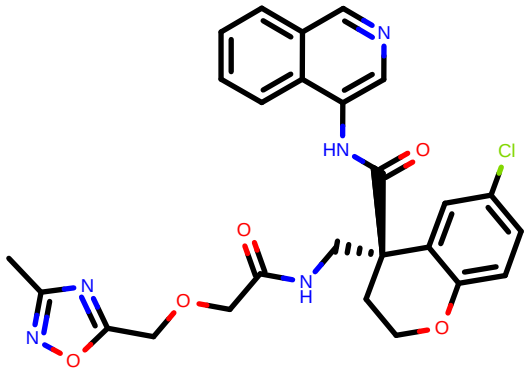
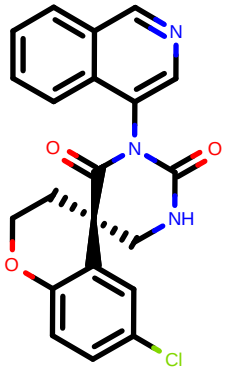
MAK-UNK-c749d764-11_1



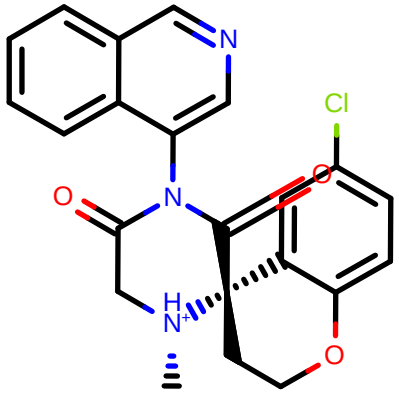
CID:	MAK-UNK-c749d764-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3O)C(F)F
RUN:	RUN949
DDG (kcal/mol):	-10.99
dDDG (kcal/mol):	0.17

LON-WEI-4d77710c-38_1



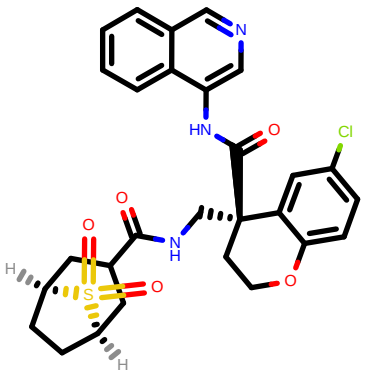
CID:	LON-WEI-4d77710c-38_1
SMILES:	CCCCN(CCCNC(=O)Nc1cn(c(=O)c2c1cccc2)CC(C)C)c3ccccc3
RUN:	RUN227
DDG (kcal/mol):	-9.94
dDDG (kcal/mol):	0.22

DAR-DIA-9e4459de-11_16



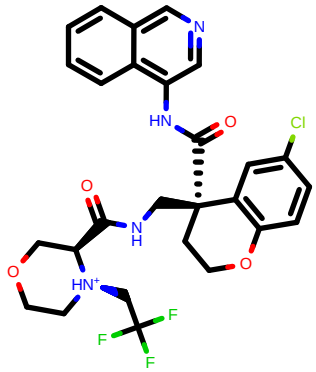
CID:	DAR-DIA-9e4459de-11_16
SMILES:	c1cc2c(c(c1)NCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1424
DDG (kcal/mol):	-9.72
dDDG (kcal/mol):	0.31

MAK-UNK-c749d764-6_1



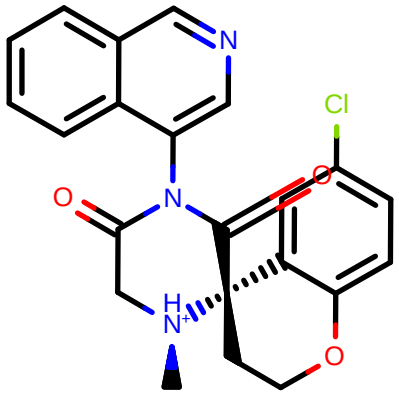
CID:	MAK-UNK-c749d764-6_1
SMILES:	C[C@@H](C[NH2+]CCCO)[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN932
DDG (kcal/mol):	-9.54
dDDG (kcal/mol):	0.20

ALP-POS-347519b5-1_34



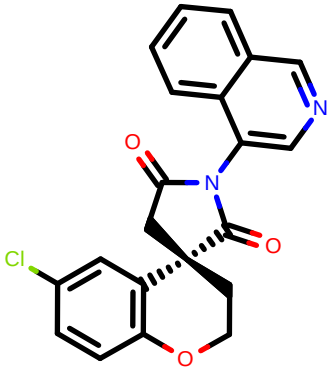
CID:	ALP-POS-347519b5-1_34
SMILES:	CS(=O)(=O)[N@]1C[C@@H]2[C@@H]3CC[C@@H](C3)[C@@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4249
DDG (kcal/mol):	-9.49
dDDG (kcal/mol):	0.20

DAR-DIA-9e4459de-11_9



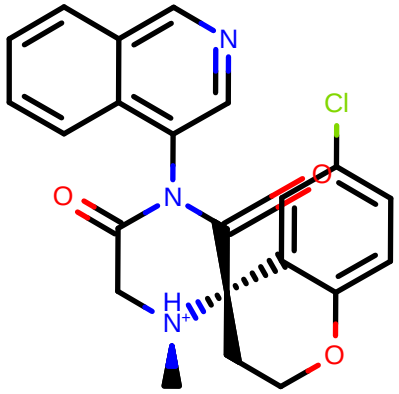
CID:	DAR-DIA-9e4459de-11_9
SMILES:	c1cc2c(c(c1)NCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5COCo6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1418
DDG (kcal/mol):	-7.52
dDDG (kcal/mol):	0.45

LON-WEI-5e7d1b3e-48_1



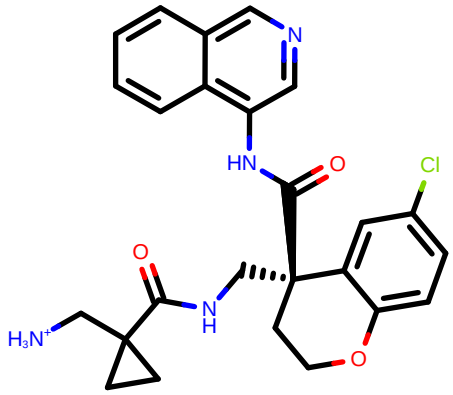
CID:	LON-WEI-5e7d1b3e-48_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3cc(ccc3OC)OC
RUN:	RUN1359
DDG (kcal/mol):	-7.48
dDDG (kcal/mol):	0.23

MAT-POS-4223bc15-21_2



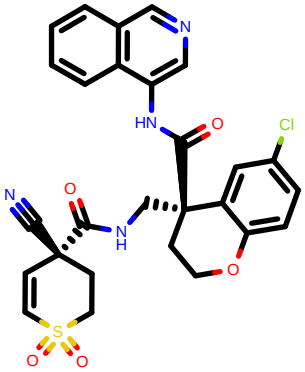
CID:	MAT-POS-4223bc15-21_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@H+](Cc4c3cc(cc4)Cl)CC(=O)[O-]
RUN:	RUN4099
DDG (kcal/mol):	-7.45
dDDG (kcal/mol):	0.32

KAD-UNI-cb0f2bbc-11_1



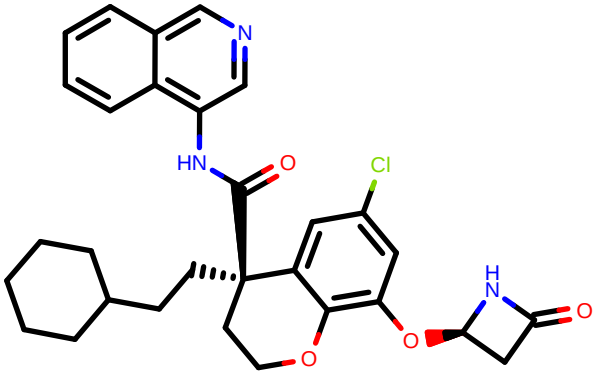
CID:	KAD-UNI-cb0f2bbc-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cnn(c5)[C@@H]6CCS(=O)(=O)C6
RUN:	RUN3693
DDG (kcal/mol):	-7.28
dDDG (kcal/mol):	0.12

EDJ-MED-611d11e7-1_1



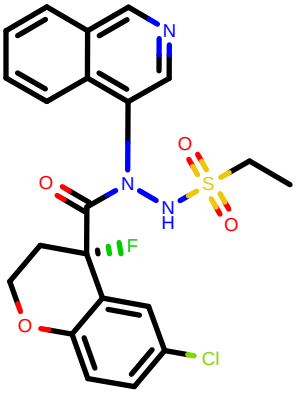
CID:	EDJ-MED-611d11e7-1_1
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cc(cc4)S(=O)(=O)C
RUN:	RUN3486
DDG (kcal/mol):	-6.95
dDDG (kcal/mol):	0.13

DAR-DIA-ecdbc7dd-14_1



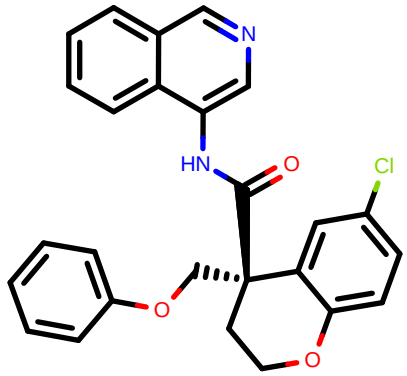
CID:	DAR-DIA-ecdbc7dd-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCNc4c3cc(cc4)Cl)C[NH+]5CC5
RUN:	RUN2900
DDG (kcal/mol):	-6.94
dDDG (kcal/mol):	0.27

ALF-EVA-b701bd13-3_1



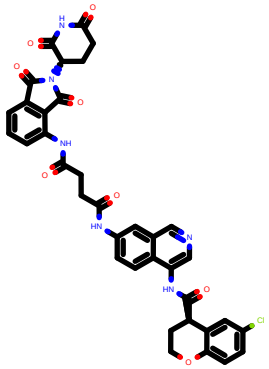
CID:	ALF-EVA-b701bd13-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNc4c3cc(c(n4)Cl)Cl
RUN:	RUN3633
DDG (kcal/mol):	-6.91
dDDG (kcal/mol):	0.14

LAU-MED-88a3970a-11_1



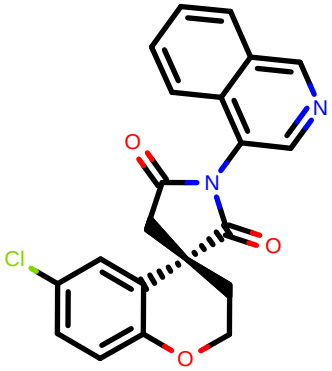
CID:	LAU-MED-88a3970a-11_1
SMILES:	C[NH2+]CCCc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1507
DDG (kcal/mol):	-6.86
dDDG (kcal/mol):	0.16

MIC-UNK-cdc2493e-4_1



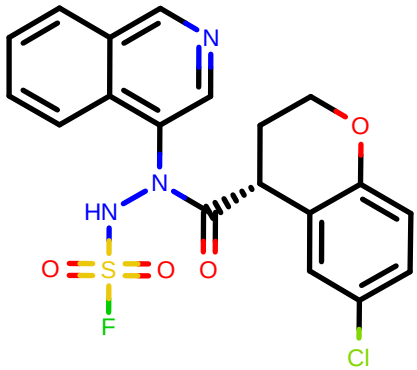
CID:	MIC-UNK-cdc2493e-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCC[C@H]5C4
RUN:	RUN527
DDG (kcal/mol):	-6.85
dDDG (kcal/mol):	0.32

EDJ-MED-ee07cf00-14_2



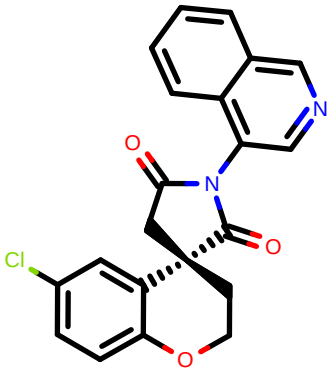
CID:	EDJ-MED-ee07cf00-14_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c(=O)n5c(n4)CCC5
RUN:	RUN2838
DDG (kcal/mol):	-6.62
dDDG (kcal/mol):	0.18

ALF-EVA-b701bd13-1_2



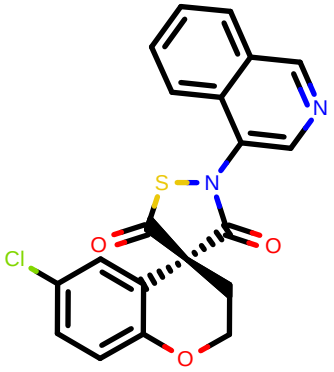
CID:	ALF-EVA-b701bd13-1_2
SMILES:	CC(=O)Nc1ccc2cncc(c2c1)NC(=O)[C@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN3631
DDG (kcal/mol):	-6.47
dDDG (kcal/mol):	0.15

MAT-POS-4223bc15-12_3



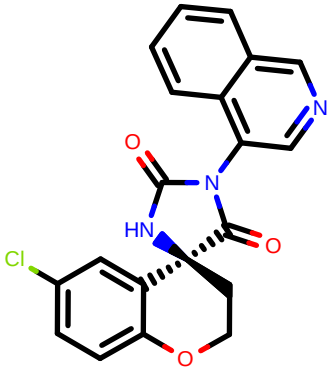
CID:	MAT-POS-4223bc15-12_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5(CCC5)C#N
RUN:	RUN4047
DDG (kcal/mol):	-6.33
dDDG (kcal/mol):	0.18

LON-WEI-5e7d1b3e-44_1



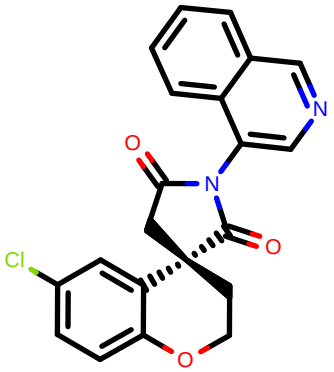
CID:	LON-WEI-5e7d1b3e-44_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCc3ccco3
RUN:	RUN1353
DDG (kcal/mol):	-6.32
dDDG (kcal/mol):	0.22

ALF-EVA-0b412456-6_1



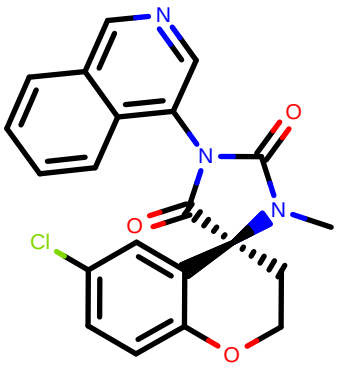
CID:	ALF-EVA-0b412456-6_1
SMILES:	CNc1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4
RUN:	RUN2760
DDG (kcal/mol):	-6.30
dDDG (kcal/mol):	0.21

VLA-UCB-1dbca3b4-10_2



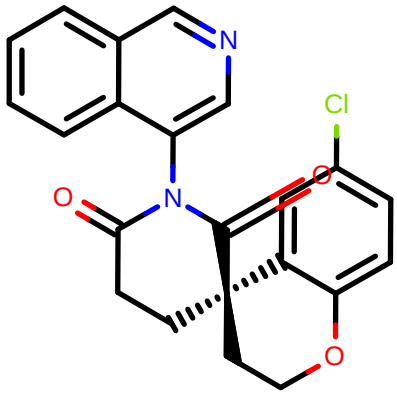
CID:	VLA-UCB-1dbca3b4-10_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN161
DDG (kcal/mol):	-6.08
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-15_1



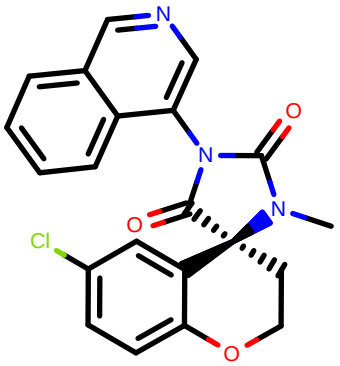
CID:	EDJ-MED-ee07cf00-15_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cc4ccc(cc4)n5cnnn5
RUN:	RUN2840
DDG (kcal/mol):	-6.02
dDDG (kcal/mol):	0.19

MAT-POS-b5746674-34_2



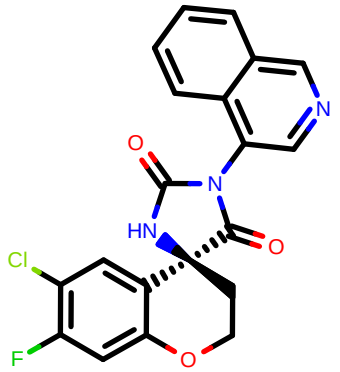
CID:	MAT-POS-b5746674-34_2
SMILES:	CCCC[N@H+](CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C)Cc3ccco3
RUN:	RUN68
DDG (kcal/mol):	-6.00
dDDG (kcal/mol):	0.20

VLA-UCB-1dbca3b4-12_1



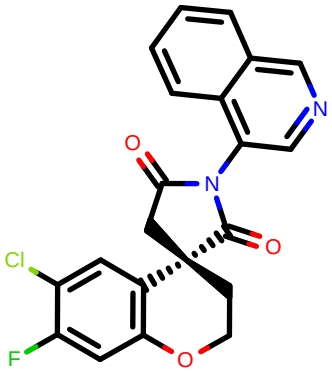
CID:	VLA-UCB-1dbca3b4-12_1
SMILES:	c1ccc2c(c1)cncc2n3c(c(n(c3=O)CC4CCCCC4)c5cccc(c5)Cl)[O-]
RUN:	RUN162
DDG (kcal/mol):	-5.95
dDDG (kcal/mol):	0.19

MAT-POS-4223bc15-24_1



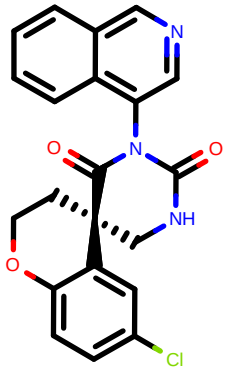
CID:	MAT-POS-4223bc15-24_1
SMILES:	CN(C)C(=O)C[N@@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4109
DDG (kcal/mol):	-5.93
dDDG (kcal/mol):	0.21

MAT-POS-4223bc15-13_11



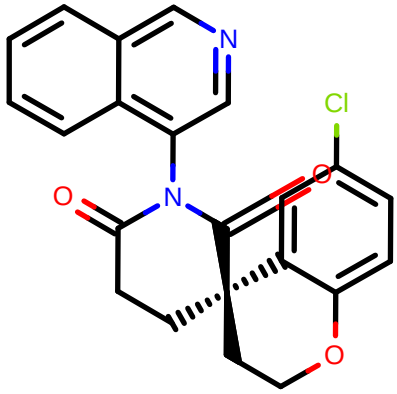
CID:	MAT-POS-4223bc15-13_11
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)[C@@H]5CC[C@H]5O
RUN:	RUN4059
DDG (kcal/mol):	-5.91
dDDG (kcal/mol):	0.17

ALF-EVA-0b412456-8_2



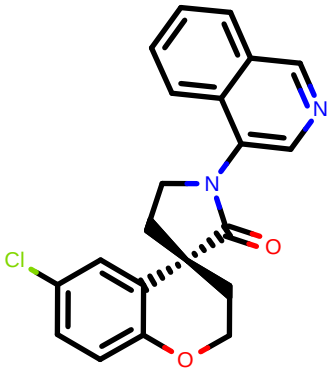
CID:	ALF-EVA-0b412456-8_2
SMILES:	c1cc2cncc(c2cc1C3C[NH2+]C3)NC(=O)Cc4cc(cc(c4)Cl)O[C@H]5CC(=O)N5
RUN:	RUN2763
DDG (kcal/mol):	-5.84
dDDG (kcal/mol):	0.15

