN300-117931_2_1
SMILES:	CC(C)(CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN5457
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.27

EN300-70487_1_1



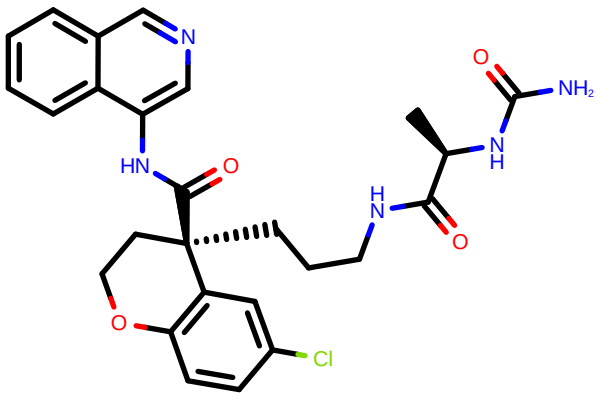
CID:	EN300-70487_1_1
SMILES:	Cc1[nH]c(nn1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6309
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.21

EN300-1268016_2_11



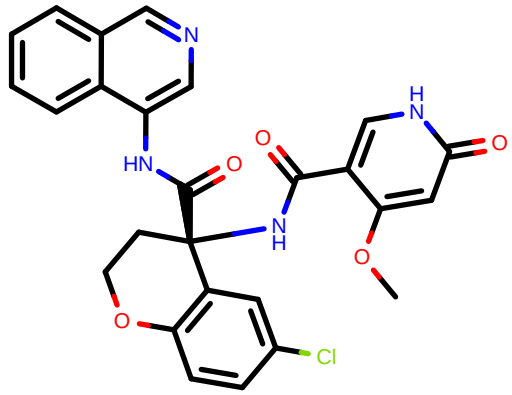
CID:	EN300-1268016_2_11
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)N[C@@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN5172
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.35

EN300-00271_4_2



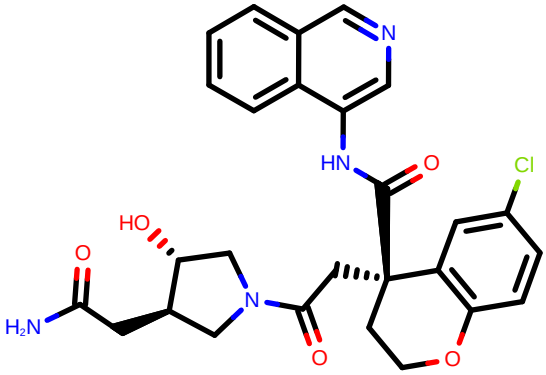
CID:	EN300-00271_4_2
SMILES:	C[C@H](C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN9801
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.36

EN300-734638_1_1



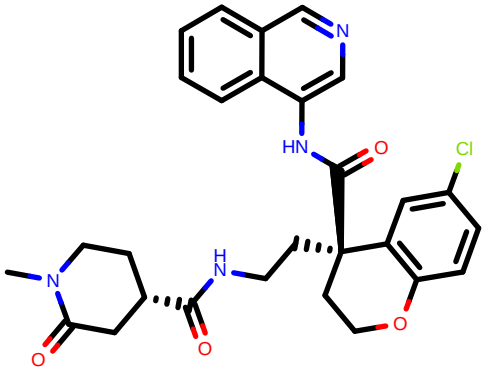
CID:	EN300-734638_1_1
SMILES:	COc1cc(=O)[nH]cc1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8186
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.32

EN300-7436546_1_1



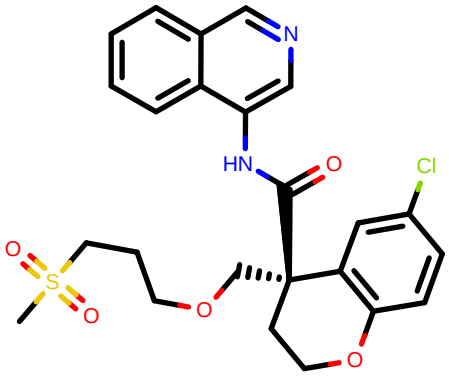
CID:	EN300-7436546_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](C[C@@H](C5)O)CC(=O)N
RUN:	RUN5346
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.35

EN300-30458_3_1



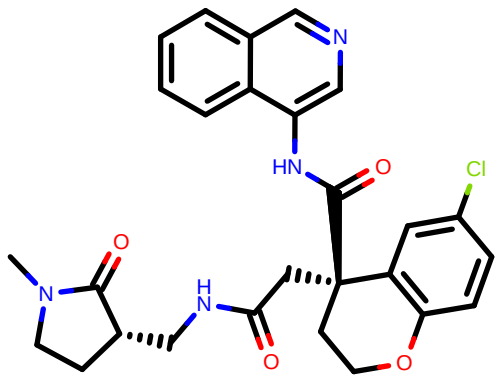
CID:	EN300-30458_3_1
SMILES:	CN1CC[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3144
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.32

EN300-68794_2_1



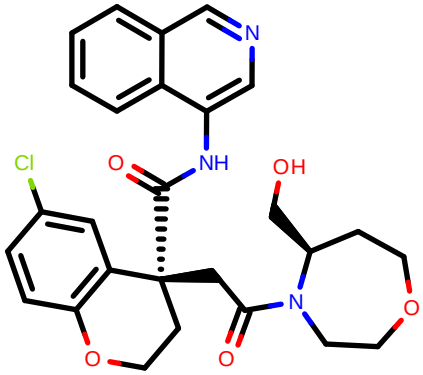
CID:	EN300-68794_2_1
SMILES:	CS(=O)(=O)CCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2085
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.35

EN300-1264816_1_2



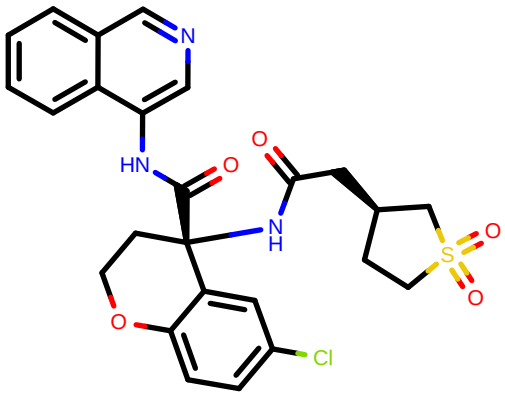
CID:	EN300-1264816_1_2
SMILES:	CN1CC[C@H](C1=O)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8180
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.30

EN300-6732376_1_1



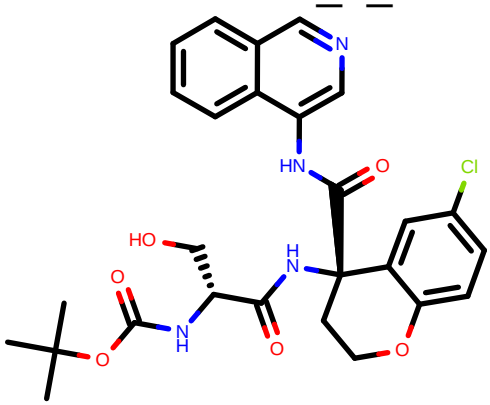
CID:	EN300-6732376_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOCC[C@@H]5CO
RUN:	RUN8880
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.34

EN300-14006_1_1



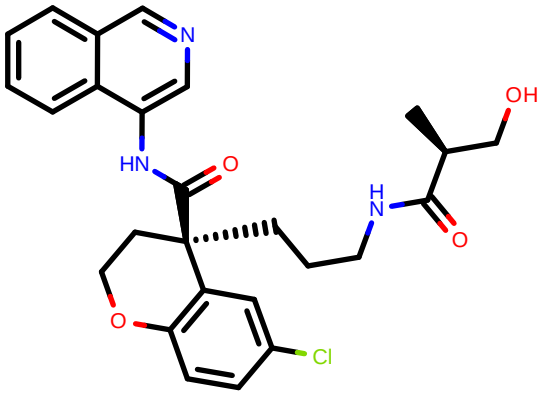
CID:	EN300-14006_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCS(=O)(=O)C5
RUN:	RUN3861
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.31

EN300-72109_1_2



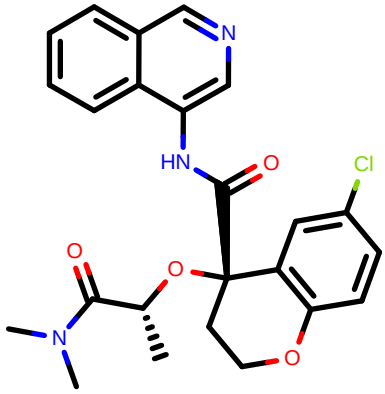
CID:	EN300-72109_1_2
SMILES:	CC(C)(C)OC(=O)N[C@H](CO)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7610
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.32

EN300-55072_4_1



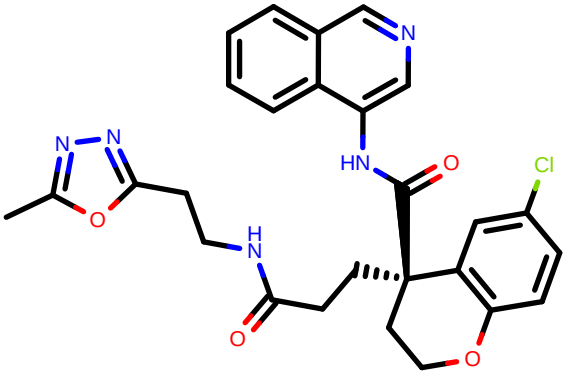
CID:	EN300-55072_4_1
SMILES:	C[C@@H](CO)C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7593
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.34

EN300-14458_1_2



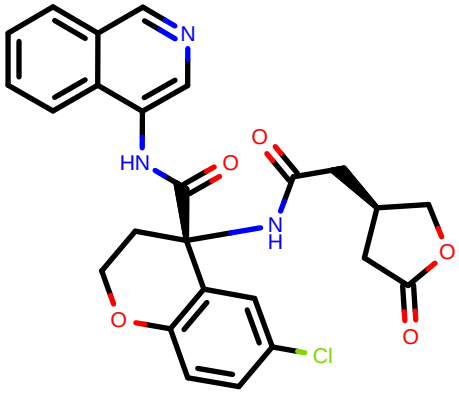
CID:	EN300-14458_1_2
SMILES:	C[C@H](C(=O)N(C)C)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1384
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.20

EN300-104896_2_1



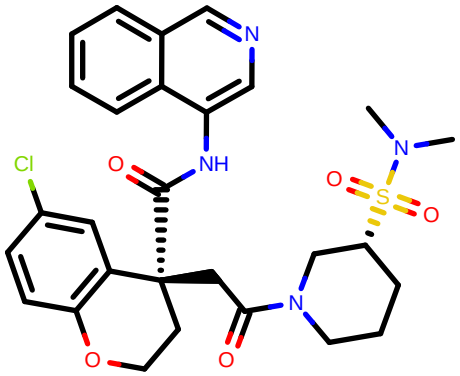
CID:	EN300-104896_2_1
SMILES:	Cc1nnc(o1)CCNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10947
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.30

EN300-109535_1_1



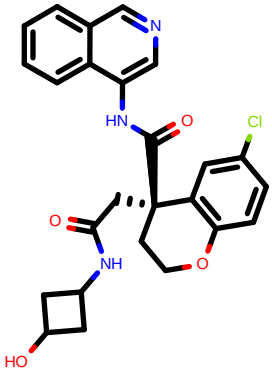
CID:	EN300-109535_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CC(=O)OC5
RUN:	RUN1245
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.26

EN300-207451_1_1



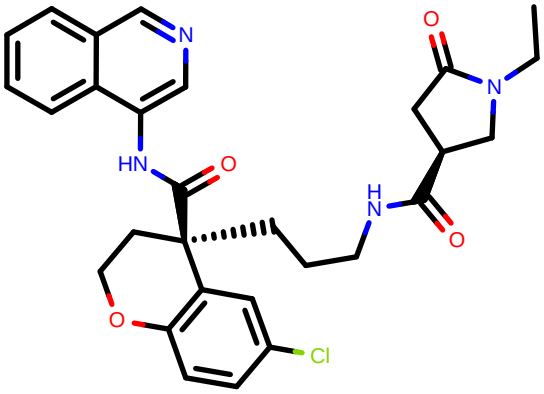
CID:	EN300-207451_1_1
SMILES:	CN(C)S(=O)(=O)[C@@H]1CCCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9163
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.44

EN300-307592_1_1



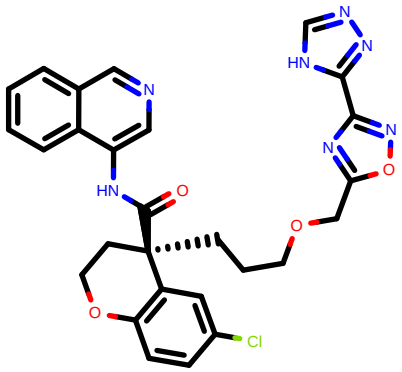
CID:	EN300-307592_1_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)CC(=O)N[C@H]5C[C@@H](C5)O)cc1
RUN:	RUN10063
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.23

EN300-33478_4_2



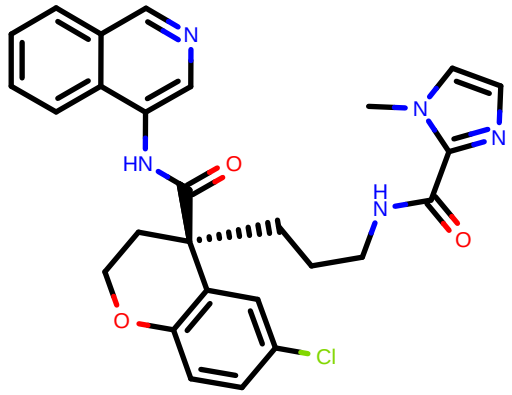
CID:	EN300-33478_4_2
SMILES:	CCN1C[C@H](CC1=O)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11113
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.40

EN300-92031_4_1



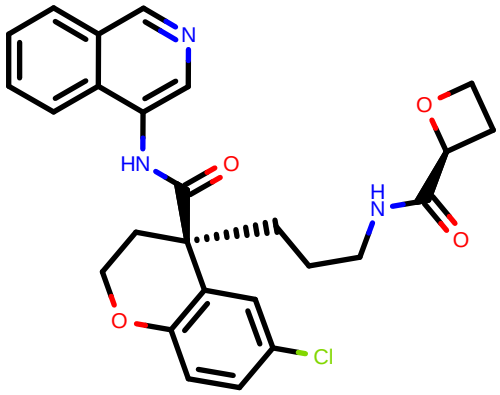
CID:	EN300-92031_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCc5nc(no5)c6[nH]cnn6
RUN:	RUN1806
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.30

EN300-1700710_4_1



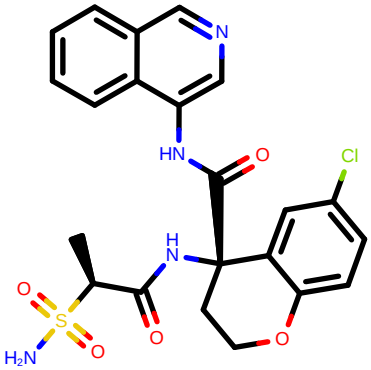
CID:	EN300-1700710_4_1
SMILES:	Cn1ccnc1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10173
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.32

EN300-85760_4_1



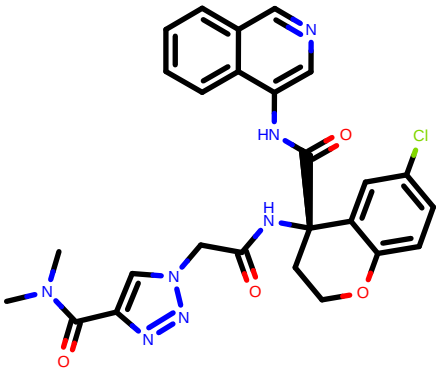
CID:	EN300-85760_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCO5
RUN:	RUN11171
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.26

EN300-132615_1_1



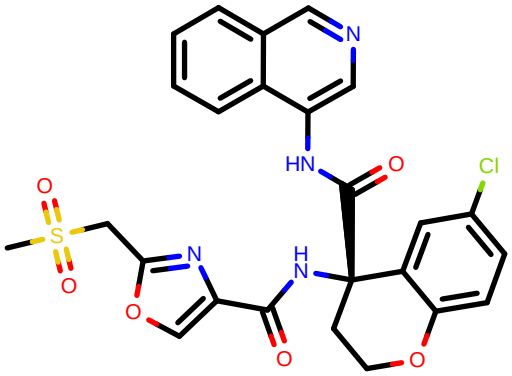
CID:	EN300-132615_1_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)N
RUN:	RUN2266
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.28

EN300-2853791_1_1



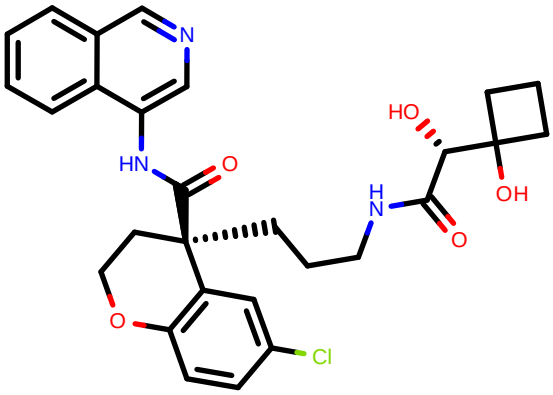
CID:	EN300-2853791_1_1
SMILES:	CN(C)C(=O)c1cn(nn1)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7926
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.26

EN300-263392_1_1



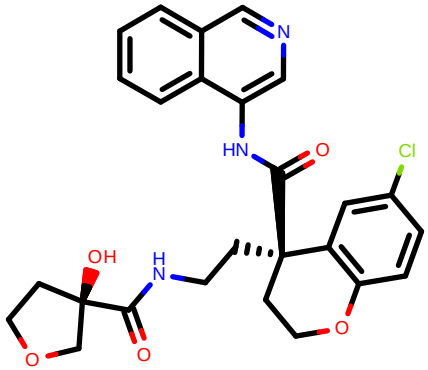
CID:	EN300-263392_1_1
SMILES:	CS(=O)(=O)Cc1nc(co1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6794
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.37

EN300-1073320_4_1



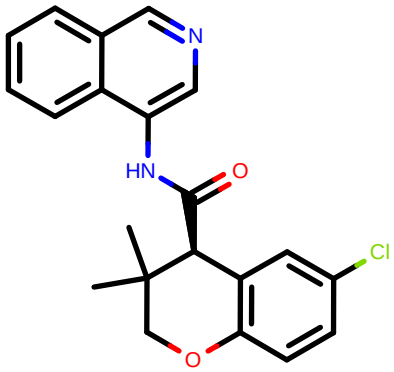
CID:	EN300-1073320_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H](C5(CCC5)O)O
RUN:	RUN9621
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.48

EN300-148421_3_2



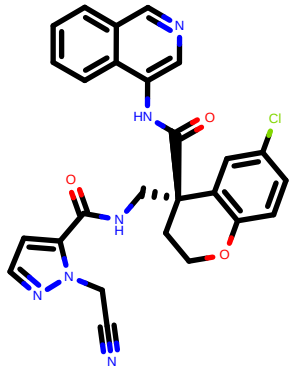
CID:	EN300-148421_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]5(CCOC5)O
RUN:	RUN5155
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.34

DAR-DIA-0d514e7d-3_1



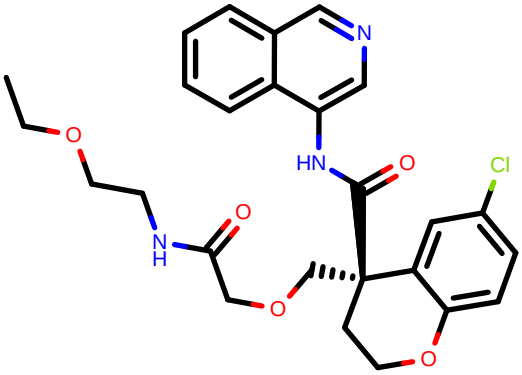
CID:	DAR-DIA-0d514e7d-3_1
SMILES:	CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C
RUN:	RUN156
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.13

EN300-373791_2_1



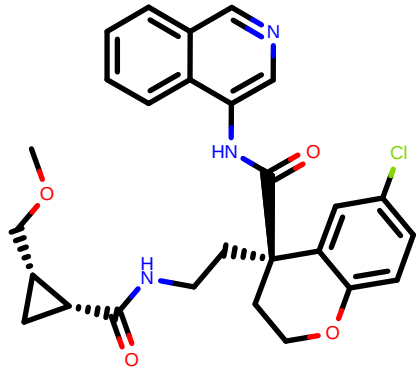
CID:	EN300-373791_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccnn5CC#N
RUN:	RUN6480
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.25

EN300-103187_2_1



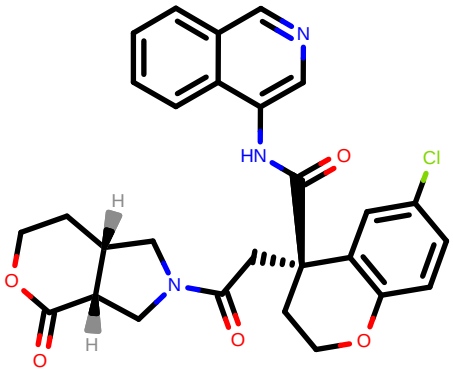
CID:	EN300-103187_2_1
SMILES:	CCOCCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN586
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.30

EN300-705381_3_1



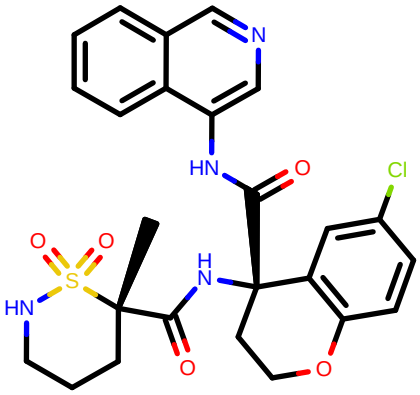
CID:	EN300-705381_3_1
SMILES:	COC[C@H]1C[C@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4743
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.27

EN300-7426520_1_1



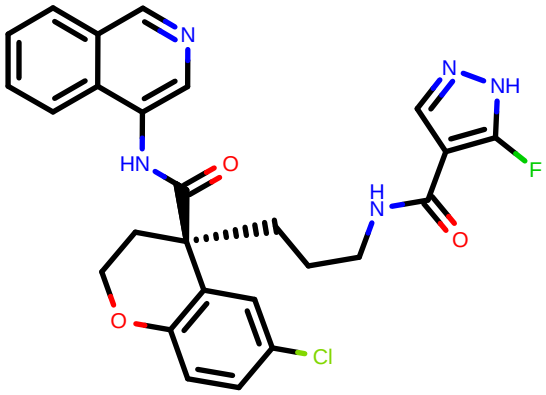
CID:	EN300-7426520_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6CCOC(=O)[C@H]6C5
RUN:	RUN4931
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.41

EN300-1709315_1_2



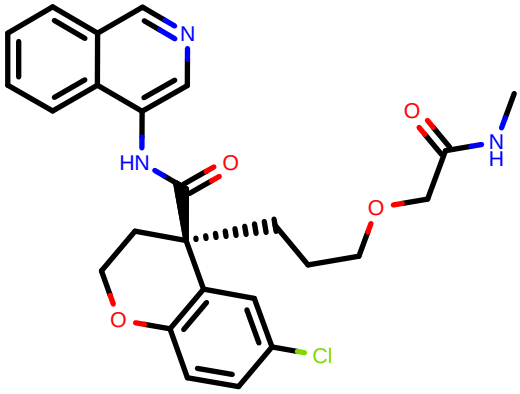
CID:	EN300-1709315_1_2
SMILES:	C[C@]1(CCCNS1(=O)=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5852
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.24

EN300-7121836_4_1



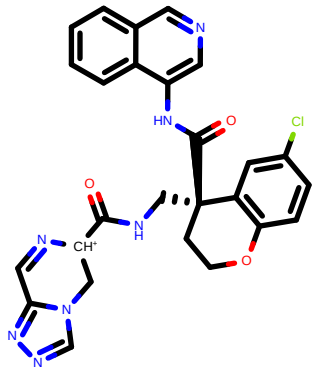
CID:	EN300-7121836_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cn[nH]c5F
RUN:	RUN9609
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.27

EN300-2977549_4_1



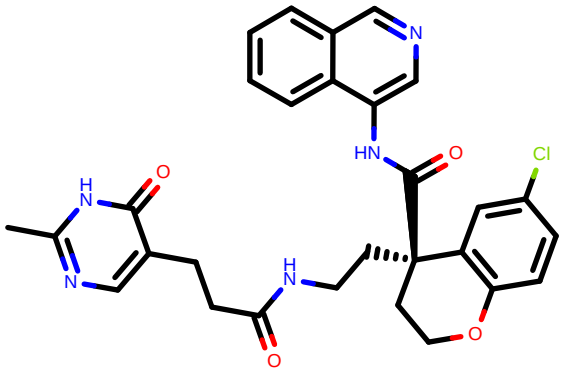
CID:	EN300-2977549_4_1
SMILES:	CNC(=O)COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN603
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.32

EN300-309106_2_1



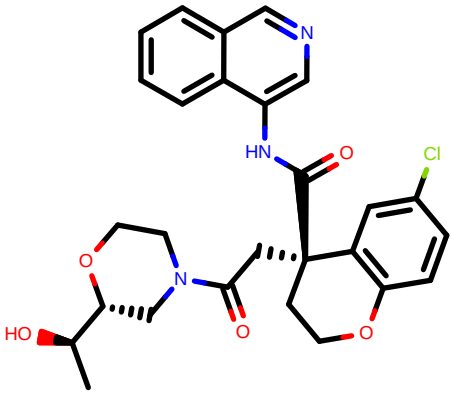
CID:	EN300-309106_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn6cnnc6cn5
RUN:	RUN8227
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.24

EN300-6734334_3_1



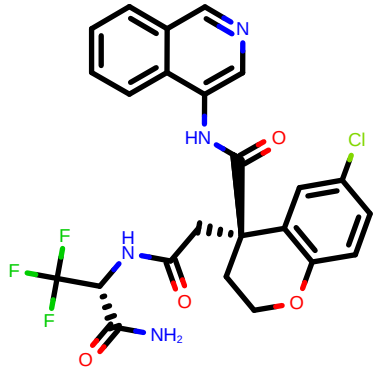
CID:	EN300-6734334_3_1
SMILES:	Cc1[nH]cc(c(=O)n1)CCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10896
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.40

EN300-254840_1_4



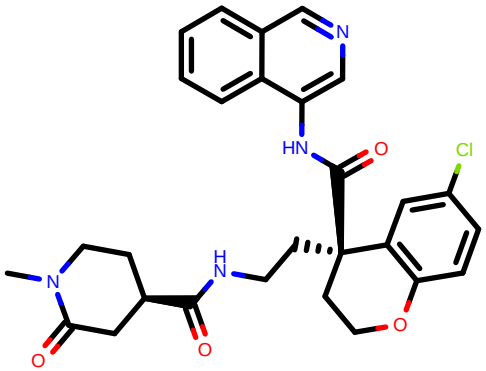
CID:	EN300-254840_1_4
SMILES:	C[C@H]([C@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10388
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.31

EN300-6763470_1_2



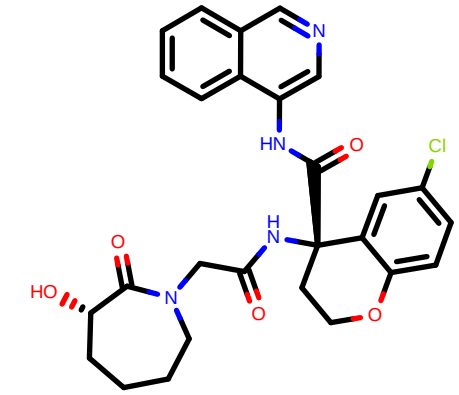
CID:	EN300-6763470_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H](C(=O)N)C(F)(F)F
RUN:	RUN9694
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.25

EN300-30458_3_2



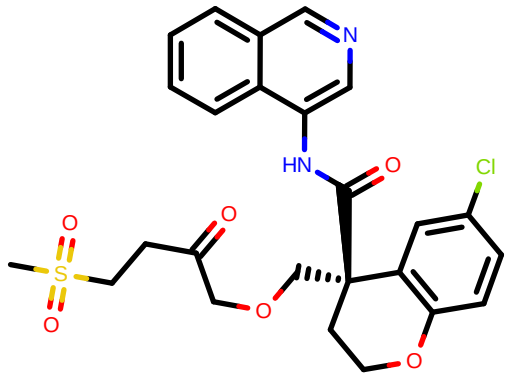
CID:	EN300-30458_3_2
SMILES:	CN1CC[C@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5039
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.30

EN300-259849_1_1



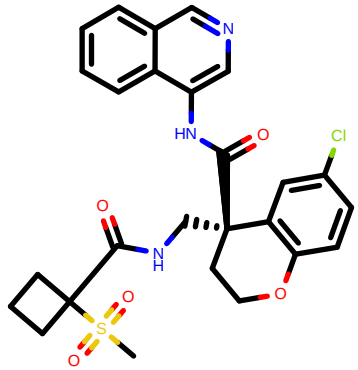
CID:	EN300-259849_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCCC[C@@H](C5=O)O
RUN:	RUN4165
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.35

EN300-1988306_2_1



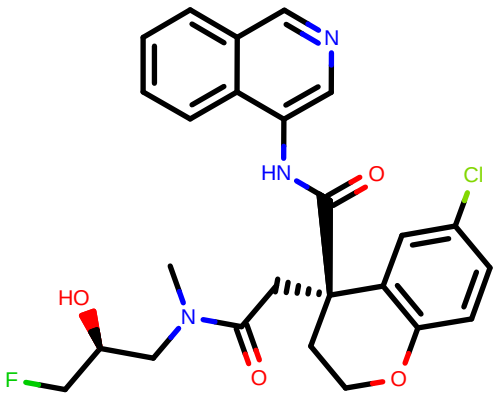
CID:	EN300-1988306_2_1
SMILES:	CS(=O)(=O)CCC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1605
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.39

EN300-191771_2_1



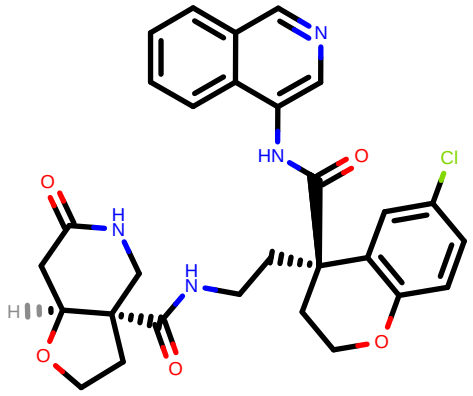
CID:	EN300-191771_2_1
SMILES:	CS(=O)(=O)C1(CCC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3651
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.50

EN300-1651623_1_1



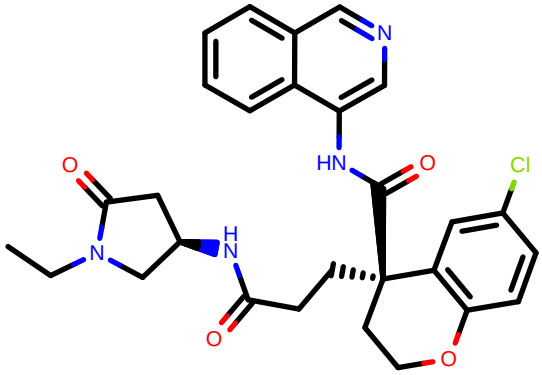
CID:	EN300-1651623_1_1
SMILES:	CN(C[C@@H](CF)O)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9874
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.30

EN300-6731226_3_1



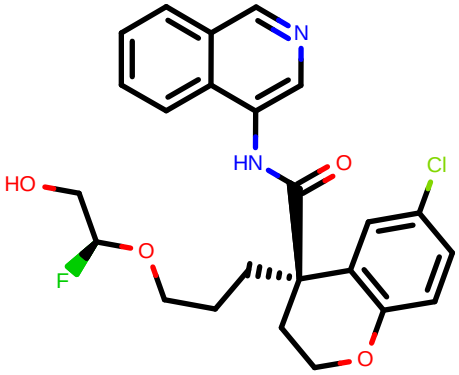
CID:	EN300-6731226_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@]56CCO[C@H]5CC(=O)NC6
RUN:	RUN4439
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.37

EN300-237952_2_1



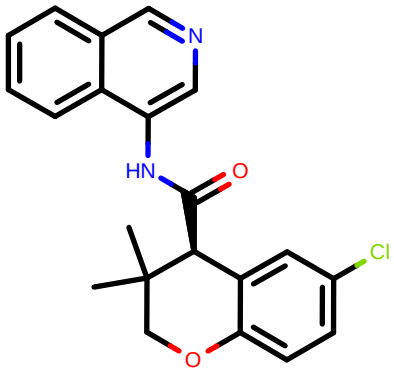
CID:	EN300-237952_2_1
SMILES:	CCN1C[C@@H](CC1=O)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5883
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.34

EN300-861925_4_2



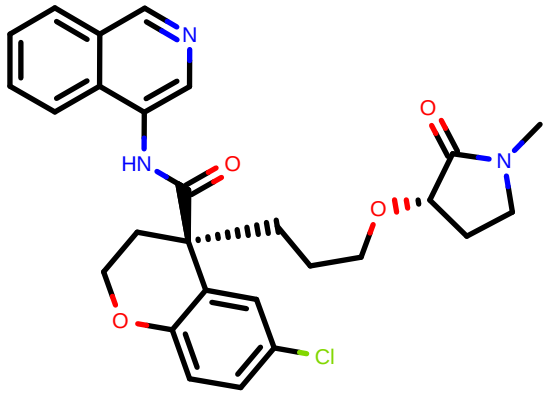
CID:	EN300-861925_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCO[C@H](CO)F
RUN:	RUN468
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.35

ADA-UCB-dc2b944c-15_1



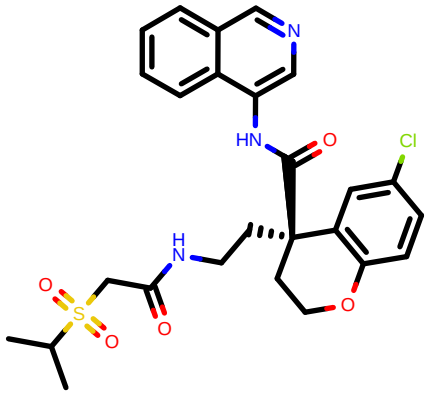
CID:	ADA-UCB-dc2b944c-15_1
SMILES:	CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C
RUN:	RUN155
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.12

EN300-98648_4_1



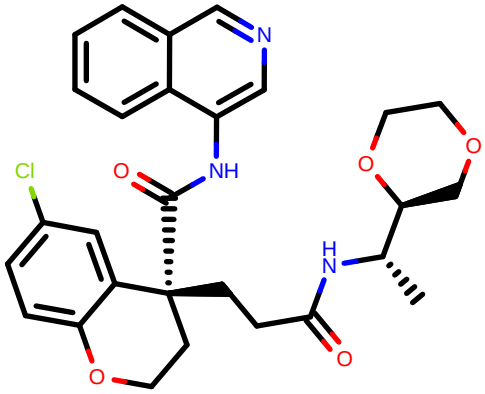
CID:	EN300-98648_4_1
SMILES:	CN1CC[C@@H](C1=O)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1926
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.33

EN300-51028_3_1



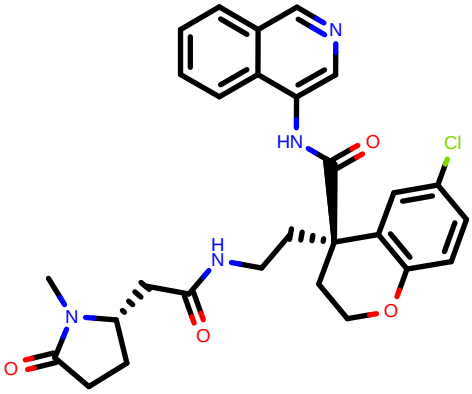
CID:	EN300-51028_3_1
SMILES:	CC(C)S(=O)(=O)CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5694
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.33

EN300-6736515_2_1



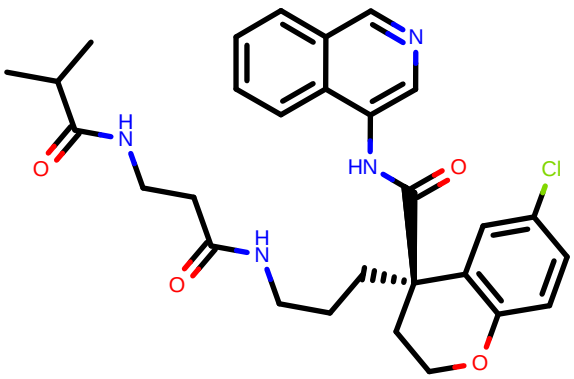
CID:	EN300-6736515_2_1
SMILES:	C[C@@H]([C@@H]1COCCO1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6750
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.29

EN300-207765_3_1



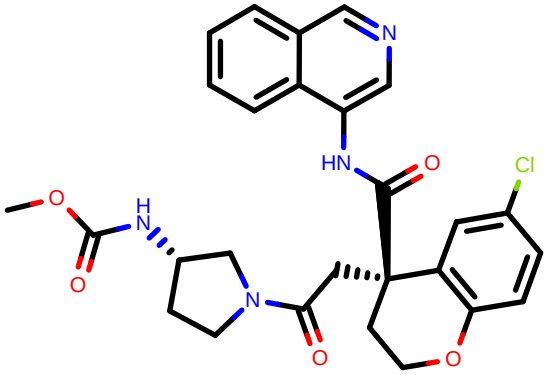
CID:	EN300-207765_3_1
SMILES:	CN1[C@@H](CCC1=O)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10736
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.37

EN300-31185_4_1



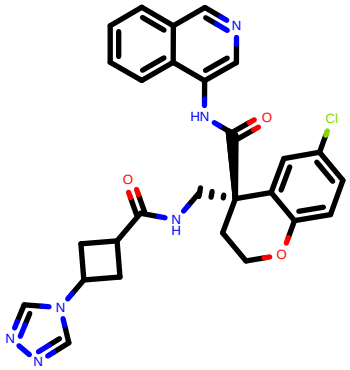
CID:	EN300-31185_4_1
SMILES:	CC(C)C(=O)NCCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10631
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.41

EN300-386187_1_1



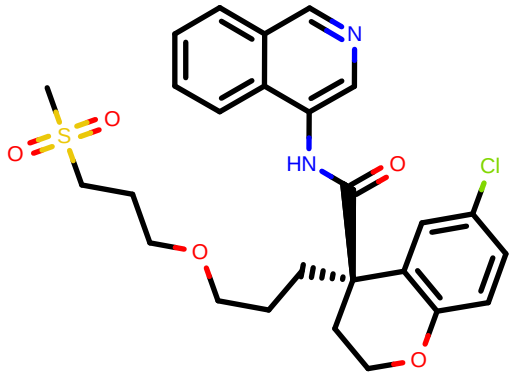
CID:	EN300-386187_1_1
SMILES:	COC(=O)N[C@H]1CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6653
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.36

EN300-1717596_2_1



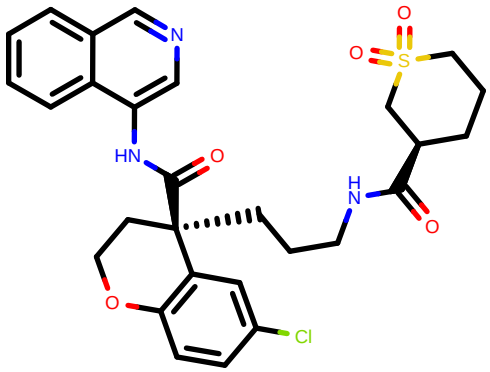
CID:	EN300-1717596_2_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)CNC(=O)[C@H]5C[C@@H](C5)n6cnnc6)cc1
RUN:	RUN7059
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.27

EN300-68794_4_1



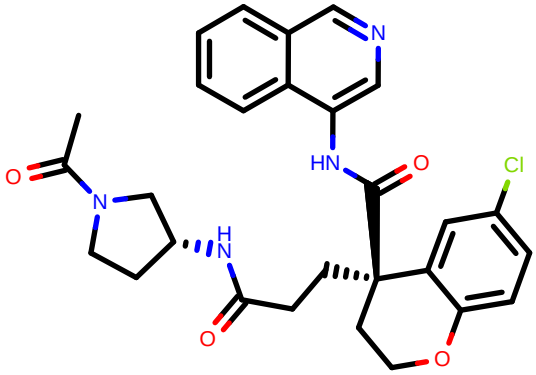
CID:	EN300-68794_4_1
SMILES:	CS(=O)(=O)CCCOCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1503
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.40

EN300-77778_4_1



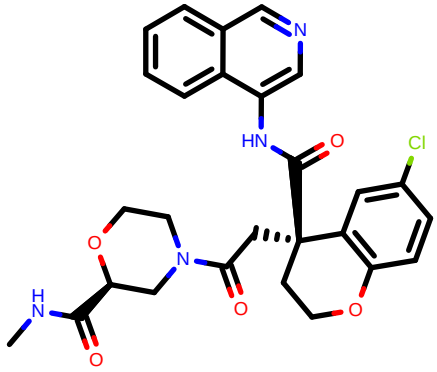
CID:	EN300-77778_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CCCS(=O)(=O)C5
RUN:	RUN10395
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.34

EN300-108407_2_2



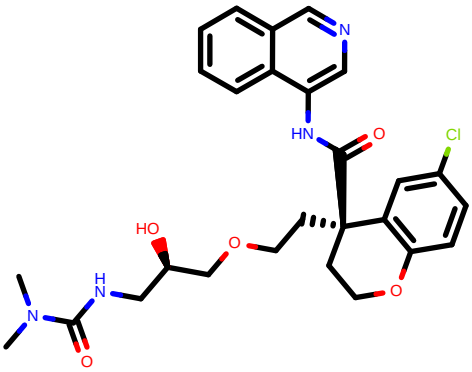
CID:	EN300-108407_2_2
SMILES:	CC(=O)N1CC[C@H](C1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5567
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.34

EN300-130644_1_1



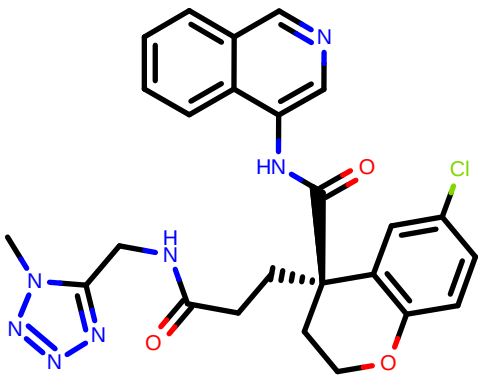
CID:	EN300-130644_1_1
SMILES:	CNC(=O)[C@@H]1CN(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2217
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.34

EN300-6501360_3_2



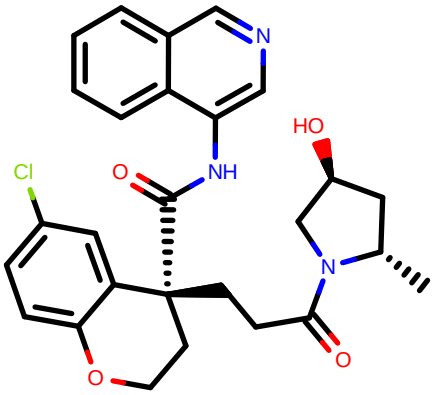
CID:	EN300-6501360_3_2
SMILES:	CN(C)C(=O)NC[C@H](COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1012
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.33

EN300-156212_2_1



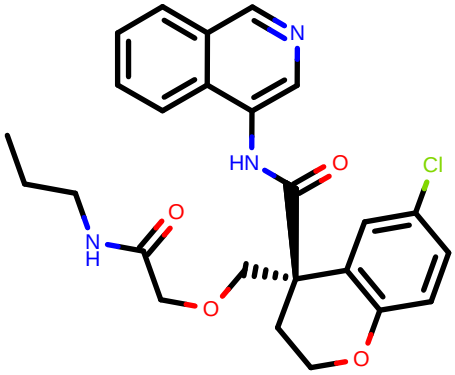
CID:	EN300-156212_2_1
SMILES:	Cn1c(nnn1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5695
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.25

EN300-173562_2_2



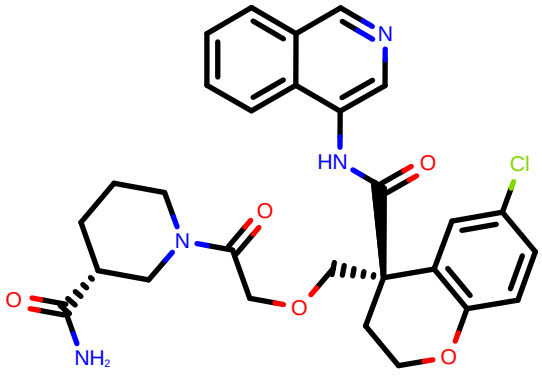
CID:	EN300-173562_2_2
SMILES:	C[C@H]1C[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4796
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.24

EN300-17184_2_1



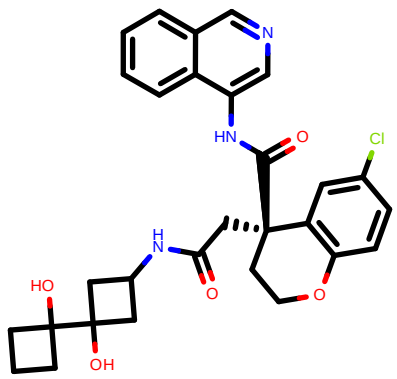
CID:	EN300-17184_2_1
SMILES:	C=CCNC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN315
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.28

EN300-22880_2_2



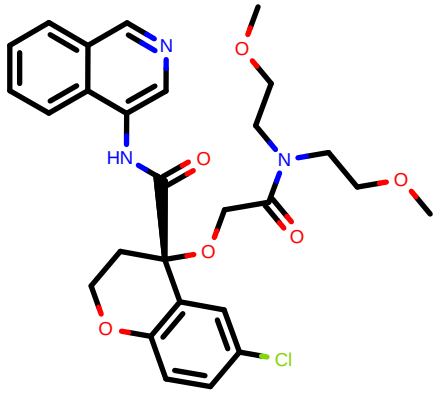
CID:	EN300-22880_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCC(=O)N5CCC[C@H](C5)C(=O)N
RUN:	RUN570
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.49

EN300-7465104_1_1



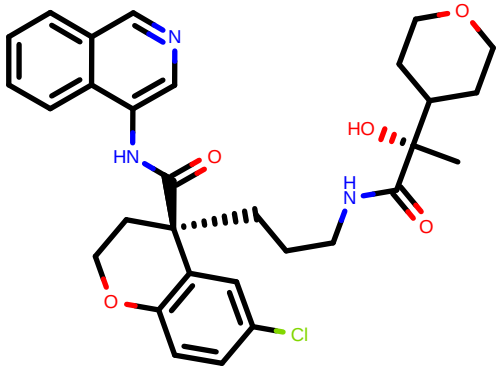
CID:	EN300-7465104_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)(C6(CCC6)O)O
RUN:	RUN4579
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.34

EN300-04491_1_1



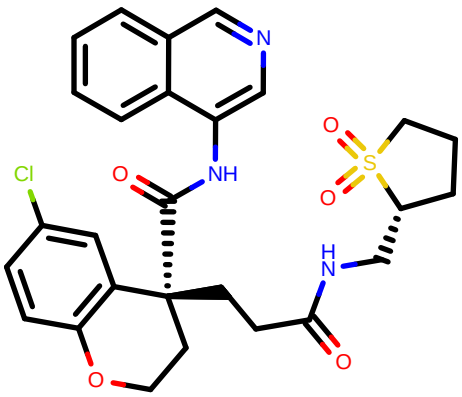
CID:	EN300-04491_1_1
SMILES:	COCCN(CCOC)C(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2007
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.53

EN300-217499_4_2



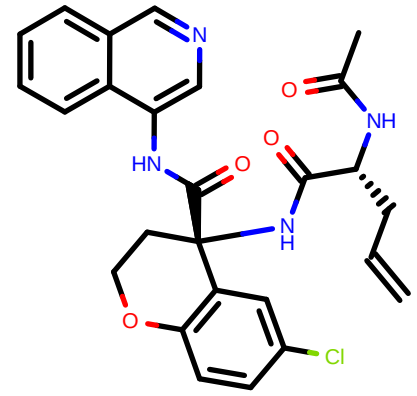
CID:	EN300-217499_4_2
SMILES:	C[C@](C1CCOCC1)(C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10635
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.43

EN300-246808_2_2



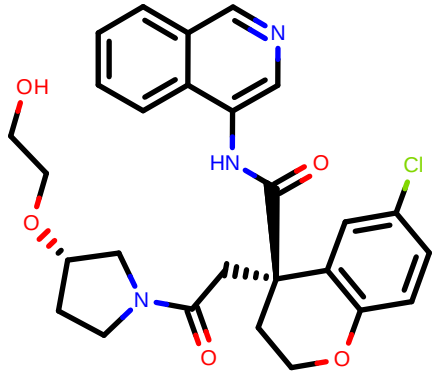
CID:	EN300-246808_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@H]5CCCS5(=O)=O
RUN:	RUN6546
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.36

EN300-43047_1_2



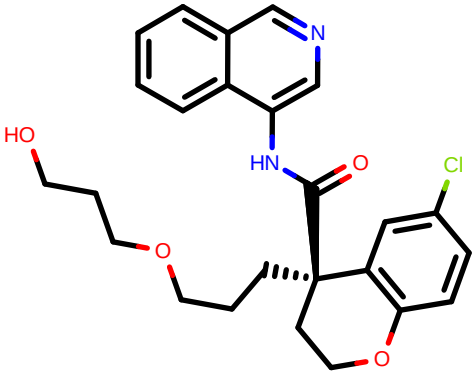
CID:	EN300-43047_1_2
SMILES:	CC(=O)N[C@H](CC=C)C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4797
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.26

EN300-6764893_1_1



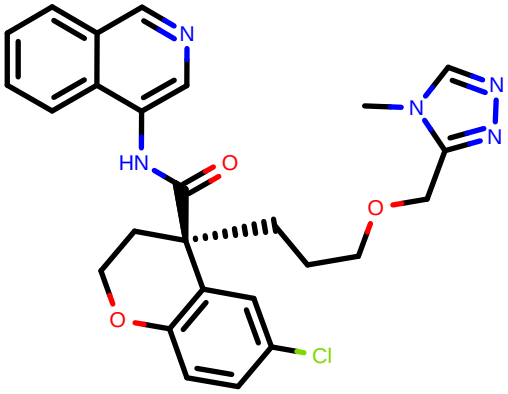
CID:	EN300-6764893_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)OCCO
RUN:	RUN9718
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.41

EN300-221518_4_1



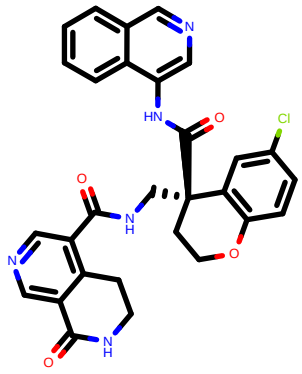
CID:	EN300-221518_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCCO
RUN:	RUN768
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.37

EN300-113112_4_1



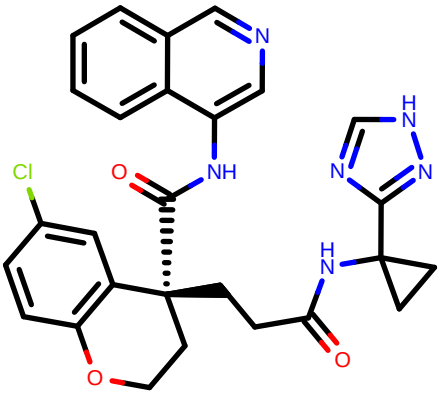
CID:	EN300-113112_4_1
SMILES:	Cn1cnnc1COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN824
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.34

EN300-314274_2_1



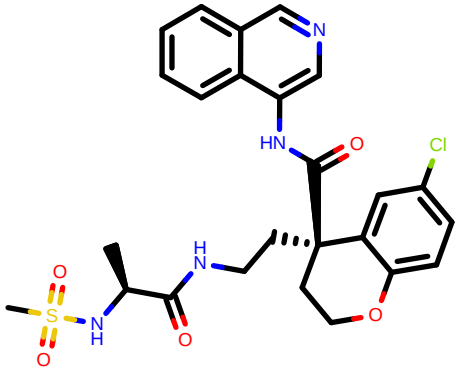
CID:	EN300-314274_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cncc6c5CCNC6=O
RUN:	RUN8411
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.38

EN300-7434398_2_1



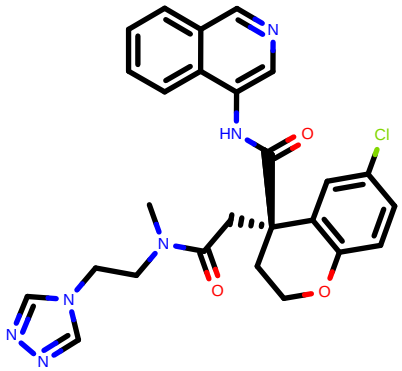
CID:	EN300-7434398_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CC5)c6[nH]cnn6
RUN:	RUN5687
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.29

EN300-31210_3_1



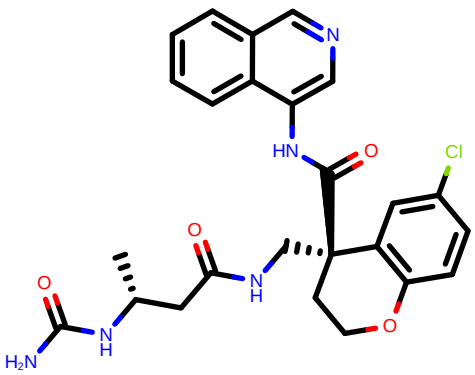
CID:	EN300-31210_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN4967
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.45

EN300-379046_1_1



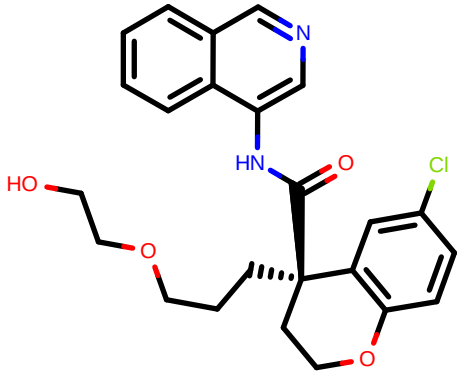
CID:	EN300-379046_1_1
SMILES:	CN(CCn1cnnc1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10840
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.27

EN300-268198_2_2



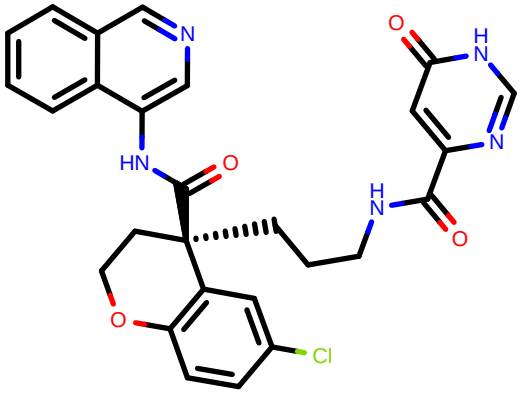
CID:	EN300-268198_2_2
SMILES:	C[C@H](CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN581
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.36

EN300-21258_4_1



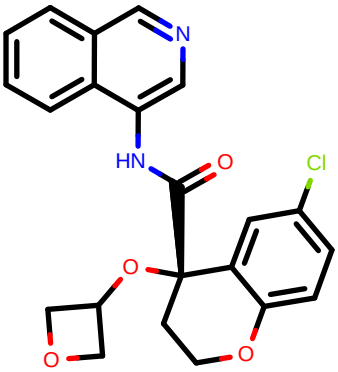
CID:	EN300-21258_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCCO
RUN:	RUN563
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.30

EN300-817811_4_1



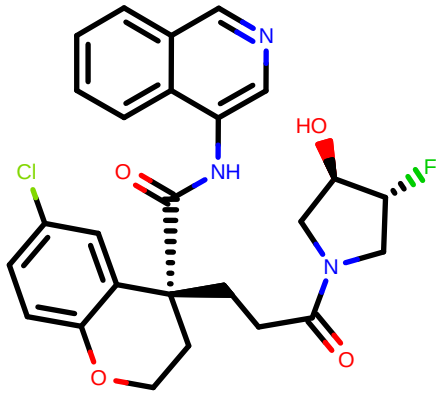
CID:	EN300-817811_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cc(=O)[nH]cn5
RUN:	RUN10144
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.33

EN300-317082_1_1



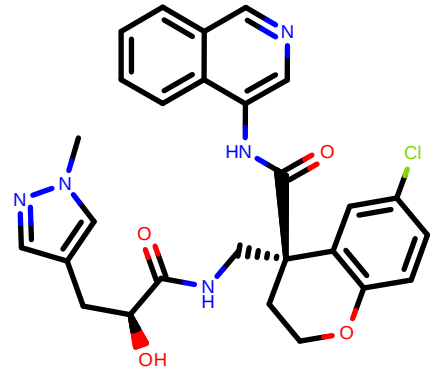
CID:	EN300-317082_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5COC5
RUN:	RUN2111
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.15

EN300-317085_2_1



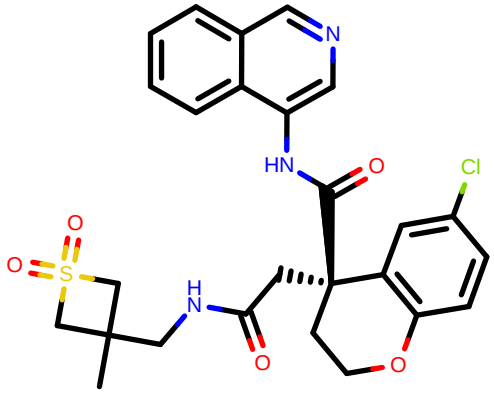
CID:	EN300-317085_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C[C@H]([C@@H](C5)F)O
RUN:	RUN3956
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.28

EN300-172020_2_1



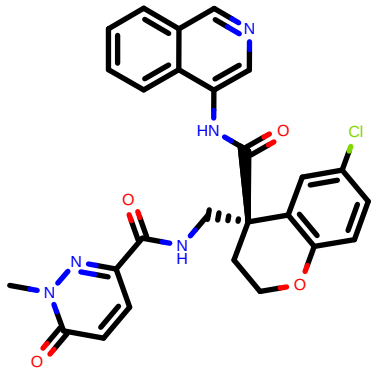
CID:	EN300-172020_2_1
SMILES:	Cn1cc(cn1)C[C@@H](C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3191
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.39

EN300-1706173_1_1



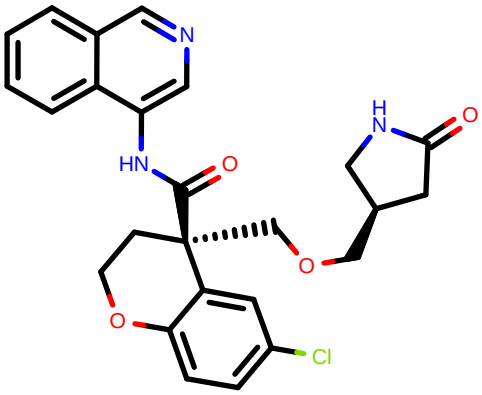
CID:	EN300-1706173_1_1
SMILES:	CC1(CS(=O)(=O)C1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5942
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.30

EN300-05798_2_1



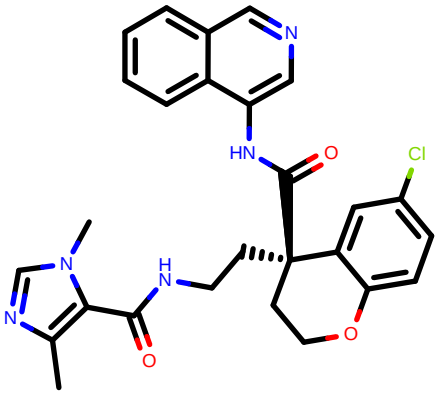
CID:	EN300-05798_2_1
SMILES:	Cn1c(=O)ccc(n1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8239
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.25

EN300-246747_2_1



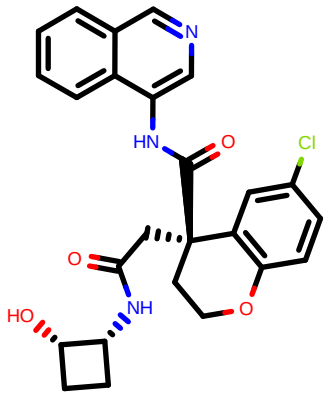
CID:	EN300-246747_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CC(=O)NC5
RUN:	RUN1861
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.23

EN300-6498351_3_1



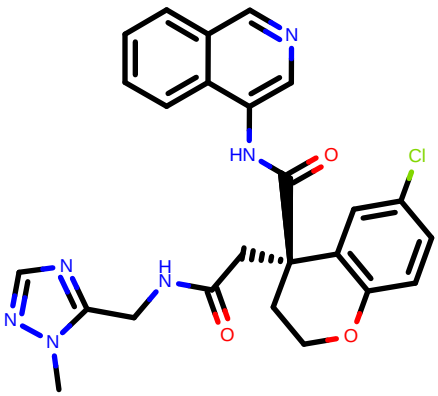
CID:	EN300-6498351_3_1
SMILES:	Cc1c(n(cn1)C)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10137
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.29

EN300-129424_1_1



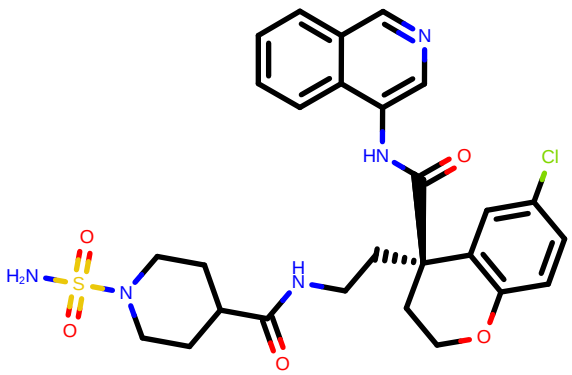
CID:	EN300-129424_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CC[C@@H]5O
RUN:	RUN9602
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.22

EN300-124063_1_1



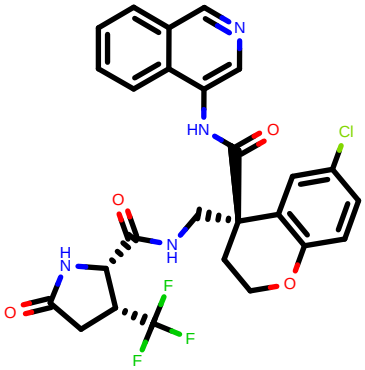
CID:	EN300-124063_1_1
SMILES:	Cn1c(ncn1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10220
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.31

EN300-31102_3_1



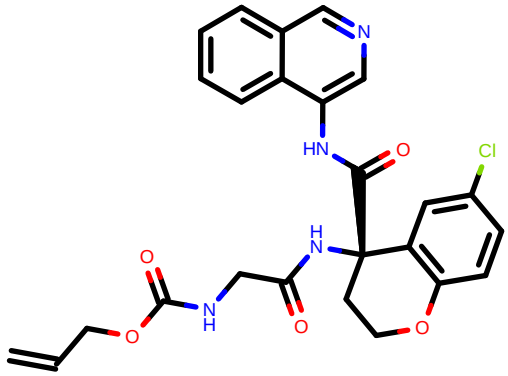
CID:	EN300-31102_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CCN(CC5)S(=O)(=O)N
RUN:	RUN4255
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.40

EN300-169955_2_1



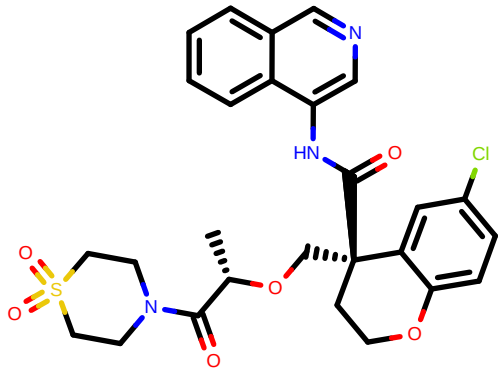
CID:	EN300-169955_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5[C@@H](CC(=O)N5)C(F)(F)F
RUN:	RUN2839
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.39

EN300-866702_1_1



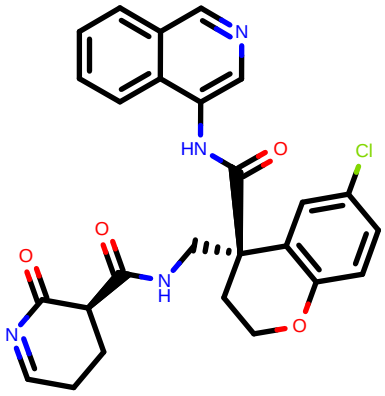
CID:	EN300-866702_1_1
SMILES:	C=CCOC(=O)NCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN5376
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.26

EN300-1265949_2_1



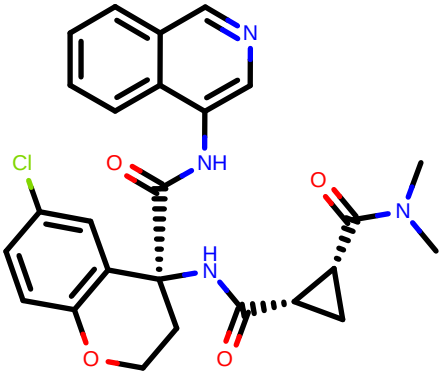
CID:	EN300-1265949_2_1
SMILES:	C[C@@H](C(=O)N1CCS(=O)(=O)CC1)OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2591
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.37

EN300-82616_2_2



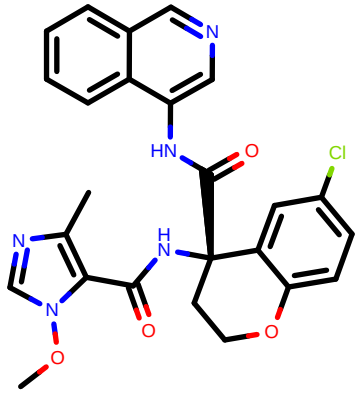
CID:	EN300-82616_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCCNC5=O
RUN:	RUN5825
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.28

EN300-253462_1_1



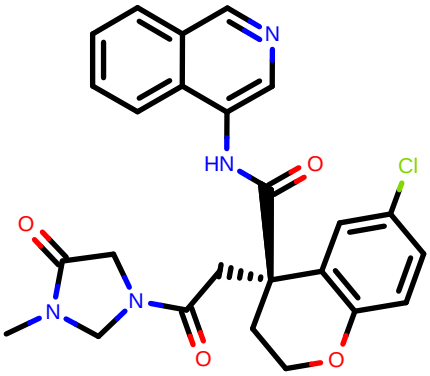
CID:	EN300-253462_1_1
SMILES:	CN(C)C(=O)[C@@H]1C[C@@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4221
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.29

EN300-7442332_1_1



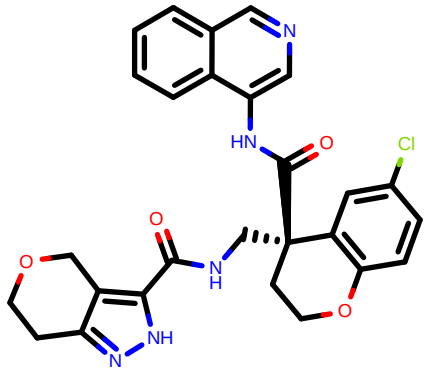
CID:	EN300-7442332_1_1
SMILES:	Cc1c(n(cn1)OC)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7566
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.32

EN300-126548_1_1



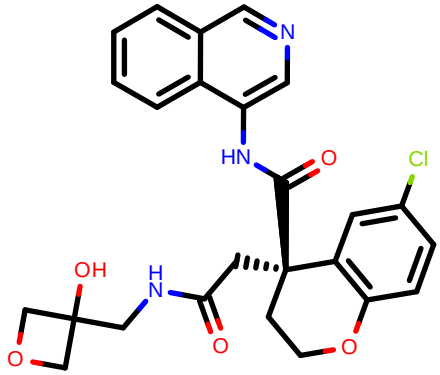
CID:	EN300-126548_1_1
SMILES:	CN1CN(CC1=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5338
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.24

EN300-103031_2_1



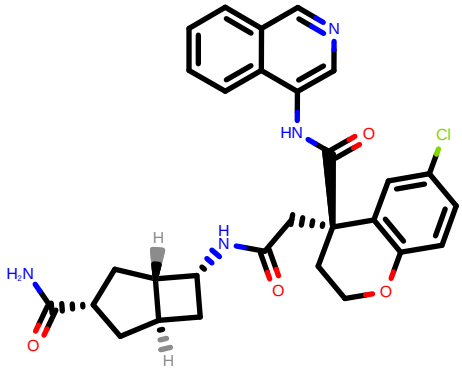
CID:	EN300-103031_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c6c([nH]n5)CCOC6
RUN:	RUN7655
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.33

EN300-1215712_1_1



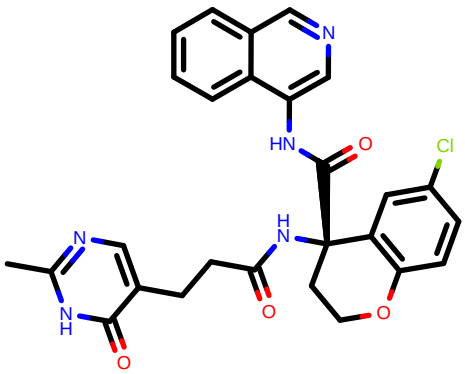
CID:	EN300-1215712_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(COC5)O
RUN:	RUN7640
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.27

EN300-1268016_1_9



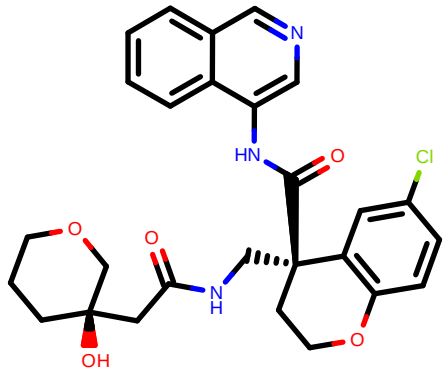
CID:	EN300-1268016_1_9
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN11290
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.32

EN300-6734334_1_1



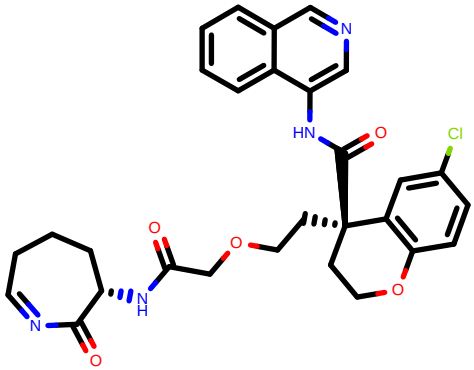
CID:	EN300-6734334_1_1
SMILES:	Cc1[nH]cc(c(=O)n1)CCC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN298
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.27

EN300-1071940_2_1



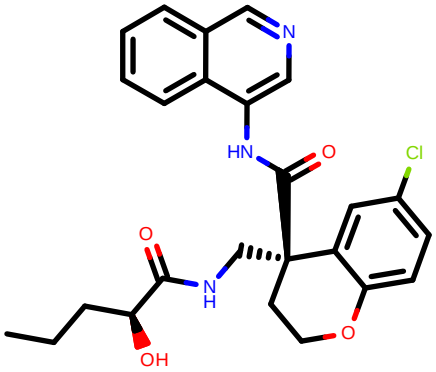
CID:	EN300-1071940_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C[C@@]5(CCCOC5)O
RUN:	RUN2479
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.31

EN300-37195_3_2



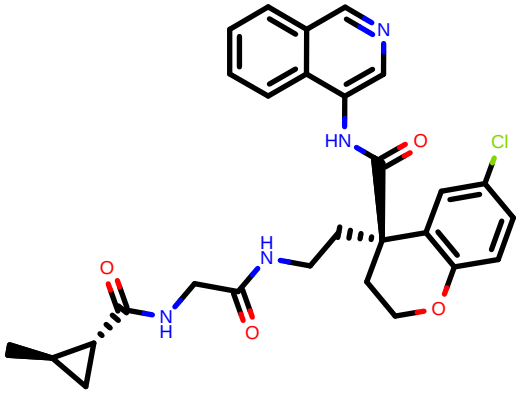
CID:	EN300-37195_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)N[C@H]5CCCCNC5=O
RUN:	RUN2530
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.31