EDG-MED-ba1ac7b9-20_1



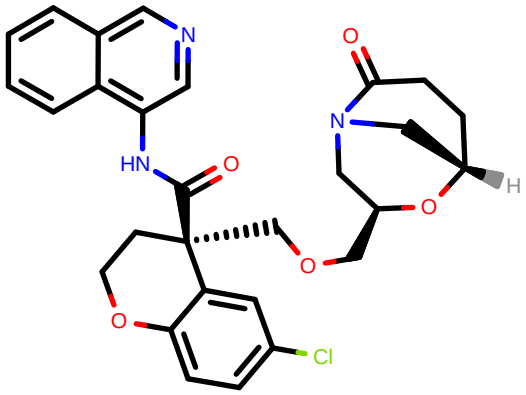
CID:	EDG-MED-ba1ac7b9-20_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@@H]5CC(F)F
RUN:	RUN2694
DDG (kcal/mol):	-5.83
dDDG (kcal/mol):	0.16

MAK-UNK-6ca90168-25_1



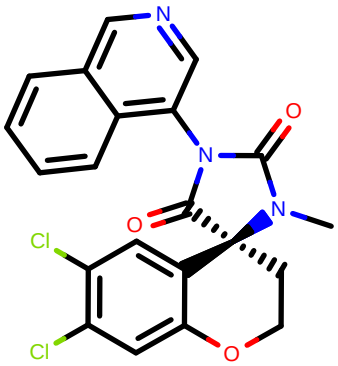
CID:	MAK-UNK-6ca90168-25_1
SMILES:	c1ccc2c(c1)cncc2C(=O)C(=O)Nc3cccc(c3)C#N
RUN:	RUN7
DDG (kcal/mol):	-5.78
dDDG (kcal/mol):	0.19

MAT-POS-a13804f0-1_3



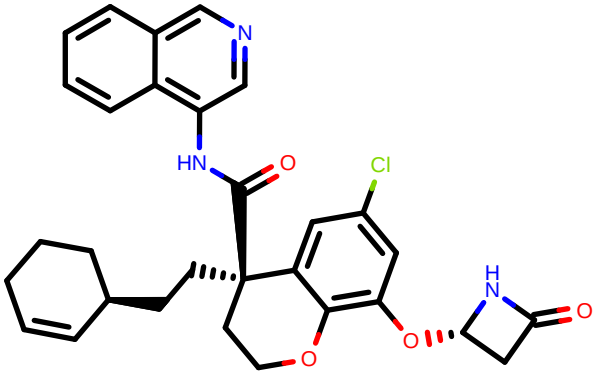
CID:	MAT-POS-a13804f0-1_3
SMILES:	Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3482
DDG (kcal/mol):	-5.69
dDDG (kcal/mol):	0.14

DAR-DIA-0d514e7d-6_1



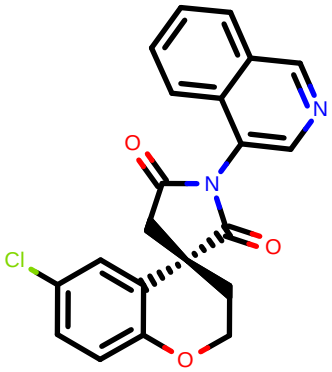
CID:	DAR-DIA-0d514e7d-6_1
SMILES:	C[C@H]1COc2c(cc(cc2OC3CC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN809
DDG (kcal/mol):	-5.65
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-5_1



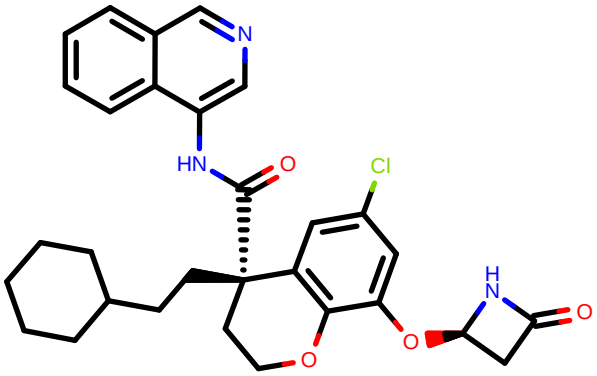
CID:	EDJ-MED-ee07cf00-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)CNC(=O)c4ccc(cc4)C#N
RUN:	RUN2810
DDG (kcal/mol):	-5.45
dDDG (kcal/mol):	0.23

JAN-GHE-f375bf5b-1_2



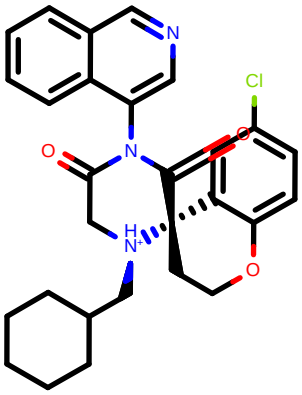
CID:	JAN-GHE-f375bf5b-1_2
SMILES:	CC(=O)N[C@@H](Cc1ccccc1)C(=O)N[C@@H](C[C@H]2CCNC2=O)C(=O)Nc3cncc4c3cccc4
RUN:	RUN16
DDG (kcal/mol):	-5.42
dDDG (kcal/mol):	0.18

ALP-POS-3b848b35-1_1



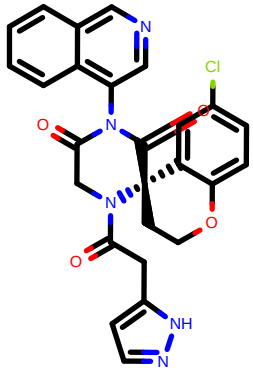
CID:	ALP-POS-3b848b35-1_1
SMILES:	COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN57
DDG (kcal/mol):	-5.38
dDDG (kcal/mol):	0.32

VLA-UCB-1dbca3b4-17_1



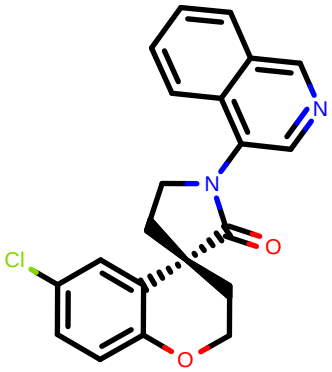
CID:	VLA-UCB-1dbca3b4-17_1
SMILES:	c1ccc2c(c1)cncc2n3c(c([nH]c3=O)c4cccc(c4)Cl)[O-]
RUN:	RUN166
DDG (kcal/mol):	-5.36
dDDG (kcal/mol):	0.37

ALF-EVA-ced740bd-2_1



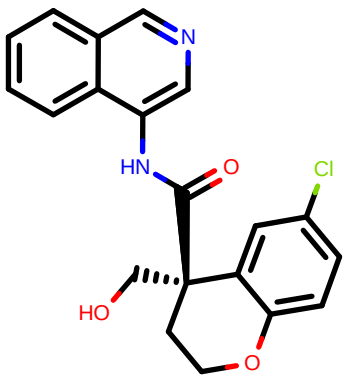
CID:	ALF-EVA-ced740bd-2_1
SMILES:	COc1cc2cncc(c2c(c1)Cl)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2791
DDG (kcal/mol):	-5.35
dDDG (kcal/mol):	0.23

EDG-MED-ba1ac7b9-15_7



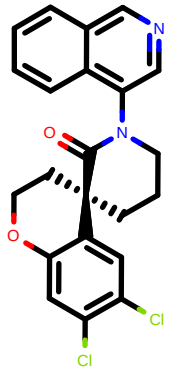
CID:	EDG-MED-ba1ac7b9-15_7
SMILES:	C[C@@H]1C[N@H+](CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2680
DDG (kcal/mol):	-5.02
dDDG (kcal/mol):	0.17

RAL-THA-4aa06b95-4_2



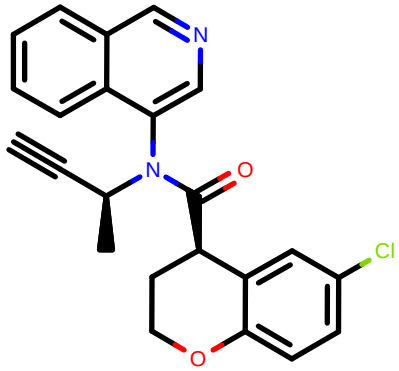
CID:	RAL-THA-4aa06b95-4_2
SMILES:	CN(C)C(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1236
DDG (kcal/mol):	-4.92
dDDG (kcal/mol):	0.11

MIC-UNK-0a05c952-1_7



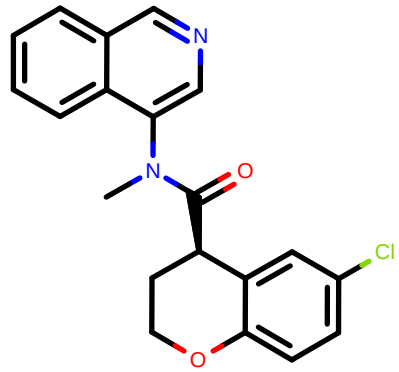
CID:	MIC-UNK-0a05c952-1_7
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](C[C@H](C3=O)c4cccc(c4)Cl)[C@H]5CO5
RUN:	RUN3503
DDG (kcal/mol):	-4.89
dDDG (kcal/mol):	0.20

LON-WEI-4d77710c-55_1



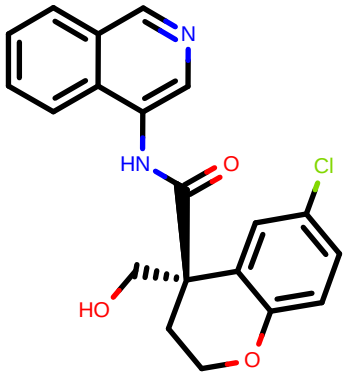
CID:	LON-WEI-4d77710c-55_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCc3ccc4c(c3)OCO4
RUN:	RUN247
DDG (kcal/mol):	-4.87
dDDG (kcal/mol):	0.24

LON-WEI-5e7d1b3e-59_1



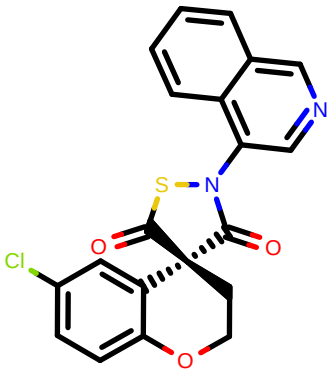
CID:	LON-WEI-5e7d1b3e-59_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N(Cc3ccco3)C[C@@H]4CCCO4
RUN:	RUN1368
DDG (kcal/mol):	-4.87
dDDG (kcal/mol):	0.20

VLA-UCB-05e51b3f-5_1



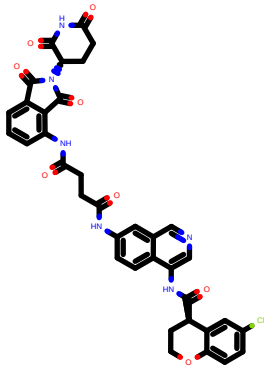
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN311
DDG (kcal/mol):	-4.83
dDDG (kcal/mol):	0.11

MAT-POS-4223bc15-18_1



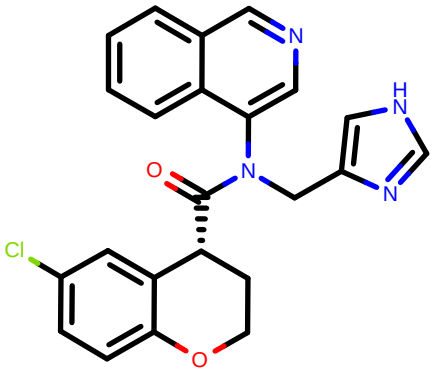
CID:	MAT-POS-4223bc15-18_1
SMILES:	CN(C)C(=O)N1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4091
DDG (kcal/mol):	-4.75
dDDG (kcal/mol):	0.19

DAR-DIA-6a508060-9_2



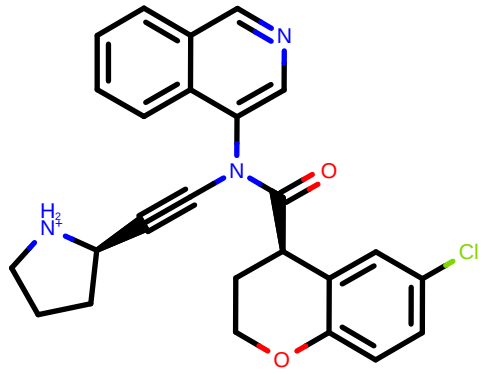
CID:	DAR-DIA-6a508060-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN350
DDG (kcal/mol):	-4.68
dDDG (kcal/mol):	0.40

ERI-UCB-ce40166b-4_1



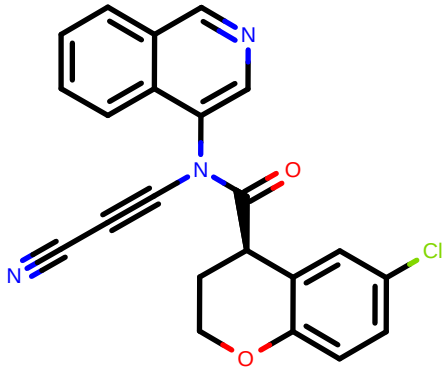
CID:	ERI-UCB-ce40166b-4_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)Oc4cccnc4
RUN:	RUN39
DDG (kcal/mol):	-4.66
dDDG (kcal/mol):	0.25

LON-WEI-4d77710c-34_1



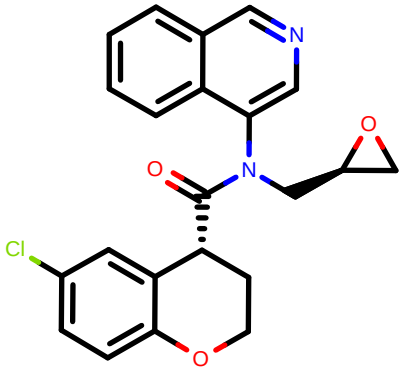
CID:	LON-WEI-4d77710c-34_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CC[C@@H](C3)c4ccccc4
RUN:	RUN216
DDG (kcal/mol):	-4.60
dDDG (kcal/mol):	0.25

LON-WEI-4d77710c-23_1



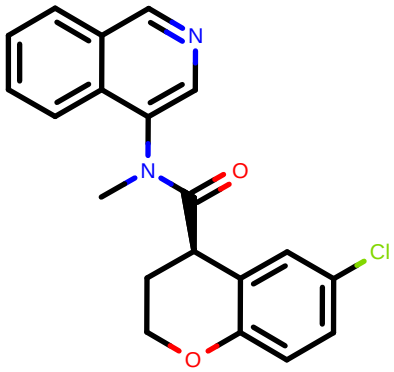
CID:	LON-WEI-4d77710c-23_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3cccc(c3)C(F)(F)F
RUN:	RUN210
DDG (kcal/mol):	-4.58
dDDG (kcal/mol):	0.21

DAR-DIA-076fb6ea-15_1



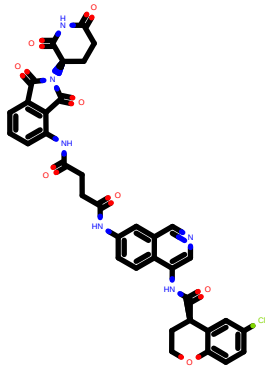
CID:	DAR-DIA-076fb6ea-15_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)N=C=S
RUN:	RUN1405
DDG (kcal/mol):	-4.52
dDDG (kcal/mol):	0.25

MAT-POS-2492181e-10_3



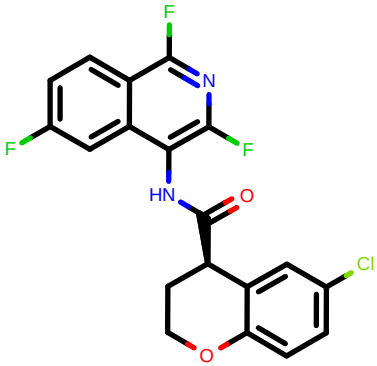
CID:	MAT-POS-2492181e-10_3
SMILES:	C[C@@H]1CCCC[N@H+]1CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN107
DDG (kcal/mol):	-4.52
dDDG (kcal/mol):	0.19

DAR-DIA-0d514e7d-31_11



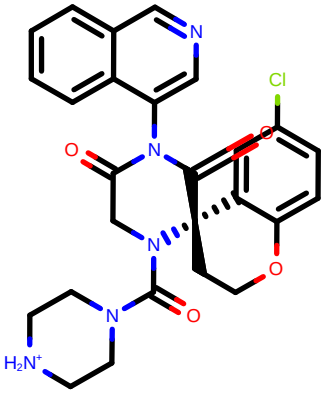
CID:	DAR-DIA-0d514e7d-31_11
SMILES:	C[C@@H]1CCO[C@H]2C=CC(=C[C@@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN844
DDG (kcal/mol):	-4.50
dDDG (kcal/mol):	0.39

VLA-UCB-05e51b3f-7_1



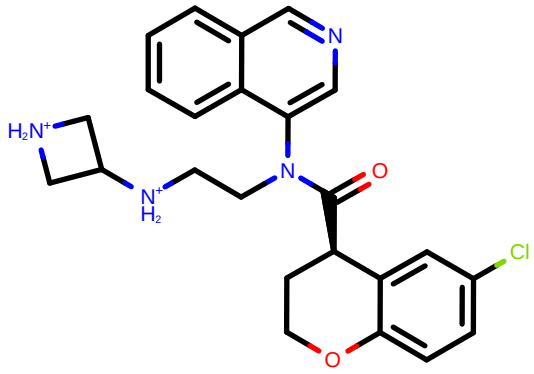
CID:	VLA-UCB-05e51b3f-7_1
SMILES:	CC(=O)N1CC[NH+](CC1)CC(=O)N(c2cncc3c2cccc3)C(=O)[C@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN322
DDG (kcal/mol):	-4.48
dDDG (kcal/mol):	0.18

MAT-POS-2492181e-6_1



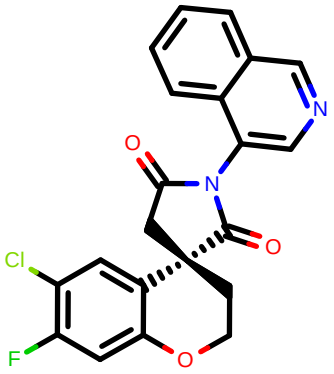
CID:	MAT-POS-2492181e-6_1
SMILES:	CC1CC[NH+](CC1)CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN101
DDG (kcal/mol):	-4.46
dDDG (kcal/mol):	0.25

MAT-POS-f7918075-2_2



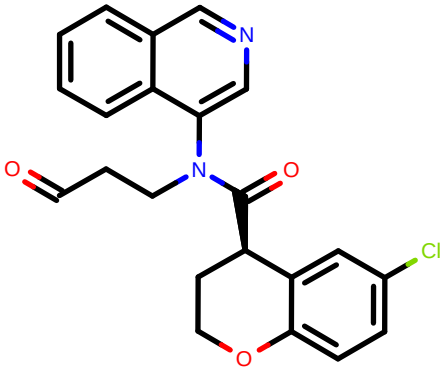
CID:	MAT-POS-f7918075-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN186
DDG (kcal/mol):	-4.45
dDDG (kcal/mol):	0.47