EN300-316679_2_1



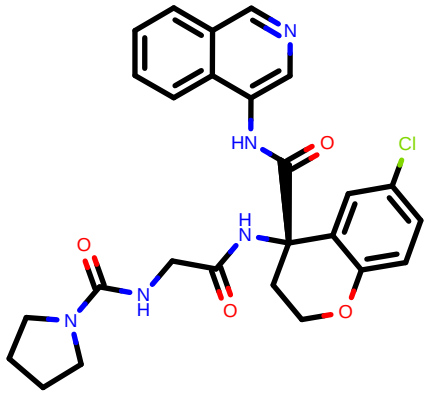
CID:	EN300-316679_2_1
SMILES:	CCC[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2959
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.40

EN300-30768_3_3



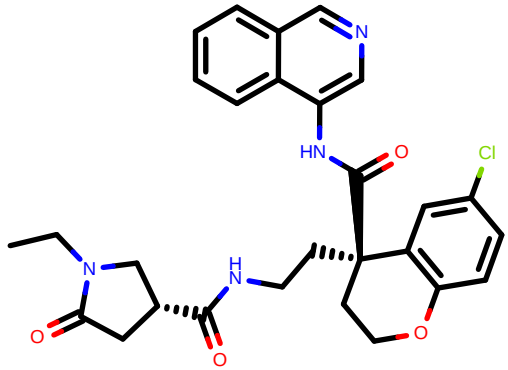
CID:	EN300-30768_3_3
SMILES:	C[C@@H]1C[C@H]1C(=O)NCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9096
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.29

EN300-383906_1_1



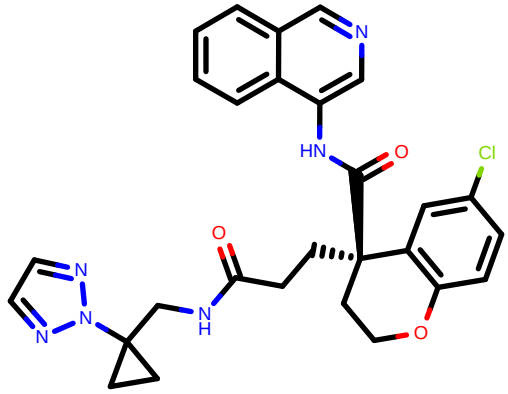
CID:	EN300-383906_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)N5CCCC5
RUN:	RUN5912
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.35

EN300-33478_3_1



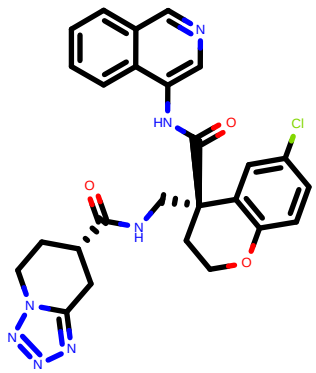
CID:	EN300-33478_3_1
SMILES:	CCN1C[C@@H](CC1=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8812
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.33

EN300-1722016_2_1



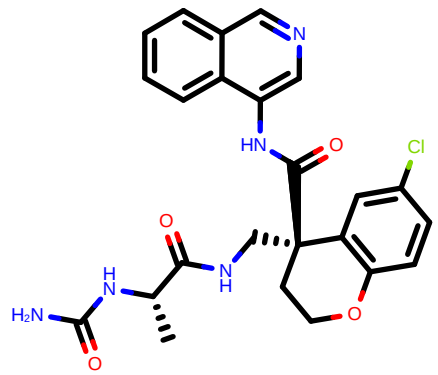
CID:	EN300-1722016_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5(CC5)n6nccn6
RUN:	RUN10813
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.24

EN300-1653482_2_2



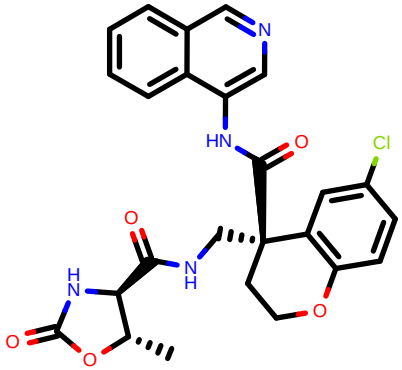
CID:	EN300-1653482_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCn6c(nnn6)C5
RUN:	RUN6225
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.30

EN300-152705_2_1



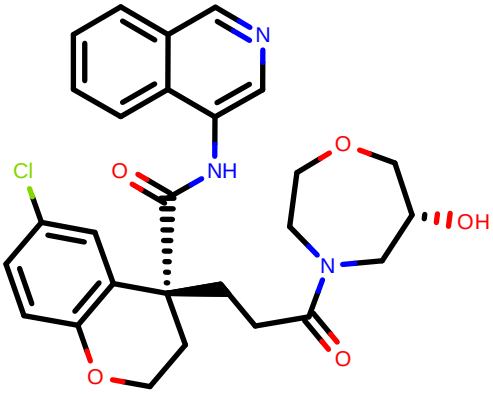
CID:	EN300-152705_2_1
SMILES:	C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN5745
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.33

EN300-172640_2_2



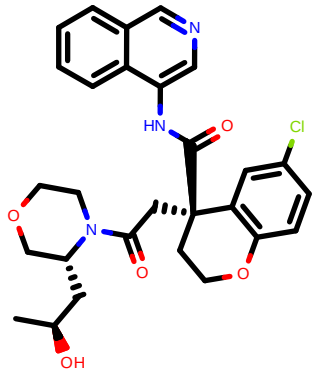
CID:	EN300-172640_2_2
SMILES:	C[C@H]1[C@@H](NC(=O)O1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5130
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.28

EN300-233951_2_1



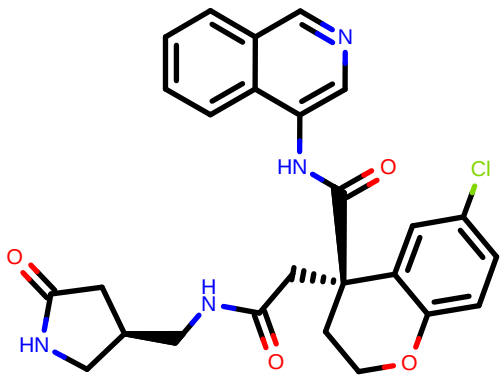
CID:	EN300-233951_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@@H](C5)O
RUN:	RUN5264
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.32

EN300-139130_1_1



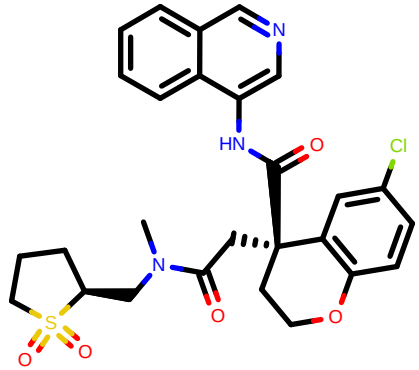
CID:	EN300-139130_1_1
SMILES:	C[C@@H](C[C@@H]1COCCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN4747
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.32

EN300-238405_1_1



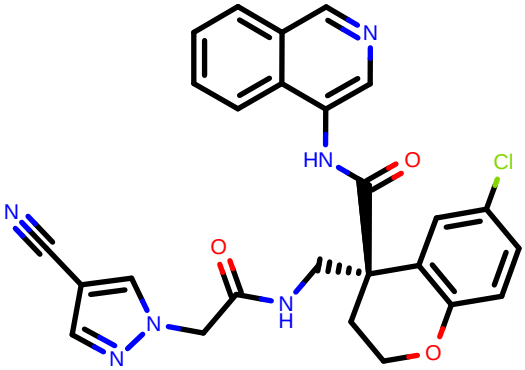
CID:	EN300-238405_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CC(=O)NC5
RUN:	RUN3672
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.28

EN300-7542465_1_1



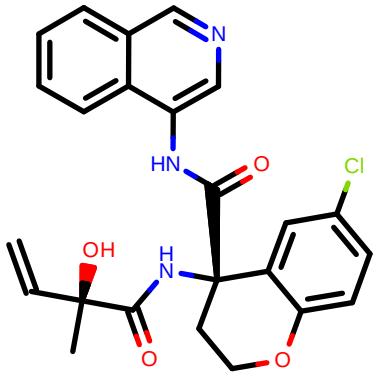
CID:	EN300-7542465_1_1
SMILES:	CN(C[C@@H]1CCCS1(=O)=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10992
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.28

EN300-1590388_2_1



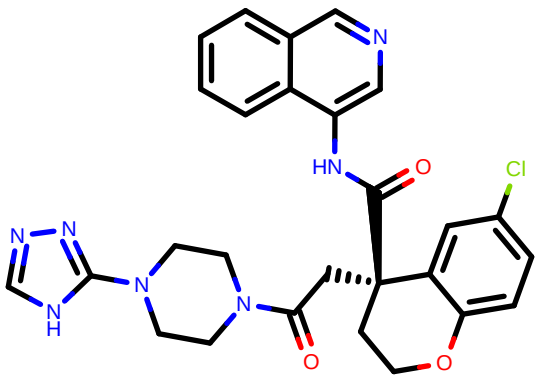
CID:	EN300-1590388_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cc(cn5)C#N
RUN:	RUN5026
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.31

EN300-248888_1_2



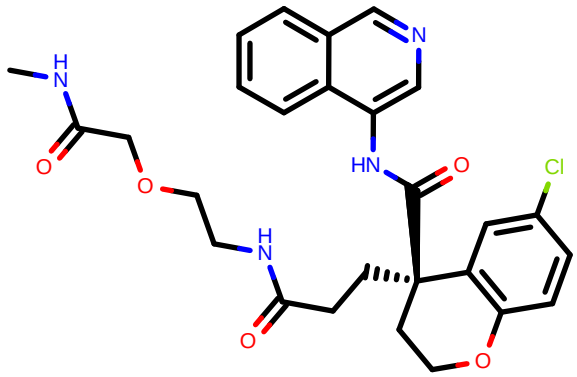
CID:	EN300-248888_1_2
SMILES:	C[C@](C=C)(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN3494
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.26

EN300-266552_1_1



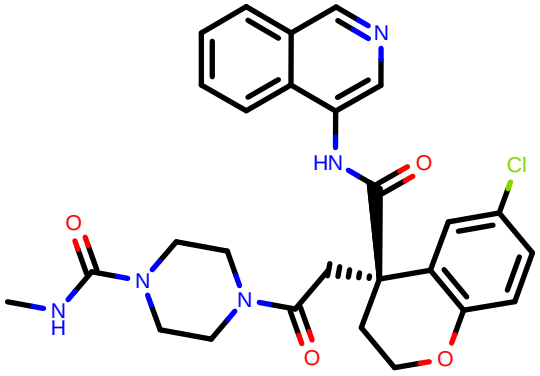
CID:	EN300-266552_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)c6[nH]cnn6
RUN:	RUN415
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.34

EN300-126575_2_1



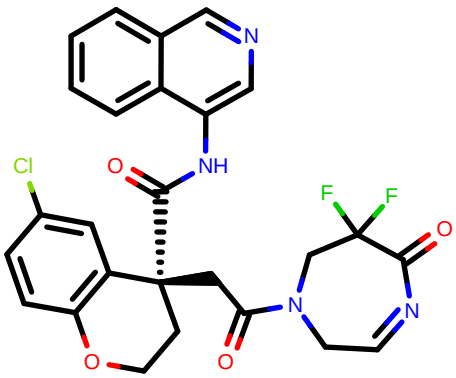
CID:	EN300-126575_2_1
SMILES:	CNC(=O)COCCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10909
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.28

EN300-147628_1_1



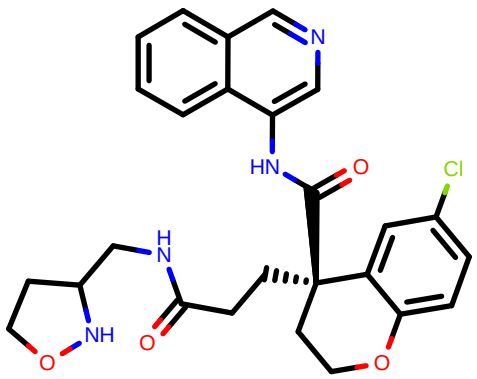
CID:	EN300-147628_1_1
SMILES:	CNC(=O)N1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2884
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.32

EN300-1083988_1_1



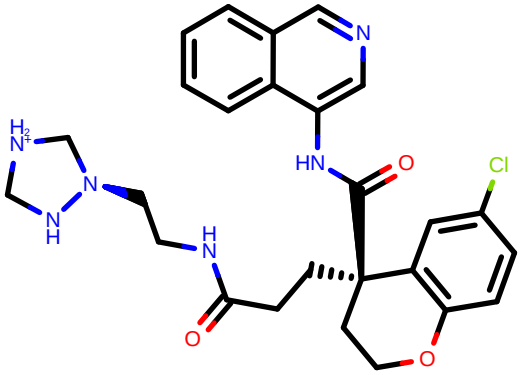
CID:	EN300-1083988_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCNC(=O)C(C5)(F)F
RUN:	RUN9570
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.28

EN300-1720418_2_1



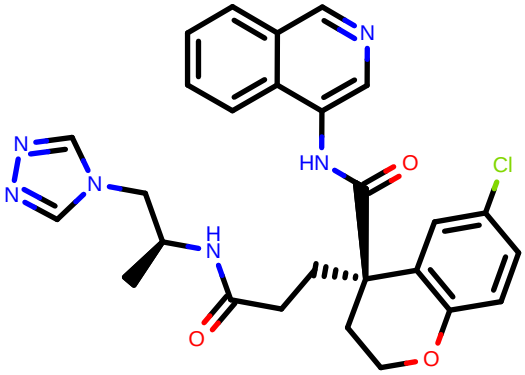
CID:	EN300-1720418_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5=NOCC5
RUN:	RUN5815
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.28

EN300-69553_2_1



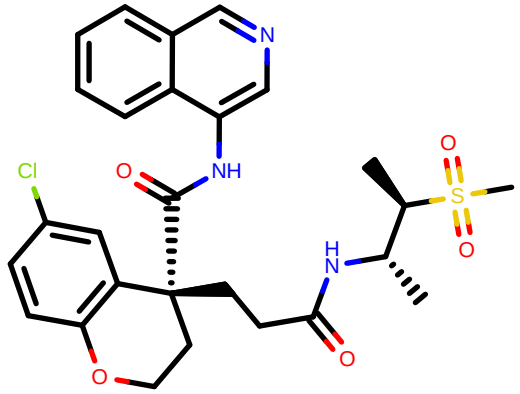
CID:	EN300-69553_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCn5cncn5
RUN:	RUN8205
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.22

EN300-7501753_2_1



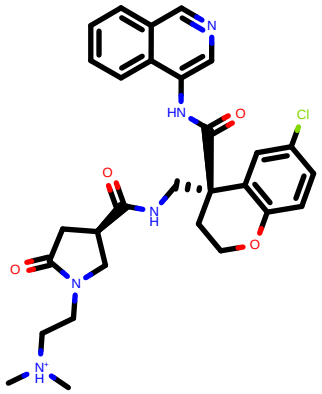
CID:	EN300-7501753_2_1
SMILES:	C[C@@H](Cn1cnnc1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4936
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.29

EN300-83434_2_1



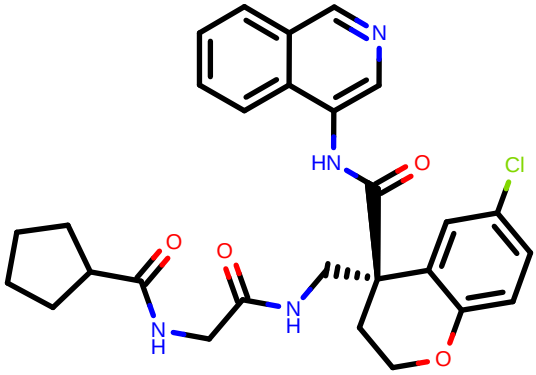
CID:	EN300-83434_2_1
SMILES:	C[C@@H]([C@@H](C)S(=O)(=O)C)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN8549
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.34

EN300-51735_2_1



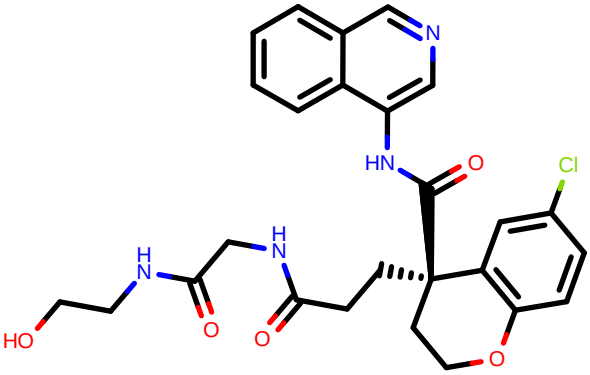
CID:	EN300-51735_2_1
SMILES:	CN(C)CCN1C[C@@H](CC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2562
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.43

EN300-36845_2_1



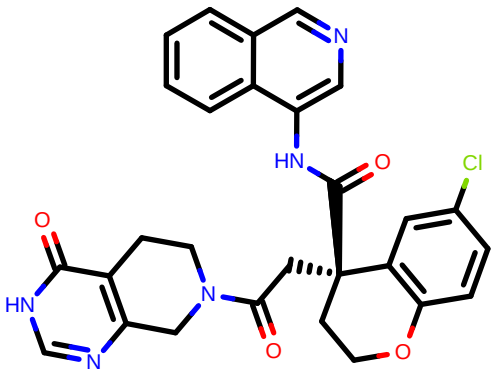
CID:	EN300-36845_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CNC(=O)C5CCCC5
RUN:	RUN2967
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.36

EN300-82181_2_1



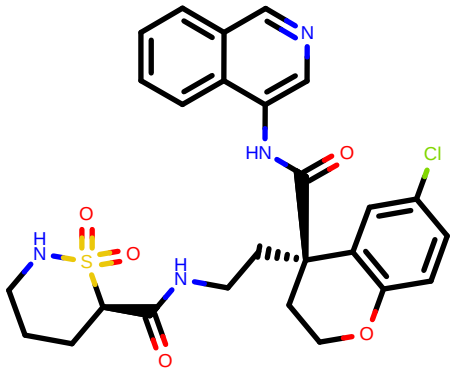
CID:	EN300-82181_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(=O)NCCO
RUN:	RUN10629
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.30

EN300-132141_1_1



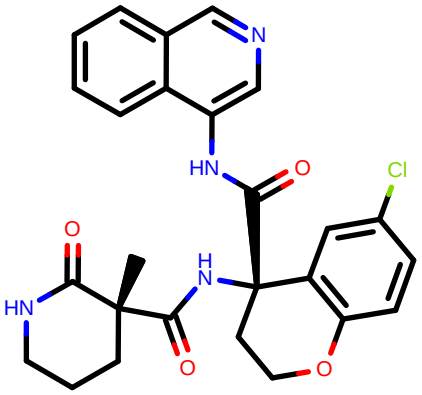
CID:	EN300-132141_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c(nc[nH]c6=O)C5
RUN:	RUN7508
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.29

EN300-1587757_3_2



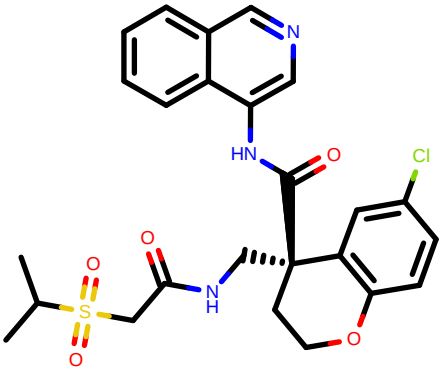
CID:	EN300-1587757_3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CCCNS5(=O)=O
RUN:	RUN3264
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.41

EN300-178876_1_2



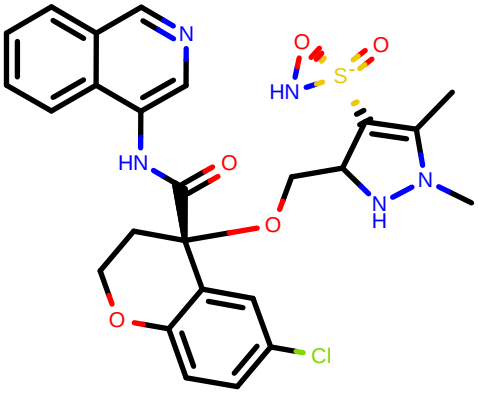
CID:	EN300-178876_1_2
SMILES:	C[C@]1(CCCNC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN6986
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.43

EN300-51028_2_1



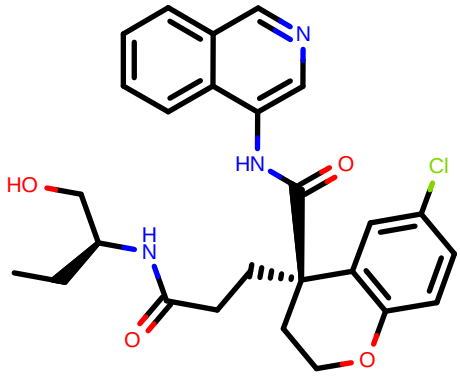
CID:	EN300-51028_2_1
SMILES:	CC(C)S(=O)(=O)CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2048
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.38

EN300-1629199_1_1



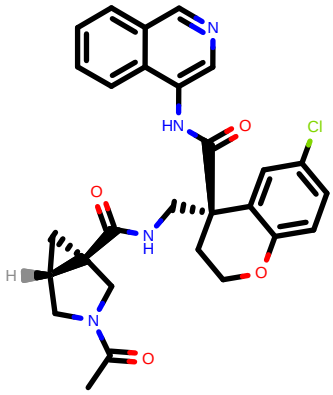
CID:	EN300-1629199_1_1
SMILES:	Cc1c(c(nn1C)CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)N
RUN:	RUN1520
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.35

EN300-157897_2_1



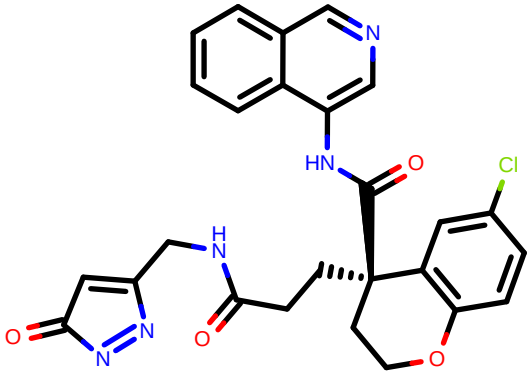
CID:	EN300-157897_2_1
SMILES:	CC[C@@H](CO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN780
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.32

EN300-313062_2_1



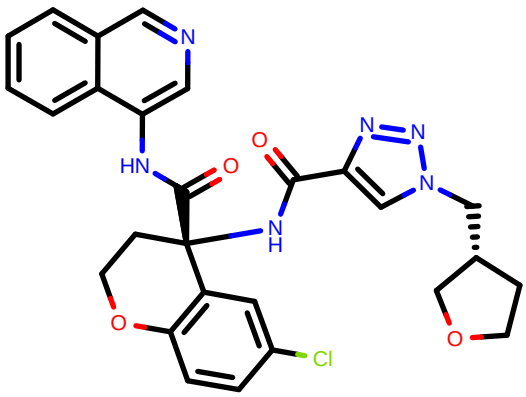
CID:	EN300-313062_2_1
SMILES:	CC(=O)N1C[C@@H]2C[C@@]2(C1)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8011
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.35

EN300-260760_2_1



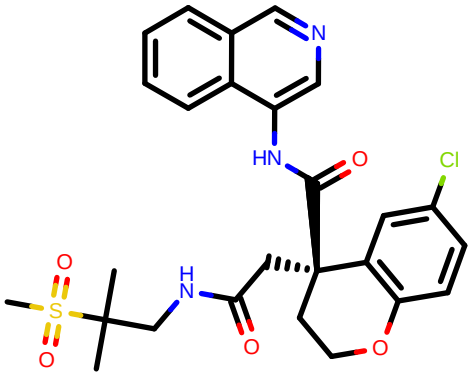
CID:	EN300-260760_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5cc(=O)[nH][nH]5
RUN:	RUN5591
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.26

EN300-317272_1_1



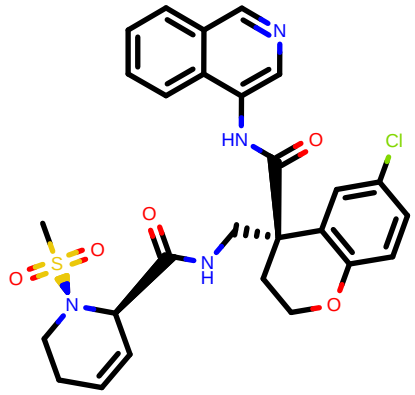
CID:	EN300-317272_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn(nn5)C[C@@H]6CCOC6
RUN:	RUN7826
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.28

EN300-100271_1_1



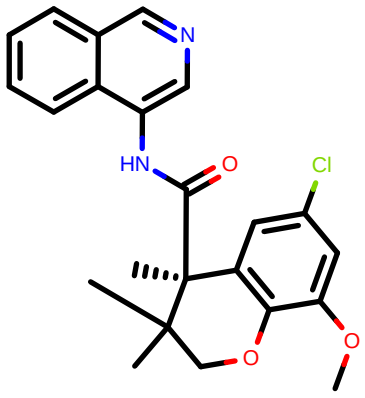
CID:	EN300-100271_1_1
SMILES:	CC(C)(CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN7280
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.32

EN300-24014_2_1



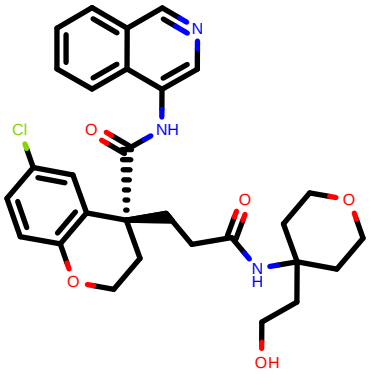
CID:	EN300-24014_2_1
SMILES:	CS(=O)(=O)N1CCCC[C@@H]1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2104
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.56

DAR-DIA-0d514e7d-27_1



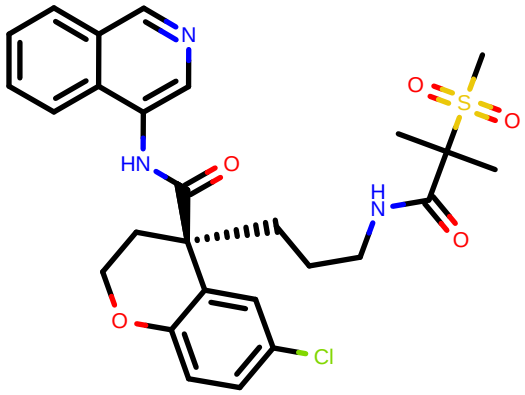
CID:	DAR-DIA-0d514e7d-27_1
SMILES:	C[C@@]1(c2cc(cc(c2OCC1(C)C)OC)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN172
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.20

EN300-300825_2_1



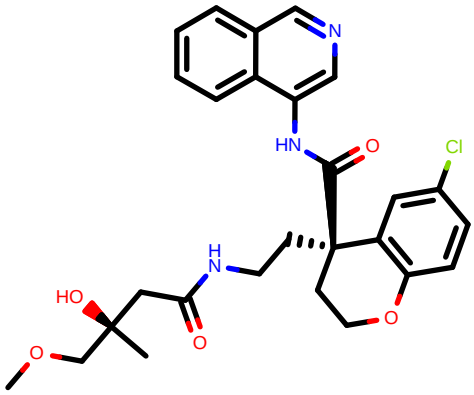
CID:	EN300-300825_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CCOCC5)CCO
RUN:	RUN5447
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.35

EN300-76205_4_1



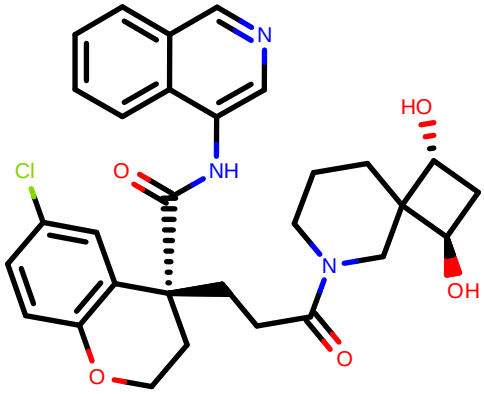
CID:	EN300-76205_4_1
SMILES:	CC(C)(C(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN9567
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.55

EN300-1296824_3_1



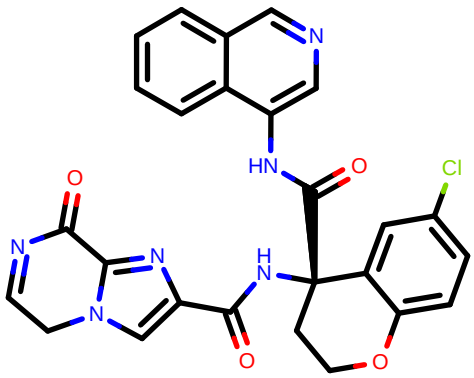
CID:	EN300-1296824_3_1
SMILES:	C[C@@](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(COC)O
RUN:	RUN2556
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.37

EN300-7445890_2_3



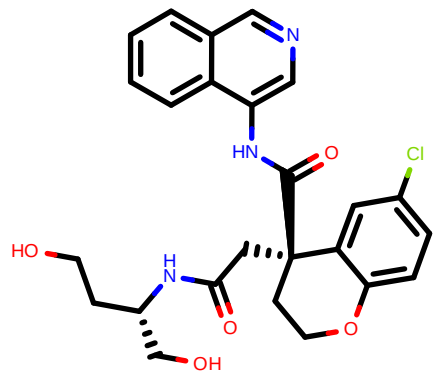
CID:	EN300-7445890_2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCC6(C5)[C@@H](C[C@H]6O)O
RUN:	RUN6853
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.38

EN300-746646_1_1



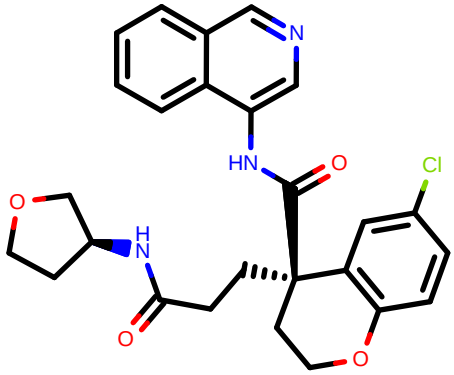
CID:	EN300-746646_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cn6cc[nH]c(=O)c6n5
RUN:	RUN8909
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.33

EN300-195790_1_1



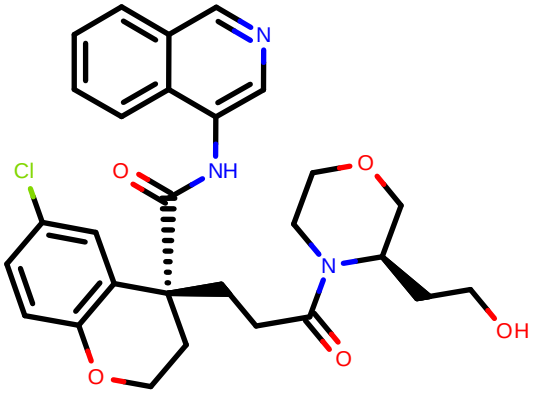
CID:	EN300-195790_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CCO)CO
RUN:	RUN7180
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.32

EN300-171752_2_2



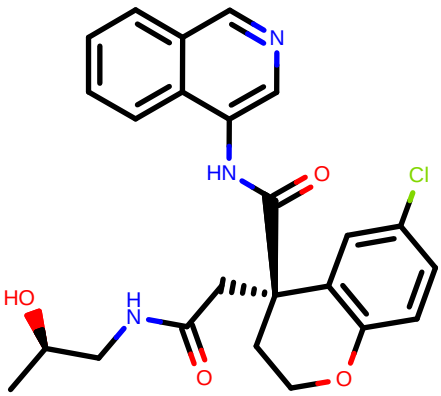
CID:	EN300-171752_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCOC5
RUN:	RUN5459
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.29

EN300-345754_2_2



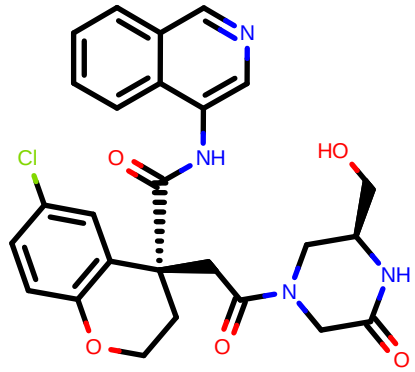
CID:	EN300-345754_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@H]5CCO
RUN:	RUN6510
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.38

EN300-117430_1_1



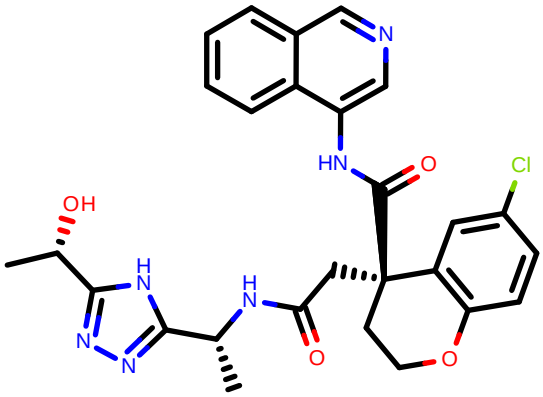
CID:	EN300-117430_1_1
SMILES:	C[C@H](CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN10111
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.34

EN300-100700_1_1



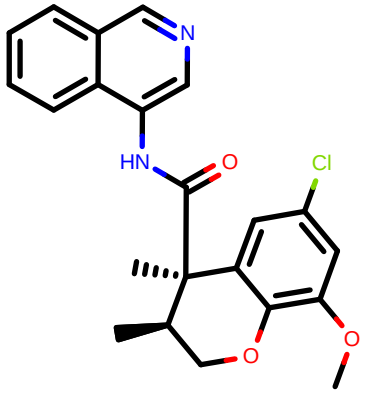
CID:	EN300-100700_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H](NC(=O)C5)CO
RUN:	RUN1218
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.33

EN300-7443527_1_4



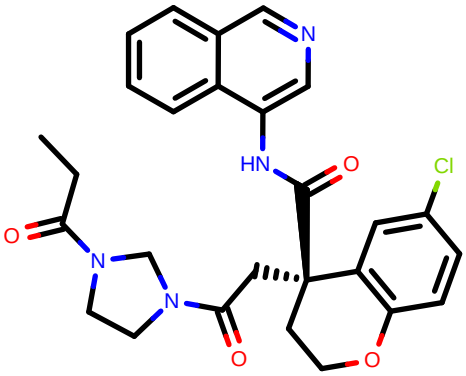
CID:	EN300-7443527_1_4
SMILES:	C[C@H](c1[nH]c(nn1)[C@H](C)O)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10250
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-26_1



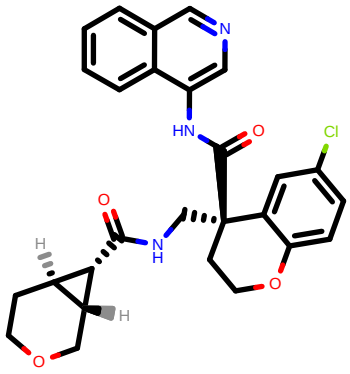
CID:	DAR-DIA-0d514e7d-26_1
SMILES:	C[C@@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN215
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.19

EN300-257790_1_1



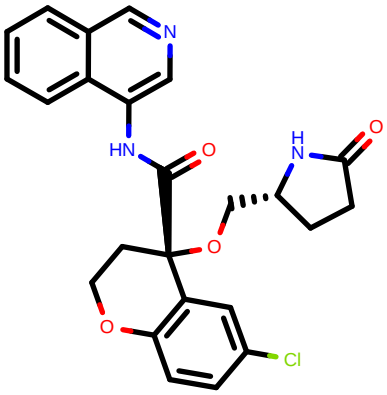
CID:	EN300-257790_1_1
SMILES:	CCC(=O)N1CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1625
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.35

EN300-1644723_2_8



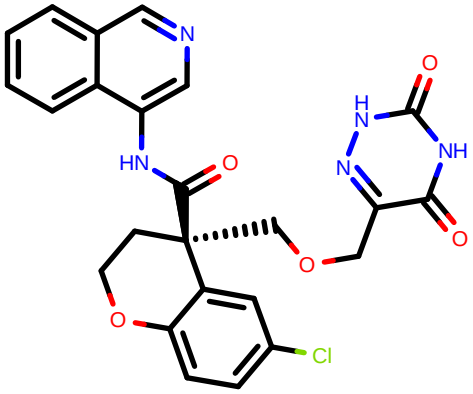
CID:	EN300-1644723_2_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5[C@H]6[C@H]5COCC6
RUN:	RUN6440
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

EN300-195756_1_2



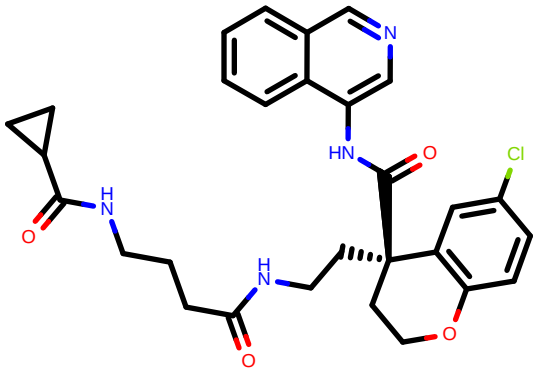
CID:	EN300-195756_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5CCC(=O)N5
RUN:	RUN2485
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.24

EN300-761746_2_1



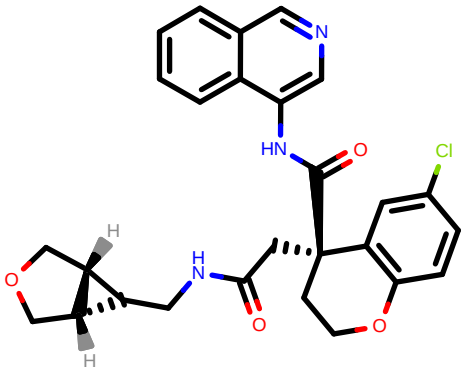
CID:	EN300-761746_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5c(=O)[nH]c(=O)[nH]n5
RUN:	RUN2330
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.30

EN300-36850_3_1



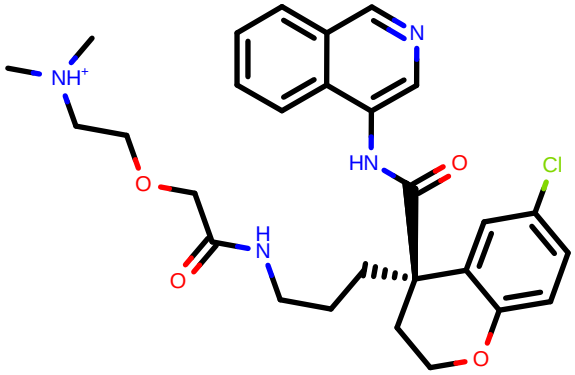
CID:	EN300-36850_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CCCNC(=O)C5CC5
RUN:	RUN10878
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.35

EN300-210089_1_2



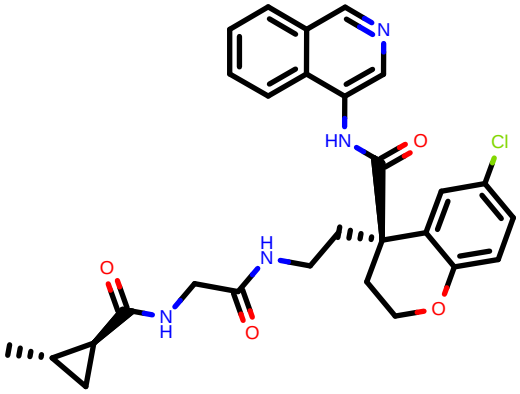
CID:	EN300-210089_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5[C@H]6[C@@H]5COC6
RUN:	RUN9117
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.25

EN300-1865348_4_1



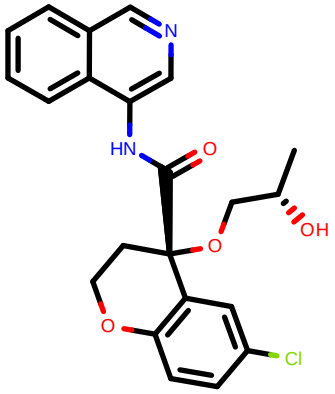
CID:	EN300-1865348_4_1
SMILES:	CN(C)CCOCC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10923
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.63

EN300-30768_3_2



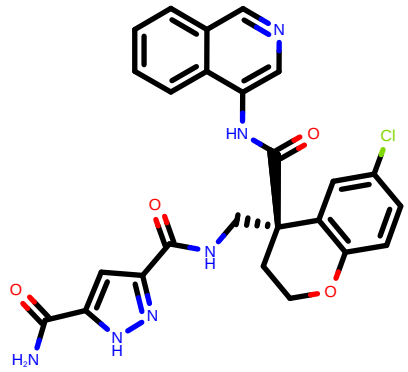
CID:	EN300-30768_3_2
SMILES:	C[C@H]1C[C@@H]1C(=O)NCC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10097
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.31

EN300-185378_1_1



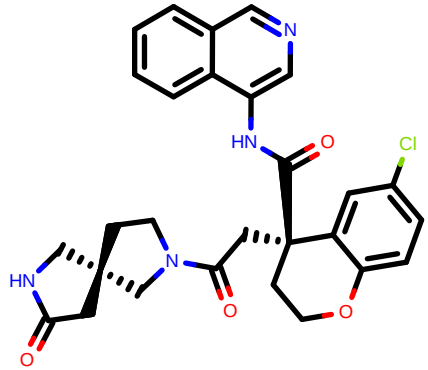
CID:	EN300-185378_1_1
SMILES:	C[C@@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1831
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

EN300-1689158_2_1



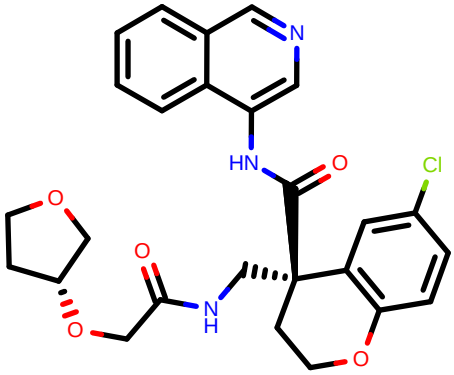
CID:	EN300-1689158_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc([nH]n5)C(=O)N
RUN:	RUN7151
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

EN300-187998_1_1



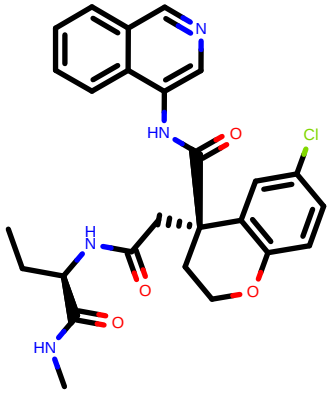
CID:	EN300-187998_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC6(C5)CC(=O)NC6
RUN:	RUN8160
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.30

EN300-99391_2_1



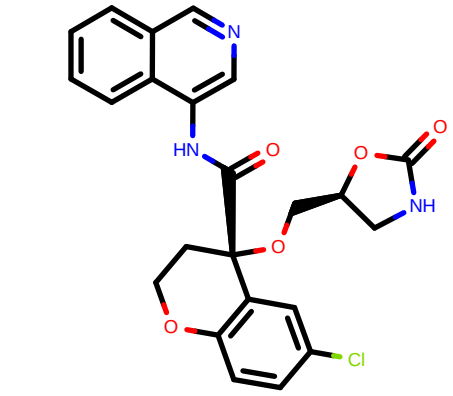
CID:	EN300-99391_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CO[C@@H]5CCOC5
RUN:	RUN716
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.29

EN300-249222_1_2



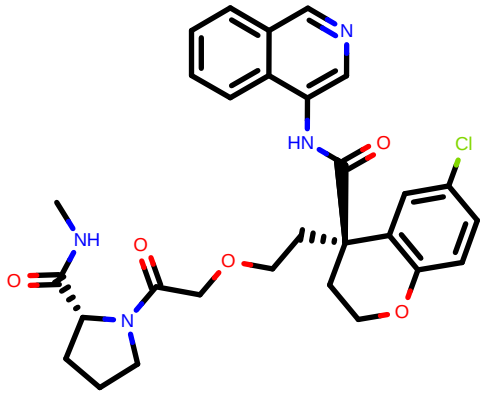
CID:	EN300-249222_1_2
SMILES:	CC[C@H](C(=O)NC)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9009
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

EN300-203293_1_1



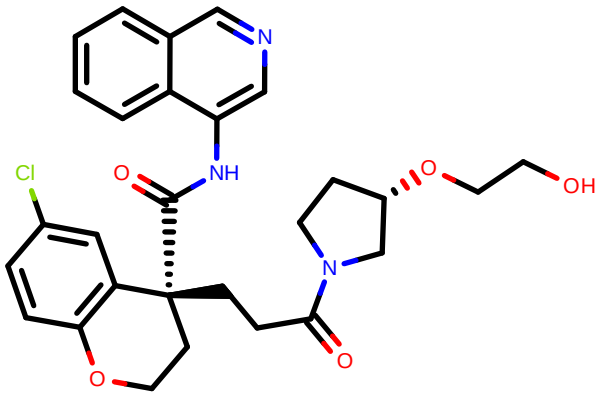
CID:	EN300-203293_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CNC(=O)O5
RUN:	RUN1847
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

EN300-48902_3_2



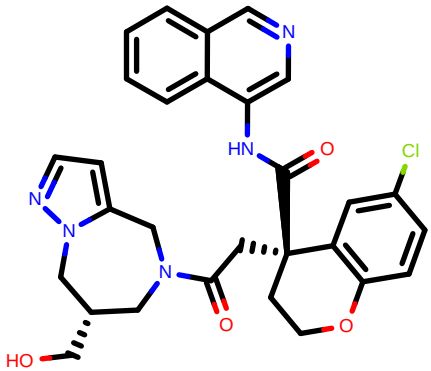
CID:	EN300-48902_3_2
SMILES:	CNC(=O)[C@H]1CCCN1C(=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1787
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.37

EN300-6764893_2_1



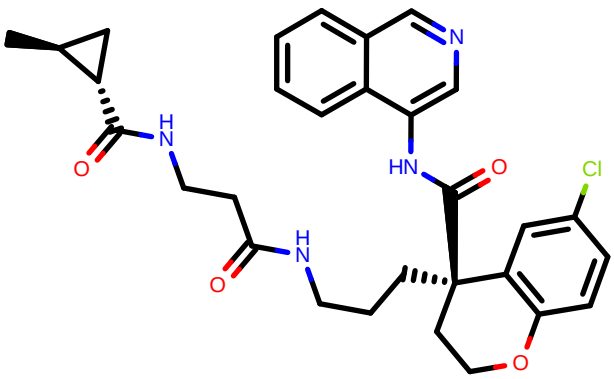
CID:	EN300-6764893_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@@H](C5)OCCO
RUN:	RUN10589
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.33

EN300-6739414_1_2



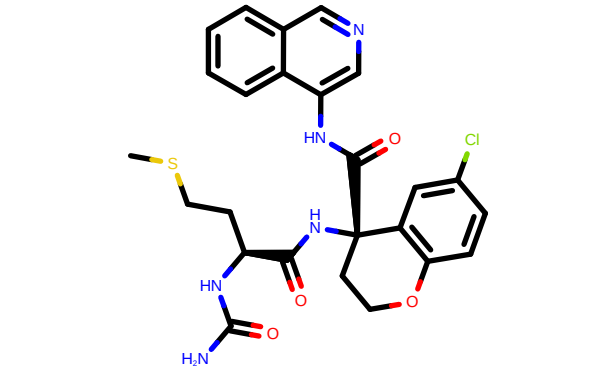
CID:	EN300-6739414_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cc6ccnn6C[C@H](C5)CO
RUN:	RUN7392
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.29

EN300-36851_4_2



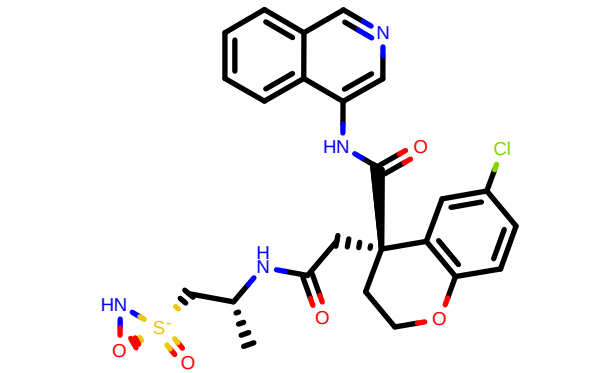
CID:	EN300-36851_4_2
SMILES:	C[C@H]1C[C@@H]1C(=O)NCCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11281
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.37

EN300-315737_1_1



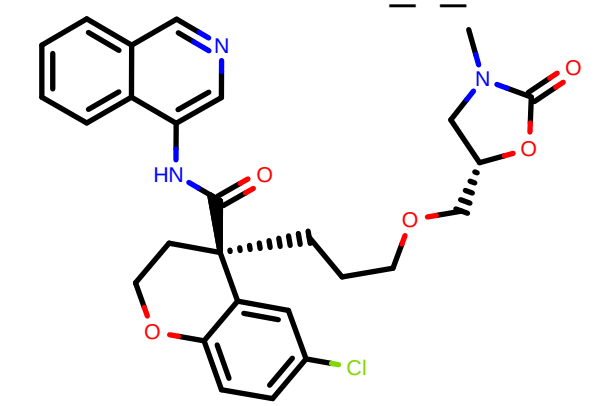
CID:	EN300-315737_1_1
SMILES:	CSCC[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)N
RUN:	RUN5956
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.36

EN300-1703559_1_1



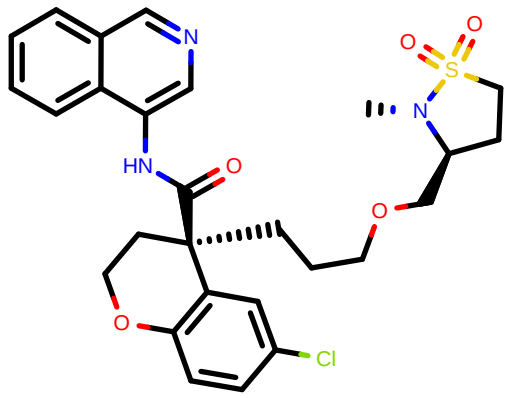
CID:	EN300-1703559_1_1
SMILES:	C[C@H](CS(=O)(=O)N)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7444
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.38

EN300-222969_4_2



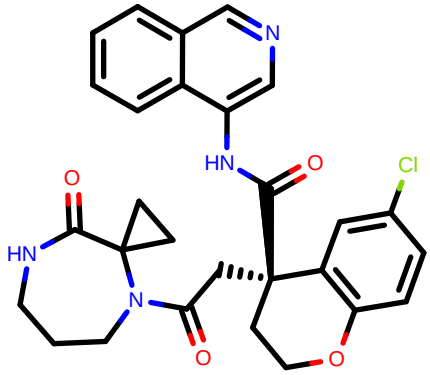
CID:	EN300-222969_4_2
SMILES:	CN1C[C@H](OC1=O)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1606
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.47

EN300-393148_4_1



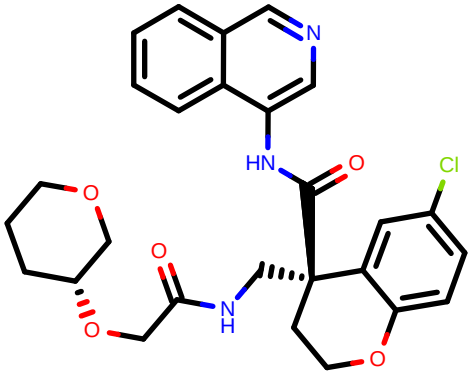
CID:	EN300-393148_4_1
SMILES:	CN1[C@@H](CCS1(=O)=O)COCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1798
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.33

EN300-716218_1_1



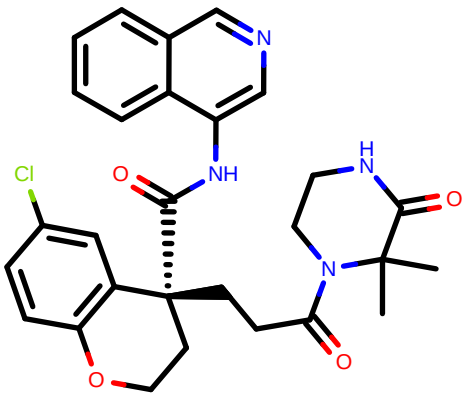
CID:	EN300-716218_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCNC(=O)C56CC6
RUN:	RUN10482
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.26

EN300-1627945_2_1



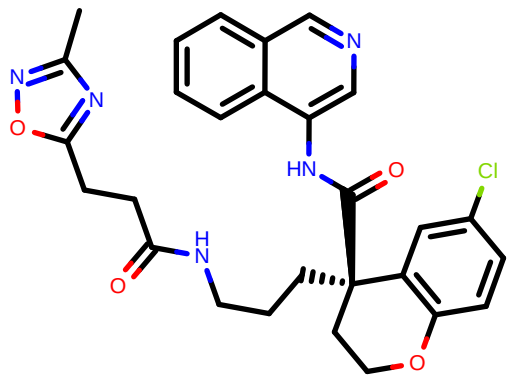
CID:	EN300-1627945_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CO[C@@H]5CCCOC5
RUN:	RUN1568
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.25

EN300-68882_2_1



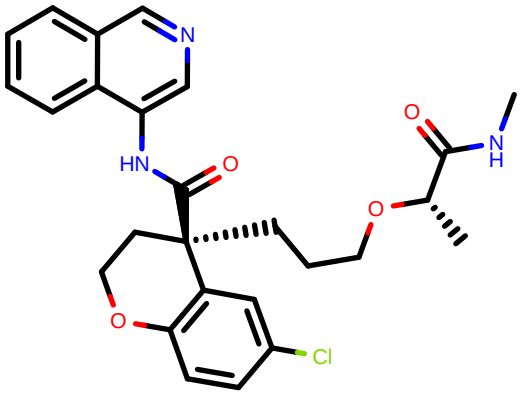
CID:	EN300-68882_2_1
SMILES:	CC1(C(=O)NCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN804
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.29

EN300-27268_4_1



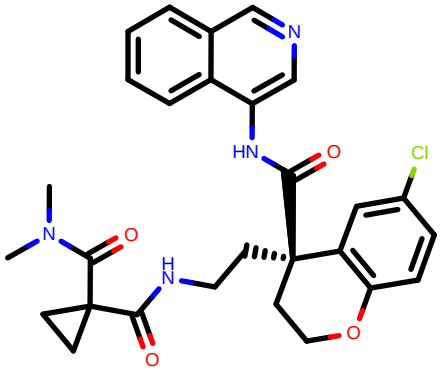
CID:	EN300-27268_4_1
SMILES:	Cc1nc(on1)CCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10070
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.31

EN300-211482_4_1



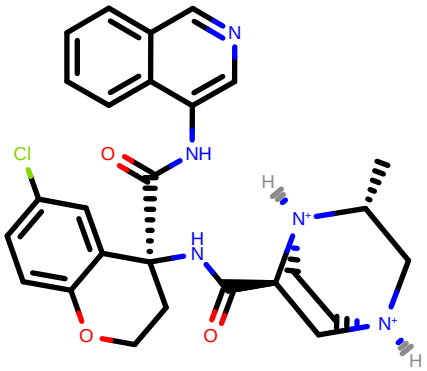
CID:	EN300-211482_4_1
SMILES:	C[C@@H](C(=O)NC)OCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1023
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.37

EN300-180875_3_1



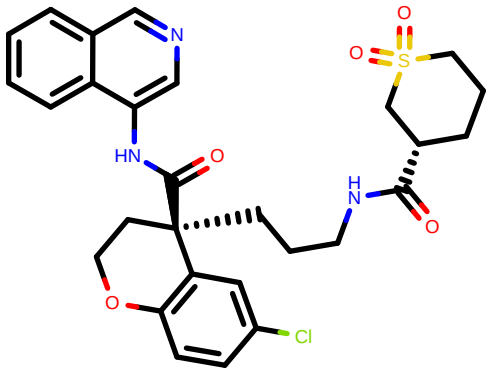
CID:	EN300-180875_3_1
SMILES:	CN(C)C(=O)C1(CC1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4299
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.33

EN300-120562_1_1



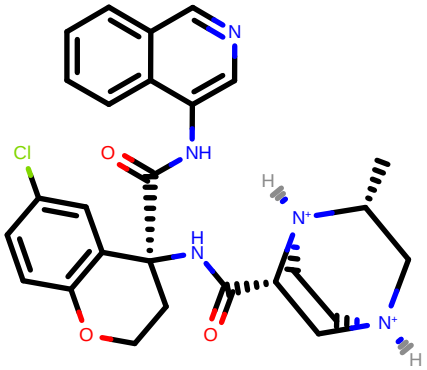
CID:	EN300-120562_1_1
SMILES:	C[C@@H]1CN2CCN1[C@@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN6008
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.30

EN300-77778_4_2



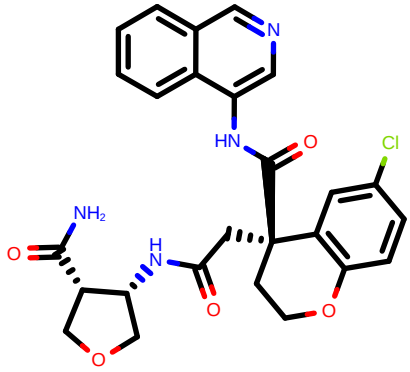
CID:	EN300-77778_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCCS(=O)(=O)C5
RUN:	RUN8477
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.46

EN300-120562_1_3



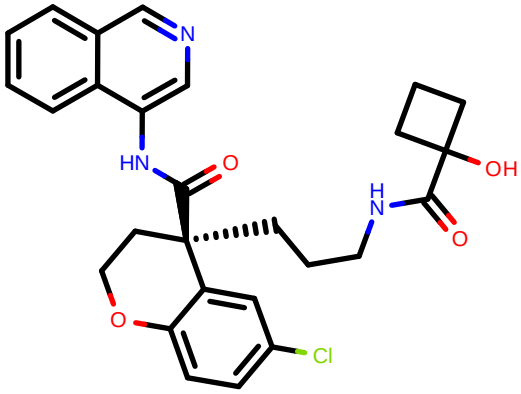
CID:	EN300-120562_1_3
SMILES:	C[C@@H]1CN2CCN1[C@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8402
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.36

EN300-7435892_1_1



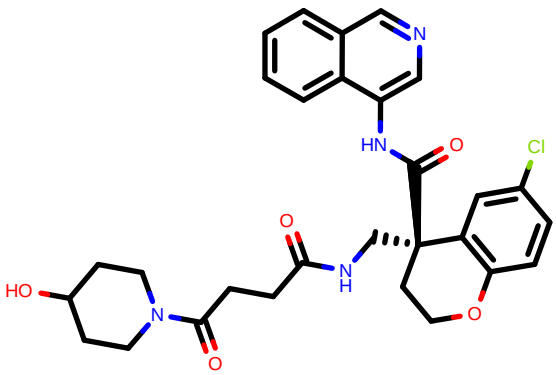
CID:	EN300-7435892_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5C(=O)N
RUN:	RUN4919
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.24

EN300-52009_4_1



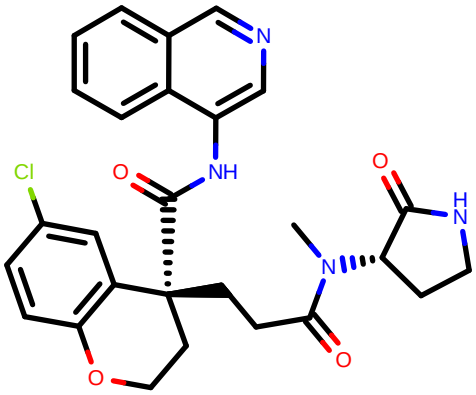
CID:	EN300-52009_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)C5(CCC5)O
RUN:	RUN9533
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.36

EN300-51889_2_1



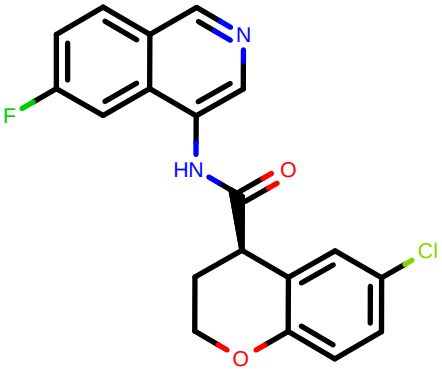
CID:	EN300-51889_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCC(=O)N5CCC(CC5)O
RUN:	RUN1409
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.36

EN300-120119_2_2



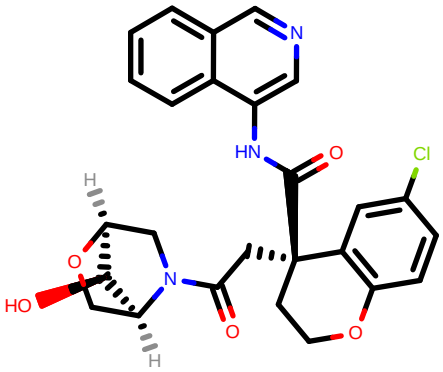
CID:	EN300-120119_2_2
SMILES:	CN([C@H]1CCNC1=O)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7653
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.34

ALP-POS-696356e4-1_1



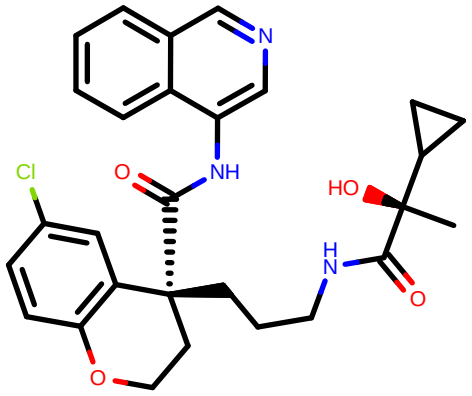
CID:	ALP-POS-696356e4-1_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN20
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.03

EN300-6493060_1_1



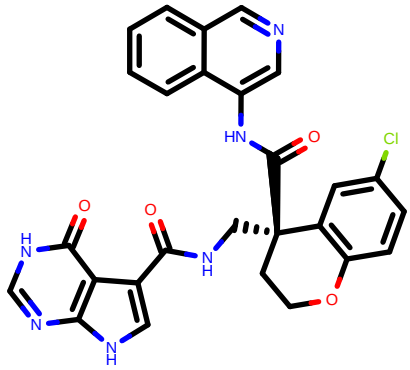
CID:	EN300-6493060_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@H]6[C@@H]([C@@H]5CO6)O
RUN:	RUN8838
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.32

EN300-118760_4_1



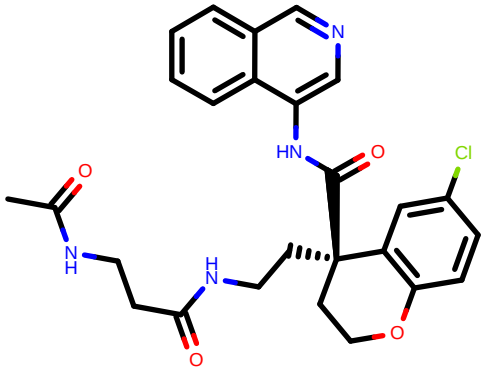
CID:	EN300-118760_4_1
SMILES:	C[C@@](C1CC1)(C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN9277
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.42

EN300-746311_2_1



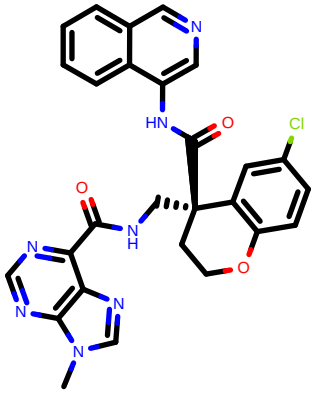
CID:	EN300-746311_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c[nH]c6c5c(=O)[nH]cn6
RUN:	RUN7491
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.29

EN300-04073_3_1



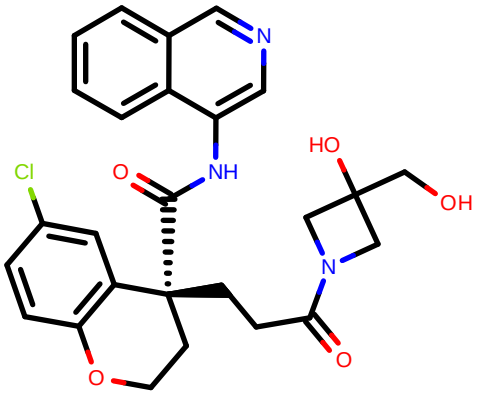
CID:	EN300-04073_3_1
SMILES:	CC(=O)NCCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7556
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.32

EN300-7434334_2_1



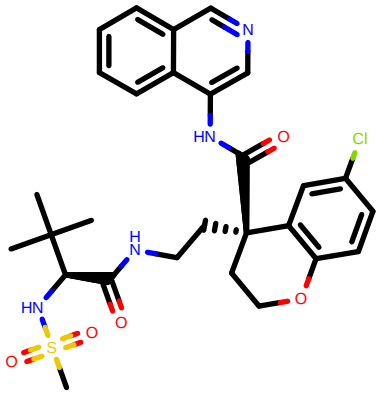
CID:	EN300-7434334_2_1
SMILES:	Cn1cnc2c1ncnc2C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN8235
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.32

EN300-226776_2_1



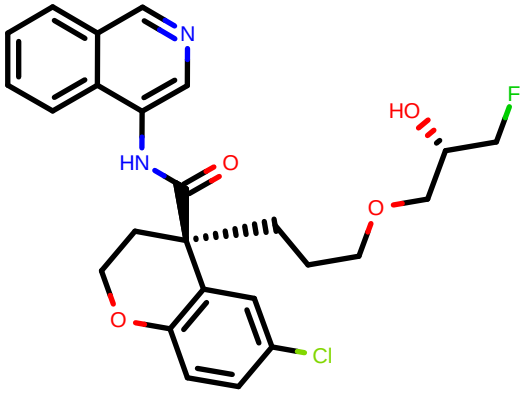
CID:	EN300-226776_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)(CO)O
RUN:	RUN4164
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.38

EN300-112872_3_1



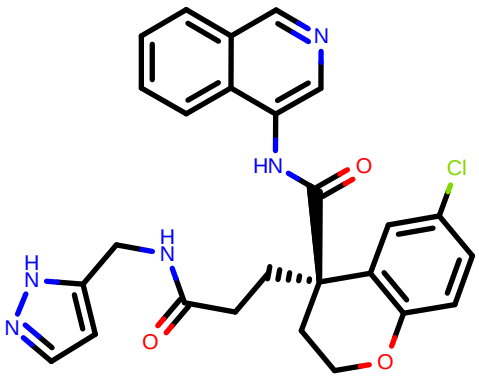
CID:	EN300-112872_3_1
SMILES:	CC(C)(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NS(=O)(=O)C
RUN:	RUN7660
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.49

EN300-1968342_4_1



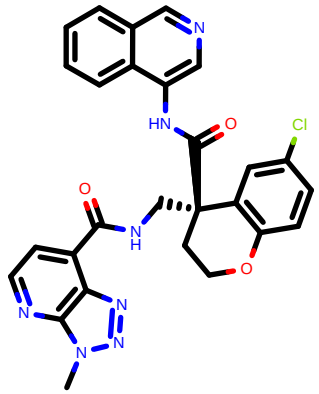
CID:	EN300-1968342_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@@H](CF)O
RUN:	RUN404
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.38

EN300-39785_2_1



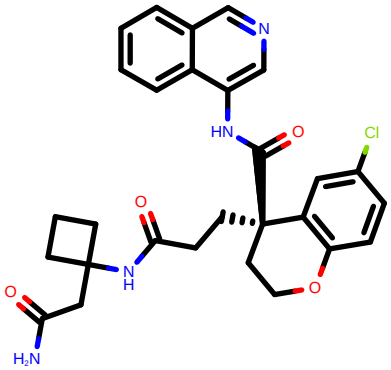
CID:	EN300-39785_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5ccn[nH]5
RUN:	RUN2210
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.33

EN300-202106_2_1



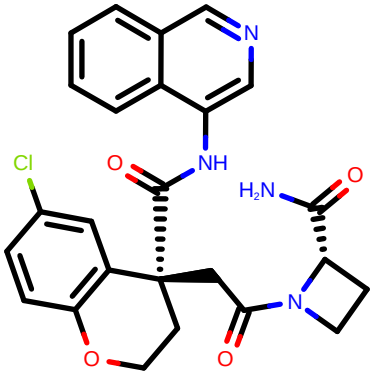
CID:	EN300-202106_2_1
SMILES:	Cn1c2c(c(ccn2)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)nn1
RUN:	RUN8299
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.30

EN300-103284_2_1



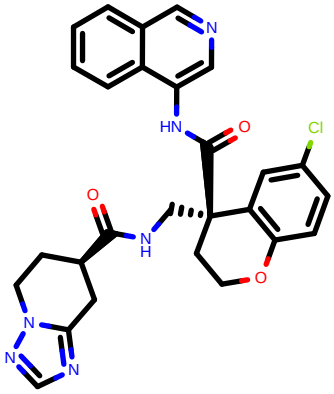
CID:	EN300-103284_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC5(CCC5)CC(=O)N
RUN:	RUN9457
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.33

EN300-862094_1_2



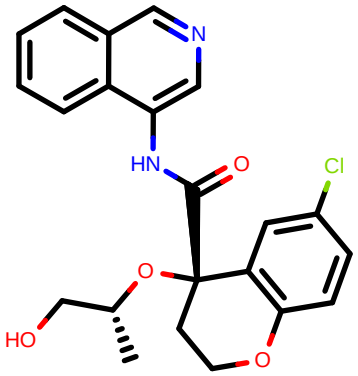
CID:	EN300-862094_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5C(=O)N
RUN:	RUN10790
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.28

EN300-1448674_2_1



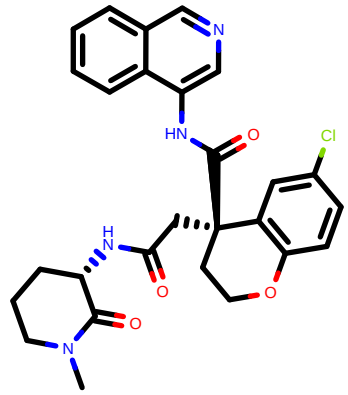
CID:	EN300-1448674_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5CCn6c(ncn6)C5
RUN:	RUN6859
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.25

EN300-175186_1_2



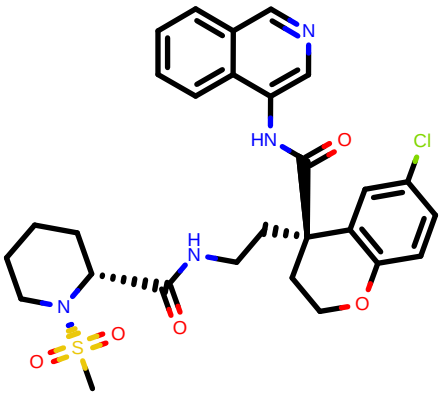
CID:	EN300-175186_1_2
SMILES:	C[C@H](CO)O[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN596
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.24

EN300-313267_1_1



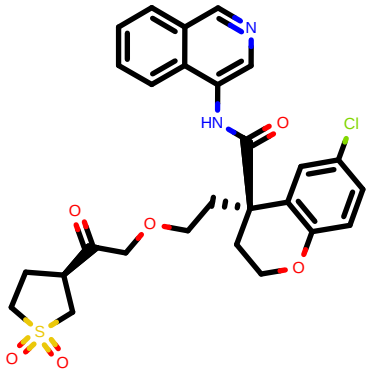
CID:	EN300-313267_1_1
SMILES:	CN1CCC[C@@H](C1=O)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10914
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.33

EN300-24014_3_1



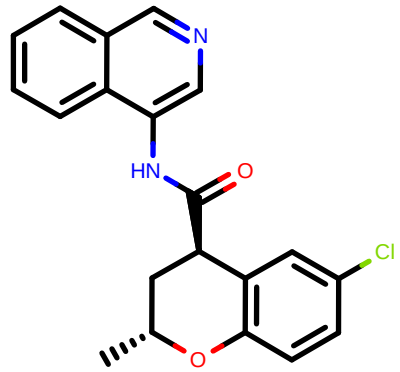
CID:	EN300-24014_3_1
SMILES:	CS(=O)(=O)N1CCCC[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3951
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.54