DAR-DIA-5ff57136-13_1



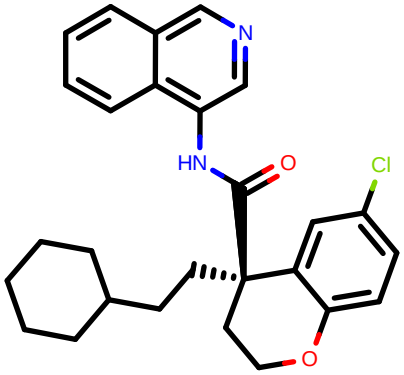
CID:	DAR-DIA-5ff57136-13_1
SMILES:	C#CCN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1380
DDG (kcal/mol):	-4.44
dDDG (kcal/mol):	0.16

BEN-DND-a7517465-5_1



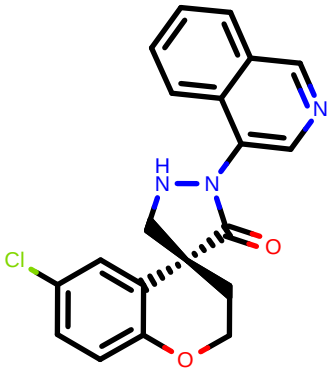
CID:	BEN-DND-a7517465-5_1
SMILES:	c1cc2cncc(c2c(c1)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1481
DDG (kcal/mol):	-4.43
dDDG (kcal/mol):	0.34

ALF-EVA-0b412456-5_2



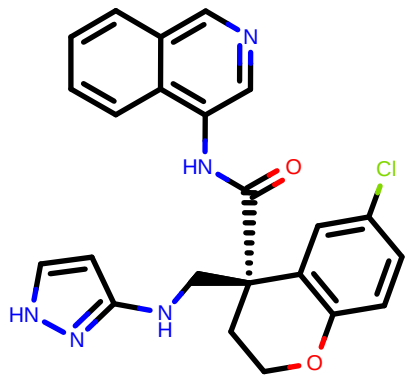
CID:	ALF-EVA-0b412456-5_2
SMILES:	c1cc2cncc(c2cc1C[NH3+])NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN2759
DDG (kcal/mol):	-4.40
dDDG (kcal/mol):	0.16

MIC-UNK-d36ab305-4_1



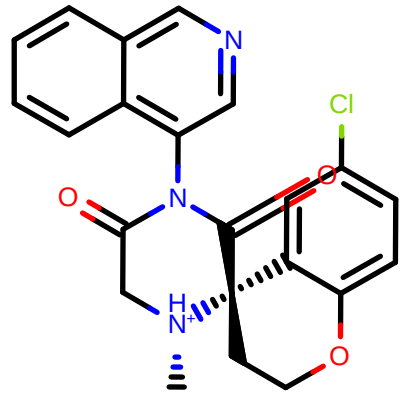
CID:	MIC-UNK-d36ab305-4_1
SMILES:	CN(C)c1ccc(cc1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN158
DDG (kcal/mol):	-4.35
dDDG (kcal/mol):	0.20

MAT-POS-4223bc15-40_1



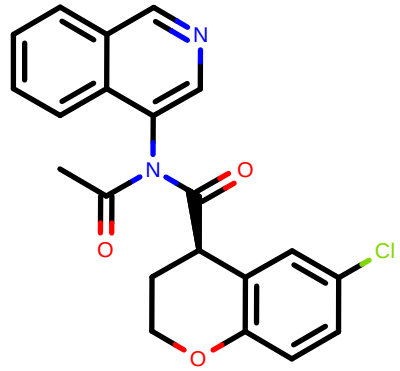
CID:	MAT-POS-4223bc15-40_1
SMILES:	Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4161
DDG (kcal/mol):	-4.34
dDDG (kcal/mol):	0.12

MAT-POS-4223bc15-22_3



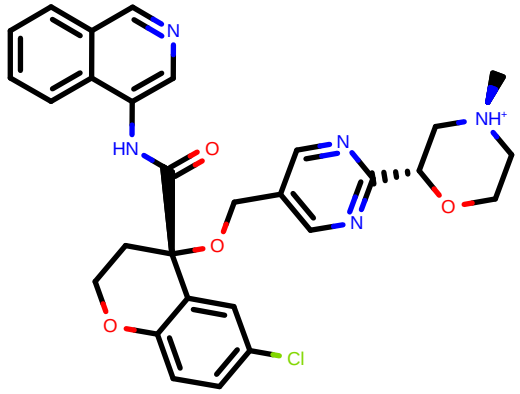
CID:	MAT-POS-4223bc15-22_3
SMILES:	COC(=O)C[N@@H+]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4103
DDG (kcal/mol):	-4.31
dDDG (kcal/mol):	0.26

MAT-POS-b5746674-98_2



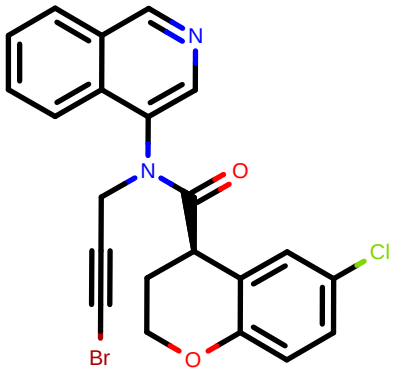
CID:	MAT-POS-b5746674-98_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCC[N@H+]3CCc4ccccc4C3
RUN:	RUN75
DDG (kcal/mol):	-4.28
dDDG (kcal/mol):	0.22

DAR-DIA-23e5a6a0-3_1



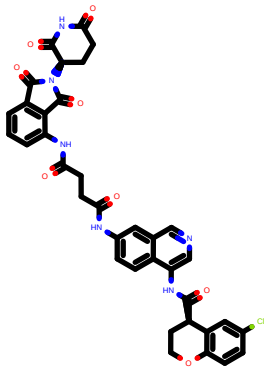
CID:	DAR-DIA-23e5a6a0-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6([NH2+]5)COC6)Cl
RUN:	RUN405
DDG (kcal/mol):	-4.24
dDDG (kcal/mol):	0.21

LON-WEI-4d77710c-37_1



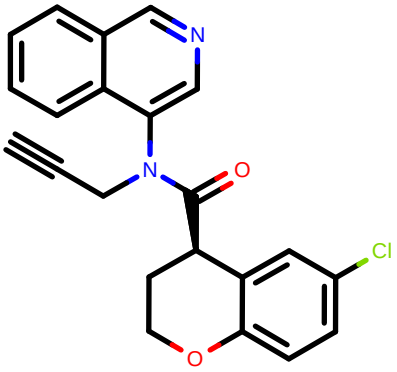
CID:	LON-WEI-4d77710c-37_1
SMILES:	CCN(CC)S(=O)(=O)c1ccc(cc1)NC(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN220
DDG (kcal/mol):	-4.20
dDDG (kcal/mol):	0.22

DAR-DIA-0f2f46c9-3_2



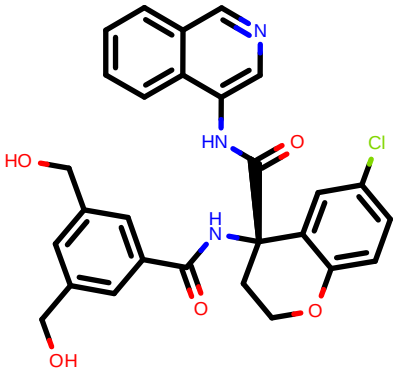
CID:	DAR-DIA-0f2f46c9-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC[N@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3227
DDG (kcal/mol):	-4.20
dDDG (kcal/mol):	0.20

LON-WEI-4d77710c-50_1



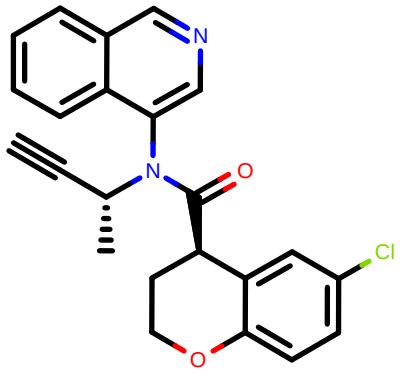
CID:	LON-WEI-4d77710c-50_1
SMILES:	CCCC[N@@H+](CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C)Cc3ccco3
RUN:	RUN242
DDG (kcal/mol):	-4.17
dDDG (kcal/mol):	0.23

JOH-UNI-f51e3bbc-2_2



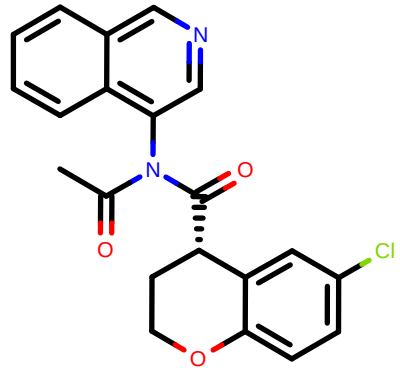
CID:	JOH-UNI-f51e3bbc-2_2
SMILES:	COc1c2ccccc2c(cn1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1162
DDG (kcal/mol):	-4.10
dDDG (kcal/mol):	0.26

LON-WEI-4d77710c-33_2



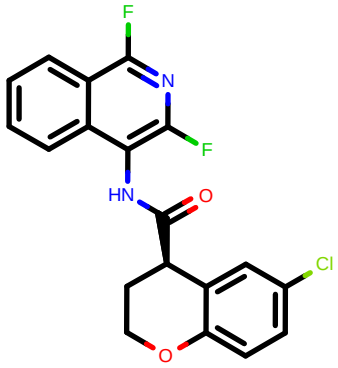
CID:	LON-WEI-4d77710c-33_2
SMILES:	C[C@H]1c2cc(c(cc2CCN1C(=O)Nc3cn(c(=O)c4c3cccc4)C)OC)OC
RUN:	RUN215
DDG (kcal/mol):	-4.07
dDDG (kcal/mol):	0.28

NIR-THE-ed286faa-2_1



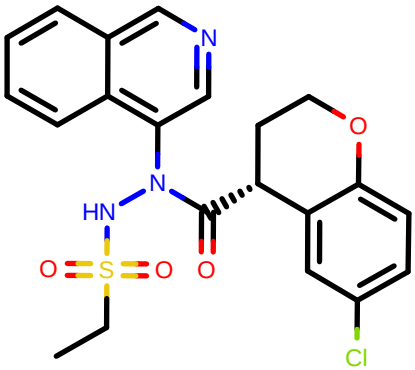
CID:	NIR-THE-ed286faa-2_1
SMILES:	CCNc1c2cc(ccc2c(cn1)C#N)N(c3cccc(c3)C(=O)N4CCSCC4)C(=O)CCl
RUN:	RUN9
DDG (kcal/mol):	-4.07
dDDG (kcal/mol):	0.28

LON-WEI-4d77710c-4_1



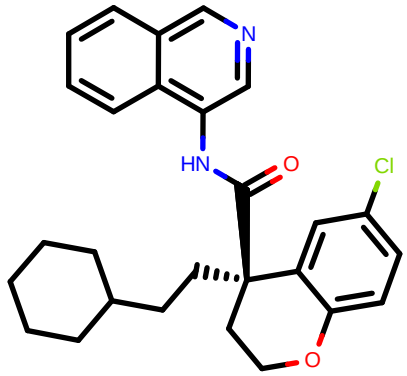
CID:	LON-WEI-4d77710c-4_1
SMILES:	Cc1ccc(c(c1)Br)NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN194
DDG (kcal/mol):	-4.03
dDDG (kcal/mol):	0.18

KAD-UNI-877d7bed-8_2



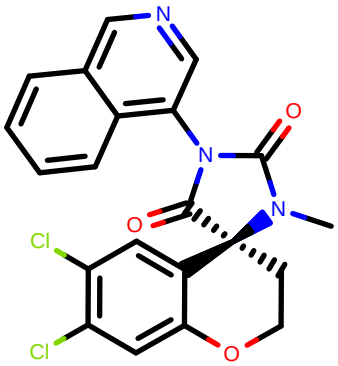
CID:	KAD-UNI-877d7bed-8_2
SMILES:	CC(=O)N1CCN(CC1)C(=O)COc2cc(cc3c2OCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3737
DDG (kcal/mol):	-4.01
dDDG (kcal/mol):	0.15

EDG-MED-ba1ac7b9-31_4



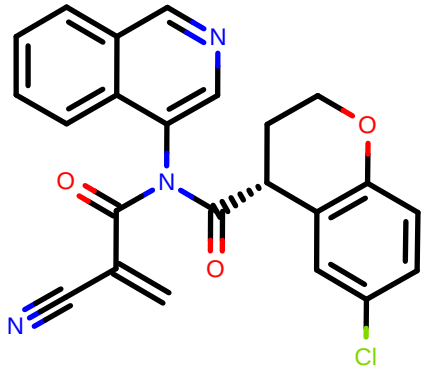
CID:	EDG-MED-ba1ac7b9-31_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@H]6CCCOC6
RUN:	RUN2743
DDG (kcal/mol):	-4.00
dDDG (kcal/mol):	0.17

MAT-POS-932d1078-1_2



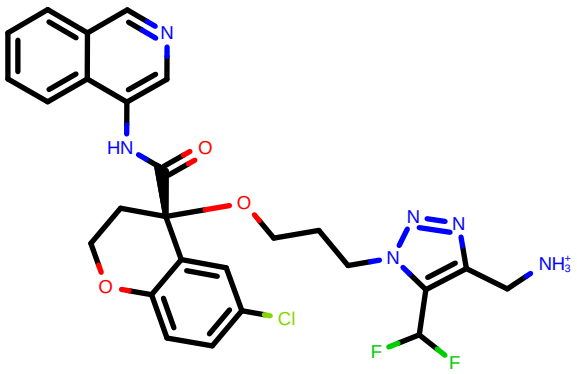
CID:	MAT-POS-932d1078-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5COCC[N@@]5CC(F)(F)F
RUN:	RUN3587
DDG (kcal/mol):	-3.95
dDDG (kcal/mol):	0.23

MIC-UNK-d36ab305-2_1



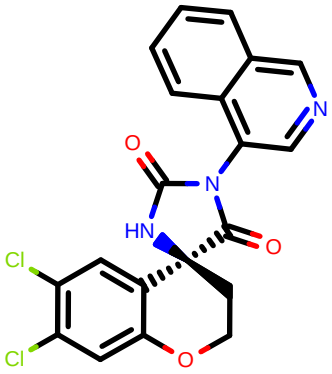
CID:	MIC-UNK-d36ab305-2_1
SMILES:	CC(=O)Nc1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN154
DDG (kcal/mol):	-3.95
dDDG (kcal/mol):	0.25

MIC-UNK-91acba05-6_3



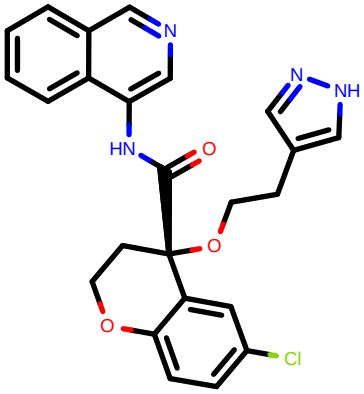
CID:	MIC-UNK-91acba05-6_3
SMILES:	CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN480
DDG (kcal/mol):	-3.93
dDDG (kcal/mol):	0.35

MAT-POS-a13804f0-3_1



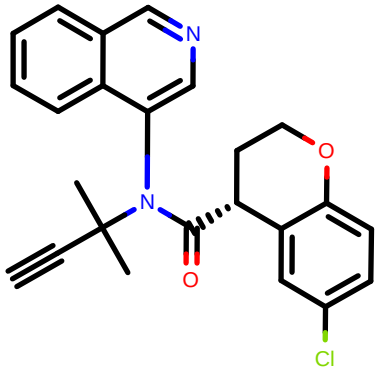
CID:	MAT-POS-a13804f0-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(c(c4)F)Cl
RUN:	RUN3484
DDG (kcal/mol):	-3.91
dDDG (kcal/mol):	0.20

EDJ-MED-28ec730d-4_1



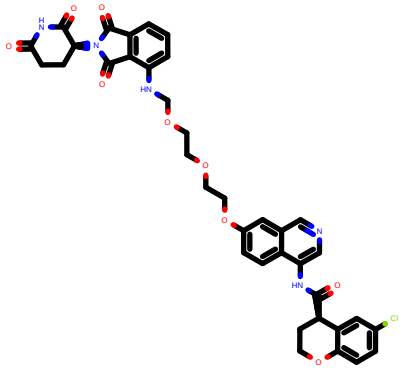
CID:	EDJ-MED-28ec730d-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5c[nH]nc5
RUN:	RUN653
DDG (kcal/mol):	-3.90
dDDG (kcal/mol):	0.26

LON-WEI-4d77710c-53_1



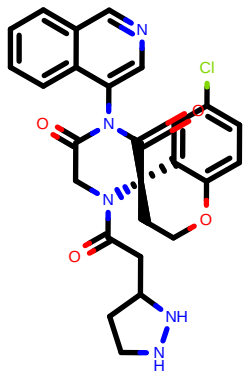
CID:	LON-WEI-4d77710c-53_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CCC[N@@H+](C3)Cc4ccccc4F
RUN:	RUN243
DDG (kcal/mol):	-3.88
dDDG (kcal/mol):	0.25

MAK-UNK-ffc90da7-9_5



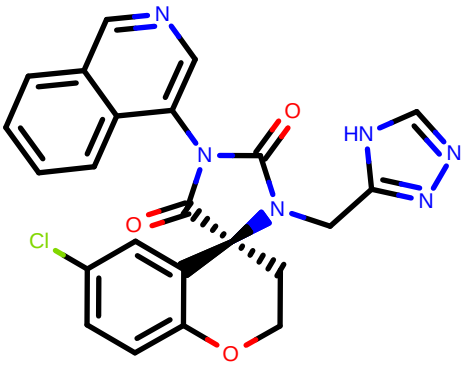
CID:	MAK-UNK-ffc90da7-9_5
SMILES:	C[C@@H]1[C@@H](CCO1)SC[C@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN716
DDG (kcal/mol):	-3.88
dDDG (kcal/mol):	0.55

MAT-POS-2492181e-3_1



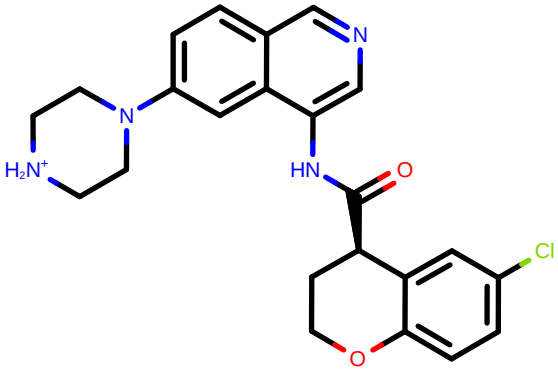
CID:	MAT-POS-2492181e-3_1
SMILES:	CCC[NH+](CCC)CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C
RUN:	RUN99
DDG (kcal/mol):	-3.88
dDDG (kcal/mol):	0.19

DAR-DIA-0d514e7d-10_1



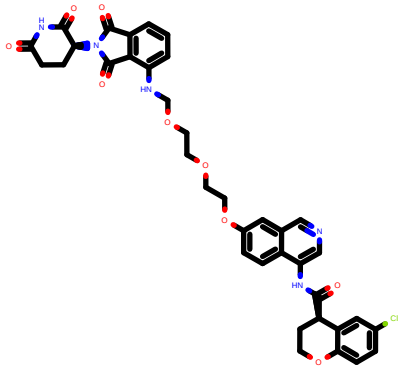
CID:	DAR-DIA-0d514e7d-10_1
SMILES:	C[C@H]1COc2c(cc(cc2Nc3cnn(c3)C)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN814
DDG (kcal/mol):	-3.85
dDDG (kcal/mol):	0.22