EN300-226314_3_1



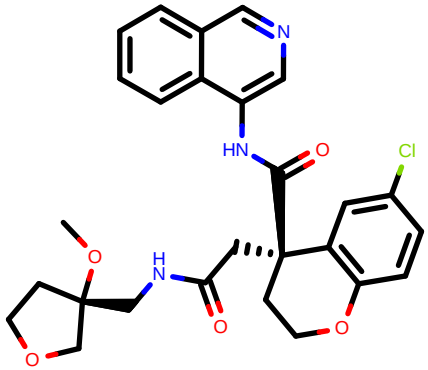
CID:	EN300-226314_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCOCC(=O)[C@@H]5CCS(=O)(=O)C5
RUN:	RUN1156
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.32

EDJ-MED-e4b030d8-2_1



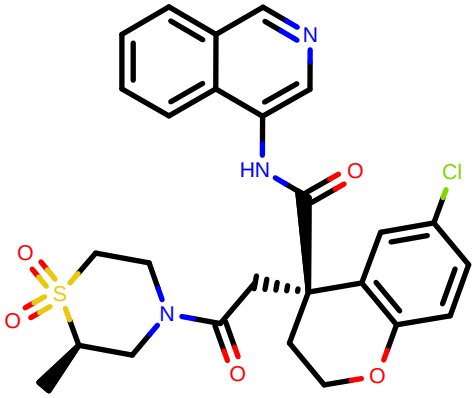
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN36
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

EN300-137255_1_2



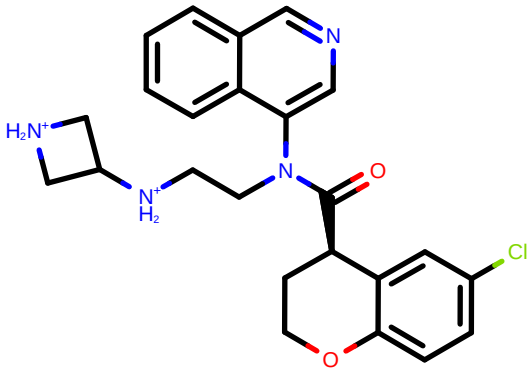
CID:	EN300-137255_1_2
SMILES:	CO[C@]1(CCOC1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4087
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.29

EN300-137734_1_1



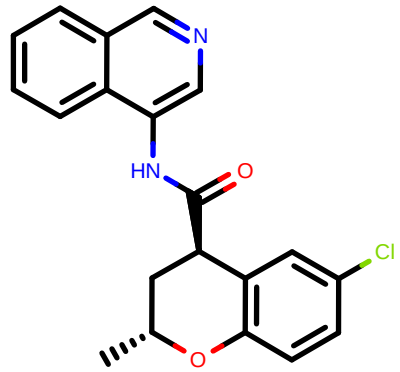
CID:	EN300-137734_1_1
SMILES:	C[C@@H]1CN(CCS1(=O)=O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4395
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.30

MAK-UNK-83e0a0b4-3_1



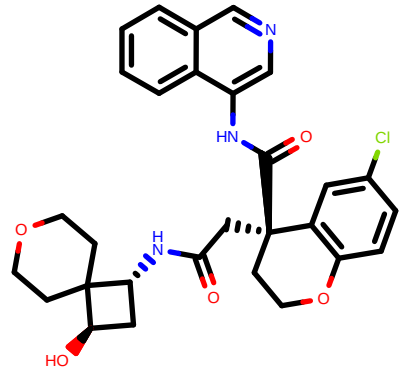
CID:	MAK-UNK-83e0a0b4-3_1
SMILES:	c1ccc2c(c1)cncc2N(CCNC3CNC3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN220
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.34

MAT-POS-8a69d52e-1_3



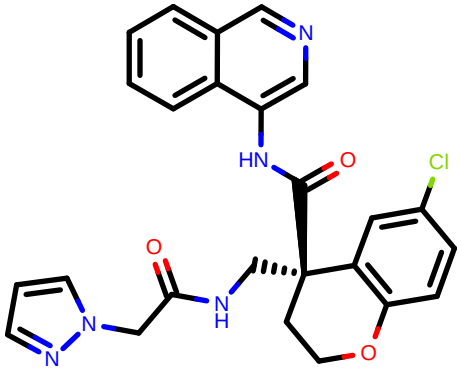
CID:	MAT-POS-8a69d52e-1_3
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN37
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.04

EN300-704039_1_3



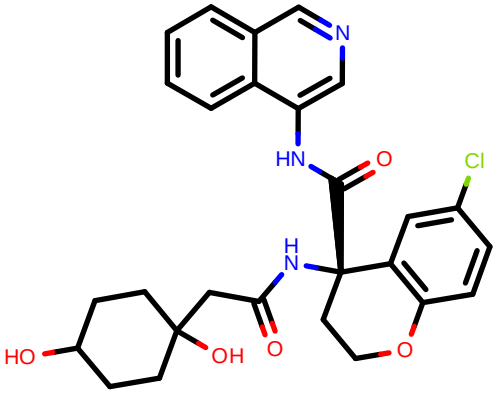
CID:	EN300-704039_1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H](C56CCOCC6)O
RUN:	RUN8931
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.35

EN300-23942_2_1



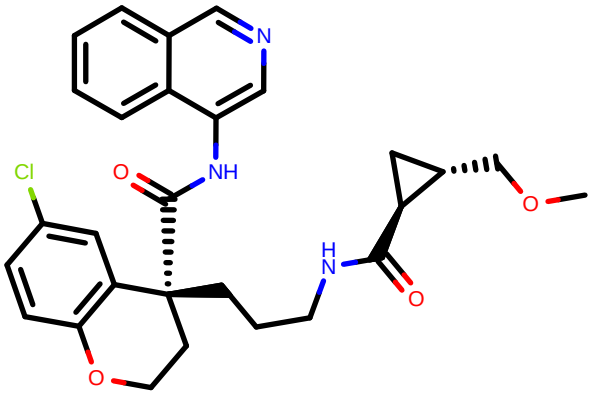
CID:	EN300-23942_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cccn5
RUN:	RUN4670
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.31

EN300-181558_1_1



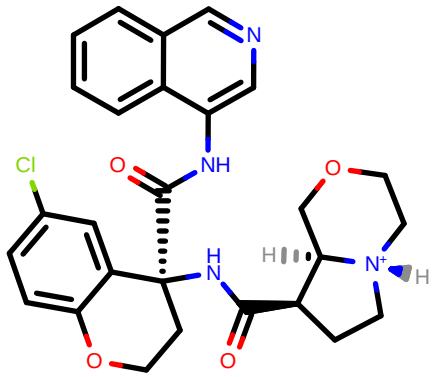
CID:	EN300-181558_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC5(CCC(CC5)O)O
RUN:	RUN1948
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.31

EN300-7352438_4_1



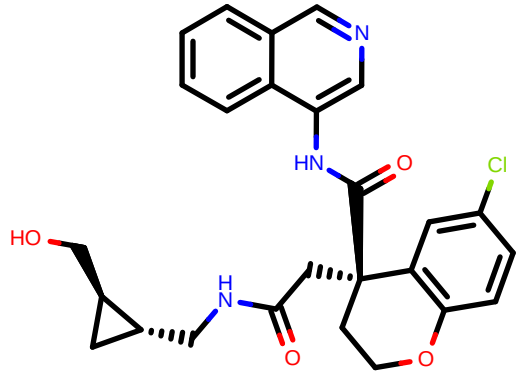
CID:	EN300-7352438_4_1
SMILES:	COC[C@H]1C[C@@H]1C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9665
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.26

EN300-1588613_1_1



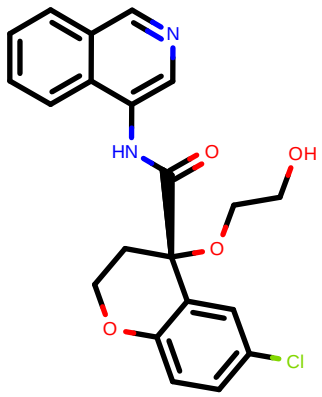
CID:	EN300-1588613_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCN6[C@@H]5COCC6
RUN:	RUN4801
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.35

EN300-1277662_1_1



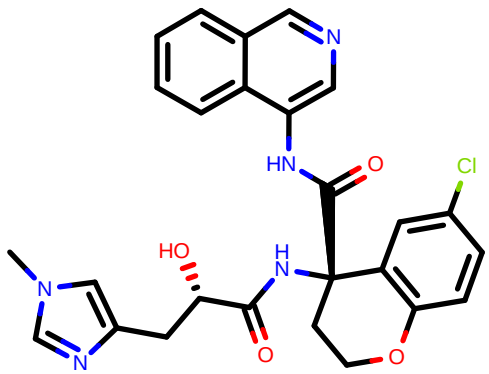
CID:	EN300-1277662_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5C[C@H]5CO
RUN:	RUN5798
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.28

EN300-21258_1_1



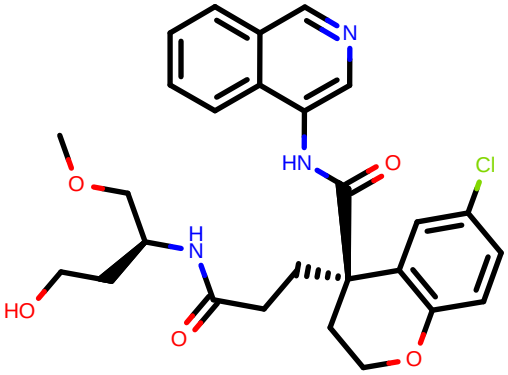
CID:	EN300-21258_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO
RUN:	RUN1799
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.22

EN300-1725538_1_1



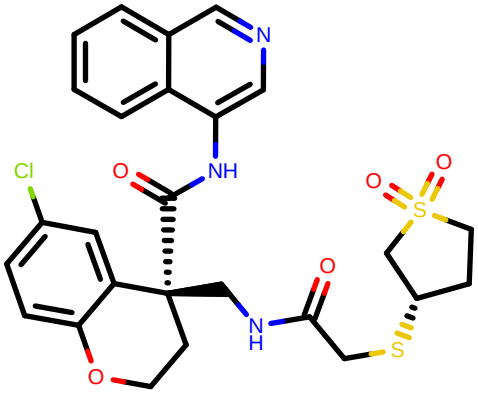
CID:	EN300-1725538_1_1
SMILES:	Cn1cc(nc1)C[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5408
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.30

EN300-83030_2_2



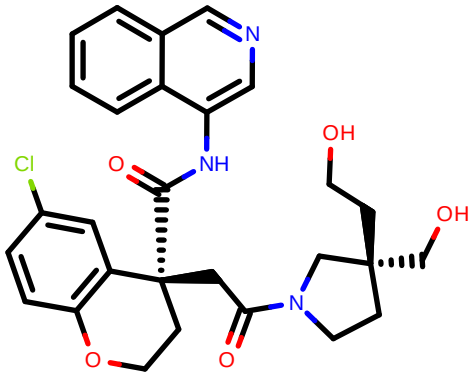
CID:	EN300-83030_2_2
SMILES:	COC[C@H](CCO)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN11185
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.27

EN300-13890_2_2



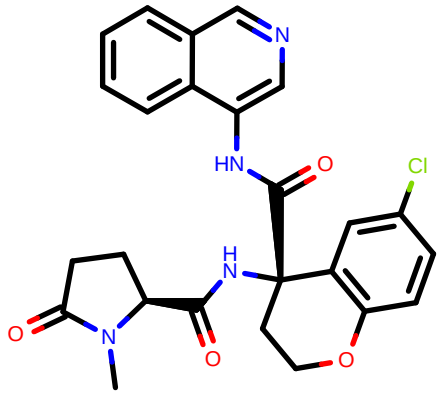
CID:	EN300-13890_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CS[C@H]5CCS(=O)(=O)C5
RUN:	RUN1313
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.31

EN300-1707870_1_1



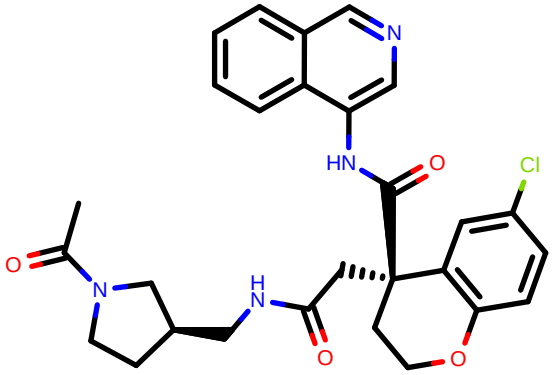
CID:	EN300-1707870_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(CCO)CO
RUN:	RUN9732
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.36

EN300-132963_1_1



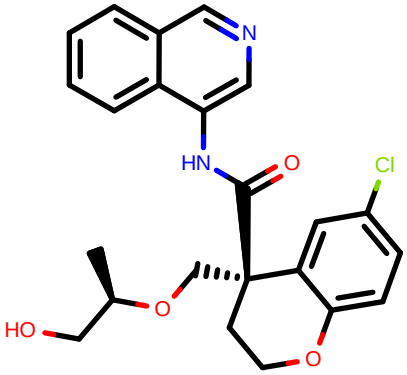
CID:	EN300-132963_1_1
SMILES:	CN1[C@@H](CCC1=O)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3498
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.29

EN300-215256_1_1



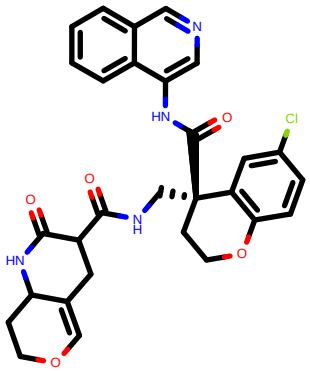
CID:	EN300-215256_1_1
SMILES:	CC(=O)N1CC[C@@H](C1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10756
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.31

EN300-175186_2_2



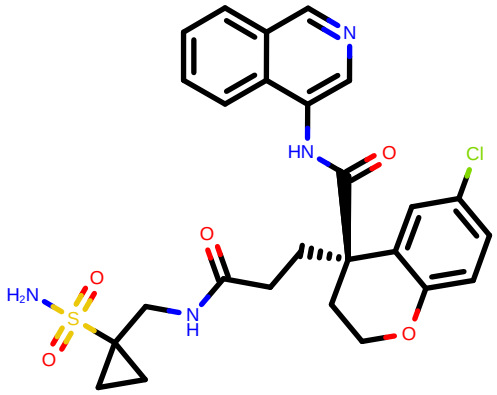
CID:	EN300-175186_2_2
SMILES:	C[C@H](CO)OC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1390
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.26

EN300-383824_2_1



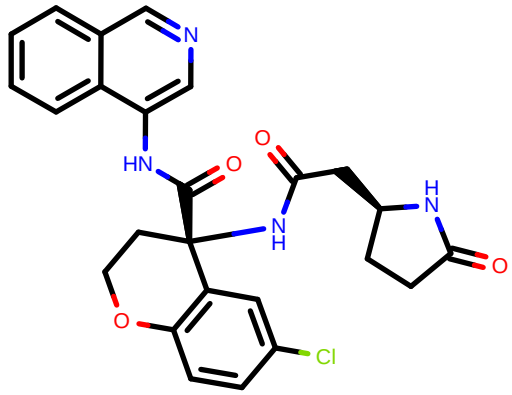
CID:	EN300-383824_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6c([nH]c5=O)CCOC6
RUN:	RUN8187
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.38

EN300-378652_2_1



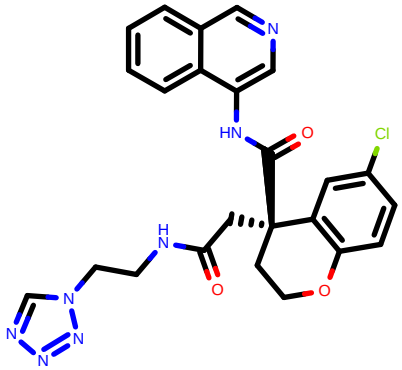
CID:	EN300-378652_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC5(CC5)S(=O)(=O)N
RUN:	RUN10977
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.37

EN300-68203_1_1



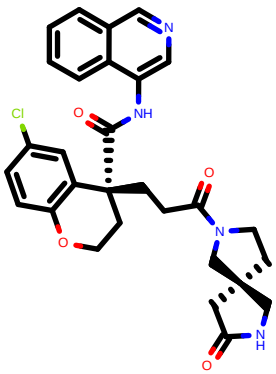
CID:	EN300-68203_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@@H]5CCC(=O)N5
RUN:	RUN2870
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.20

EN300-108022_1_1



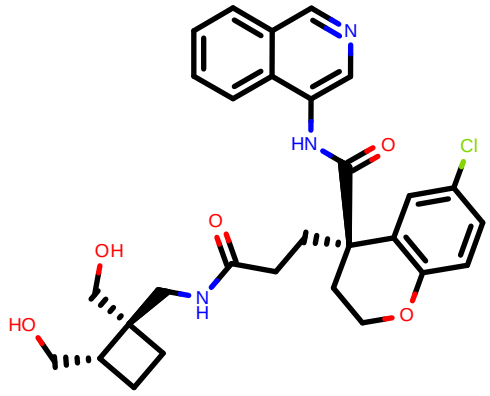
CID:	EN300-108022_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCCn5cnnn5
RUN:	RUN9102
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.31

EN300-187998_2_1



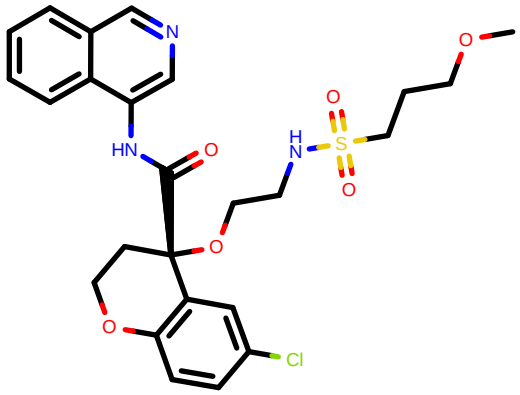
CID:	EN300-187998_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC6(C5)CC(=O)NC6
RUN:	RUN4200
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.30

EN300-1692359_2_2



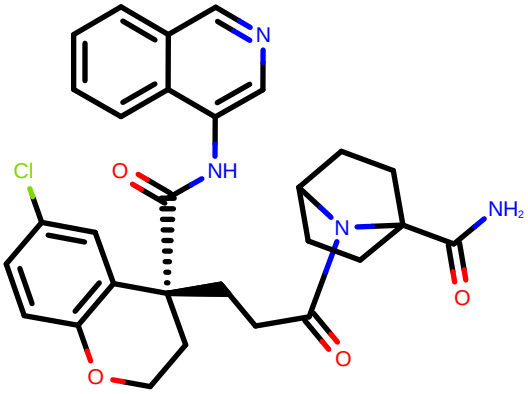
CID:	EN300-1692359_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@]5(CC[C@@H]5CO)CO
RUN:	RUN10377
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.24

EN300-97453_1_1



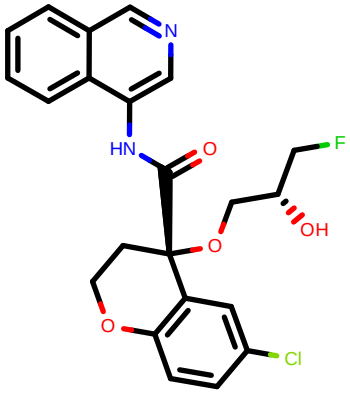
CID:	EN300-97453_1_1
SMILES:	COCCCS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2592
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.43

EN300-637522_2_1



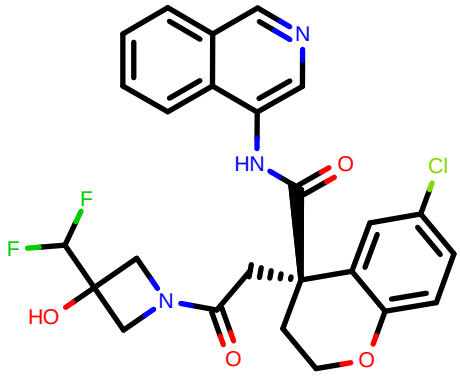
CID:	EN300-637522_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5C6CCC5(CC6)C(=O)N
RUN:	RUN6490
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.34

EN300-1968342_1_2



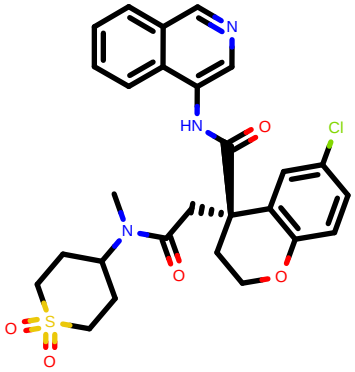
CID:	EN300-1968342_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CF)O
RUN:	RUN2071
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.33

EN300-249245_1_1



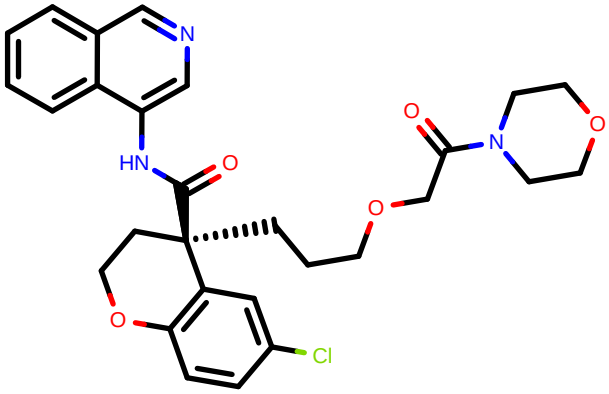
CID:	EN300-249245_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)(C(F)F)O
RUN:	RUN5810
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.22

EN300-95152_1_1



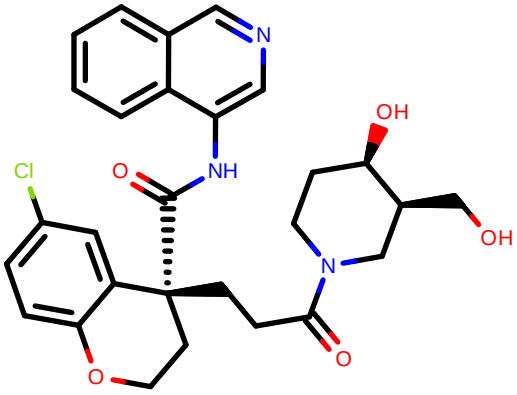
CID:	EN300-95152_1_1
SMILES:	CN(C1CCS(=O)(=O)CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11120
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.28

EN300-1241327_4_1



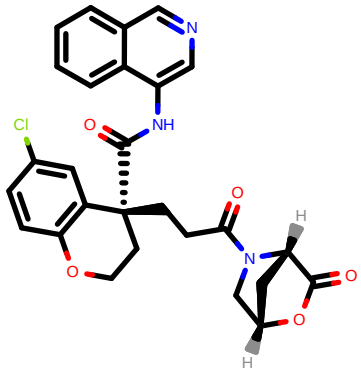
CID:	EN300-1241327_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOCC(=O)N5CCOCC5
RUN:	RUN1183
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.38

EN300-233678_2_4



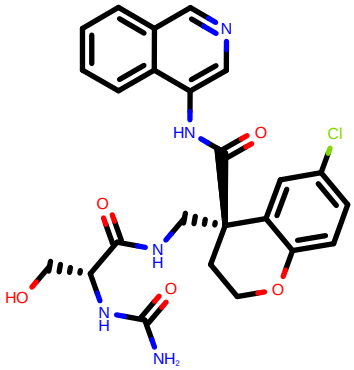
CID:	EN300-233678_2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC[C@H]([C@H](C5)CO)O
RUN:	RUN4236
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.29

EN300-233821_2_1



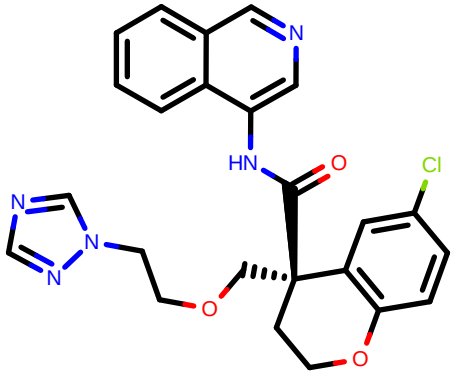
CID:	EN300-233821_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6CC5C(=O)O6
RUN:	RUN5747
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.26

EN300-10170_2_1



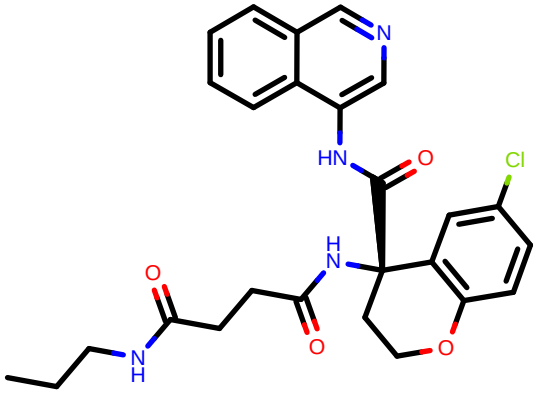
CID:	EN300-10170_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H](CO)NC(=O)N
RUN:	RUN1449
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.35

EN300-6255179_2_1



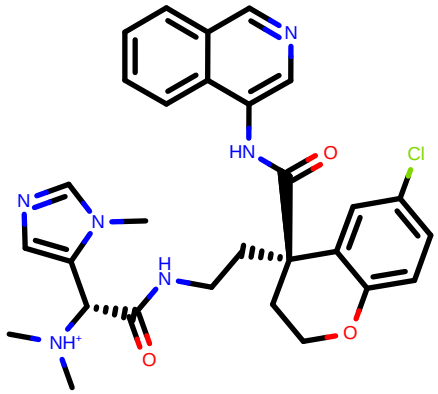
CID:	EN300-6255179_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCCn5cncn5
RUN:	RUN1566
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.23

EN300-68740_1_1



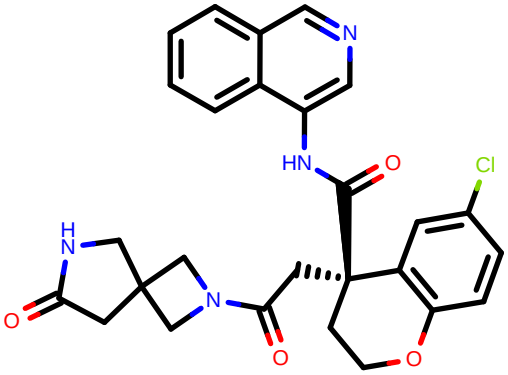
CID:	EN300-68740_1_1
SMILES:	CCCNC(=O)CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1229
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.32

EN300-192809_3_2



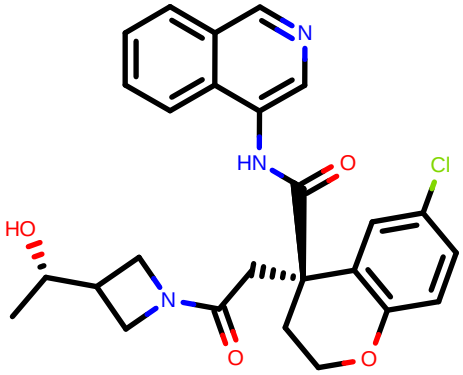
CID:	EN300-192809_3_2
SMILES:	Cn1cncc1[C@H](C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)N(C)C
RUN:	RUN2081
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.51

EN300-1722713_1_1



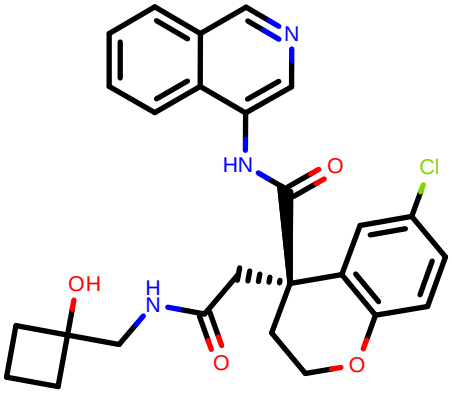
CID:	EN300-1722713_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC6(C5)CC(=O)NC6
RUN:	RUN279
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.31

EN300-365650_1_1



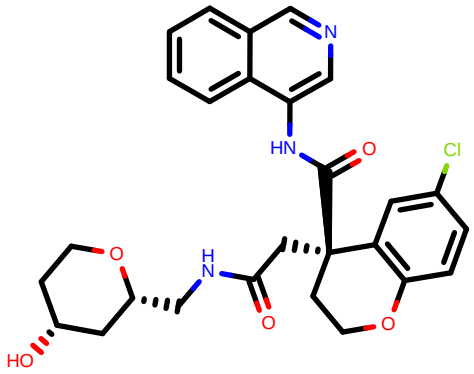
CID:	EN300-365650_1_1
SMILES:	C[C@@H](C1CN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN3388
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.24

EN300-70656_1_1



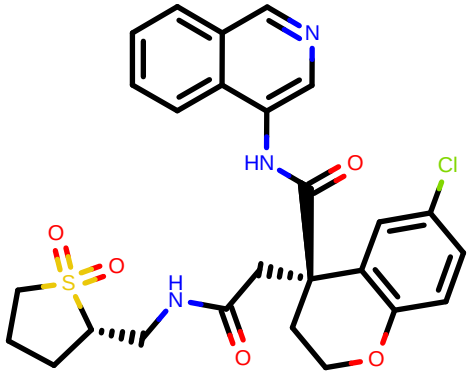
CID:	EN300-70656_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC5(CCC5)O
RUN:	RUN3424
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.30

EN300-1708899_1_1



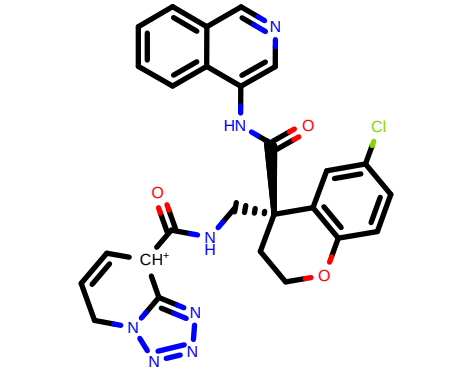
CID:	EN300-1708899_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5C[C@@H](CCO5)O
RUN:	RUN4799
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.29

EN300-246808_1_1



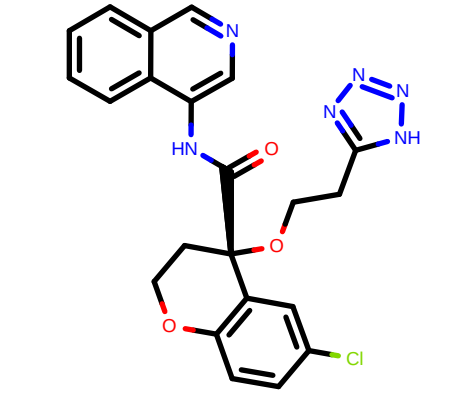
CID:	EN300-246808_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCCS5(=O)=O
RUN:	RUN6473
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.35

EN300-305984_2_1



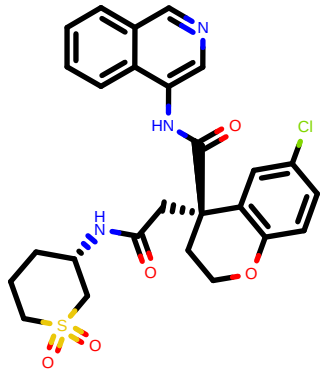
CID:	EN300-305984_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cccn6c5nnn6
RUN:	RUN8207
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.28

EN300-183231_1_1



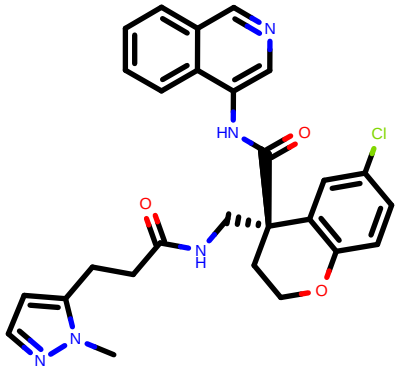
CID:	EN300-183231_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5[nH]nnn5
RUN:	RUN2721
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.31

EN300-74856_1_2



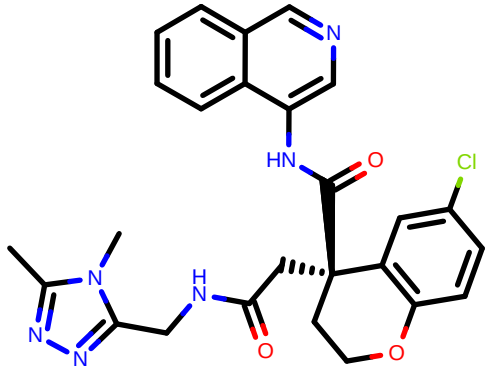
CID:	EN300-74856_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCCS(=O)(=O)C5
RUN:	RUN9730
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.33

EN300-92662_2_1



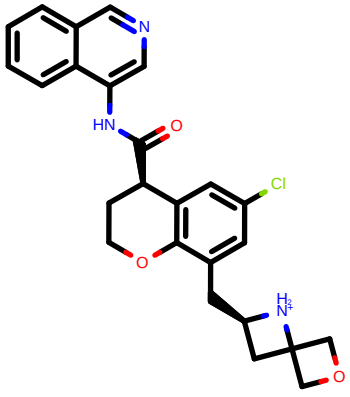
CID:	EN300-92662_2_1
SMILES:	Cn1c(ccn1)CCC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4070
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.34

EN300-70323_1_1



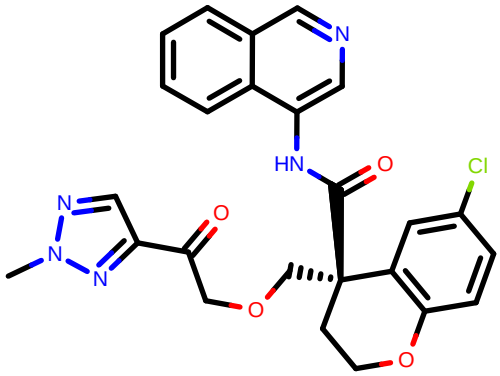
CID:	EN300-70323_1_1
SMILES:	Cc1nnc(n1C)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7168
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.24

DAR-DIA-23e5a6a0-8_1



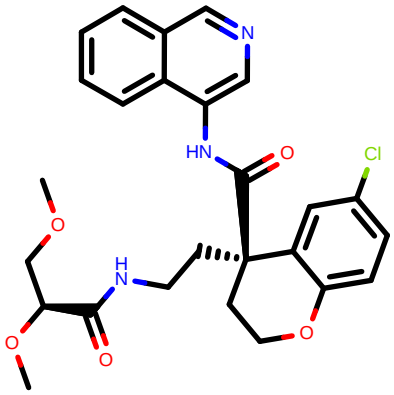
CID:	DAR-DIA-23e5a6a0-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6(N5)COC6)Cl
RUN:	RUN222
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.30

EN300-204935_2_1



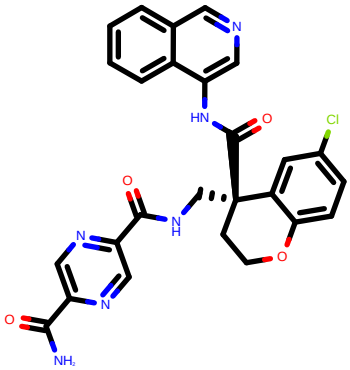
CID:	EN300-204935_2_1
SMILES:	Cn1ncc(n1)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2093
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.27

EN300-305282_3_1



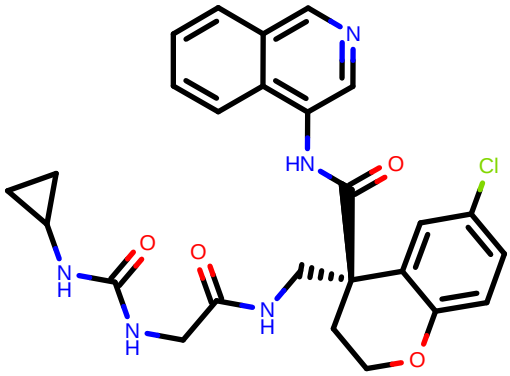
CID:	EN300-305282_3_1
SMILES:	COC[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN5938
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.40

EN300-1273172_2_1



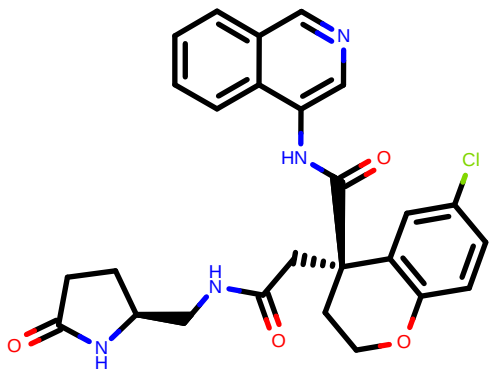
CID:	EN300-1273172_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnc(cn5)C(=O)N
RUN:	RUN7871
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.26

EN300-42591_2_1



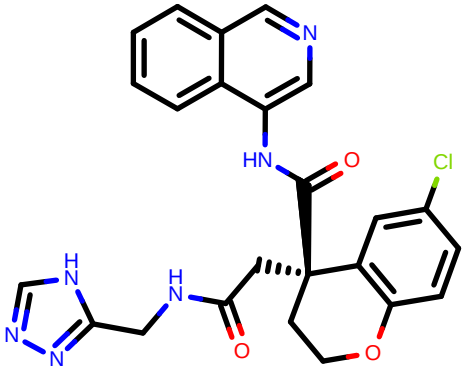
CID:	EN300-42591_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CNC(=O)NC5CC5
RUN:	RUN5162
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.25

EN300-297937_1_1



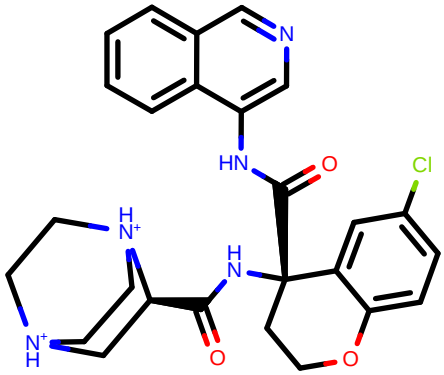
CID:	EN300-297937_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H]5CCC(=O)N5
RUN:	RUN9414
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.27

EN300-43972_1_1



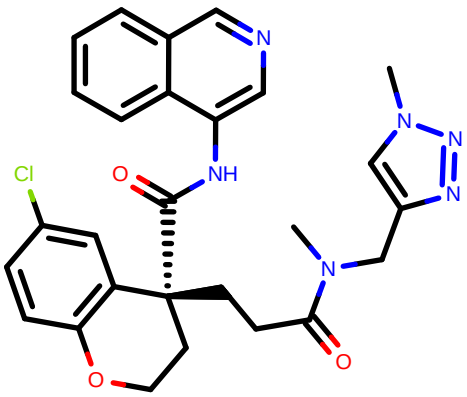
CID:	EN300-43972_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCc5[nH]cnn5
RUN:	RUN7068
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.26

EN300-1605566_1_2



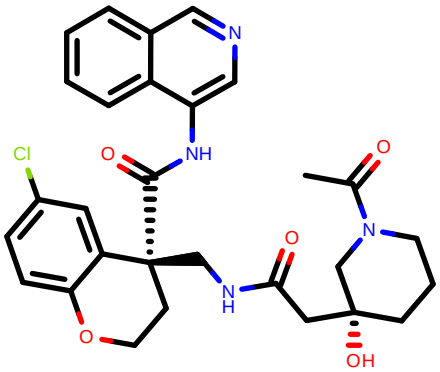
CID:	EN300-1605566_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CN6CCN5CC6
RUN:	RUN8250
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.30

EN300-304051_2_1



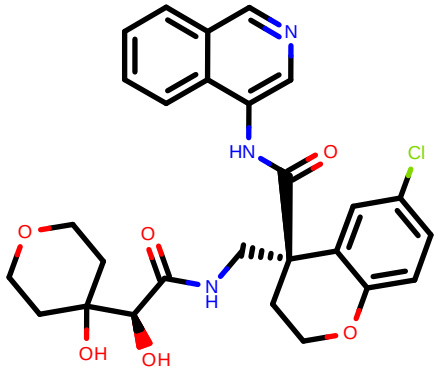
CID:	EN300-304051_2_1
SMILES:	Cn1cc(nn1)CN(C)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7793
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.24

EN300-259063_2_2



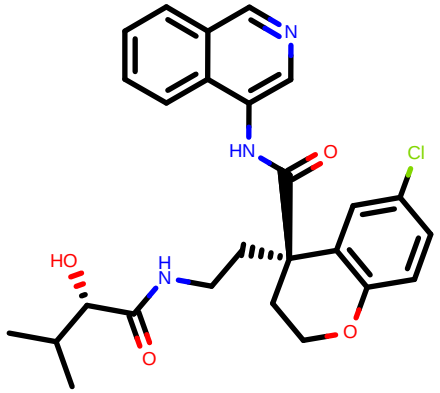
CID:	EN300-259063_2_2
SMILES:	CC(=O)N1CCC[C@](C1)(CC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN905
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.35

EN300-749499_2_2



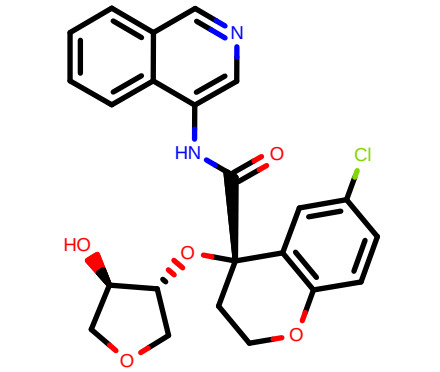
CID:	EN300-749499_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H](C5(CCOCC5)O)O
RUN:	RUN2416
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.29

EN300-199359_3_1



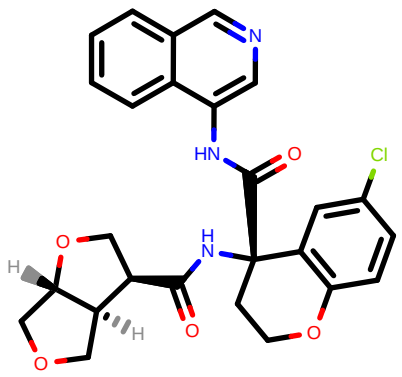
CID:	EN300-199359_3_1
SMILES:	CC(C)[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2333
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.31

EN300-331828_1_1



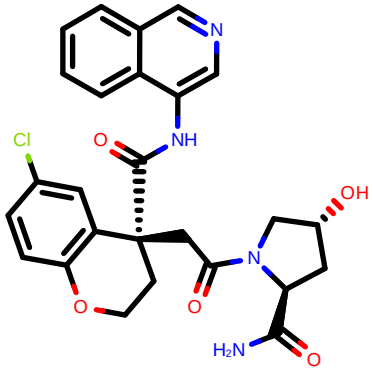
CID:	EN300-331828_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H]5COC[C@H]5O
RUN:	RUN1591
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.20

EN300-6482296_1_1



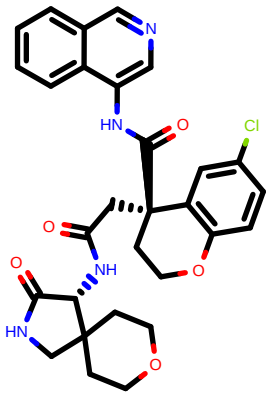
CID:	EN300-6482296_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CO[C@@H]6[C@@H]5COC6
RUN:	RUN5544
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.23

EN300-314410_1_1



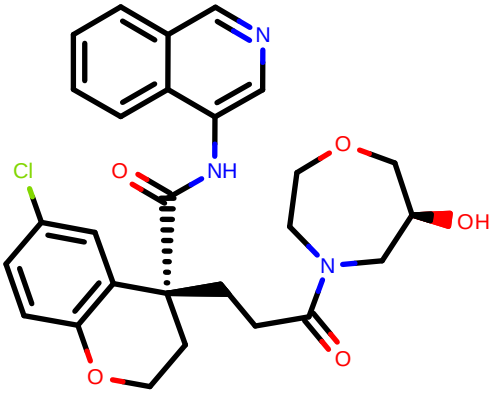
CID:	EN300-314410_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H](C[C@H]5C(=O)N)O
RUN:	RUN11124
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.31

EN300-310254_1_2



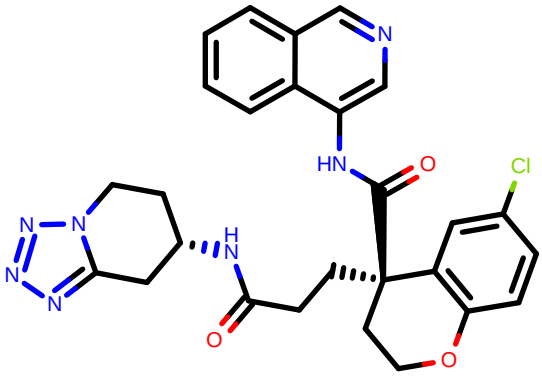
CID:	EN300-310254_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C(=O)NCC56CCOCC6
RUN:	RUN4467
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.38

EN300-233951_2_2



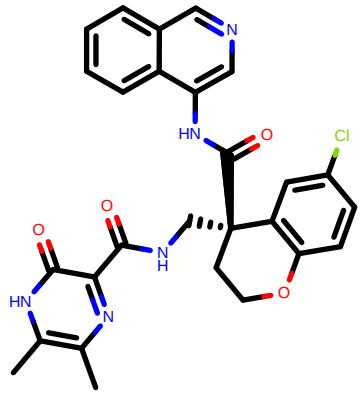
CID:	EN300-233951_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCOC[C@H](C5)O
RUN:	RUN2138
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.34

EN300-7438451_2_2



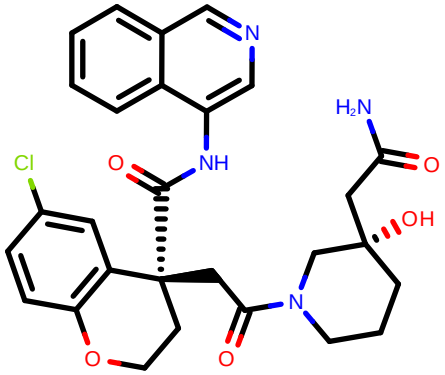
CID:	EN300-7438451_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCn6c(nnn6)C5
RUN:	RUN2292
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.31

EN300-116885_2_1



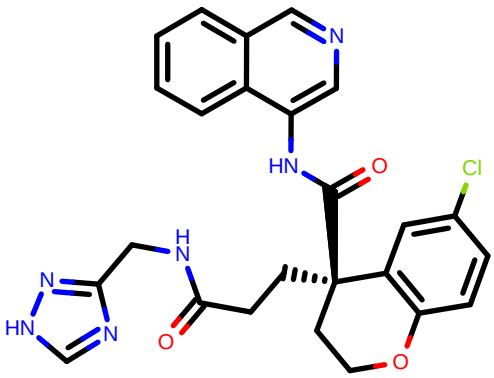
CID:	EN300-116885_2_1
SMILES:	Cc1c(nc(c(=O)[nH]1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN8007
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.28

EN300-259060_1_1



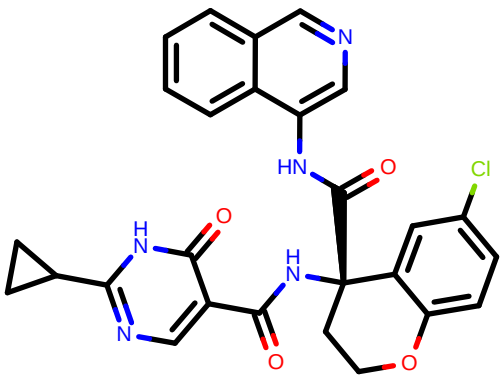
CID:	EN300-259060_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@](C5)(CC(=O)N)O
RUN:	RUN2249
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.40

EN300-43972_2_1



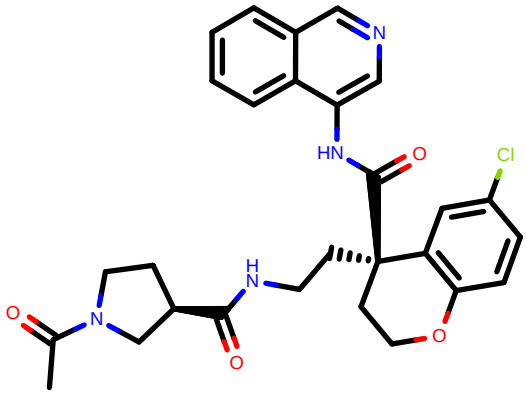
CID:	EN300-43972_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5[nH]cnn5
RUN:	RUN2917
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.26

EN300-118045_1_1



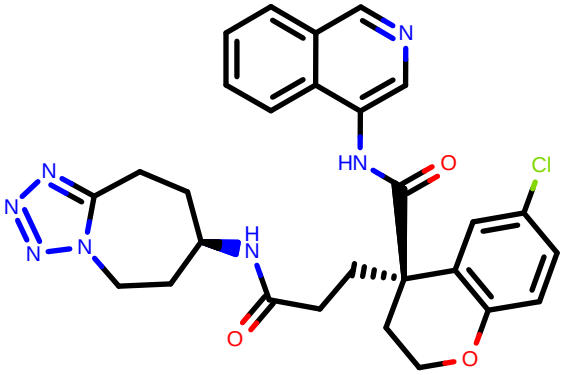
CID:	EN300-118045_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cnc([nH]c5=O)C6CC6
RUN:	RUN8927
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.37

EN300-100180_3_2



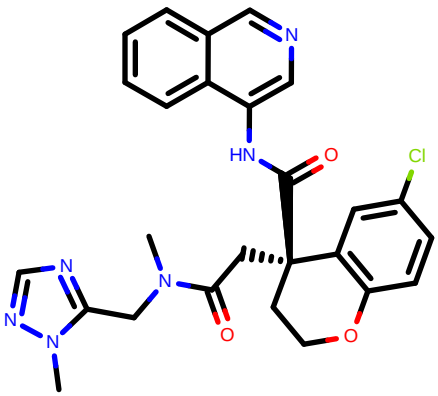
CID:	EN300-100180_3_2
SMILES:	CC(=O)N1CC[C@H](C1)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10830
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.48

EN300-256798_2_1



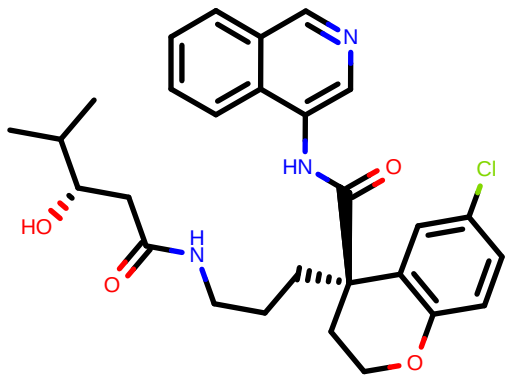
CID:	EN300-256798_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@@H]5CCc6nnnn6CC5
RUN:	RUN6710
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.27

EN300-7444635_1_1



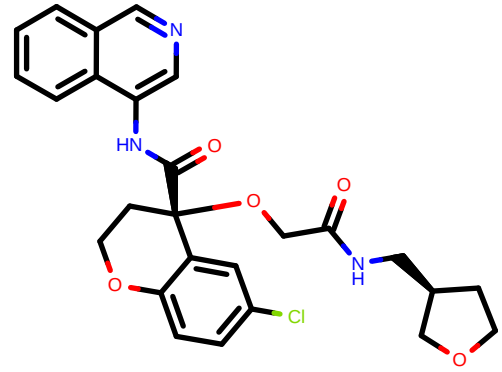
CID:	EN300-7444635_1_1
SMILES:	Cn1c(ncn1)CN(C)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8847
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.40

EN300-155498_4_1



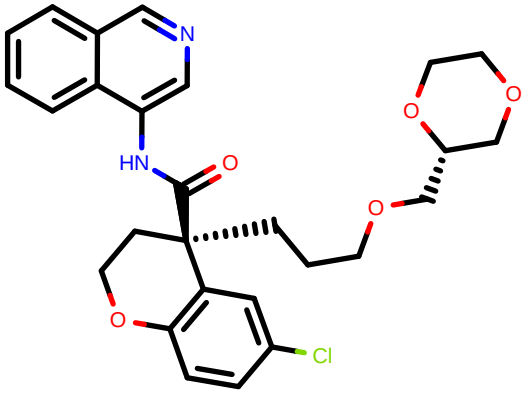
CID:	EN300-155498_4_1
SMILES:	CC(=C)[C@H](CC(=O)NCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN10187
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.22

EN300-46832_1_2



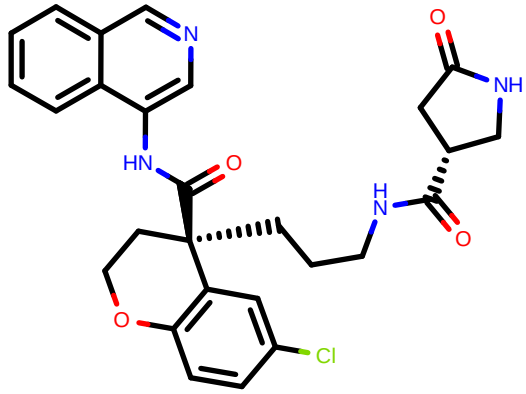
CID:	EN300-46832_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NC[C@H]5CCOC5
RUN:	RUN1440
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

EN300-139167_4_2



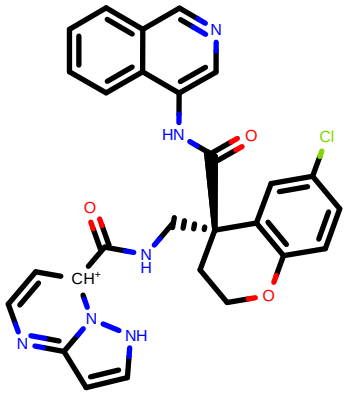
CID:	EN300-139167_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5COCCO5
RUN:	RUN1143
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.47

EN300-59487_4_1



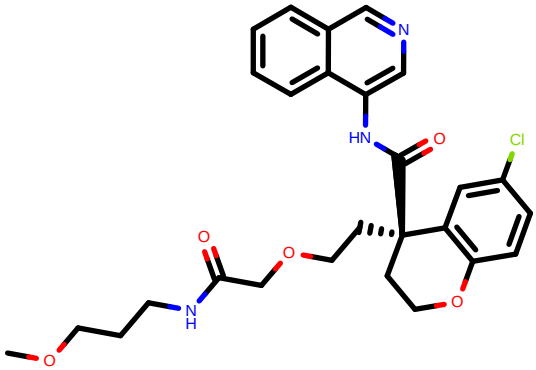
CID:	EN300-59487_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@@H]5CC(=O)NC5
RUN:	RUN9004
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.33

EN300-322100_2_1



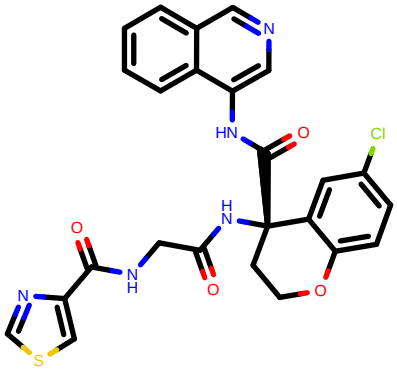
CID:	EN300-322100_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccnc6n5ncc6
RUN:	RUN8515
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.33

EN300-04492_3_1



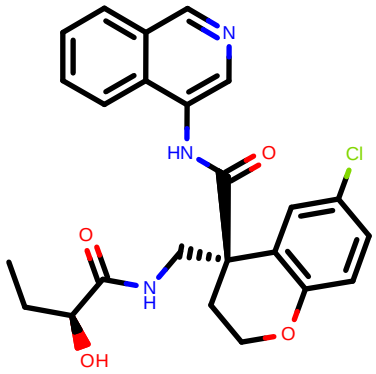
CID:	EN300-04492_3_1
SMILES:	COCCCNC(=O)COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1651
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.29

EN300-182084_1_1



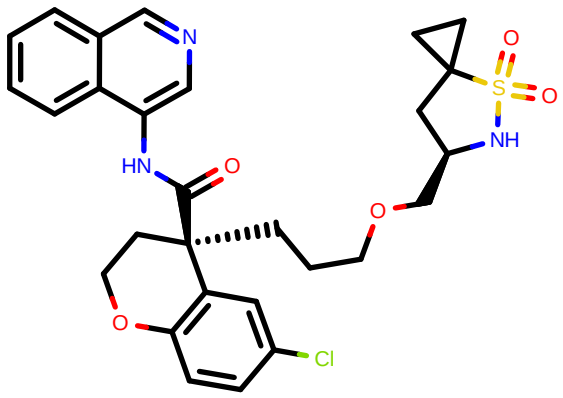
CID:	EN300-182084_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CNC(=O)c5cscn5
RUN:	RUN6575
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.32

EN300-181492_2_1



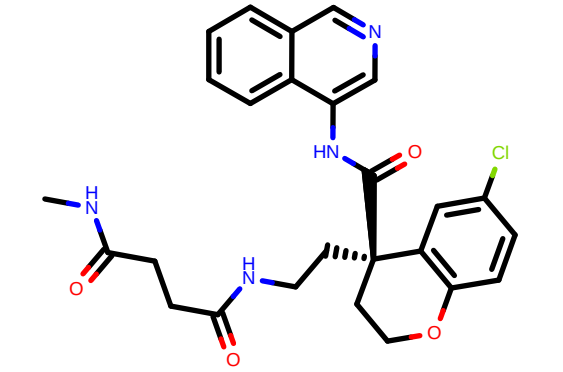
CID:	EN300-181492_2_1
SMILES:	C=C[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN4846
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.27

EN300-6504697_4_2



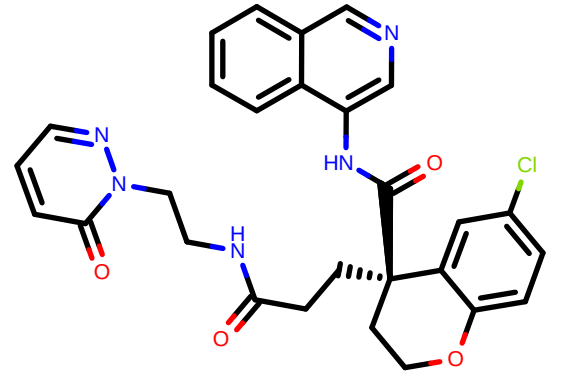
CID:	EN300-6504697_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCOC[C@H]5CC6(CC6)S(=O)(=O)N5
RUN:	RUN1622
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.43

EN300-1081277_3_1



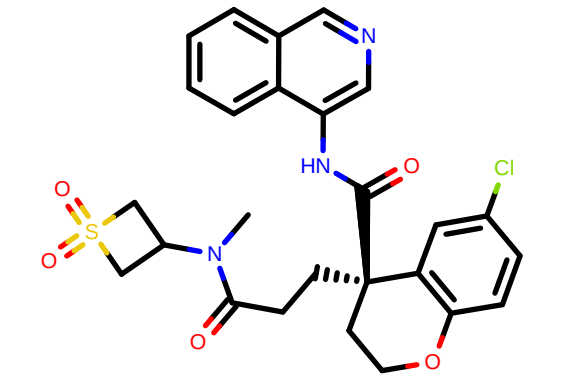
CID:	EN300-1081277_3_1
SMILES:	CNC(=O)CCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1146
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.30

EN300-239233_2_1



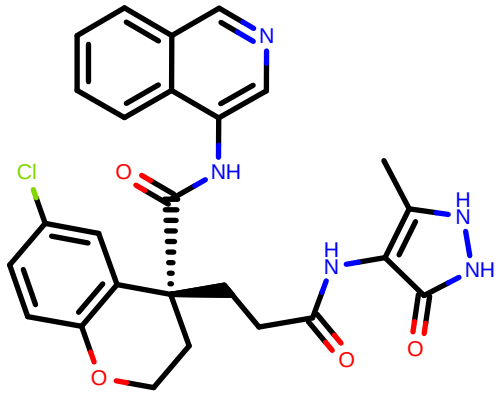
CID:	EN300-239233_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCCn5c(=O)cccn5
RUN:	RUN8529
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.27

EN300-318341_2_1



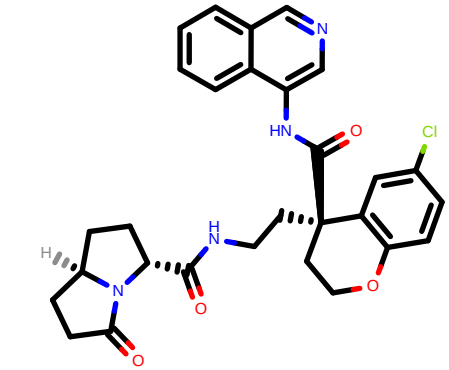
CID:	EN300-318341_2_1
SMILES:	CN(C1CS(=O)(=O)C1)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10024
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.27

EN300-260642_2_1



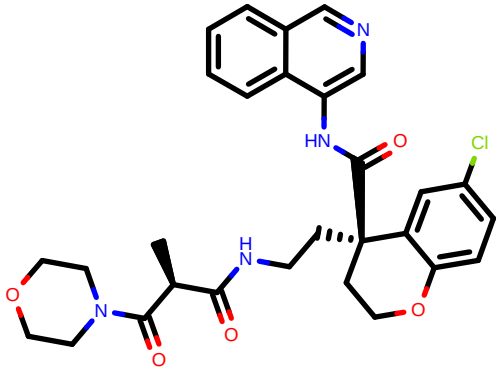
CID:	EN300-260642_2_1
SMILES:	Cc1c(c(=O)[nH][nH]1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8947
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.26

EN300-6479181_3_4



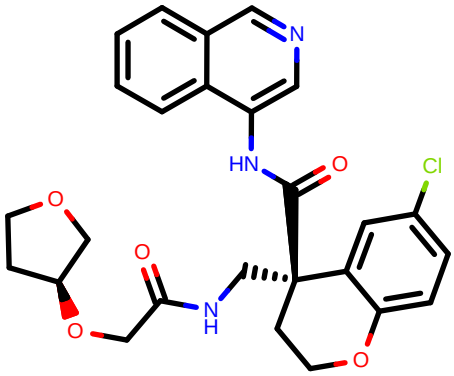
CID:	EN300-6479181_3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5CC[C@H]6N5C(=O)CC6
RUN:	RUN10960
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.49

EN300-2855057_3_1



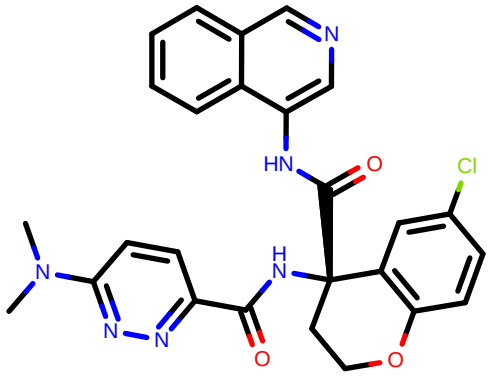
CID:	EN300-2855057_3_1
SMILES:	C[C@@H](C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C(=O)N5CCOCC5
RUN:	RUN3044
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.39

EN300-99391_2_2



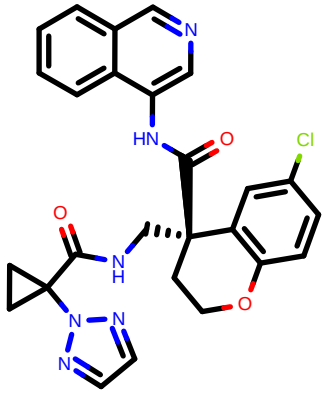
CID:	EN300-99391_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CO[C@H]5CCOC5
RUN:	RUN826
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.25

EN300-7535922_1_1



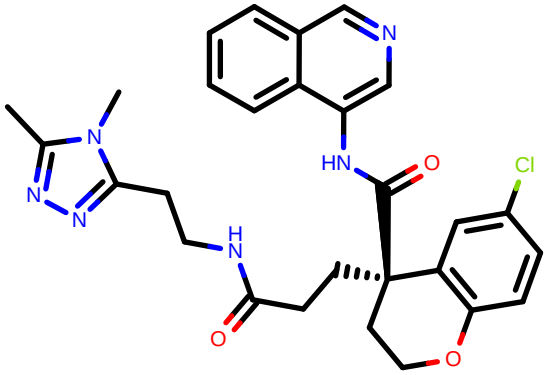
CID:	EN300-7535922_1_1
SMILES:	CN(C)c1ccc(nn1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8843
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.27

EN300-1722017_2_1



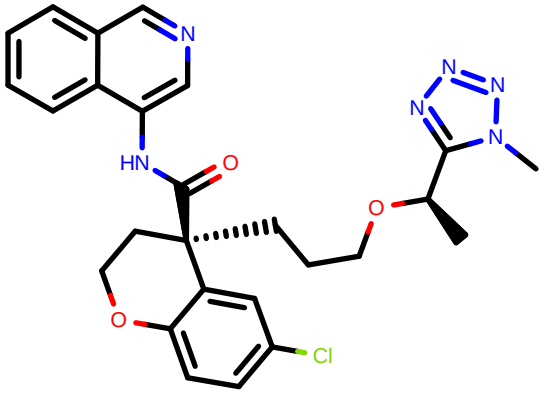
CID:	EN300-1722017_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CC5)n6nccn6
RUN:	RUN4834
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.29

EN300-172485_2_1



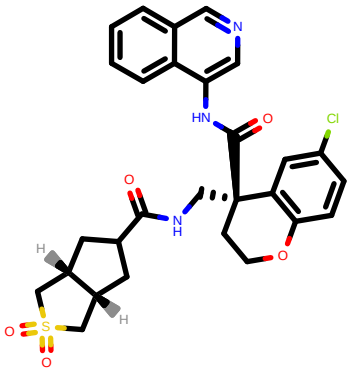
CID:	EN300-172485_2_1
SMILES:	Cc1nnc(n1C)CCNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9097
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.32

EN300-173006_4_2



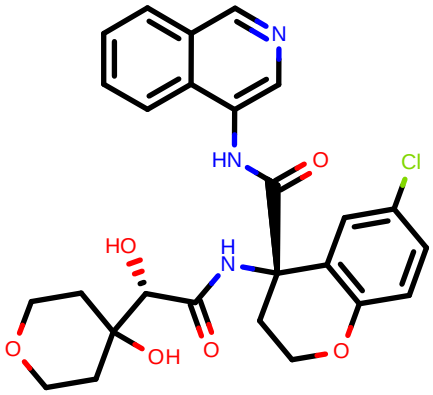
CID:	EN300-173006_4_2
SMILES:	C[C@H](c1nnnn1C)OCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1279
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.34

EN300-7438088_2_1



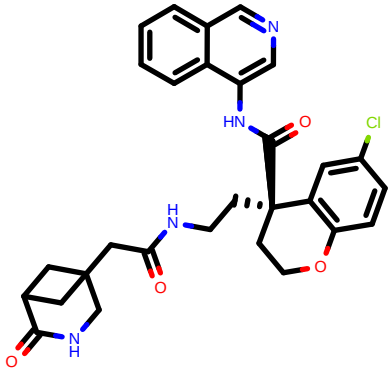
CID:	EN300-7438088_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5C[C@@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN5449
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.23

EN300-749499_1_2



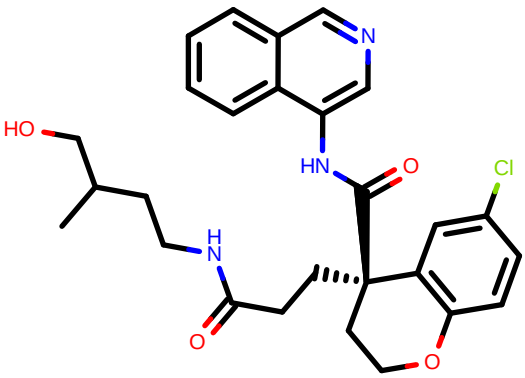
CID:	EN300-749499_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H](C5(CCOCC5)O)O
RUN:	RUN2392
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.32

EN300-6487134_3_1



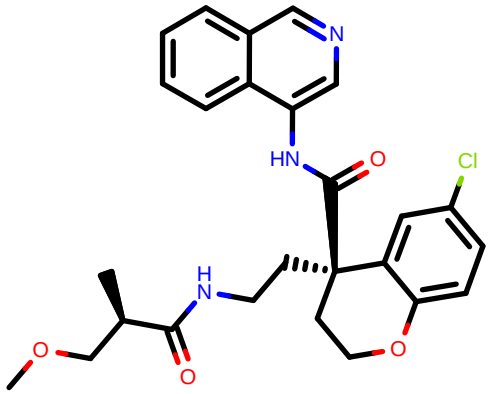
CID:	EN300-6487134_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)CC56CC(C5)C(=O)NC6
RUN:	RUN3616
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.40

EN300-7540675_2_1



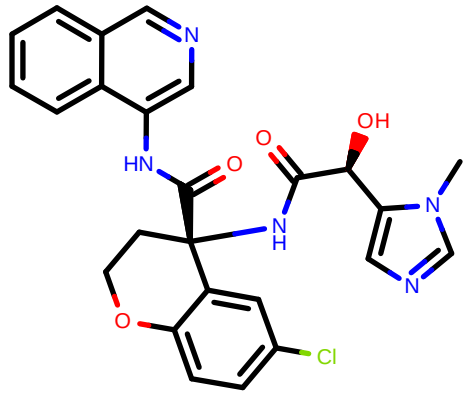
CID:	EN300-7540675_2_1
SMILES:	C=C(CCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)CO
RUN:	RUN11197
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.26

EN300-69162_3_2



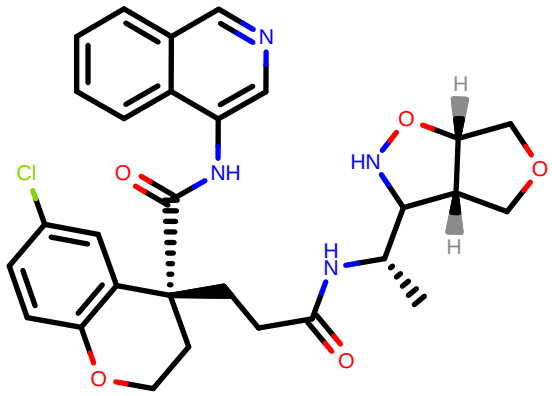
CID:	EN300-69162_3_2
SMILES:	C[C@H](COC)C(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1585
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.31

EN300-190283_1_1



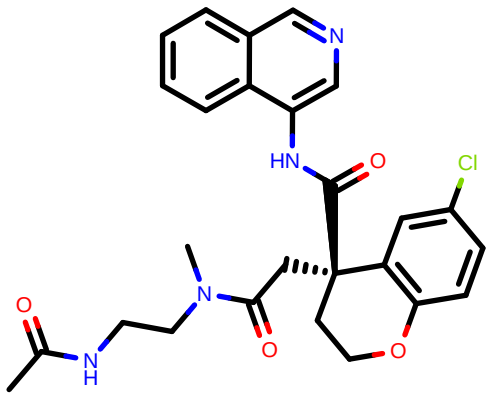
CID:	EN300-190283_1_1
SMILES:	Cn1cncc1[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7338
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.35

EN300-7438575_2_1



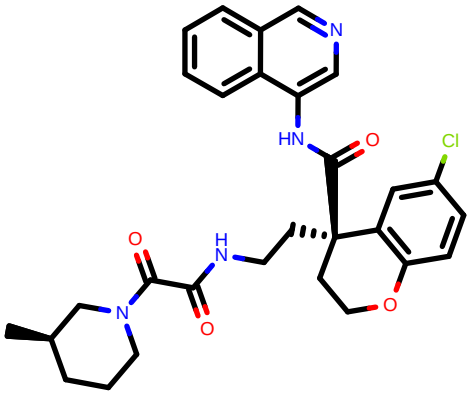
CID:	EN300-7438575_2_1
SMILES:	C[C@@H](C1=NO[C@H]2[C@@H]1COC2)NC(=O)CC[C@]3(CCOc4cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN7561
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.29

EN300-150022_1_1



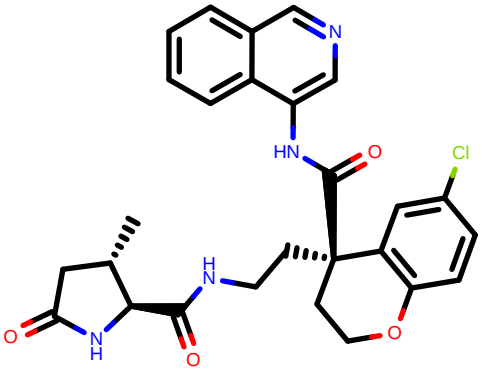
CID:	EN300-150022_1_1
SMILES:	CC(=O)NCCN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN7832
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.26