MAT-POS-af71705c-2_1



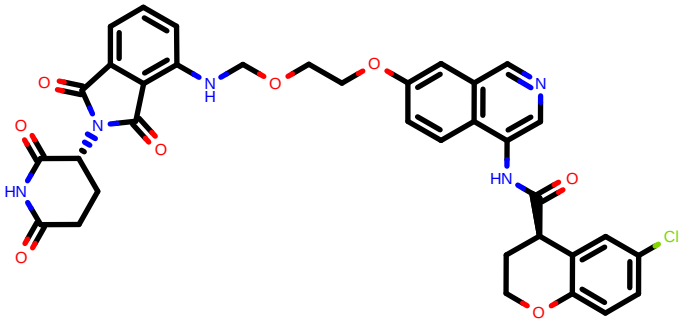
CID:	MAT-POS-af71705c-2_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NC3=[NH+]N(CC3)c4ccccc4
RUN:	RUN56
DDG (kcal/mol):	-3.85
dDDG (kcal/mol):	0.24

MAT-POS-11b63608-1_1



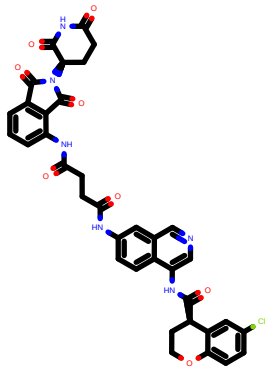
CID:	MAT-POS-11b63608-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Br
RUN:	RUN281
DDG (kcal/mol):	-3.82
dDDG (kcal/mol):	0.52

VLA-UCB-50c39ae8-9_2



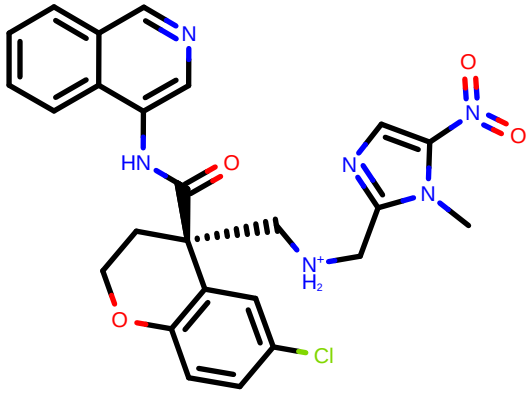
CID:	VLA-UCB-50c39ae8-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O[C@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN396
DDG (kcal/mol):	-3.82
dDDG (kcal/mol):	0.46

MAK-UNK-8be7dca9-8_2



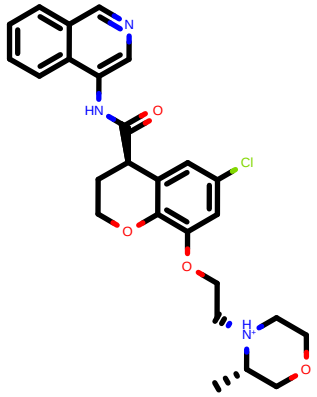
CID:	MAK-UNK-8be7dca9-8_2
SMILES:	c1cc2cncc(c2cc1CC(=O)[O-])NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN509
DDG (kcal/mol):	-3.77
dDDG (kcal/mol):	0.46

ALP-UNI-76695c4f-2_1



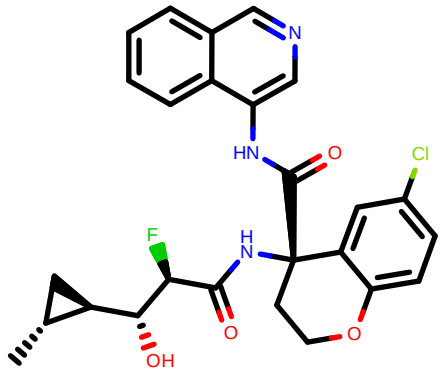
CID:	ALP-UNI-76695c4f-2_1
SMILES:	Cn1c(nnn1)C2CCN(CC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2164
DDG (kcal/mol):	-3.76
dDDG (kcal/mol):	0.31

EDG-MED-ba1ac7b9-13_3



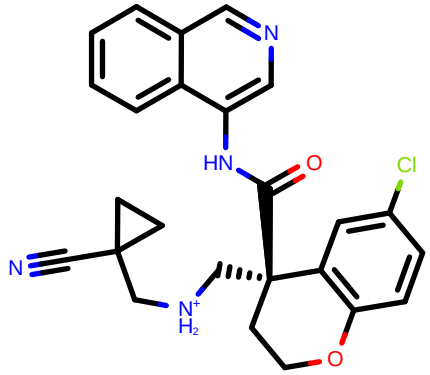
CID:	EDG-MED-ba1ac7b9-13_3
SMILES:	C[N@@H+]1C[C@@H]2C[C@H]1CN2C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2664
DDG (kcal/mol):	-3.72
dDDG (kcal/mol):	0.42

MAK-UNK-ffc90da7-5_2



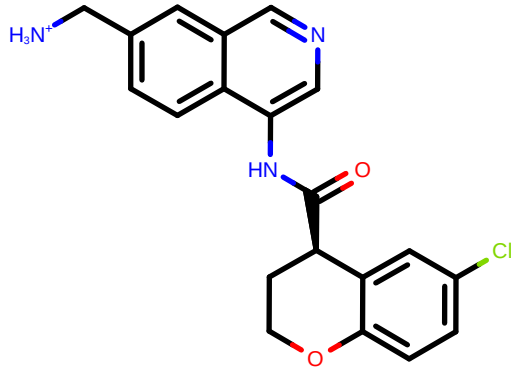
CID:	MAK-UNK-ffc90da7-5_2
SMILES:	C[C@](CO)(c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C4CC4
RUN:	RUN701
DDG (kcal/mol):	-3.68
dDDG (kcal/mol):	0.20

EDG-MED-4c68219f-1_4



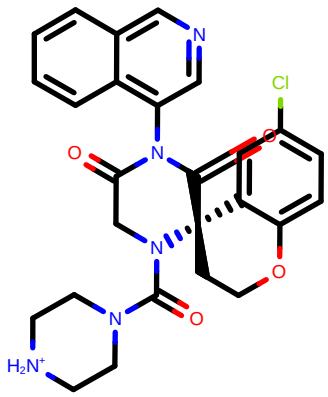
CID:	EDG-MED-4c68219f-1_4
SMILES:	C[C@H](CN1C(=O)[C@H](CO1)[NH3+])CO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1640
DDG (kcal/mol):	-3.67
dDDG (kcal/mol):	0.23

MAT-POS-f7918075-2_1



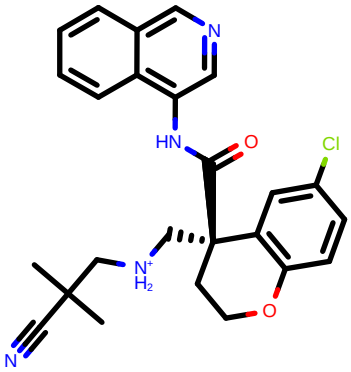
CID:	MAT-POS-f7918075-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN185
DDG (kcal/mol):	-3.65
dDDG (kcal/mol):	0.24

ALP-UNI-dbbfd3db-18_1



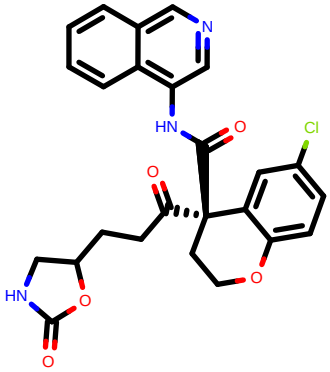
CID:	ALP-UNI-dbbfd3db-18_1
SMILES:	Cn1c(=O)ccn(c1=O)CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2790
DDG (kcal/mol):	-3.65
dDDG (kcal/mol):	0.21

DAR-DIA-9e4459de-13_7



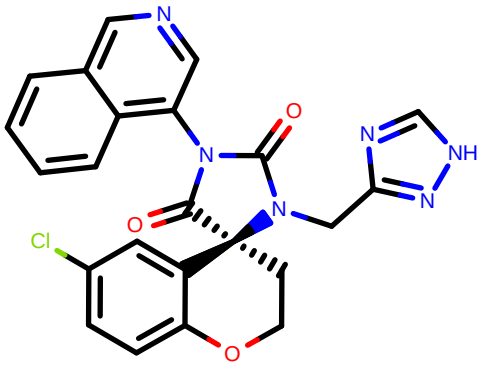
CID:	DAR-DIA-9e4459de-13_7
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O))[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1431
DDG (kcal/mol):	-3.61
dDDG (kcal/mol):	0.24

EDJ-MED-ee07cf00-1_1



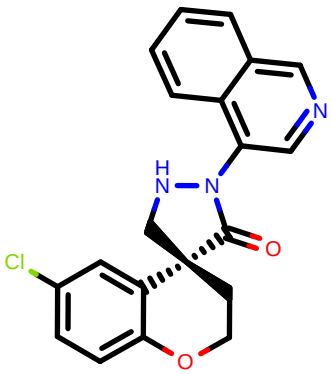
CID:	EDJ-MED-ee07cf00-1_1
SMILES:	Cn1c(=O)ccn(c1=O)CC(=O)N[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2800
DDG (kcal/mol):	-3.60
dDDG (kcal/mol):	0.16

MAT-POS-a13804f0-4_1



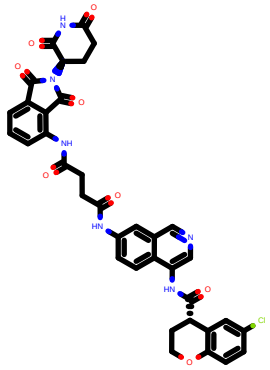
CID:	MAT-POS-a13804f0-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN3490
DDG (kcal/mol):	-3.59
dDDG (kcal/mol):	0.18

DAR-DIA-ecdbc7dd-2_1



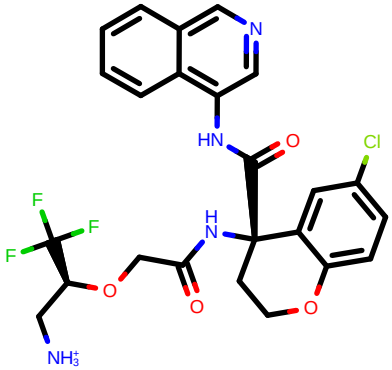
CID:	DAR-DIA-ecdbc7dd-2_1
SMILES:	CN1CC[NH+](CC1)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2877
DDG (kcal/mol):	-3.56
dDDG (kcal/mol):	0.24

MAK-UNK-8be7dca9-3_1



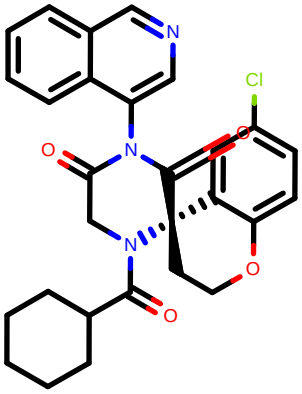
CID:	MAK-UNK-8be7dca9-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4OC[C@@H]3C[NH3+])Cl
RUN:	RUN495
DDG (kcal/mol):	-3.54
dDDG (kcal/mol):	0.32

DAR-DIA-f6ee7aeb-2_3



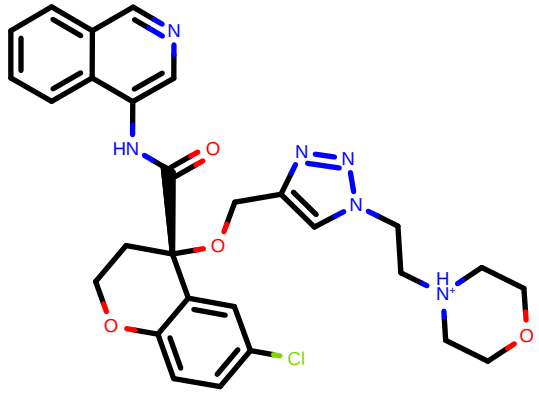
CID:	DAR-DIA-f6ee7aeb-2_3
SMILES:	c1ccc2c(c1)cncc2N3C[C@@H]([C@H](CC3=O)c4cc(cc(c4)Cl)OCCC(F)(F)F)c5ccccc5C#N
RUN:	RUN3404
DDG (kcal/mol):	-3.52
dDDG (kcal/mol):	0.38

MAT-POS-b5746674-108_3



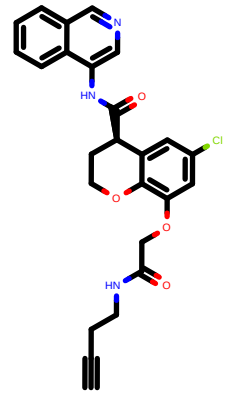
CID:	MAT-POS-b5746674-108_3
SMILES:	Cc1ccc(cc1)C[N@@H+]2CC[C@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN93
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.28

RAL-THA-1d44ff04-7_1



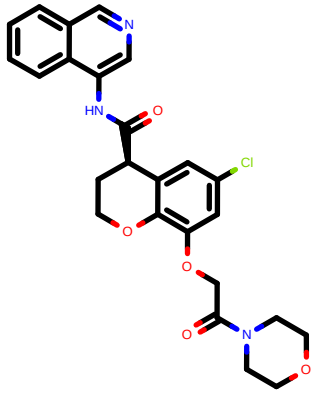
CID:	RAL-THA-1d44ff04-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)c4[nH]ccn4
RUN:	RUN441
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.36

JOH-UNI-ea72002d-1_2



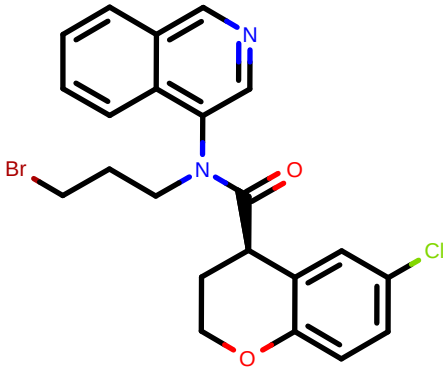
CID:	JOH-UNI-ea72002d-1_2
SMILES:	c1ccc2c(c1)cncc2N(C(=O)[C@H]3CCOc4c3cc(cc4)Cl)N5C(=O)C=CC5=O
RUN:	RUN2482
DDG (kcal/mol):	-3.51
dDDG (kcal/mol):	0.32

EDG-MED-ba1ac7b9-9_2



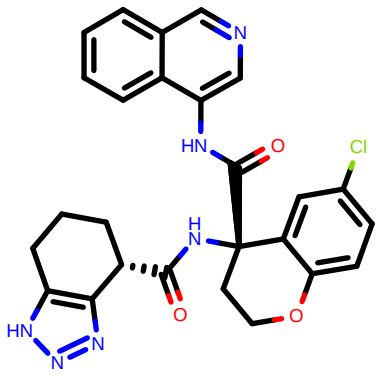
CID:	EDG-MED-ba1ac7b9-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5c6[nH]ncn6
RUN:	RUN2647
DDG (kcal/mol):	-3.50
dDDG (kcal/mol):	0.35

ALP-UNI-8e43a71e-15_31



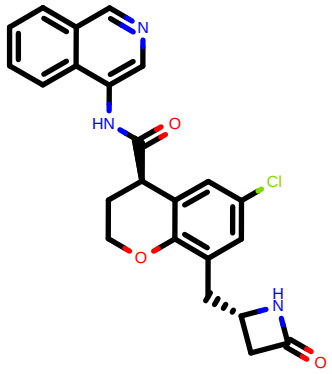
CID:	ALP-UNI-8e43a71e-15_31
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]6[C@H]5C[C@H](C6)C(=O)N
RUN:	RUN3017
DDG (kcal/mol):	-3.44
dDDG (kcal/mol):	0.13

MAK-UNK-c749d764-33_8



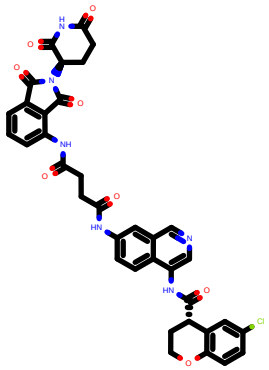
CID:	MAK-UNK-c749d764-33_8
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1087
DDG (kcal/mol):	-3.41
dDDG (kcal/mol):	0.23

DAR-DIA-0cde14eb-55_2



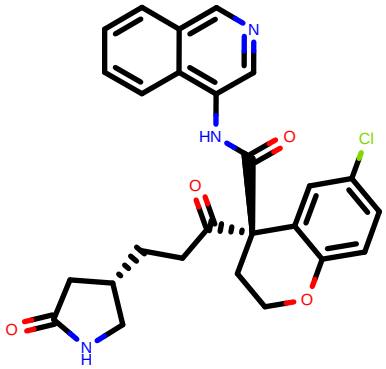
CID:	DAR-DIA-0cde14eb-55_2
SMILES:	C[C@H](c1cccc(c1)C2(CC2)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN22
DDG (kcal/mol):	-3.40
dDDG (kcal/mol):	0.30

MIC-UNK-cdc2493e-5_3



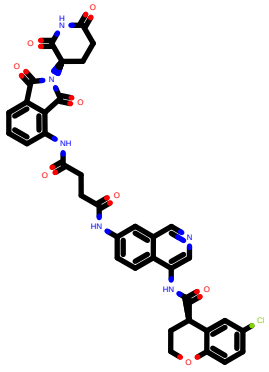
CID:	MIC-UNK-cdc2493e-5_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@@H]5CCCC[C@H]5C4
RUN:	RUN535
DDG (kcal/mol):	-3.39
dDDG (kcal/mol):	0.26

DAR-DIA-ecdbc7dd-18_2



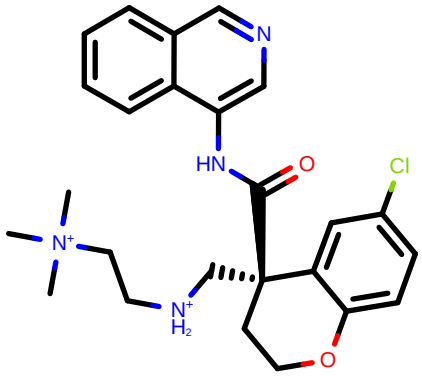
CID:	DAR-DIA-ecdbc7dd-18_2
SMILES:	CC(=O)N1CC[NH+](CC1)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2912
DDG (kcal/mol):	-3.39
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-10_1



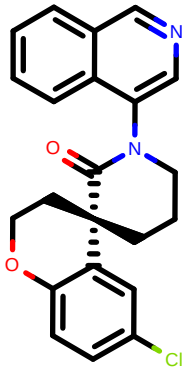
CID:	EDJ-MED-e4b030d8-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3c(c(cc4)Cl)Cl
RUN:	RUN293
DDG (kcal/mol):	-3.36
dDDG (kcal/mol):	0.45

EDG-MED-90036822-8_1



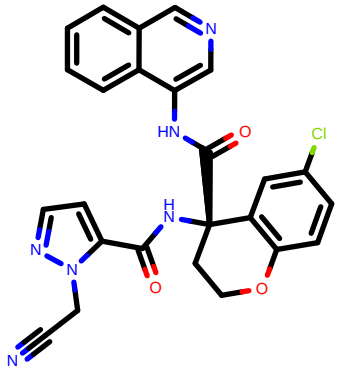
CID:	EDG-MED-90036822-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5c[nH]nc5)F
RUN:	RUN1662
DDG (kcal/mol):	-3.35
dDDG (kcal/mol):	0.24