EN300-137786_3_1



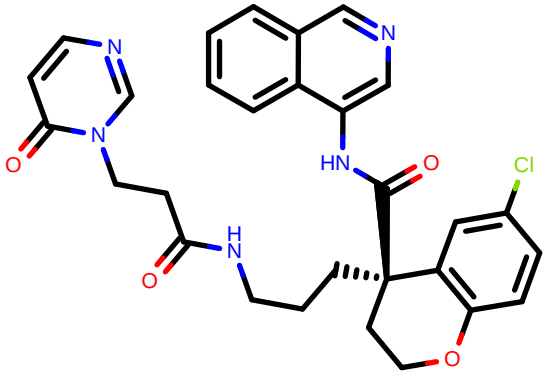
CID:	EN300-137786_3_1
SMILES:	C[C@@H]1CCCN(C1)C(=O)C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9520
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.32

EN300-155362_3_2



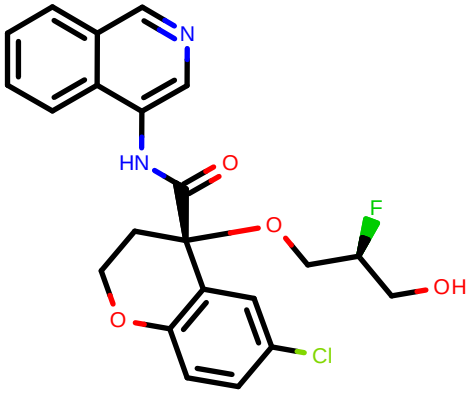
CID:	EN300-155362_3_2
SMILES:	C[C@H]1CC(=O)N[C@@H]1C(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10304
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.28

EN300-219609_4_1



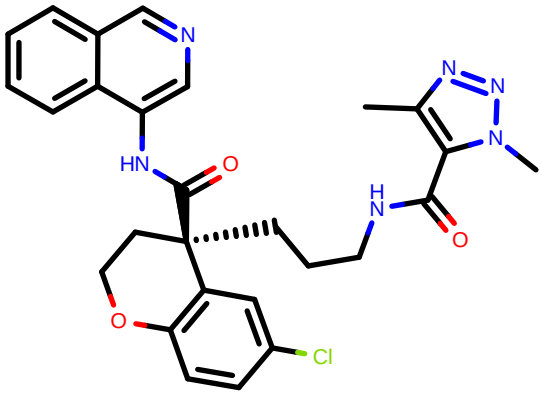
CID:	EN300-219609_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)CCn5cnccc5=O
RUN:	RUN10673
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.35

EN300-1600517_1_2



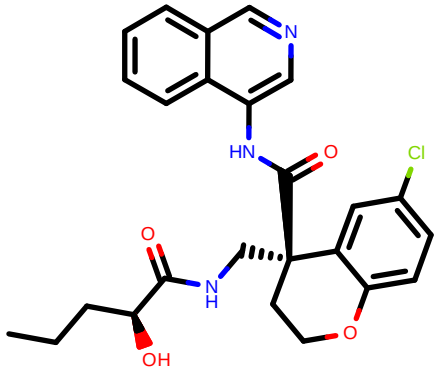
CID:	EN300-1600517_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CO)F
RUN:	RUN1208
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.29

EN300-649738_4_1



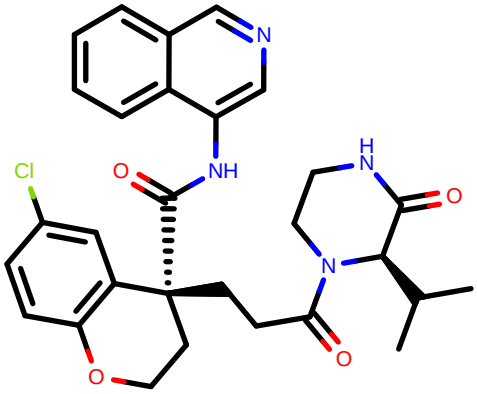
CID:	EN300-649738_4_1
SMILES:	Cc1c(n(nn1)C)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9115
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.34

EN300-219531_2_1



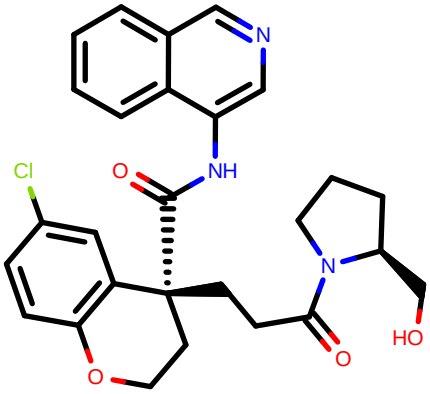
CID:	EN300-219531_2_1
SMILES:	CCC[C@@H](C(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN2955
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.37

EN300-67791_2_1



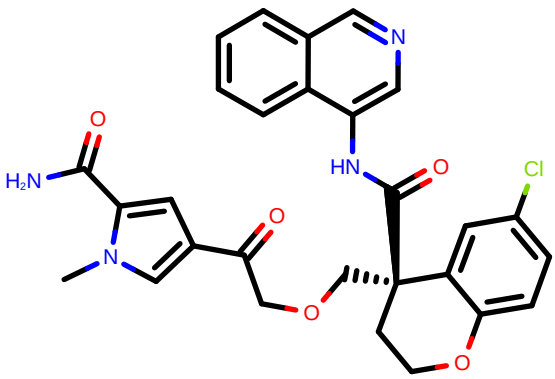
CID:	EN300-67791_2_1
SMILES:	CC(C)[C@@H]1C(=O)NCCN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7345
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.26

EN300-55109_2_2



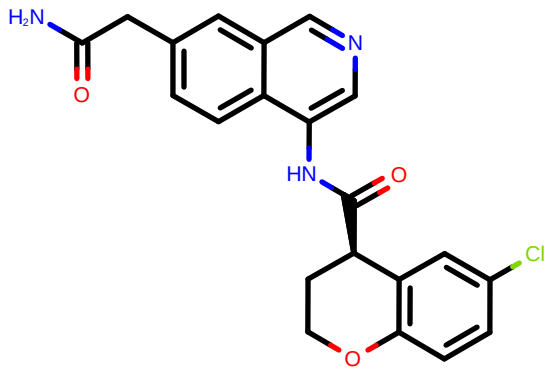
CID:	EN300-55109_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCC[C@H]5CO
RUN:	RUN1890
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.27

EN300-35592_2_1



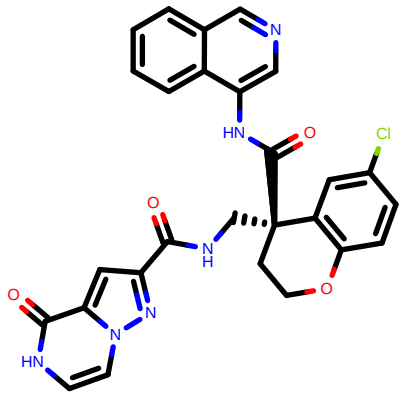
CID:	EN300-35592_2_1
SMILES:	Cn1cc(cc1C(=O)N)C(=O)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1366
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.29

MAK-UNK-8be7dca9-2_1



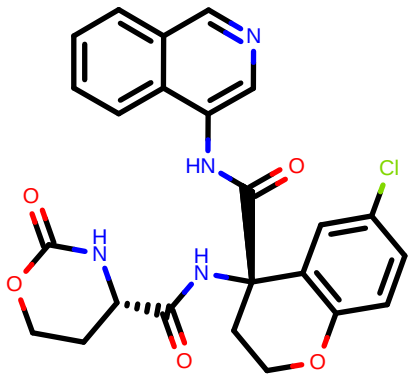
CID:	MAK-UNK-8be7dca9-2_1
SMILES:	c1cc2c(cc1CC(=O)N)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN59
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.09

EN300-393121_2_1



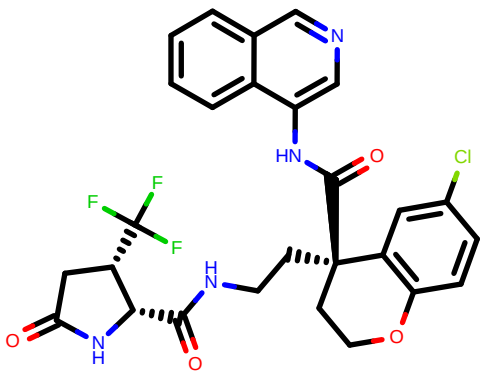
CID:	EN300-393121_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6c(=O)[nH]ccn6n5
RUN:	RUN8499
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.26

EN300-249804_1_1



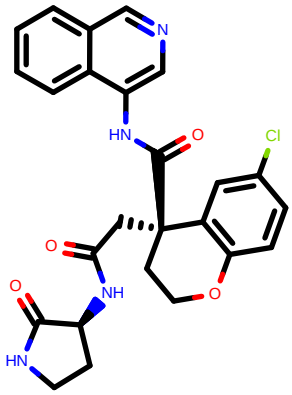
CID:	EN300-249804_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]5CCOC(=O)N5
RUN:	RUN4833
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.26

EN300-169955_3_4



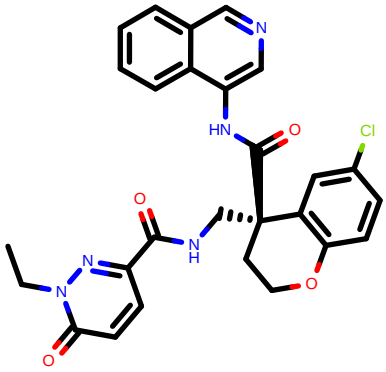
CID:	EN300-169955_3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5[C@H](CC(=O)N5)C(F)(F)F
RUN:	RUN7600
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.38

EN300-307333_1_1



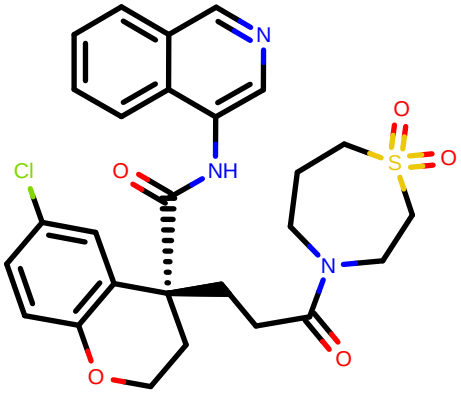
CID:	EN300-307333_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCNC5=O
RUN:	RUN10105
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.21

EN300-74314_2_1



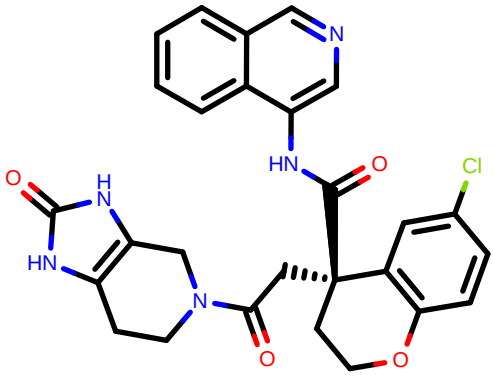
CID:	EN300-74314_2_1
SMILES:	CCn1c(=O)ccc(n1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7543
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.27

EN300-73620_2_1



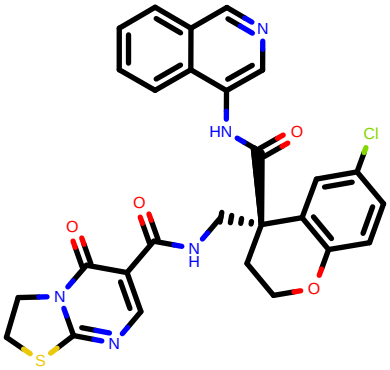
CID:	EN300-73620_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCCS(=O)(=O)CC5
RUN:	RUN6051
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.45

EN300-7237143_1_1



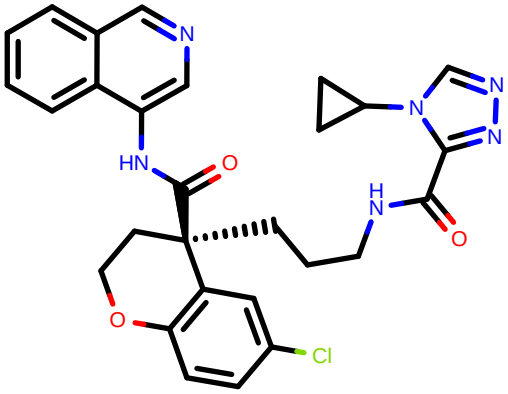
CID:	EN300-7237143_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCc6c([nH]c(=O)[nH]6)C5
RUN:	RUN5930
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.28

EN300-14405_2_1



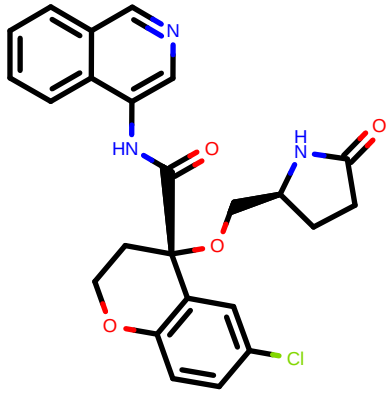
CID:	EN300-14405_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnc6n(c5=O)CCS6
RUN:	RUN7547
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.32

EN300-6745581_4_1



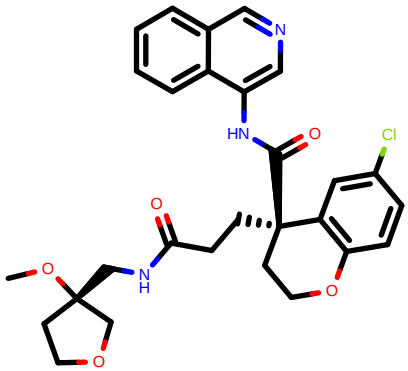
CID:	EN300-6745581_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5nncn5C6CC6
RUN:	RUN11291
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.44

EN300-264301_1_1



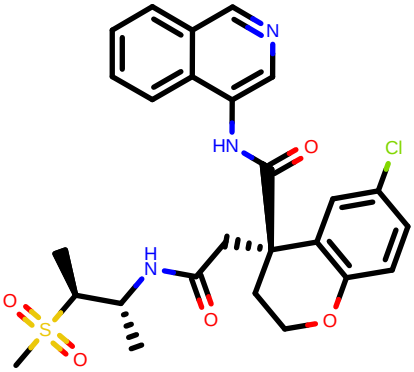
CID:	EN300-264301_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCC(=O)N5
RUN:	RUN2119
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.26

EN300-137255_2_2



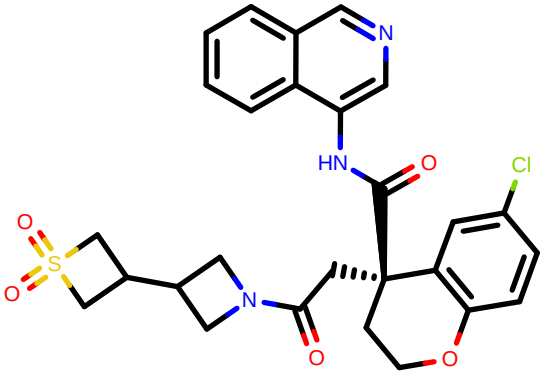
CID:	EN300-137255_2_2
SMILES:	CO[C@]1(CCOC1)CNC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4276
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.26

EN300-83434_1_4



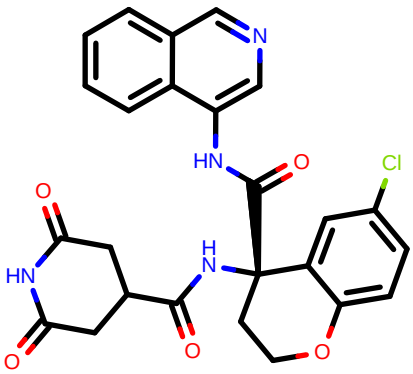
CID:	EN300-83434_1_4
SMILES:	C[C@H]([C@H](C)S(=O)(=O)C)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9268
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.34

EN300-246501_1_1



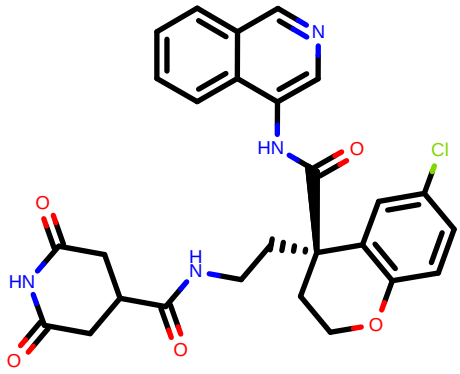
CID:	EN300-246501_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)C6CS(=O)(=O)C6
RUN:	RUN7064
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.31

EN300-62192_1_1



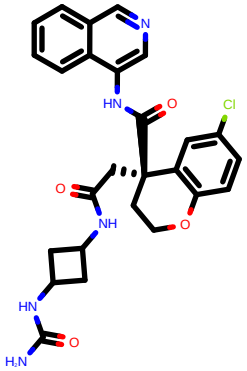
CID:	EN300-62192_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5CC(=O)NC(=O)C5
RUN:	RUN7018
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.29

EN300-62192_3_1



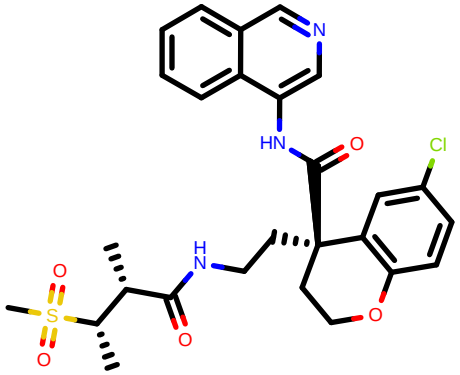
CID:	EN300-62192_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5CC(=O)NC(=O)C5
RUN:	RUN9608
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.26

EN300-1702911_1_1



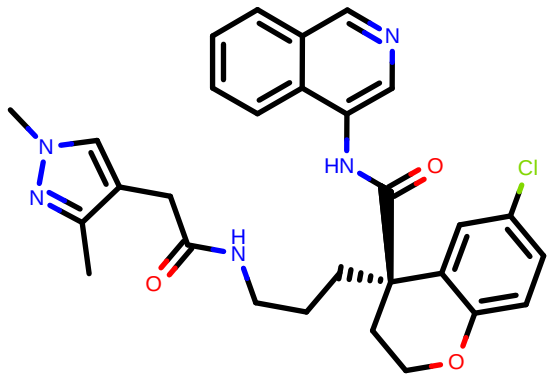
CID:	EN300-1702911_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC5CC(C5)NC(=O)N
RUN:	RUN7076
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.32

EN300-182725_3_3



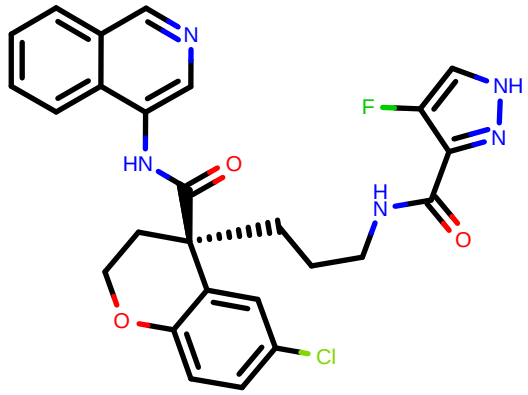
CID:	EN300-182725_3_3
SMILES:	C[C@@H]([C@H](C)S(=O)(=O)C)C(=O)NCC[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2417
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.46

EN300-245061_4_1



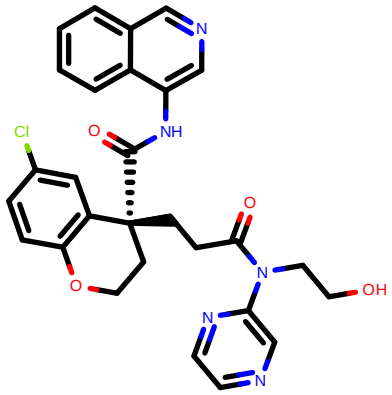
CID:	EN300-245061_4_1
SMILES:	Cc1c(cn(n1)C)CC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10827
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.33

EN300-98143_4_1



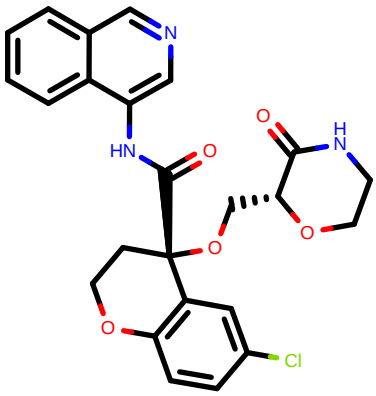
CID:	EN300-98143_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5c(cn[nH]5)F
RUN:	RUN9501
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.28

EN300-370792_2_1



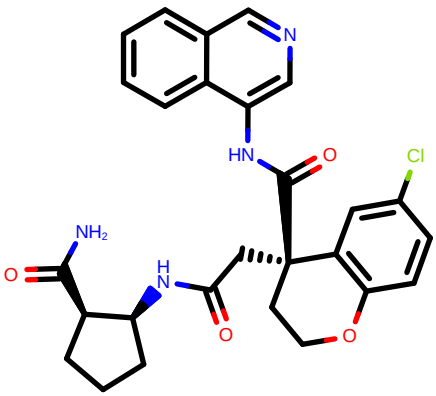
CID:	EN300-370792_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N(CCO)c5cnccn5
RUN:	RUN9978
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.27

EN300-1706036_1_1



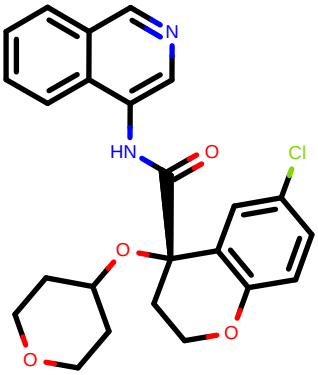
CID:	EN300-1706036_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C(=O)NCCO5
RUN:	RUN2031
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.27

EN300-90531_1_4



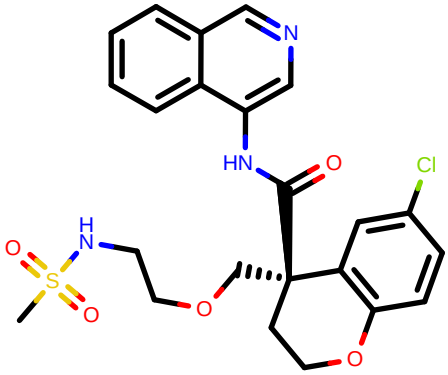
CID:	EN300-90531_1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCC[C@H]5C(=O)N
RUN:	RUN8400
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.35

EDJ-MED-28ec730d-3_1



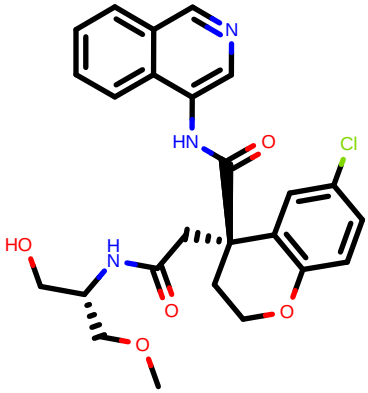
CID:	EDJ-MED-28ec730d-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5CCOCC5
RUN:	RUN169
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.25

EN300-1238839_2_1



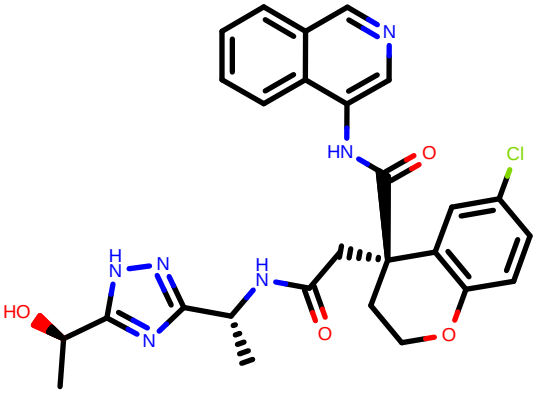
CID:	EN300-1238839_2_1
SMILES:	CS(=O)(=O)NCCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN283
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.30

EN300-216674_1_1



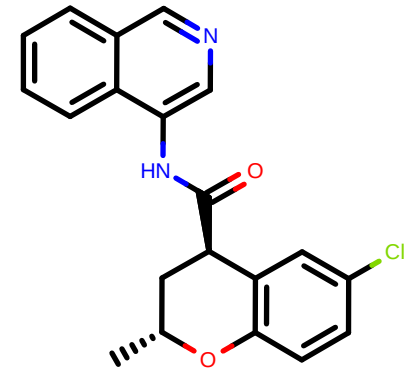
CID:	EN300-216674_1_1
SMILES:	COC[C@H](CO)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN9864
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.35

EN300-7443527_1_2



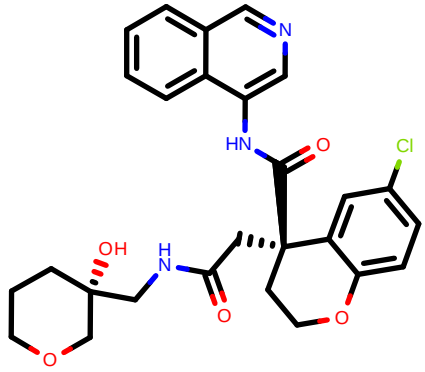
CID:	EN300-7443527_1_2
SMILES:	C[C@H](c1[nH]c(nn1)[C@@H](C)O)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9622
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.30

ALP-POS-d3acb8cc-4_1



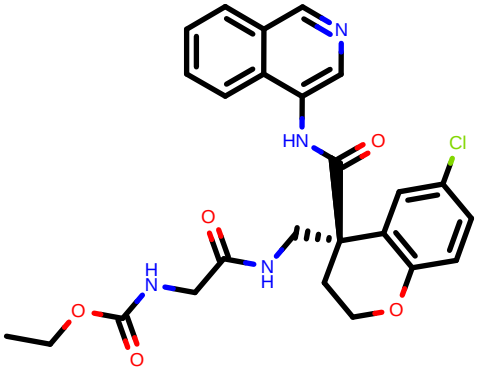
CID:	ALP-POS-d3acb8cc-4_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN38
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.05

EN300-193679_1_1



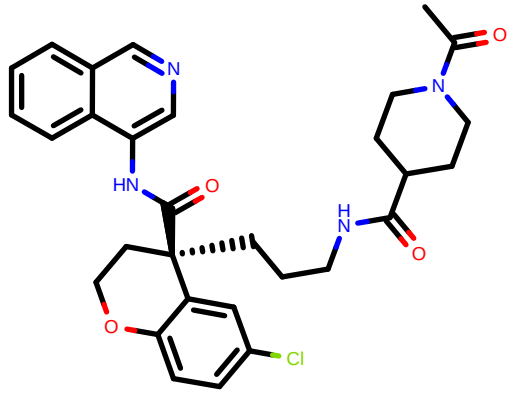
CID:	EN300-193679_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@]5(CCCOC5)O
RUN:	RUN4319
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.39

EN300-36390_2_1



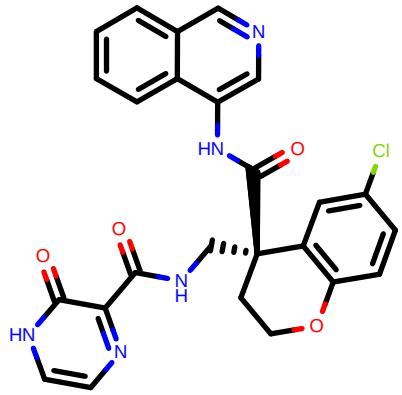
CID:	EN300-36390_2_1
SMILES:	CCOC(=O)NCC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4130
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

EN300-18557_4_1



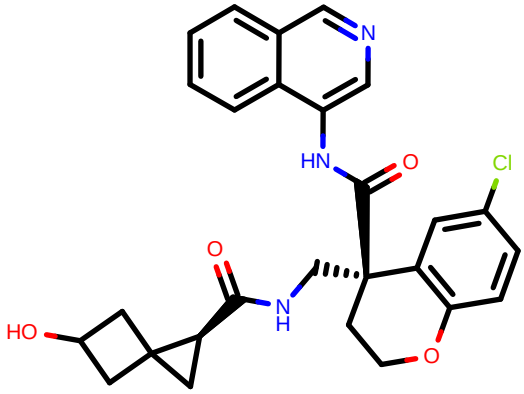
CID:	EN300-18557_4_1
SMILES:	CC(=O)N1CCC(CC1)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN11125
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.38

EN300-97055_2_1



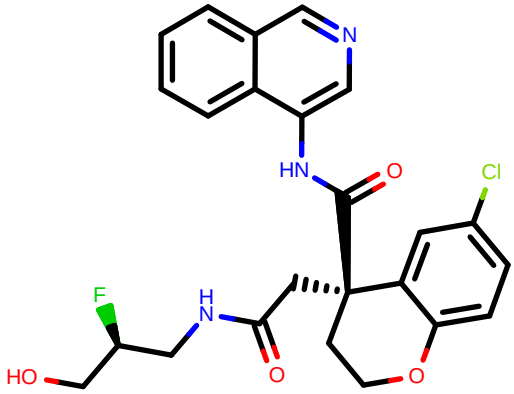
CID:	EN300-97055_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5c(=O)[nH]ccn5
RUN:	RUN8039
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.24

EN300-1717166_2_2



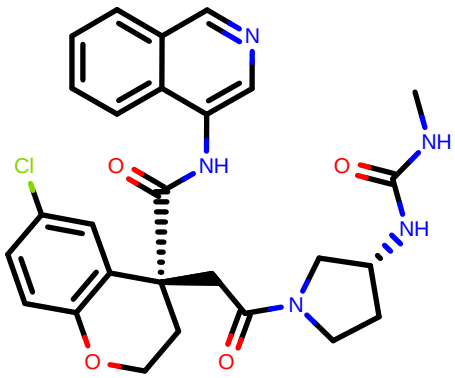
CID:	EN300-1717166_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CC56CC(C6)O
RUN:	RUN5841
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.19

EN300-7353971_1_1



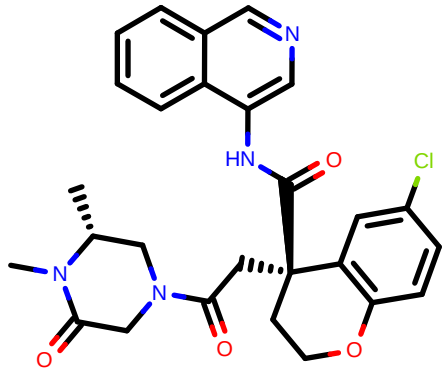
CID:	EN300-7353971_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NC[C@@H](CO)F
RUN:	RUN5071
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.29

EN300-139629_1_1



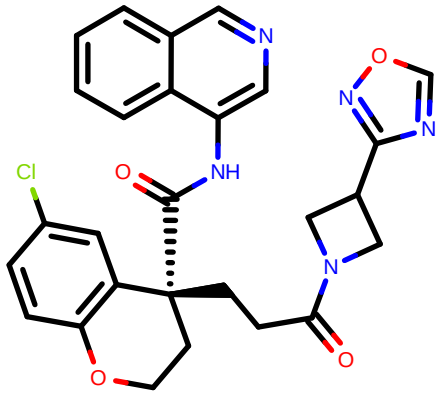
CID:	EN300-139629_1_1
SMILES:	CNC(=O)N[C@@H]1CCN(C1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9740
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

EN300-6482634_1_1



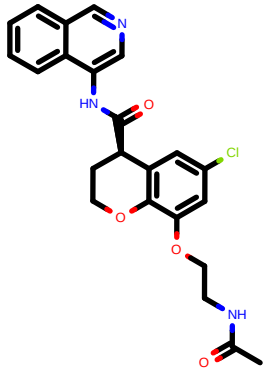
CID:	EN300-6482634_1_1
SMILES:	C[C@@H]1CN(CC(=O)N1C)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN930
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.32

EN300-1700143_2_1



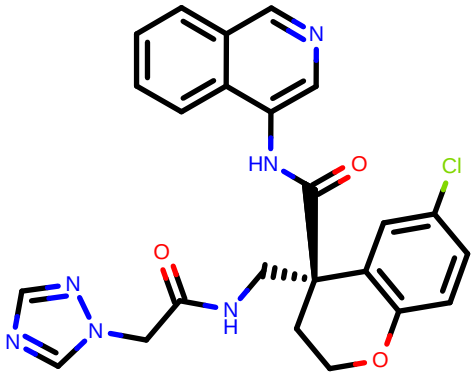
CID:	EN300-1700143_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC(C5)c6ncon6
RUN:	RUN812
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.27

NAU-LAT-0543f7f2-10_2



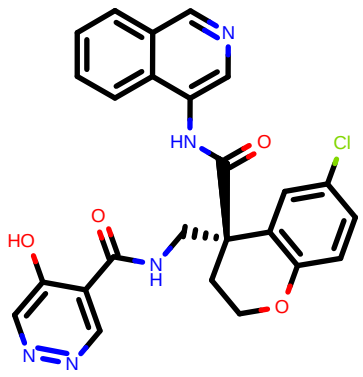
CID:	NAU-LAT-0543f7f2-10_2
SMILES:	CC(=O)NCCOc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN60
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.33

EN300-06654_2_1



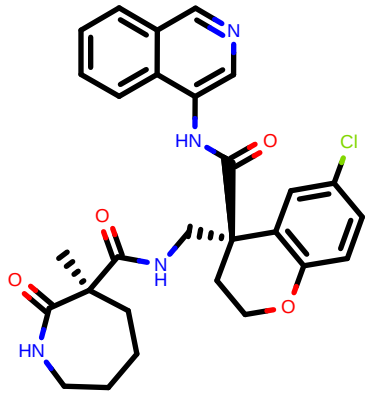
CID:	EN300-06654_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5cncn5
RUN:	RUN4826
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.26

EN300-243828_2_1



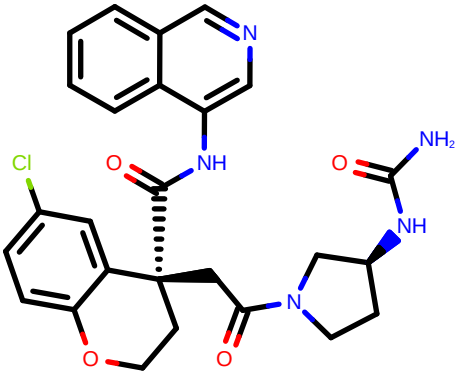
CID:	EN300-243828_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnncc5O
RUN:	RUN6720
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.37

EN300-6745081_2_1



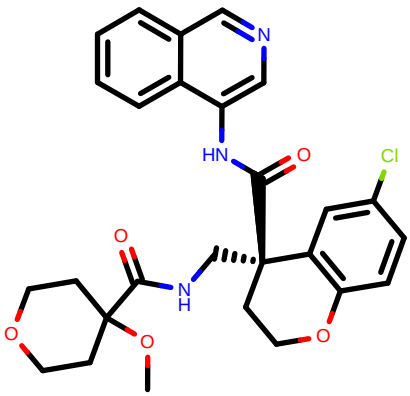
CID:	EN300-6745081_2_1
SMILES:	C[C@@]1(CCCCNC1=O)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4566
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.50

EN300-118869_1_1



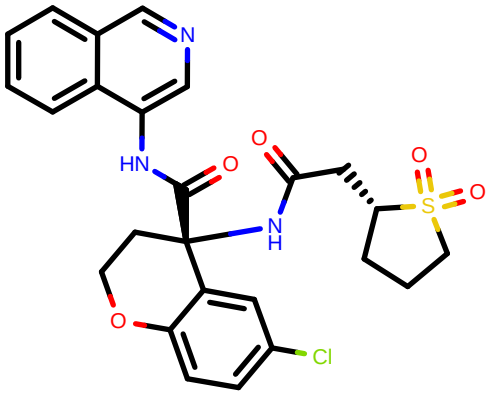
CID:	EN300-118869_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H](C5)NC(=O)N
RUN:	RUN4719
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.30