DAR-DIA-23aa0b97-20_1



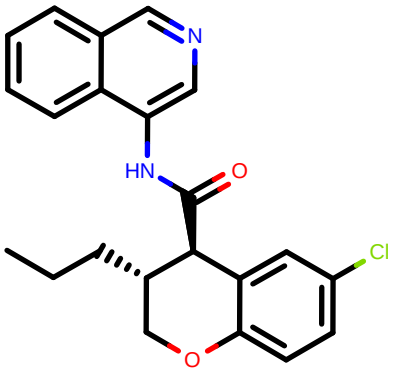
CID:	DAR-DIA-23aa0b97-20_1
SMILES:	c1ccc(cc1)NC(=O)Cc2cncc3c2cccc3
RUN:	RUN0
DDG (kcal/mol):	-3.35
dDDG (kcal/mol):	0.18

GIA-UNK-80c9bc96-1_2



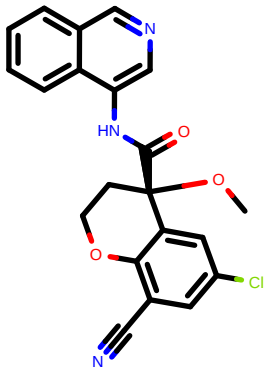
CID:	GIA-UNK-80c9bc96-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN1103
DDG (kcal/mol):	-3.34
dDDG (kcal/mol):	0.25

DAR-DIA-0cde14eb-49_1



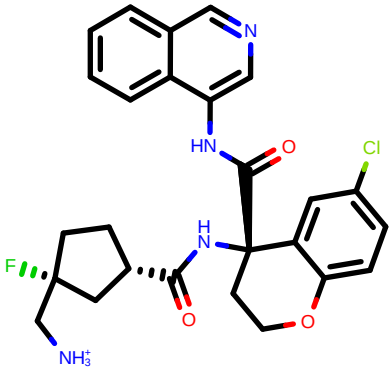
CID:	DAR-DIA-0cde14eb-49_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)C4(CC4)I
RUN:	RUN13
DDG (kcal/mol):	-3.32
dDDG (kcal/mol):	0.20

DAR-DIA-5ff57136-14_1



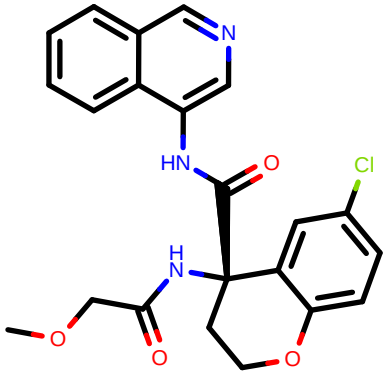
CID:	DAR-DIA-5ff57136-14_1
SMILES:	CC(C)(C#C)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1381
DDG (kcal/mol):	-3.29
dDDG (kcal/mol):	0.19

ADA-UCB-dc2b944c-5_1



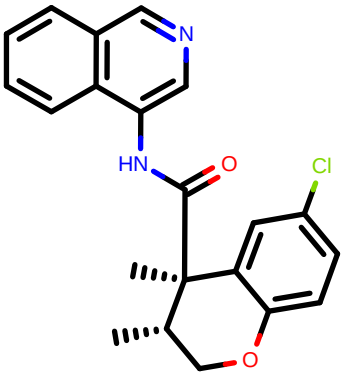
CID:	ADA-UCB-dc2b944c-5_1
SMILES:	Cc1ccc2c(c1)[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4
RUN:	RUN601
DDG (kcal/mol):	-3.28
dDDG (kcal/mol):	0.39

MIC-UNK-bcd487e9-10_1



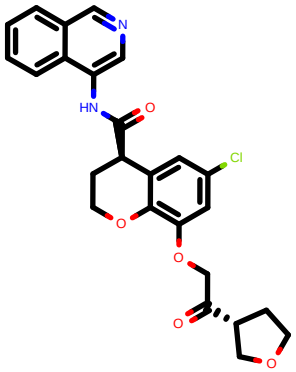
CID:	MIC-UNK-bcd487e9-10_1
SMILES:	Cn1cnc(n1)CN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN599
DDG (kcal/mol):	-3.28
dDDG (kcal/mol):	0.26

MIC-UNK-d36ab305-6_1



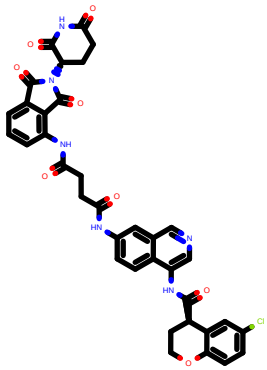
CID:	MIC-UNK-d36ab305-6_1
SMILES:	CN(C)c1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Cc3cncc4c3cccc4
RUN:	RUN155
DDG (kcal/mol):	-3.26
dDDG (kcal/mol):	0.18

ALP-UNI-0676e700-18_1



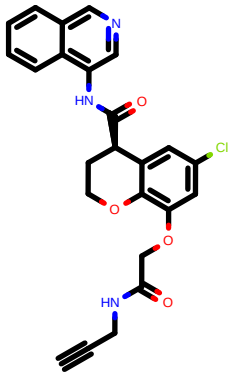
CID:	ALP-UNI-0676e700-18_1
SMILES:	Cc1nnc2n1C[C@@H][N@@H+](C2)C)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2462
DDG (kcal/mol):	-3.25
dDDG (kcal/mol):	0.36

VLA-UCB-50c39ae8-3_1



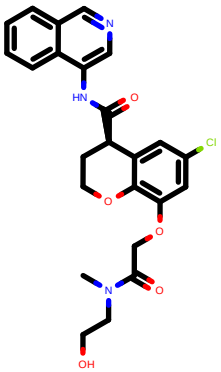
CID:	VLA-UCB-50c39ae8-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN379
DDG (kcal/mol):	-3.25
dDDG (kcal/mol):	0.41

ALP-POS-2da19ca7-5_1



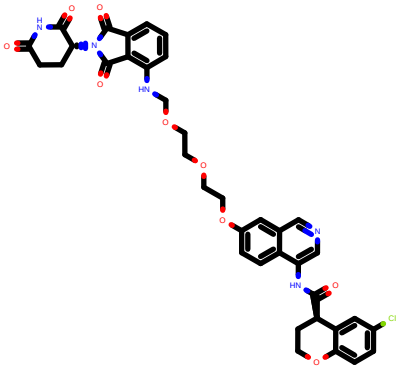
CID:	ALP-POS-2da19ca7-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)c6n[n-]nn6
RUN:	RUN2379
DDG (kcal/mol):	-3.23
dDDG (kcal/mol):	0.37

ALP-UNI-3496895b-10_1



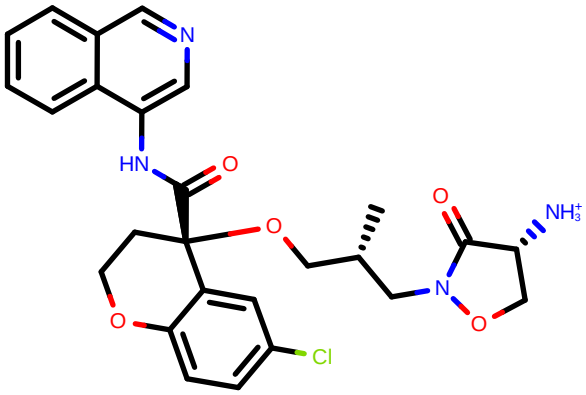
CID:	ALP-UNI-3496895b-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)CC(CO)(F)F
RUN:	RUN2532
DDG (kcal/mol):	-3.23
dDDG (kcal/mol):	0.38

MIC-UNK-9582b2c5-1_8



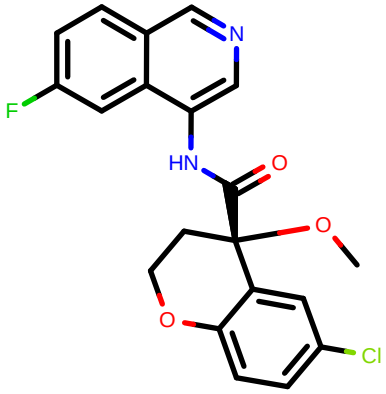
CID:	MIC-UNK-9582b2c5-1_8
SMILES:	CC(=O)N1CC[C@H]2[C@H](C1)CN(C(=O)[C@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN261
DDG (kcal/mol):	-3.22
dDDG (kcal/mol):	0.53

NIR-WEI-acbd6416-1_1



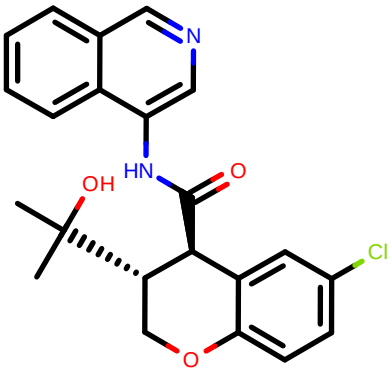
CID:	NIR-WEI-acbd6416-1_1
SMILES:	C=C(c1cncc2c1cccc2)C(=O)N3CCOc4c3cc(cc4)Cl
RUN:	RUN455
DDG (kcal/mol):	-3.22
dDDG (kcal/mol):	0.35

LAU-MED-88a3970a-10_1



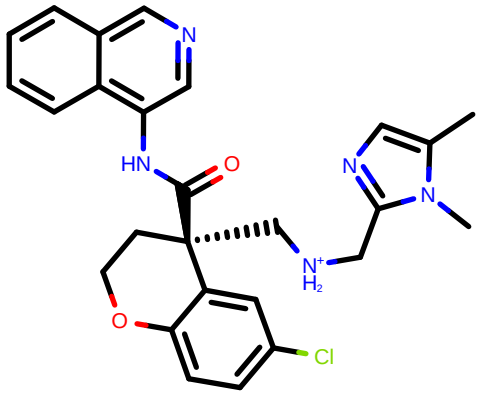
CID:	LAU-MED-88a3970a-10_1
SMILES:	CS(=O)(=O)CCc1cc(cc2c1OCC[C@@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1506
DDG (kcal/mol):	-3.22
dDDG (kcal/mol):	0.24

LON-WEI-4d77710c-56_1



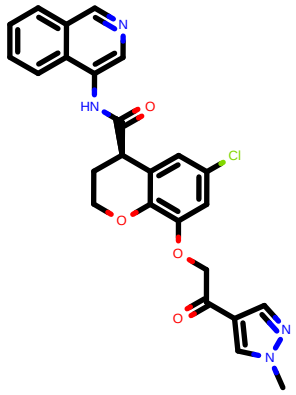
CID:	LON-WEI-4d77710c-56_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccsc3C(=O)OC
RUN:	RUN248
DDG (kcal/mol):	-3.21
dDDG (kcal/mol):	0.17

EDG-MED-90036822-77_1



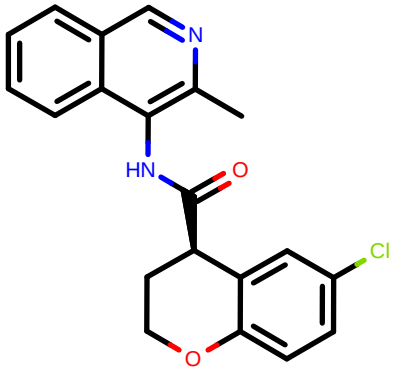
CID:	EDG-MED-90036822-77_1
SMILES:	c1cc2c(c(cnc2)NC(=O)[C@]3(c4c(ccc(c4)Cl)OCC3)NC(=O)[C@H]5C[C@](C5)(F)CO)cc1
RUN:	RUN1773
DDG (kcal/mol):	-3.21
dDDG (kcal/mol):	0.24

MAT-POS-89e65850-1_1



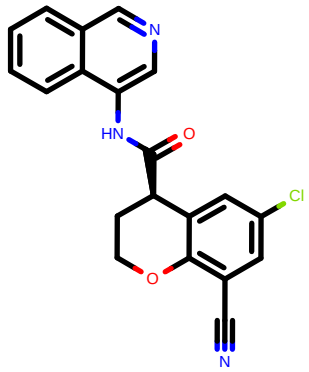
CID:	MAT-POS-89e65850-1_1
SMILES:	CO[C@@]1(CC(=O)Nc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2184
DDG (kcal/mol):	-3.19
dDDG (kcal/mol):	0.31

MAT-POS-b5746674-108_2



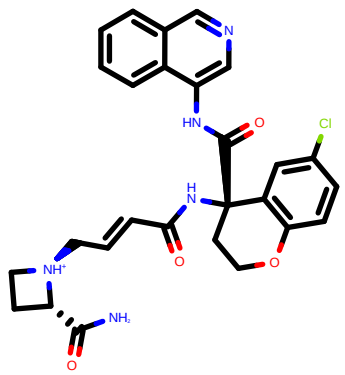
CID:	MAT-POS-b5746674-108_2
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN89
DDG (kcal/mol):	-3.19
dDDG (kcal/mol):	0.18

MAK-UNK-ffc90da7-4_7



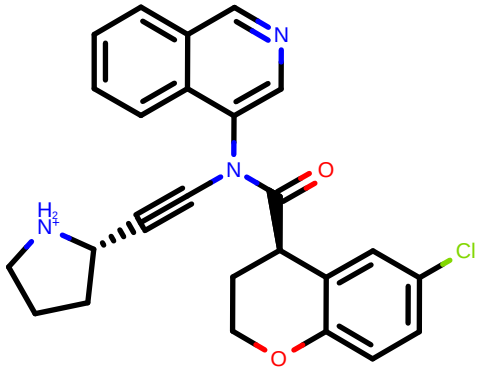
CID:	MAK-UNK-ffc90da7-4_7
SMILES:	C[C@@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN704
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.19

MAK-UNK-83e0a0b4-4_2



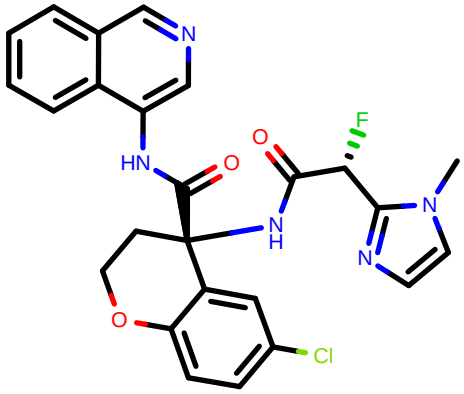
CID:	MAK-UNK-83e0a0b4-4_2
SMILES:	CCCCc1ccc2c(c1)[C@H](CCO2)C(=O)N(CCNC3C[NH2+]C3)c4cncc5c4cccc5
RUN:	RUN734
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.42

MIC-UNK-9582b2c5-2_3



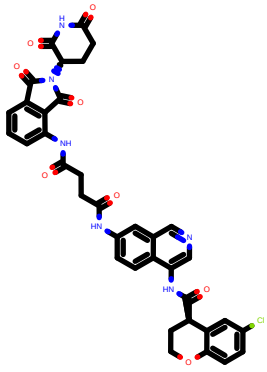
CID:	MIC-UNK-9582b2c5-2_3
SMILES:	CC(=O)N1CC[C@@H]2[C@H](C1)C[C@@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN264
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.24

MIC-UNK-cdc2493e-13_1



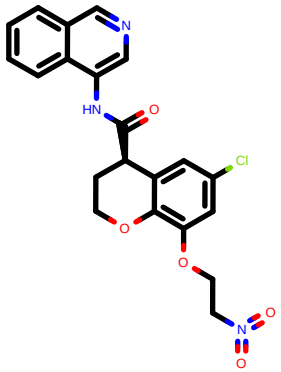
CID:	MIC-UNK-cdc2493e-13_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4CCC(CC4)[NH+]5CCCCC5
RUN:	RUN555
DDG (kcal/mol):	-3.18
dDDG (kcal/mol):	0.25

EDJ-MED-50011917-2_1



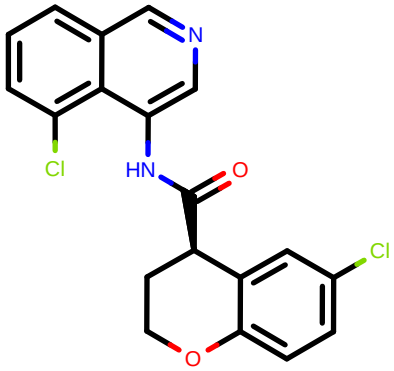
CID:	EDJ-MED-50011917-2_1
SMILES:	Cc1c(cc(cc1O[C@@H]2CC(=O)N2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN373
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.45

ALP-POS-2da19ca7-7_3



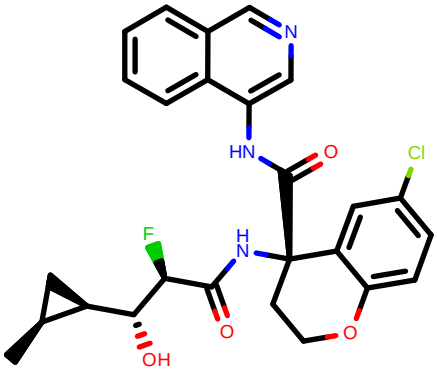
CID:	ALP-POS-2da19ca7-7_3
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)S(=O)(=O)C
RUN:	RUN2384
DDG (kcal/mol):	-3.17
dDDG (kcal/mol):	0.37

MAT-POS-bbbbc21a-3_1



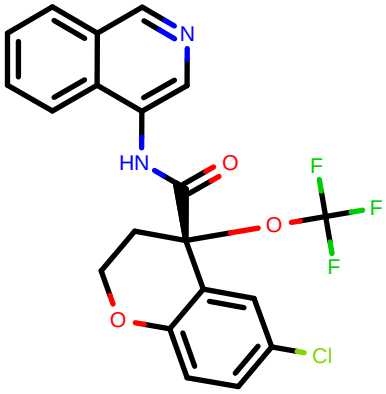
CID:	MAT-POS-bbbbc21a-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc4c3OCC4)Cl
RUN:	RUN280
DDG (kcal/mol):	-3.16
dDDG (kcal/mol):	0.14

ADA-UCB-dc2b944c-11_1



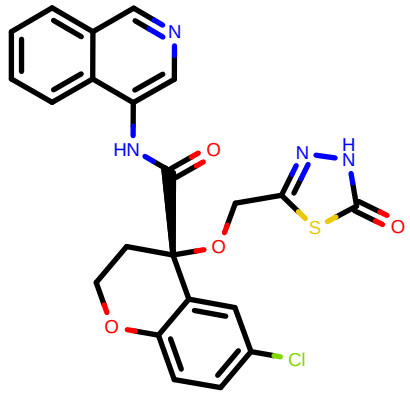
CID:	ADA-UCB-dc2b944c-11_1
SMILES:	c1ccc2c(c1)c(cnc2Br)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN610
DDG (kcal/mol):	-3.16
dDDG (kcal/mol):	0.30

MAK-UNK-c749d764-8_8



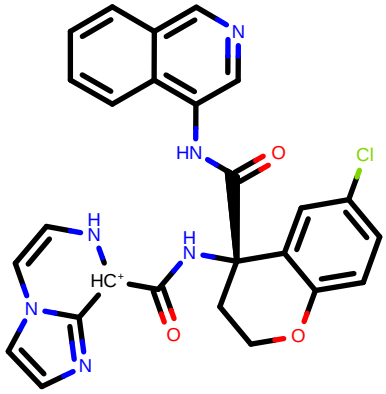
CID:	MAK-UNK-c749d764-8_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN940
DDG (kcal/mol):	-3.16
dDDG (kcal/mol):	0.21

VLA-UCB-34f3ed0c-17_1



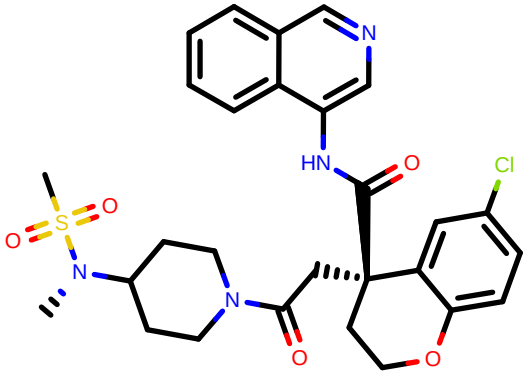
CID:	VLA-UCB-34f3ed0c-17_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CN([C@@]4(C3=O)CCOc5c4cc(cc5)Cl)C(=O)C6CCCCC6
RUN:	RUN641
DDG (kcal/mol):	-3.16
dDDG (kcal/mol):	0.22

KAD-UNI-877d7bed-11_3



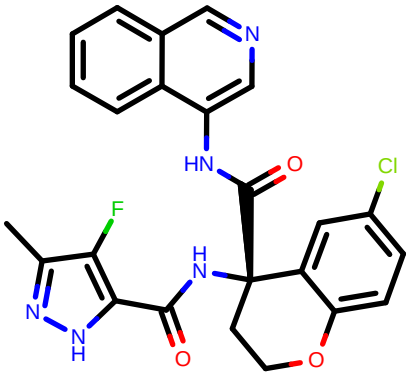
CID:	KAD-UNI-877d7bed-11_3
SMILES:	CC(C)[C@@H]1CCN(C1)C(=O)COc2cc(cc3c2OCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl)O
RUN:	RUN3749
DDG (kcal/mol):	-3.15
dDDG (kcal/mol):	0.15

MAK-UNK-c749d764-26_4



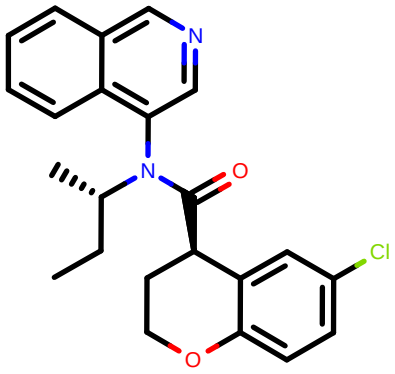
CID:	MAK-UNK-c749d764-26_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCCC[C@H]([C@@H]3O)Cl
RUN:	RUN1049
DDG (kcal/mol):	-3.15
dDDG (kcal/mol):	0.27

MIC-UNK-bcd487e9-4_1



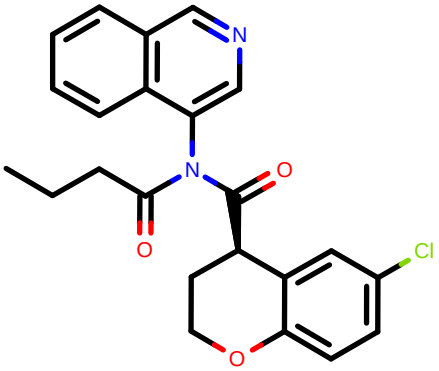
CID:	MIC-UNK-bcd487e9-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(C[C@@H]3CCCO3)c4cccc(c4)Cl
RUN:	RUN589
DDG (kcal/mol):	-3.15
dDDG (kcal/mol):	0.23

DAR-DIA-ecdbc7dd-11_1



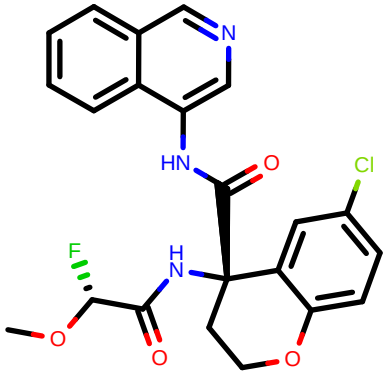
CID:	DAR-DIA-ecdbc7dd-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH+]5CCCCC5
RUN:	RUN2897
DDG (kcal/mol):	-3.15
dDDG (kcal/mol):	0.11

LON-WEI-4d77710c-28_1



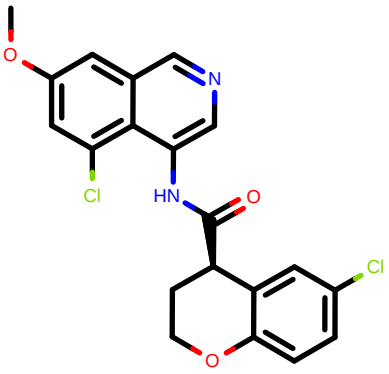
CID:	LON-WEI-4d77710c-28_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCc3cc(ccc3OC)OC
RUN:	RUN218
DDG (kcal/mol):	-3.15
dDDG (kcal/mol):	0.28

MAK-UNK-919546f0-5_1



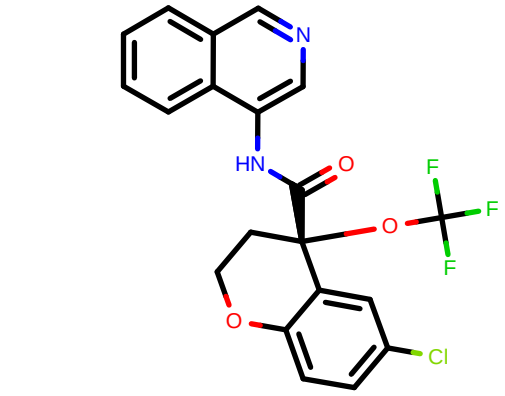
CID:	MAK-UNK-919546f0-5_1
SMILES:	CN(CC(=O)Nc1cncc2c1cccc2)C=O
RUN:	RUN485
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.25

RAL-THA-8416115c-2_1



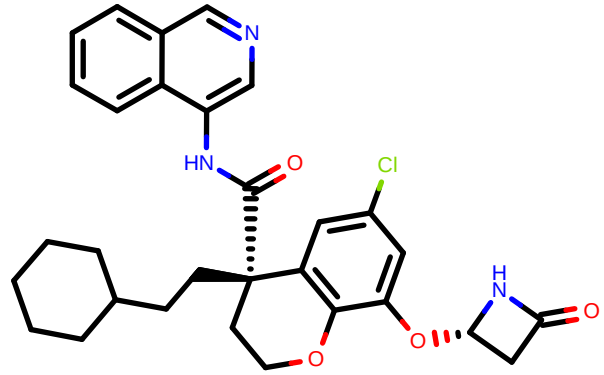
CID:	RAL-THA-8416115c-2_1
SMILES:	CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1251
DDG (kcal/mol):	-3.14
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-15_12



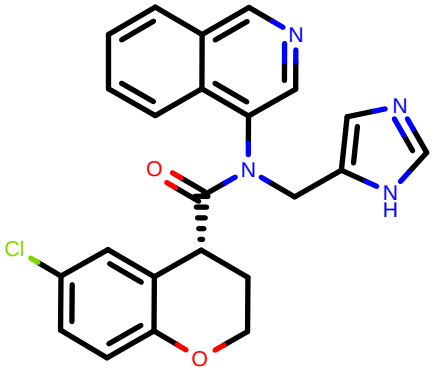
CID:	MAK-UNK-c749d764-15_12
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN967
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.20

VLA-UCB-1dbca3b4-16_1



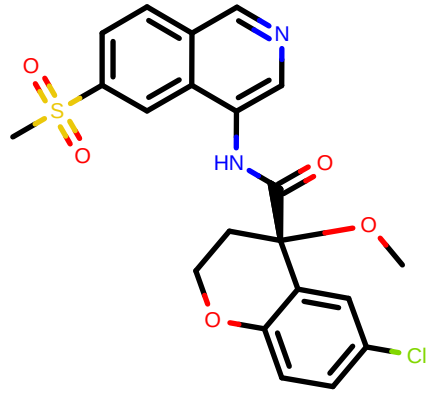
CID:	VLA-UCB-1dbca3b4-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3=C(COc4c3cc(cc4)Cl)O
RUN:	RUN169
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.29

EDG-MED-ba1ac7b9-25_4



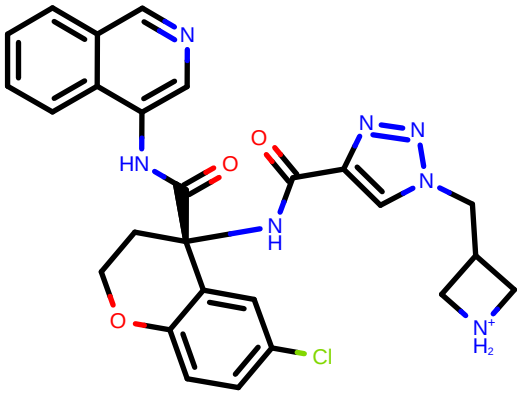
CID:	EDG-MED-ba1ac7b9-25_4
SMILES:	C[C@H]1CN(CC[N@H+]1CCO)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2714
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.14

ALP-POS-fab80cf2-1_1



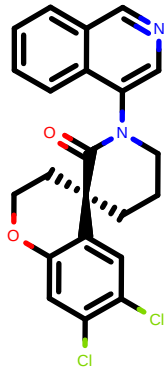
CID:	ALP-POS-fab80cf2-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C([C@@H]4CC(=O)N4)(F)F
RUN:	RUN1514
DDG (kcal/mol):	-3.13
dDDG (kcal/mol):	0.21

NAU-LAT-b7d8c353-8_1



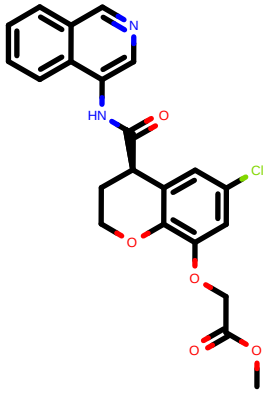
CID:	NAU-LAT-b7d8c353-8_1
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)C[NH3+]
RUN:	RUN456
DDG (kcal/mol):	-3.12
dDDG (kcal/mol):	0.28

DAR-DIA-0d514e7d-31_2



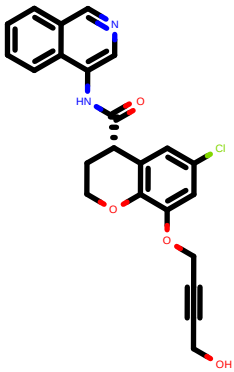
CID:	DAR-DIA-0d514e7d-31_2
SMILES:	C[C@H]1CCO[C@@H]2C=CC(=C[C@@H]2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN833
DDG (kcal/mol):	-3.11
dDDG (kcal/mol):	0.31

MAT-POS-f9802937-9_1



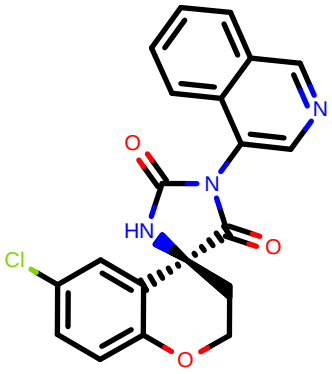
CID:	MAT-POS-f9802937-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN2403
DDG (kcal/mol):	-3.11
dDDG (kcal/mol):	0.31

ALP-POS-2da19ca7-1_1



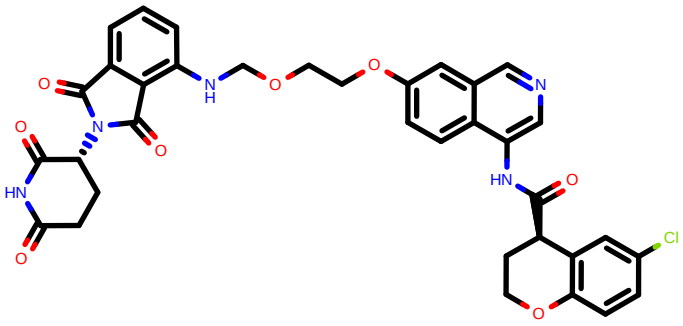
CID:	ALP-POS-2da19ca7-1_1
SMILES:	CCNC(=O)C[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2382
DDG (kcal/mol):	-3.11
dDDG (kcal/mol):	0.15

MAT-POS-b5746674-105_1



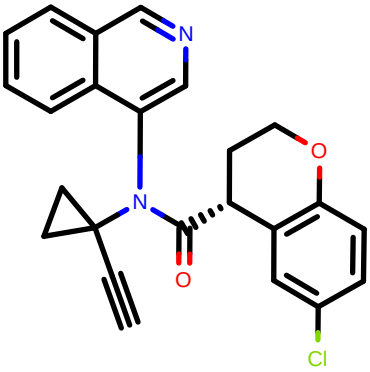
CID:	MAT-POS-b5746674-105_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NC3CC[NH+](CC3)Cc4ccccc4
RUN:	RUN82
DDG (kcal/mol):	-3.11
dDDG (kcal/mol):	0.20

MAT-POS-bbbbc21a-1_1



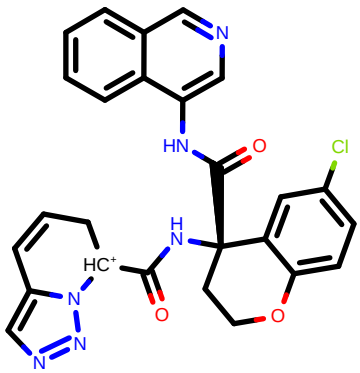
CID:	MAT-POS-bbbbc21a-1_1
SMILES:	COc1ccc(cc1CC(=O)Nc2cncc3c2cccc3)Cl
RUN:	RUN275
DDG (kcal/mol):	-3.09
dDDG (kcal/mol):	0.48

LON-WEI-4d77710c-54_1



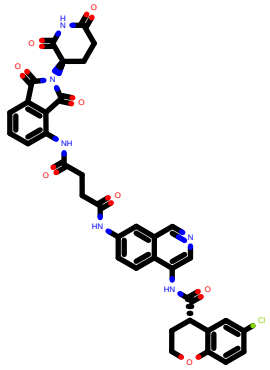
CID:	LON-WEI-4d77710c-54_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CCC(CC3)Cc4ccccc4
RUN:	RUN244
DDG (kcal/mol):	-3.09
dDDG (kcal/mol):	0.24

JOH-SUS-a69c159d-6_2



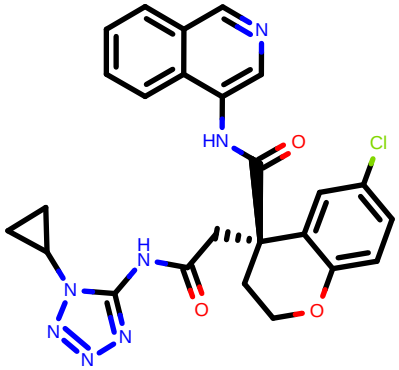
CID:	JOH-SUS-a69c159d-6_2
SMILES:	c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1127
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.23

FRA-DIA-0fa076fe-2_1



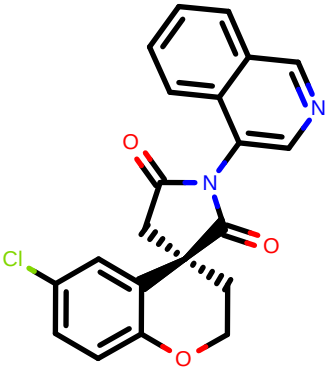
CID:	FRA-DIA-0fa076fe-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cc(cc4Cl)O
RUN:	RUN422
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.27

MAK-UNK-c749d764-33_4



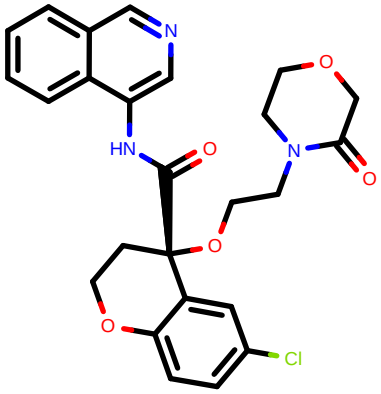
CID:	MAK-UNK-c749d764-33_4
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1082
DDG (kcal/mol):	-3.07
dDDG (kcal/mol):	0.33

LON-WEI-adc59df6-52_2



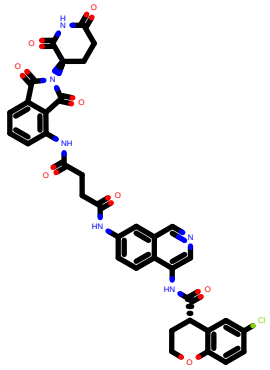
CID:	LON-WEI-adc59df6-52_2
SMILES:	CC(C)(C)c1ccc(cc1)N([C@H](c2cncc3c2cccc3)C(=O)NC(C)(C)C)C(=O)C=C
RUN:	RUN3
DDG (kcal/mol):	-3.06
dDDG (kcal/mol):	0.25

VLA-UCB-34f3ed0c-19_1



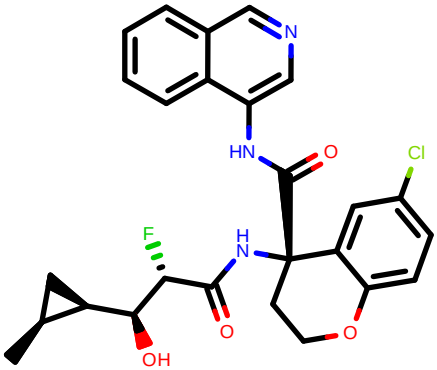
CID:	VLA-UCB-34f3ed0c-19_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)c3ccco3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN646
DDG (kcal/mol):	-3.05
dDDG (kcal/mol):	0.28

ALP-UNI-44c99a80-4_1



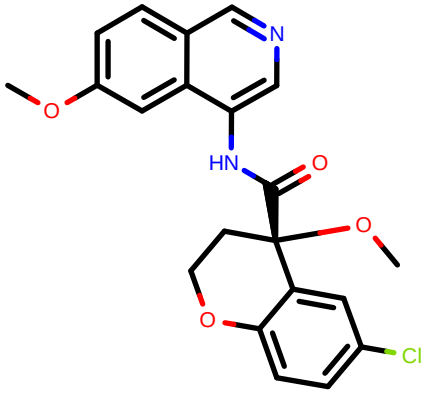
CID:	ALP-UNI-44c99a80-4_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)Cc4cccc(c4)Cl
RUN:	RUN459
DDG (kcal/mol):	-3.05
dDDG (kcal/mol):	0.28

EDJ-MED-28ec730d-2_1



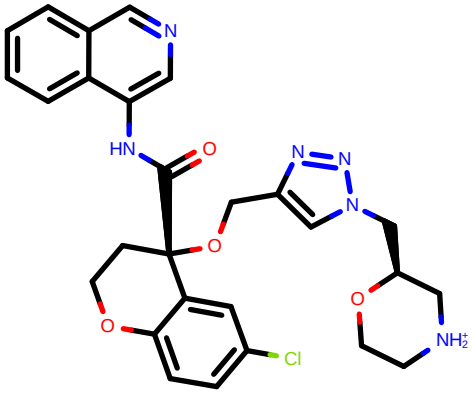
CID:	EDJ-MED-28ec730d-2_1
SMILES:	COCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN650
DDG (kcal/mol):	-3.05
dDDG (kcal/mol):	0.23

ED_-GRI-5b13fbe2-63_1



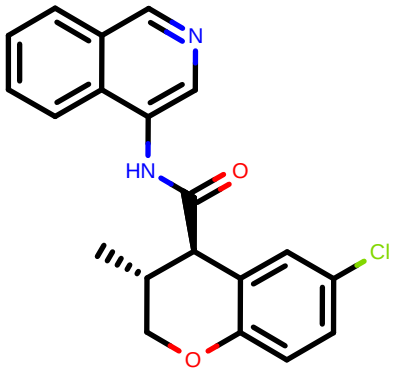
CID:	ED_-GRI-5b13fbe2-63_1
SMILES:	Cc1c(nnn1CCCCO[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C[NH3+]
RUN:	RUN1617
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.20