EN300-204133_2_1



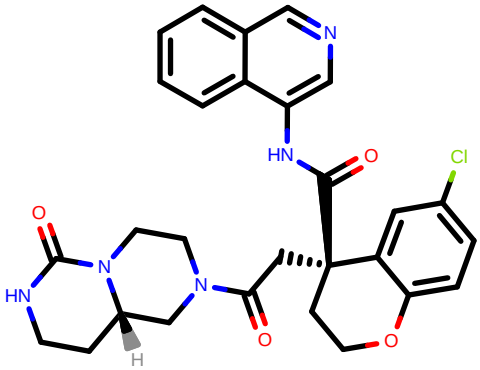
CID:	EN300-204133_2_1
SMILES:	COC1(CCOCC1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3523
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.36

EN300-155176_1_2



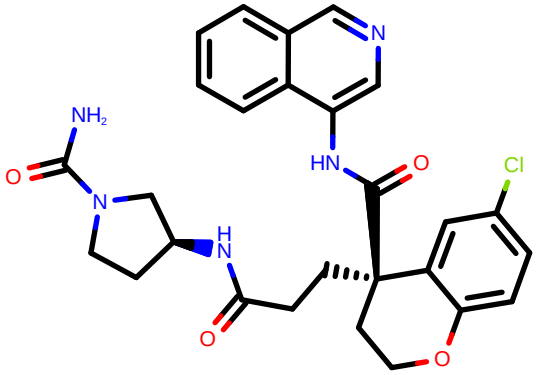
CID:	EN300-155176_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[C@H]5CCCS5(=O)=O
RUN:	RUN2308
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.28

EN300-6474647_1_2



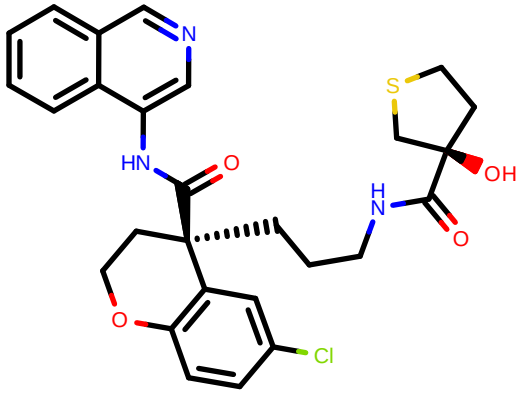
CID:	EN300-6474647_1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN6[C@H](C5)CCNC6=O
RUN:	RUN4159
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.28

EN300-75402_2_2



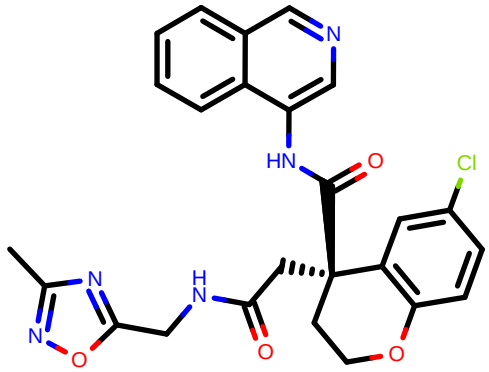
CID:	EN300-75402_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N[C@H]5CCN(C5)C(=O)N
RUN:	RUN3661
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.35

EN300-122656_4_2



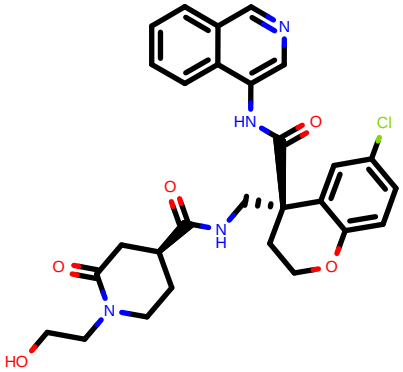
CID:	EN300-122656_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@]5(CCSC5)O
RUN:	RUN7737
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.50

EN300-50657_1_1



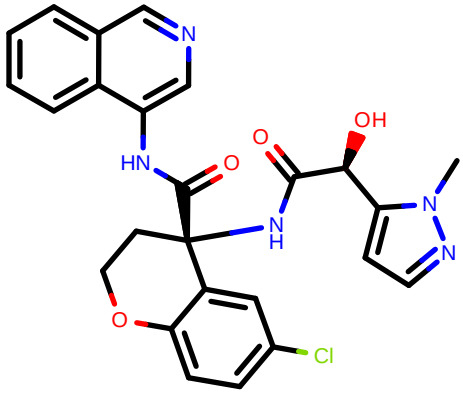
CID:	EN300-50657_1_1
SMILES:	Cc1nc(on1)CNC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7936
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.27

EN300-1723663_2_2



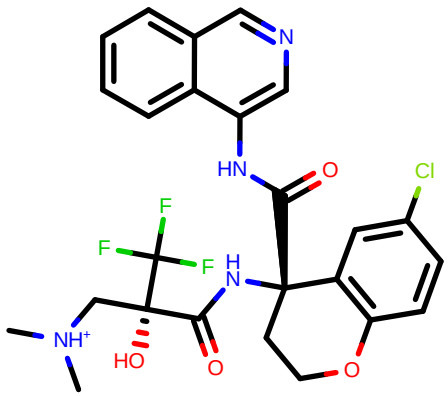
CID:	EN300-1723663_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5CCN(C(=O)C5)CCO
RUN:	RUN358
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.34

EN300-6473273_1_1



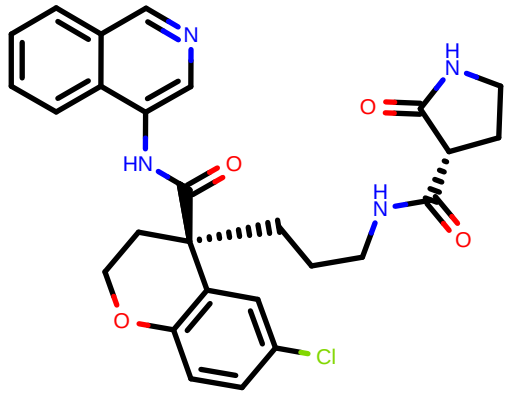
CID:	EN300-6473273_1_1
SMILES:	Cn1c(ccn1)[C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN7426
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.27

EN300-7459545_1_2



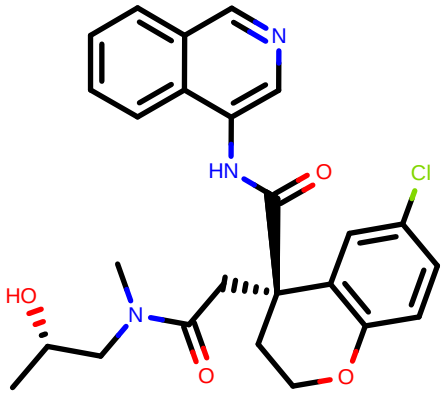
CID:	EN300-7459545_1_2
SMILES:	CN(C)C[C@](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C(F)(F)F)O
RUN:	RUN7002
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.31

EN300-94945_4_2



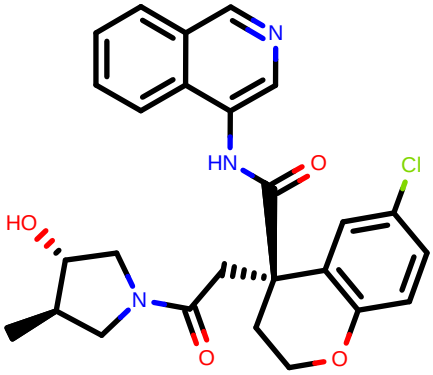
CID:	EN300-94945_4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)[C@H]5CCNC5=O
RUN:	RUN9225
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.35

EN300-55145_1_1



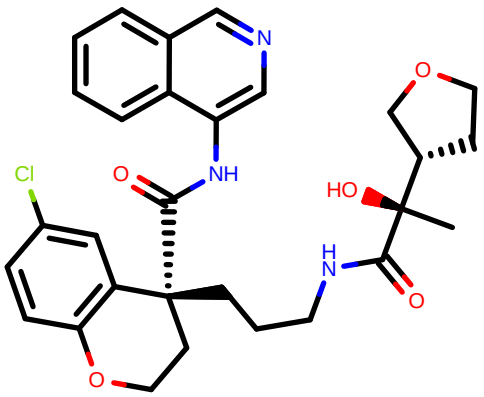
CID:	EN300-55145_1_1
SMILES:	C[C@@H](CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN6285
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.28

EN300-6497226_1_1



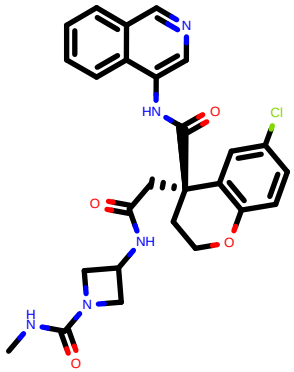
CID:	EN300-6497226_1_1
SMILES:	C[C@@H]1CN(C[C@H]1O)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4727
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.25

EN300-217494_4_3



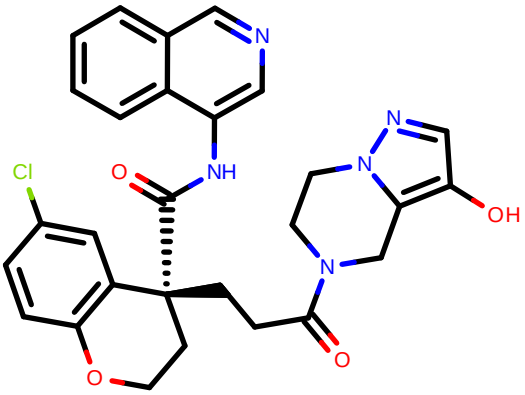
CID:	EN300-217494_4_3
SMILES:	C[C@@]([C@H]1CCOC1)(C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN10627
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.28

EN300-6474575_1_1



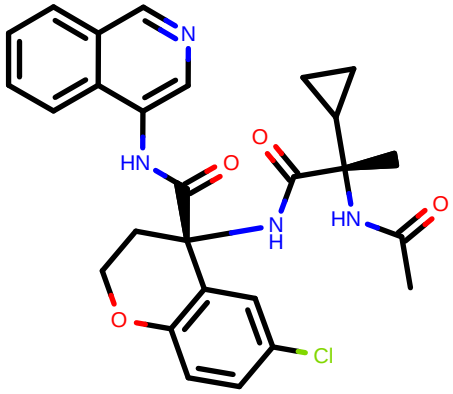
CID:	EN300-6474575_1_1
SMILES:	CNC(=O)N1CC(C1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN10682
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.28

EN300-7355835_2_1



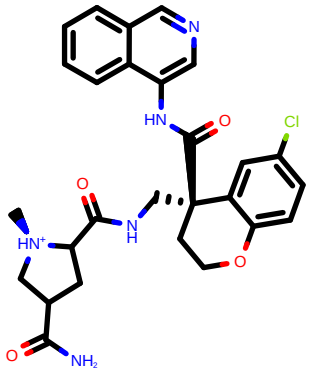
CID:	EN300-7355835_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CCn6c(c(cn6)O)C5
RUN:	RUN4480
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.30

EN300-67073_1_1



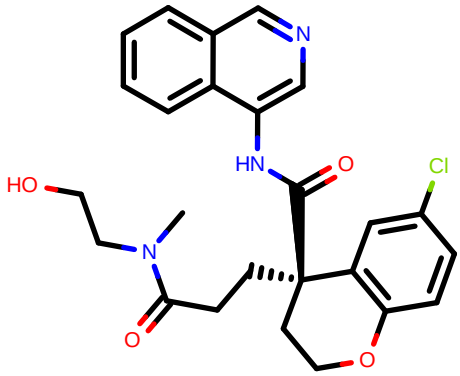
CID:	EN300-67073_1_1
SMILES:	CC(=O)N[C@@](C)(C1CC1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7494
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.27

EN300-105081_2_1



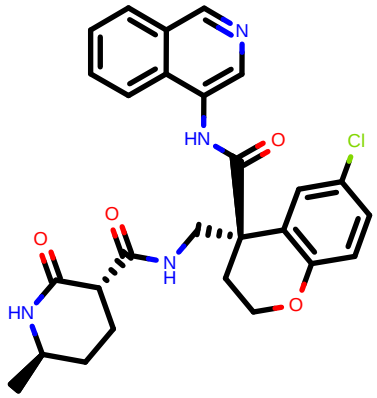
CID:	EN300-105081_2_1
SMILES:	Cn1cc(cc1C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C(=O)N
RUN:	RUN8303
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.28

EN300-19342_2_1



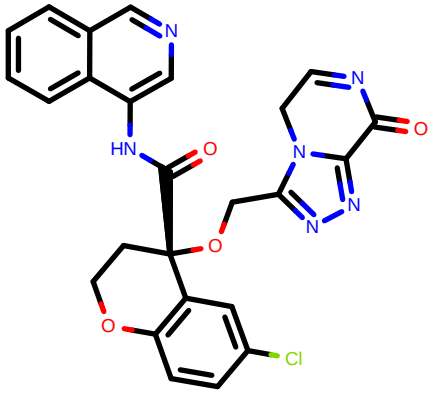
CID:	EN300-19342_2_1
SMILES:	CN(CCO)C(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1722
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.30

EN300-6505003_2_3



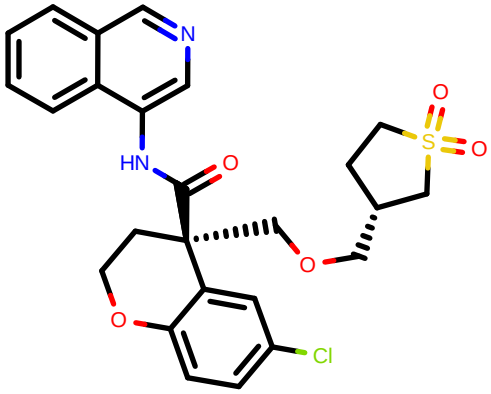
CID:	EN300-6505003_2_3
SMILES:	C[C@@H]1CC[C@H](C(=O)N1)C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5881
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.29

EN300-378316_1_1



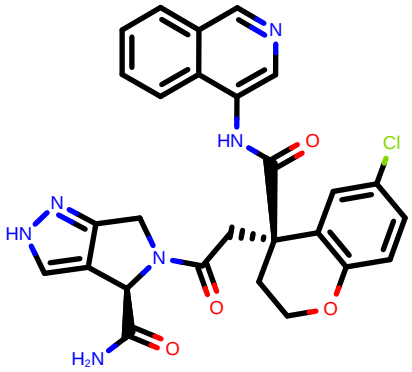
CID:	EN300-378316_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nnc6n5cc[nH]c6=O
RUN:	RUN1160
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.26

EN300-1448603_2_1



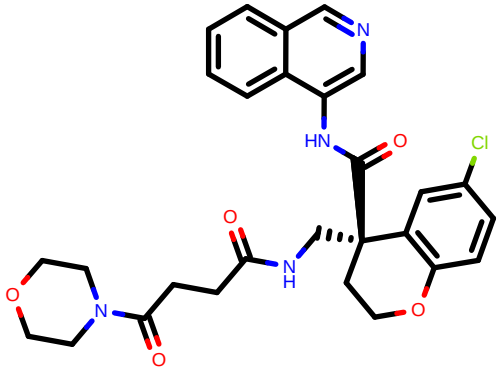
CID:	EN300-1448603_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CCS(=O)(=O)C5
RUN:	RUN2181
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.36

EN300-1704047_1_1



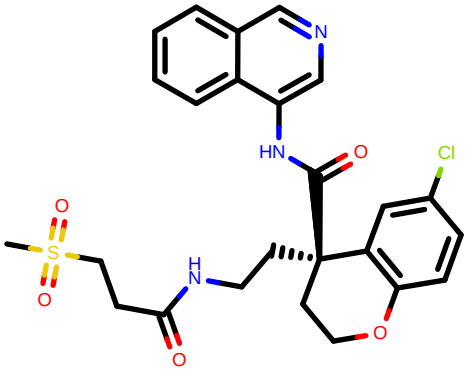
CID:	EN300-1704047_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cc6c(cn[nH]6)[C@@H]5C(=O)N
RUN:	RUN11052
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.38

EN300-05277_2_1



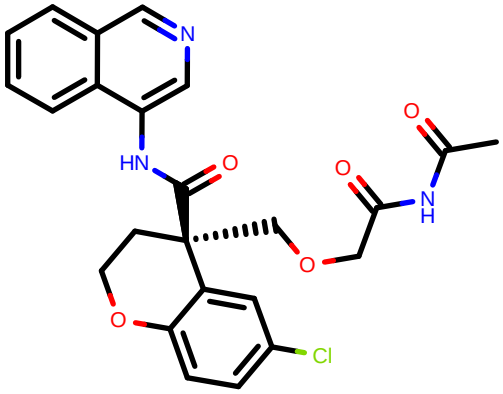
CID:	EN300-05277_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)CCC(=O)N5CCOCC5
RUN:	RUN278
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.31

EN300-31387_3_1



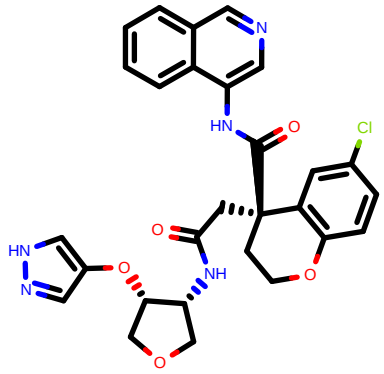
CID:	EN300-31387_3_1
SMILES:	CS(=O)(=O)CCC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4175
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.29

EN300-249475_2_1



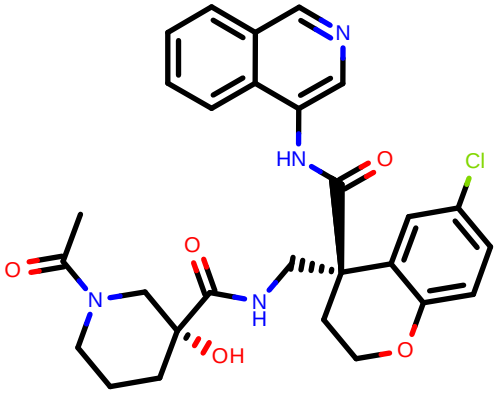
CID:	EN300-249475_2_1
SMILES:	CC(=O)NC(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1214
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.23

EN300-716163_1_1



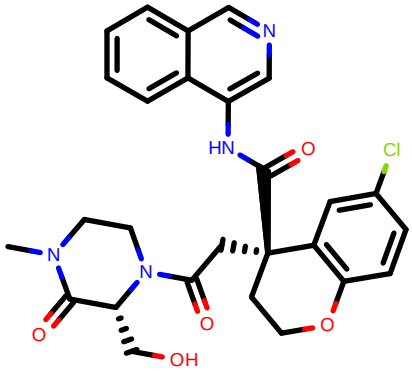
CID:	EN300-716163_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4cc3cc(cc4)Cl)CC(=O)N[C@@H]5COC[C@@H]5Oc6c[nH]nc6
RUN:	RUN9794
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.39

EN300-210552_2_1



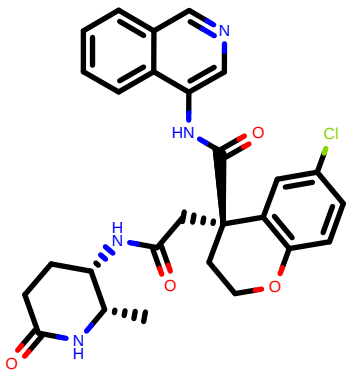
CID:	EN300-210552_2_1
SMILES:	CC(=O)N1CCC[C@@](C1)(C(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN5929
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.55

EN300-1724997_1_1



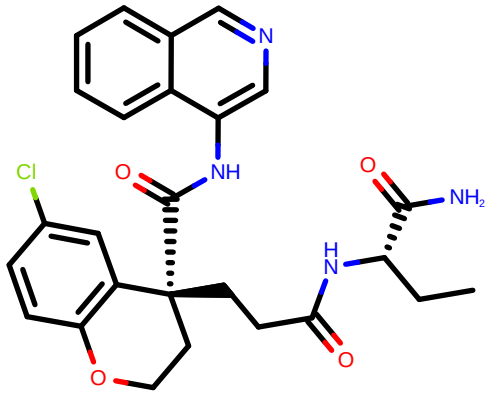
CID:	EN300-1724997_1_1
SMILES:	CN1CCN([C@@H](C1=O)CO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN7584
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.32

EN300-199449_1_4



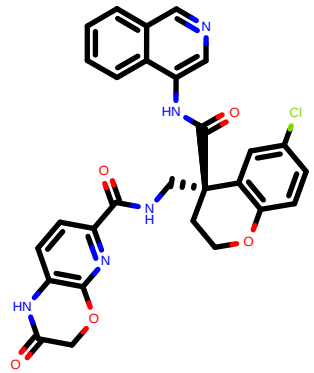
CID:	EN300-199449_1_4
SMILES:	C[C@H]1[C@H](CCC(=O)N1)NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN8348
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.29

EN300-218962_2_1



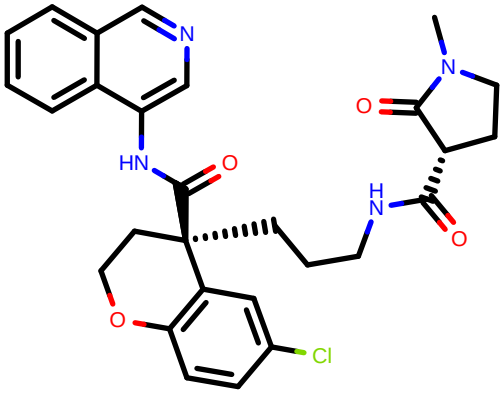
CID:	EN300-218962_2_1
SMILES:	CC[C@@H](C(=O)N)NC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1075
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.28

EN300-2726690_2_1



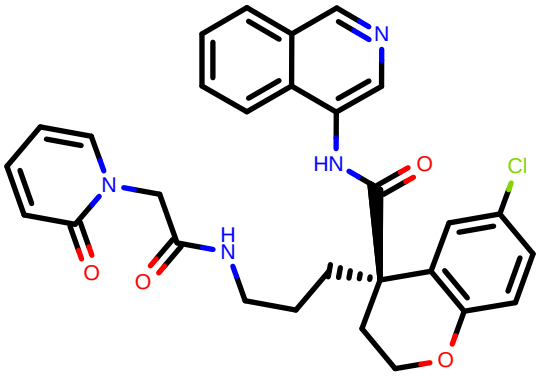
CID:	EN300-2726690_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6c(n5)OCC(=O)N6
RUN:	RUN8815
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.31

EN300-141695_4_1



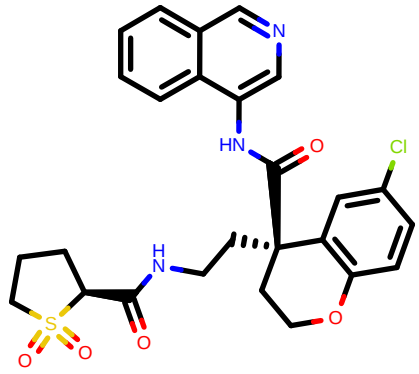
CID:	EN300-141695_4_1
SMILES:	CN1CC[C@@H](C1=O)C(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN9218
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.39

EN300-11714_4_1



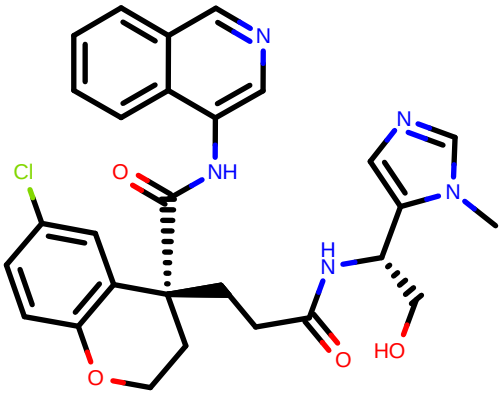
CID:	EN300-11714_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)Cn5ccccc5=O
RUN:	RUN11285
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.29

EN300-88656_3_1



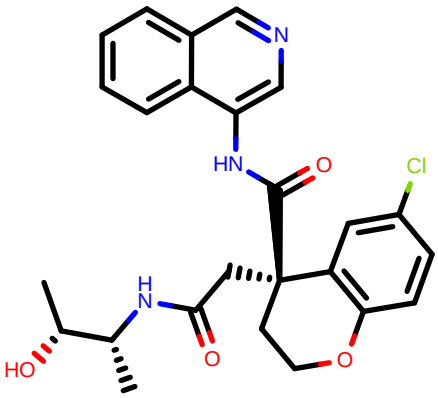
CID:	EN300-88656_3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@@H]5CCCS5(=O)=O
RUN:	RUN4463
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.33

EN300-305343_2_2



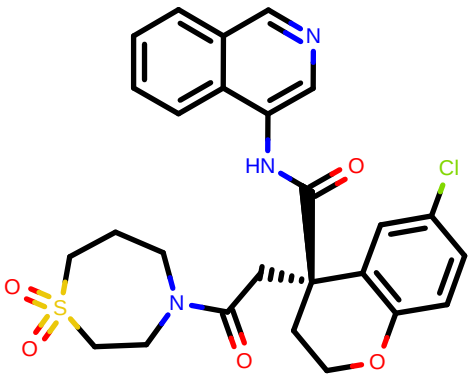
CID:	EN300-305343_2_2
SMILES:	Cn1cncc1[C@H](CO)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5915
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.31

EN300-72272_1_2



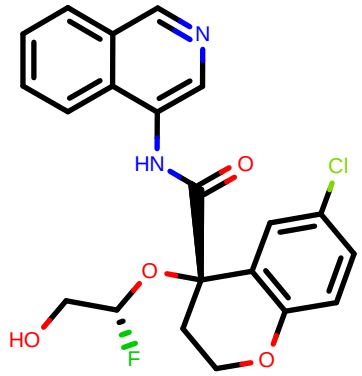
CID:	EN300-72272_1_2
SMILES:	C[C@H]([C@@H](C)O)NC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN10484
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.26

EN300-73620_1_1



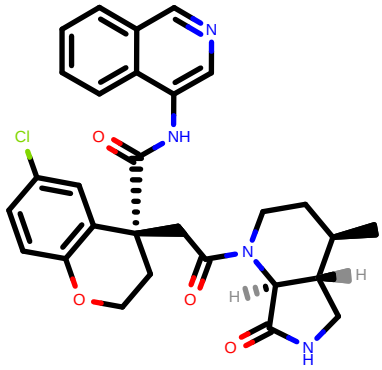
CID:	EN300-73620_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCS(=O)(=O)CC5
RUN:	RUN2912
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.38

EN300-861925_1_1



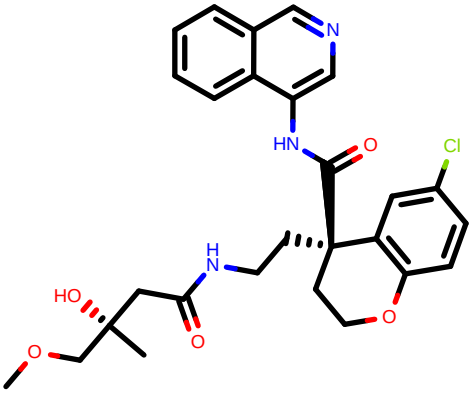
CID:	EN300-861925_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@@H](CO)F
RUN:	RUN1711
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.25

EN300-6739879_1_7



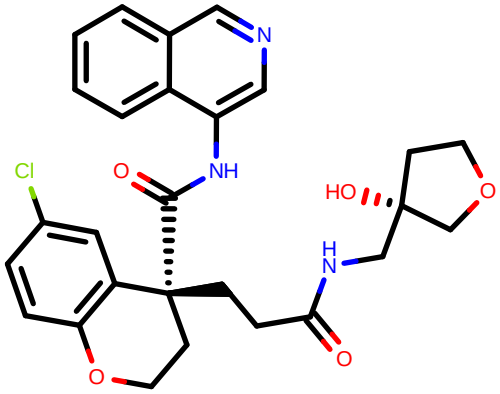
CID:	EN300-6739879_1_7
SMILES:	C[C@@H]1CCN([C@H]2[C@H]1CNC2=O)C(=O)C[C@]3(CCOc4c3ccc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN10384
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.26

EN300-1296824_3_2



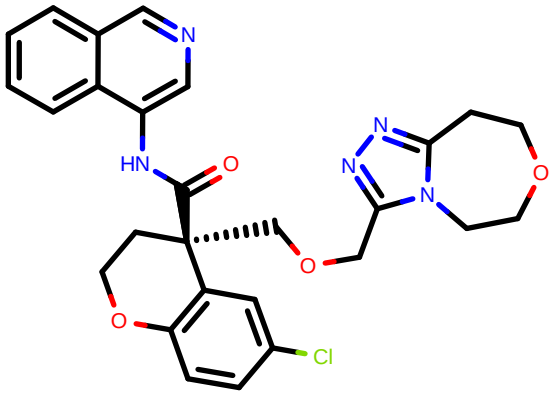
CID:	EN300-1296824_3_2
SMILES:	C[C@](CC(=O)NCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(COC)O
RUN:	RUN3560
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.38

EN300-200699_2_2



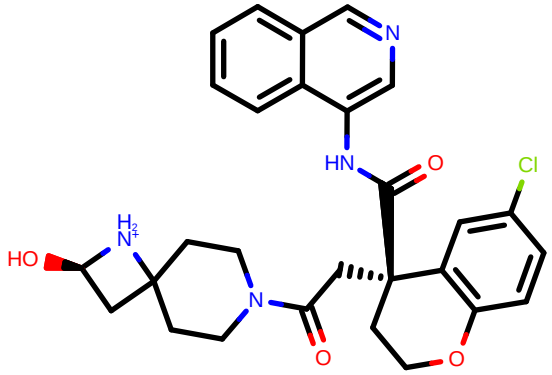
CID:	EN300-200699_2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NC[C@]5(CCOC5)O
RUN:	RUN2719
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.33

EN300-310888_2_1



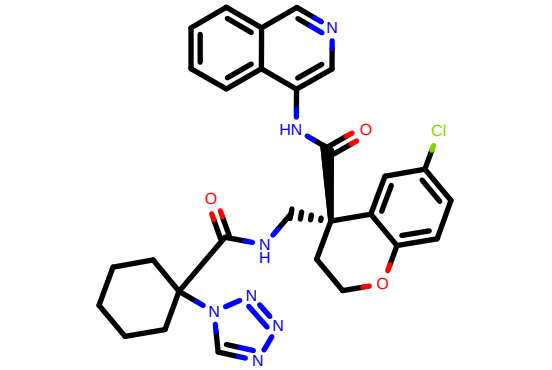
CID:	EN300-310888_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5nnc6n5CCOCC6
RUN:	RUN2109
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.31

EN300-52210_1_1



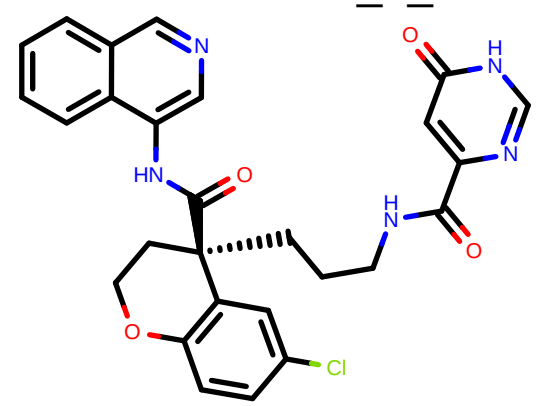
CID:	EN300-52210_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC6(CC5)CC(=O)N6
RUN:	RUN4615
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.25

EN300-186536_2_1



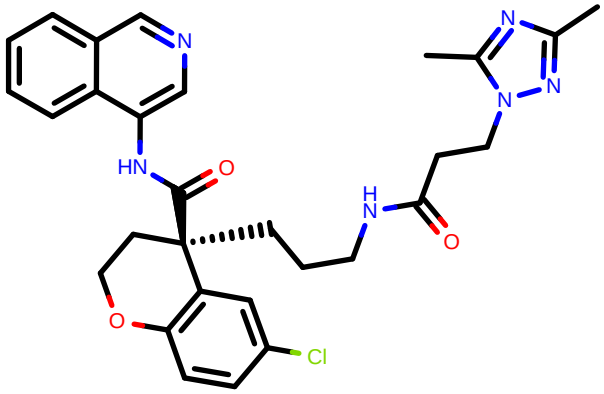
CID:	EN300-186536_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCCCC5)n6cnnn6
RUN:	RUN5837
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.55

EN300-817811_4_1



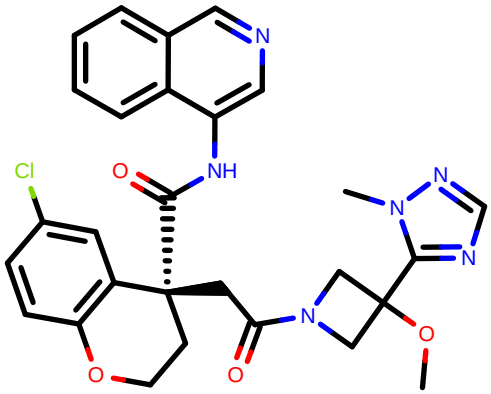
CID:	EN300-817811_4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCNC(=O)c5cc(=O)[nH]cn5
RUN:	RUN10146
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.31

EN300-41366_4_1



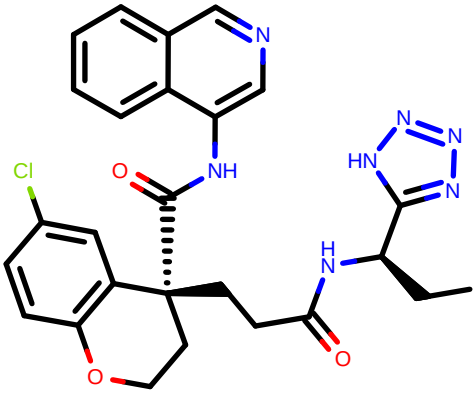
CID:	EN300-41366_4_1
SMILES:	Cc1nc(n(n1)CCC(=O)NCCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN9897
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.42

EN300-1725234_1_1



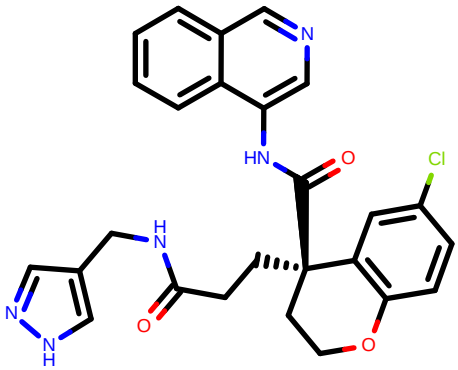
CID:	EN300-1725234_1_1
SMILES:	Cn1c(ncn1)C2(CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6)OC
RUN:	RUN10037
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.31

EN300-73861_2_2



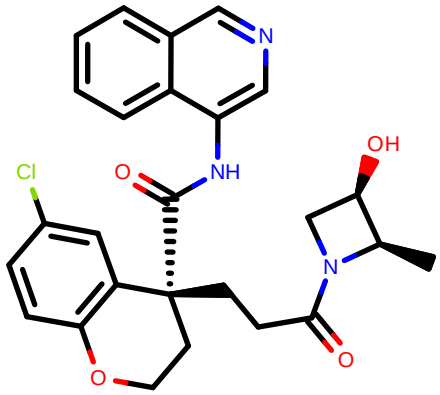
CID:	EN300-73861_2_2
SMILES:	CC[C@H](c1[nH]nnn1)NC(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4952
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.27

EN300-31562_2_1



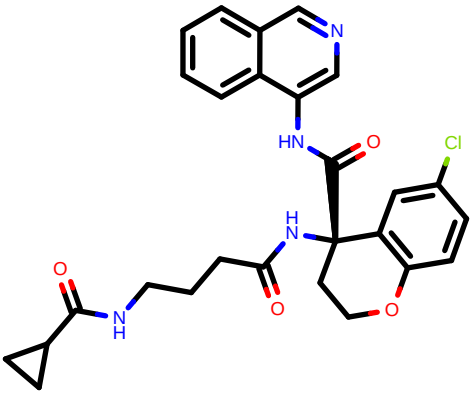
CID:	EN300-31562_2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCc5c[nH]nc5
RUN:	RUN1051
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.30

EN300-7471076_2_1



CID:	EN300-7471076_2_1
SMILES:	C[C@@H]1[C@@H](CN1C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2034
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.27

EN300-36850_1_1



CID:	EN300-36850_1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CCCNC(=O)C5CC5
RUN:	RUN410
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.33