MAR-UCB-f313ec4d-2_1



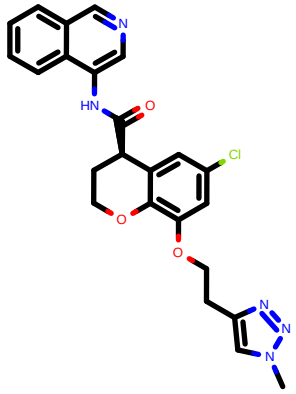
CID:	MAR-UCB-f313ec4d-2_1
SMILES:	COc1ccccc1OCCNC(=O)c2cncc3c2cccc3
RUN:	RUN326
DDG (kcal/mol):	-3.03
dDDG (kcal/mol):	0.40

MIC-UNK-d36ab305-5_1



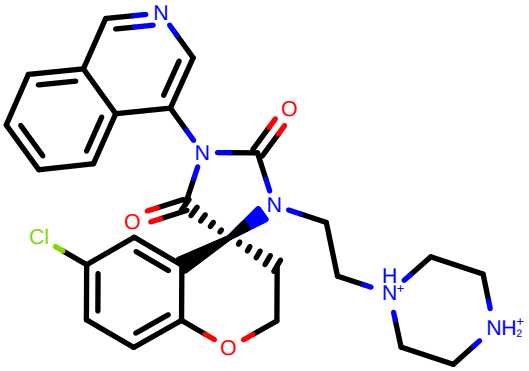
CID:	MIC-UNK-d36ab305-5_1
SMILES:	CN(C)c1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN165
DDG (kcal/mol):	-3.02
dDDG (kcal/mol):	0.17

MAT-POS-e9e99895-13_2



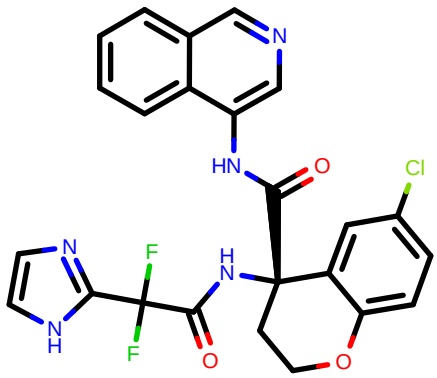
CID:	MAT-POS-e9e99895-13_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CC[N@@H+](C4)C
RUN:	RUN2268
DDG (kcal/mol):	-3.00
dDDG (kcal/mol):	0.35

DAR-DIA-0d514e7d-32_7



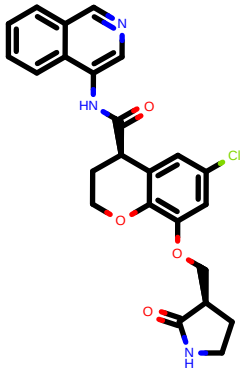
CID:	DAR-DIA-0d514e7d-32_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@H]4C[C@H]4CO[C@@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN856
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.23

MIC-UNK-50cce87d-11_2



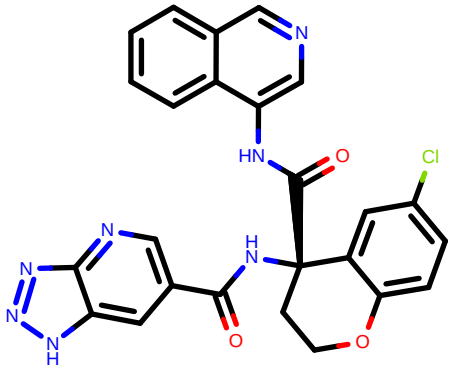
CID:	MIC-UNK-50cce87d-11_2
SMILES:	Cc1cccc2c1c(cnc2)N3CCC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN678
DDG (kcal/mol):	-2.99
dDDG (kcal/mol):	0.25

EDG-MED-5d232de5-8_1



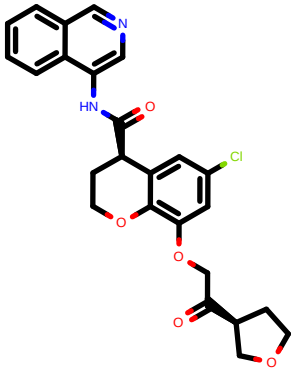
CID:	EDG-MED-5d232de5-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN2370
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.42

MAK-UNK-c749d764-29_5



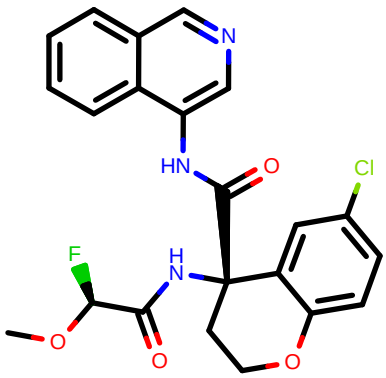
CID:	MAK-UNK-c749d764-29_5
SMILES:	c1ccc2c(c1)cncc2N(C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F)C(=O)ON
RUN:	RUN1066
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.26

EDG-MED-ba1ac7b9-5_1



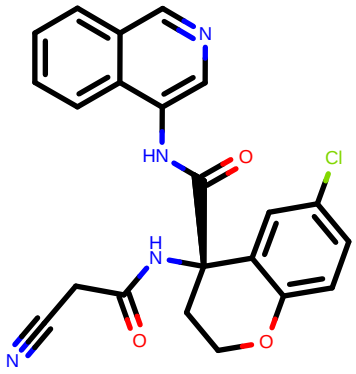
CID:	EDG-MED-ba1ac7b9-5_1
SMILES:	CC[C@@H](CO)[NH+]1CCN(CC1)C(=O)C[C@@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2634
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.48

MAK-UNK-8be7dca9-3_2



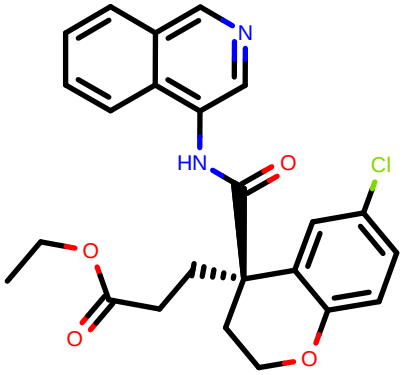
CID:	MAK-UNK-8be7dca9-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4OC[C@@H]3C[NH3+])Cl
RUN:	RUN496
DDG (kcal/mol):	-2.97
dDDG (kcal/mol):	0.22

MIC-UNK-cdc2493e-8_6



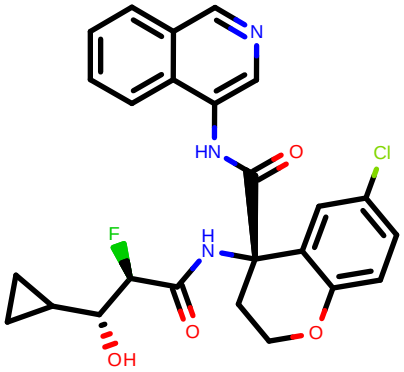
CID:	MIC-UNK-cdc2493e-8_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@H]4CC[C@@H]5CCCC[C@H]5C4
RUN:	RUN541
DDG (kcal/mol):	-2.96
dDDG (kcal/mol):	0.23

ALP-UNI-8e43a71e-1_2



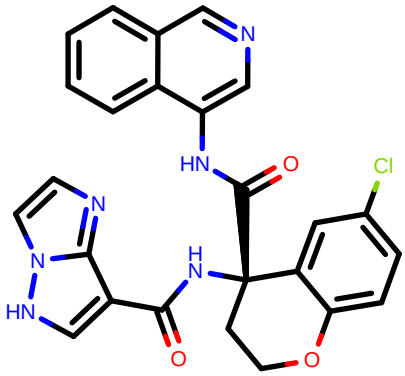
CID:	ALP-UNI-8e43a71e-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)[N@@]6[C@@H]5CCCC6
RUN:	RUN2919
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.12

MIC-UNK-cdc2493e-20_1



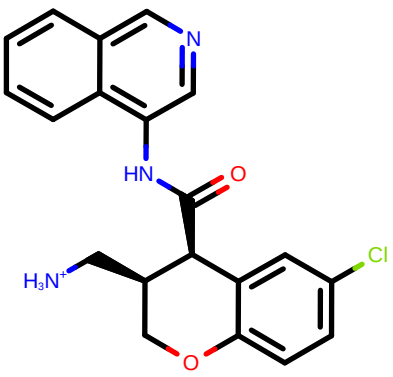
CID:	MIC-UNK-cdc2493e-20_1
SMILES:	CC(=O)N(C)C1CCC(CC1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN565
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.23

JOH-SUS-a69c159d-6_1



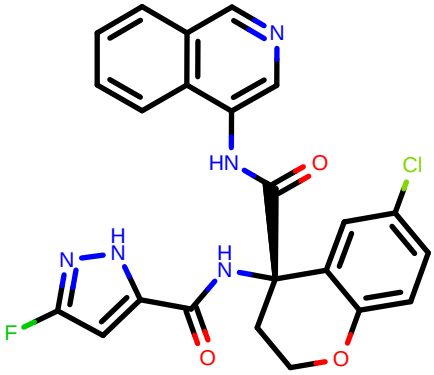
CID:	JOH-SUS-a69c159d-6_1
SMILES:	c1ccc2c(c1)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1126
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.23

ALF-EVA-650655fc-4_5



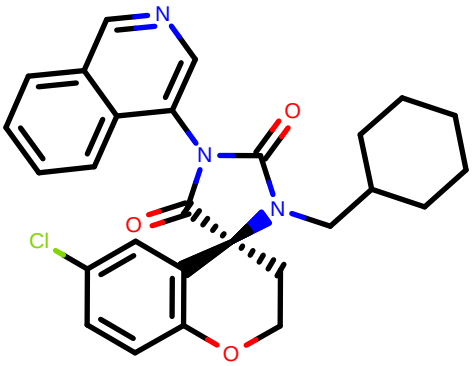
CID:	ALF-EVA-650655fc-4_5
SMILES:	C[N@@H+]1CC[C@@H](C1)CCN(c2cc(cc(c2)Cl)O[C@H]3CC(=O)N3)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2861
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-3_1



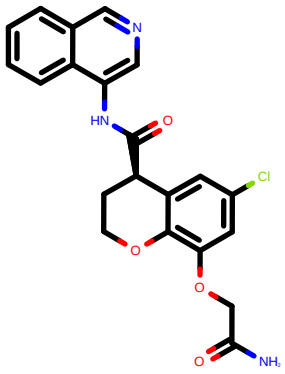
CID:	MIC-UNK-5a93dd5f-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN740
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.22

LON-WEI-4d77710c-51_1



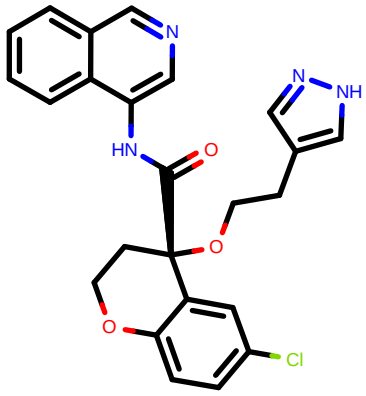
CID:	LON-WEI-4d77710c-51_1
SMILES:	Cc1c(c(on1)C)CCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN241
DDG (kcal/mol):	-2.93
dDDG (kcal/mol):	0.22

MAT-POS-e9e99895-13_1



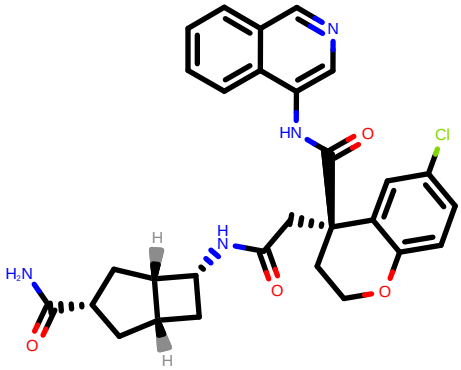
CID:	MAT-POS-e9e99895-13_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CC[N@@H+](C4)C
RUN:	RUN2267
DDG (kcal/mol):	-2.92
dDDG (kcal/mol):	0.27

MAT-POS-3b92565d-3_2



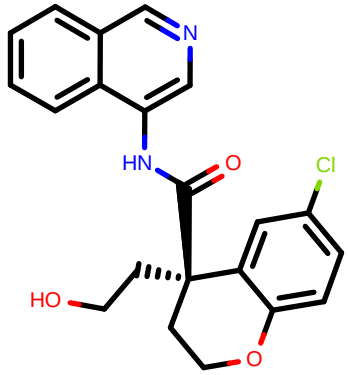
CID:	MAT-POS-3b92565d-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN112
DDG (kcal/mol):	-2.91
dDDG (kcal/mol):	0.32

MAK-UNK-c749d764-24_3



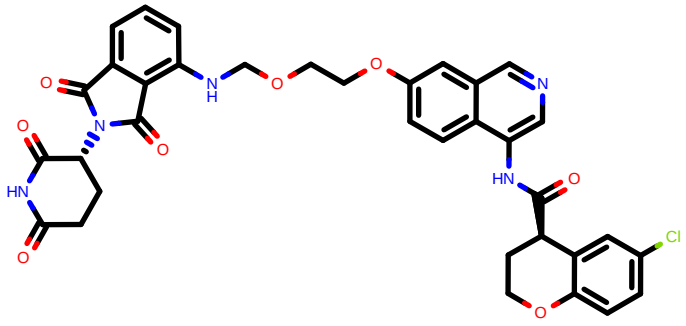
CID:	MAK-UNK-c749d764-24_3
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1032
DDG (kcal/mol):	-2.91
dDDG (kcal/mol):	0.33

MAT-POS-173a45da-1_1



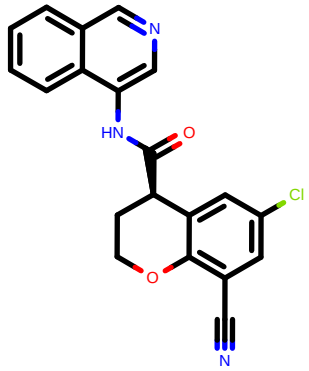
CID:	MAT-POS-173a45da-1_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)N(CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN310
DDG (kcal/mol):	-2.90
dDDG (kcal/mol):	0.23

RAL-THA-1d44ff04-5_1



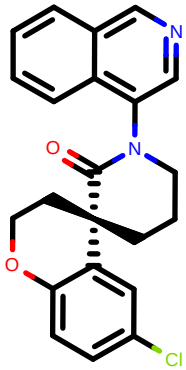
CID:	RAL-THA-1d44ff04-5_1
SMILES:	CNC(=O)c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN440
DDG (kcal/mol):	-2.90
dDDG (kcal/mol):	0.45

LON-WEI-5e7d1b3e-56_1



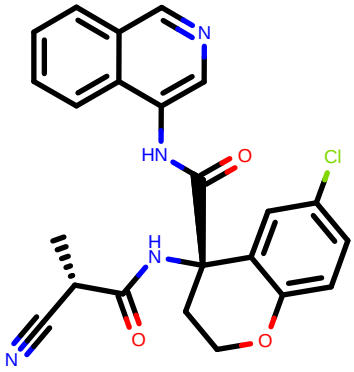
CID:	LON-WEI-5e7d1b3e-56_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccsc3C(=O)OC
RUN:	RUN1367
DDG (kcal/mol):	-2.88
dDDG (kcal/mol):	0.22

MIC-UNK-0a05c952-2_4



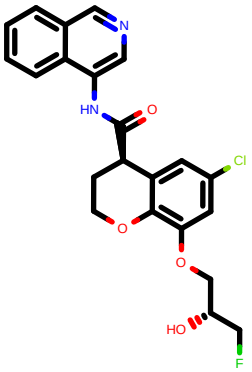
CID:	MIC-UNK-0a05c952-2_4
SMILES:	c1ccc2c(c1)cncc2N3[C@H](CC[C@H](C3=O)c4cccc(c4Cl)[C@@H]5CO5
RUN:	RUN3508
DDG (kcal/mol):	-2.88
dDDG (kcal/mol):	0.17

ADA-UCB-dc2b944c-14_1



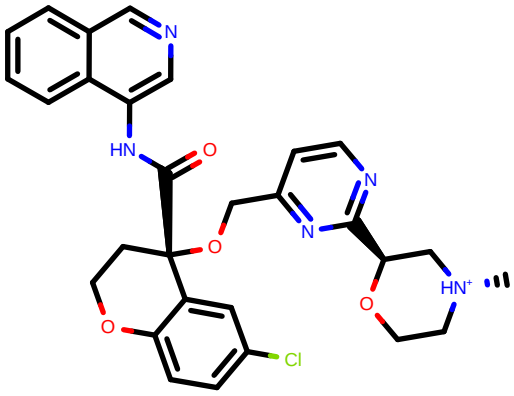
CID:	ADA-UCB-dc2b944c-14_1
SMILES:	C[C@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN612
DDG (kcal/mol):	-2.87
dDDG (kcal/mol):	0.24

KAD-UNI-80f122c8-5_2



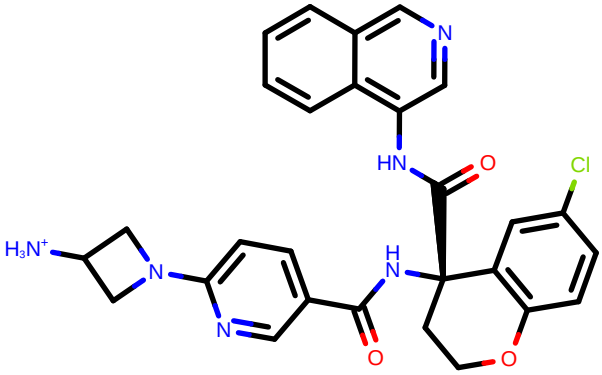
CID:	KAD-UNI-80f122c8-5_2
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2302
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.36

MIC-UNK-644c43c7-3_1



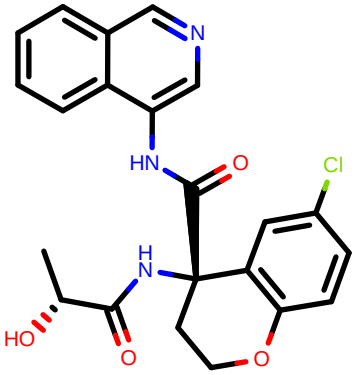
CID:	MIC-UNK-644c43c7-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CNCC(F)(F)F
RUN:	RUN431
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.19

VLA-UCB-34f3ed0c-12_1



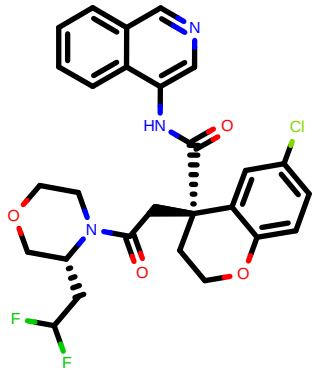
CID:	VLA-UCB-34f3ed0c-12_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CNC3=O
RUN:	RUN632
DDG (kcal/mol):	-2.86
dDDG (kcal/mol):	0.35

MAK-UNK-f481d203-3_1



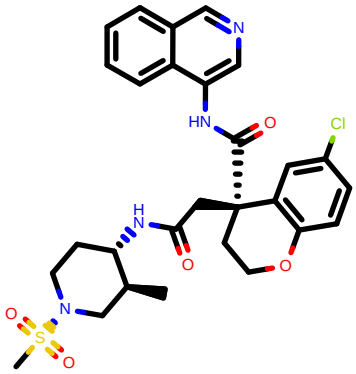
CID:	MAK-UNK-f481d203-3_1
SMILES:	c1ccc(cc1)[C@H](C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN486
DDG (kcal/mol):	-2.85
dDDG (kcal/mol):	0.26

RAL-THA-4aa06b95-4_1



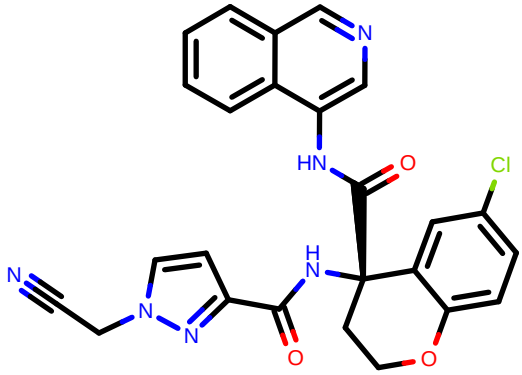
CID:	RAL-THA-4aa06b95-4_1
SMILES:	CN(C)C(=O)N1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1235
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.30

MAK-UNK-c749d764-2_7



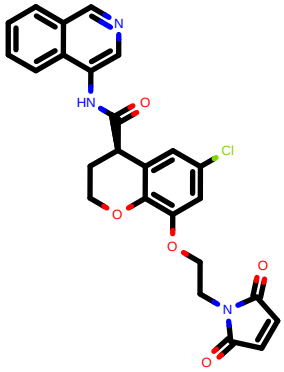
CID:	MAK-UNK-c749d764-2_7
SMILES:	CC[C@@H]1CCC[C@H]([C@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN903
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-31_6



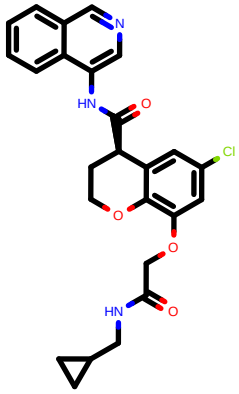
CID:	MAK-UNK-c749d764-31_6
SMILES:	CC/C=C(/c1cncc2c1cccc2)\C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1076
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.23

ALP-UNI-0676e700-24_2



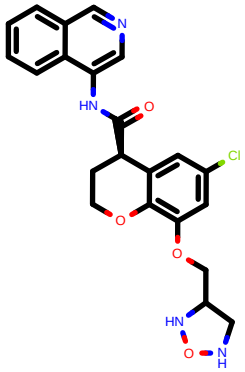
CID:	ALP-UNI-0676e700-24_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5[C@H](CC(=O)N5)C(F)(F)F
RUN:	RUN2473
DDG (kcal/mol):	-2.83
dDDG (kcal/mol):	0.37

ALP-UNI-0676e700-11_1



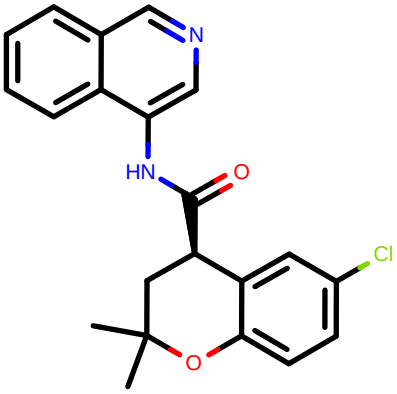
CID:	ALP-UNI-0676e700-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cc5)CC(=O)N
RUN:	RUN2460
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.33

ALP-POS-e0fe77e5-7_1



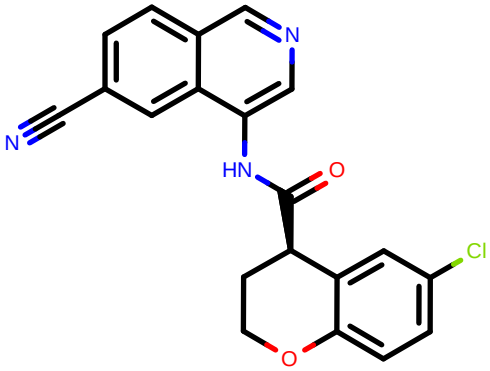
CID:	ALP-POS-e0fe77e5-7_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN2325
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.34

MAT-POS-2492181e-9_1



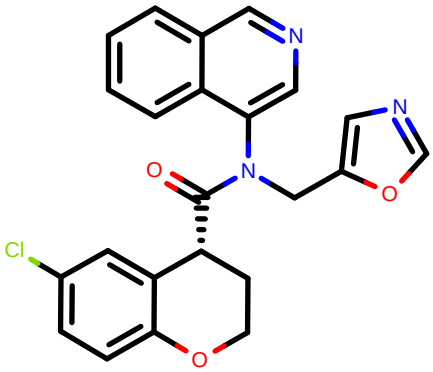
CID:	MAT-POS-2492181e-9_1
SMILES:	CC1CC[NH+](CC1)Cc2ccc(cc2)NC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN102
DDG (kcal/mol):	-2.82
dDDG (kcal/mol):	0.22

ALP-POS-f13221e1-3_1



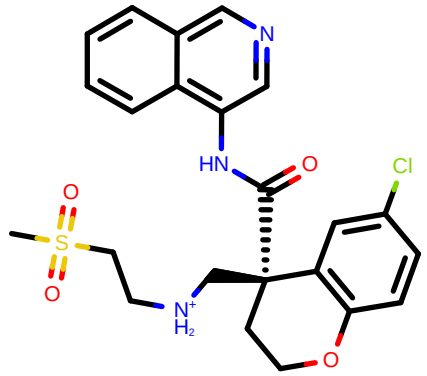
CID:	ALP-POS-f13221e1-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)CCc3cccc(c3)Cl
RUN:	RUN184
DDG (kcal/mol):	-2.81
dDDG (kcal/mol):	0.19

MIC-UNK-d36ab305-4_2



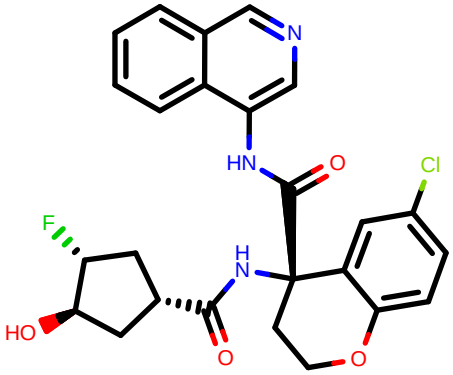
CID:	MIC-UNK-d36ab305-4_2
SMILES:	CN(C)c1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN159
DDG (kcal/mol):	-2.81
dDDG (kcal/mol):	0.29

PET-UNK-1b92fa34-4_1



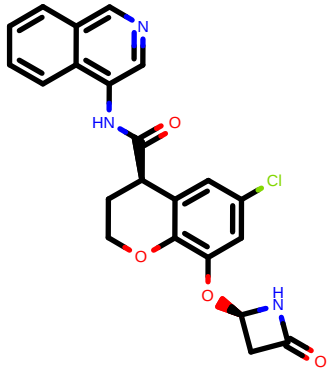
CID:	PET-UNK-1b92fa34-4_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CS(=O)(=O)Cc4c3cc(c(c4)F)Cl
RUN:	RUN4172
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.28

MIC-UNK-cdc2493e-22_1



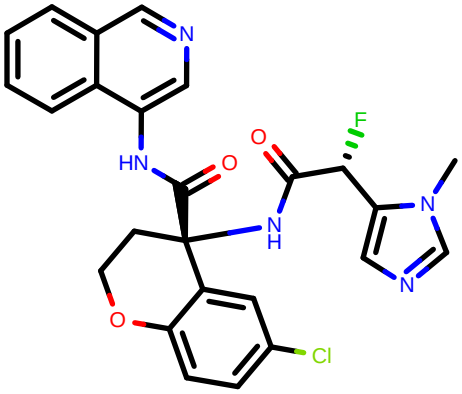
CID:	MIC-UNK-cdc2493e-22_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCn3ccnn3)c4cccc(c4)Cl
RUN:	RUN574
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.28

EDG-MED-ba1ac7b9-28_3



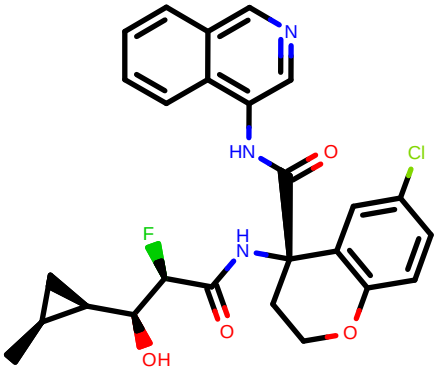
CID:	EDG-MED-ba1ac7b9-28_3
SMILES:	C[N@@H+](CCO)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2734
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.17

MIC-UNK-cdc2493e-5_2



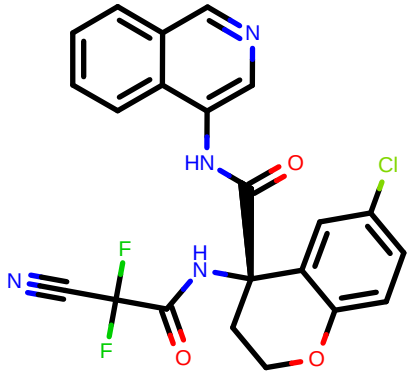
CID:	MIC-UNK-cdc2493e-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCCC[C@@H]5C4
RUN:	RUN533
DDG (kcal/mol):	-2.80
dDDG (kcal/mol):	0.26

VLA-UCB-34f3ed0c-6_1



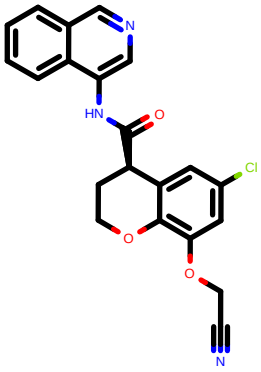
CID:	VLA-UCB-34f3ed0c-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C(=O)CC4CCCCC4
RUN:	RUN630
DDG (kcal/mol):	-2.79
dDDG (kcal/mol):	0.25

MIC-UNK-cdc2493e-21_4



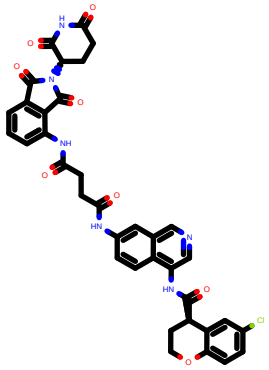
CID:	MIC-UNK-cdc2493e-21_4
SMILES:	CC(=O)N(C)[C@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN572
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.24

MAT-POS-e9e99895-2_3



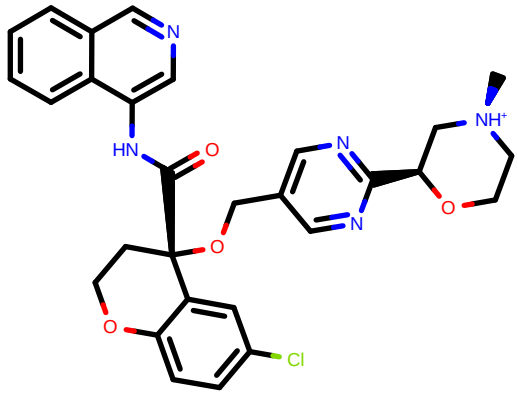
CID:	MAT-POS-e9e99895-2_3
SMILES:	CC(C)[N@@H+]1CCO[C@H](C1)C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2236
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.27

ALP-UNI-8e43a71e-5_14



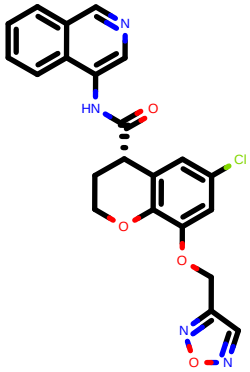
CID:	ALP-UNI-8e43a71e-5_14
SMILES:	C[C@H]1C[N@@](CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2958
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.24

MIC-UNK-cdc2493e-3_1



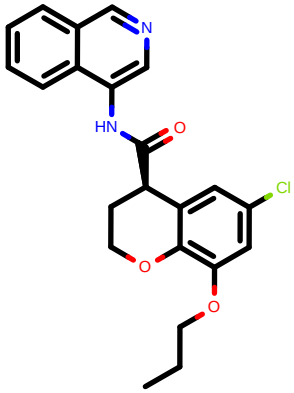
CID:	MIC-UNK-cdc2493e-3_1
SMILES:	c1ccc(cc1)CCN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN523
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.30

ALP-POS-e0fe77e5-4_1



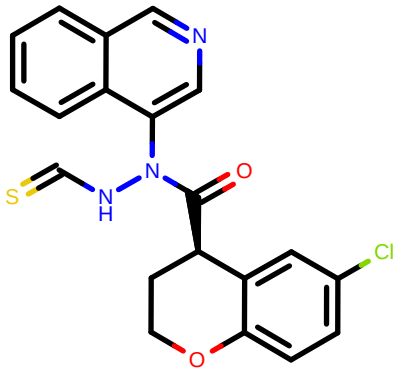
CID:	ALP-POS-e0fe77e5-4_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@@]4(C3=O)CCOc5c4cc(c(c5)Cl)Cl
RUN:	RUN2324
DDG (kcal/mol):	-2.78
dDDG (kcal/mol):	0.24

DAR-DIA-9e4459de-15_1



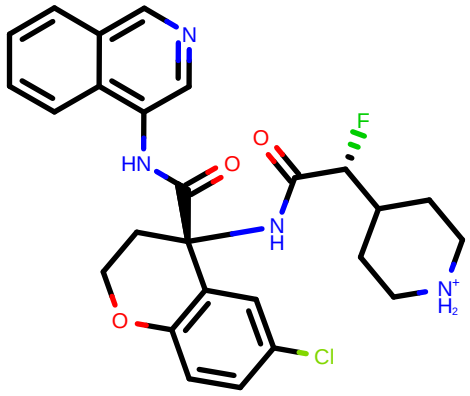
CID:	DAR-DIA-9e4459de-15_1
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1441
DDG (kcal/mol):	-2.77
dDDG (kcal/mol):	0.33

LON-WEI-4d77710c-29_1



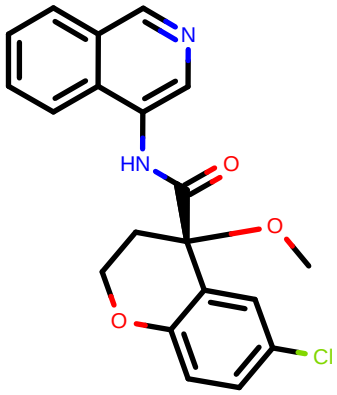
CID:	LON-WEI-4d77710c-29_1
SMILES:	CCOC(=O)Cc1csc(n1)NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN221
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-7_2



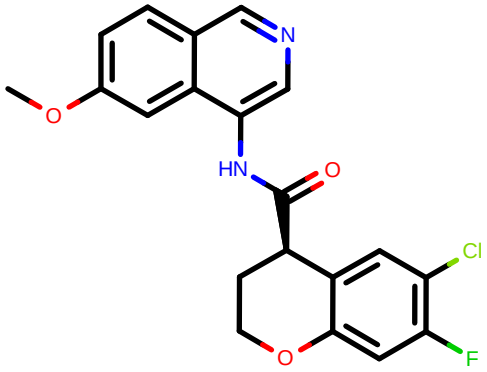
CID:	MIC-UNK-5a93dd5f-7_2
SMILES:	CC(=O)N(C)[C@H]1CC[N@@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN769
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.25

DAR-DIA-0d514e7d-31_6



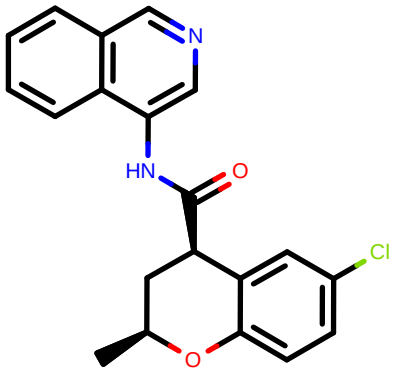
CID:	DAR-DIA-0d514e7d-31_6
SMILES:	C[C@H]1CCO[C@@H]2C=CC(=C[C@H]2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN839
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.19

LAU-MED-88a3970a-14_1



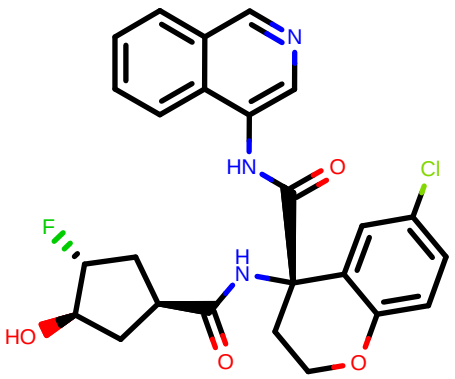
CID:	LAU-MED-88a3970a-14_1
SMILES:	COCCCc1cc(cc2c1OCC[C@@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1510
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.21

ERI-UCB-ce40166b-10_1



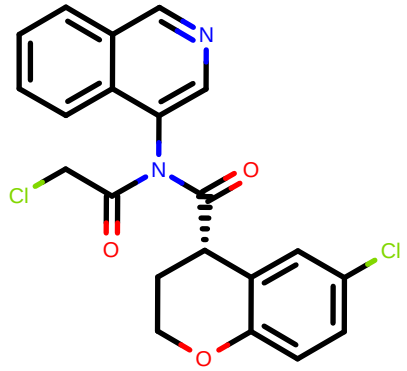
CID:	ERI-UCB-ce40166b-10_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)O[C@@H]4CCC(=O)N4)C#N
RUN:	RUN48
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.20

MAK-UNK-ffc90da7-9_1



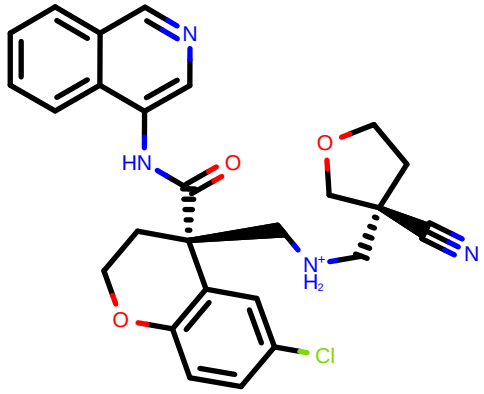
CID:	MAK-UNK-ffc90da7-9_1
SMILES:	C[C@@H]1[C@@H](CCO1)SC[C@@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN709
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.25

LON-WEI-af038623-3_1



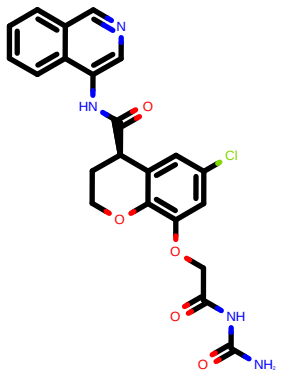
CID:	LON-WEI-af038623-3_1
SMILES:	C=CC(=O)Nc1cncc2c1cccc2
RUN:	RUN34
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.25

MAT-POS-4223bc15-26_2



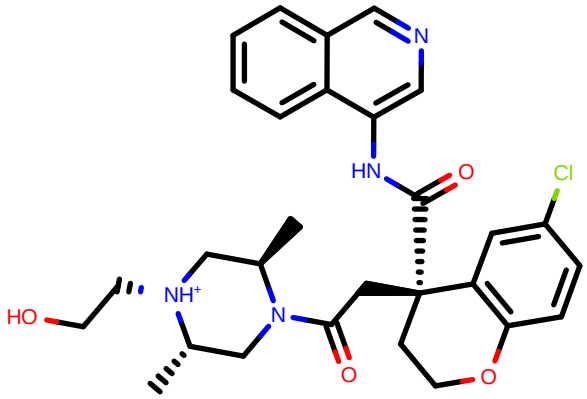
CID:	MAT-POS-4223bc15-26_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)CC(F)(F)F
RUN:	RUN4118
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.20

KAD-UNI-8a629cb0-2_1



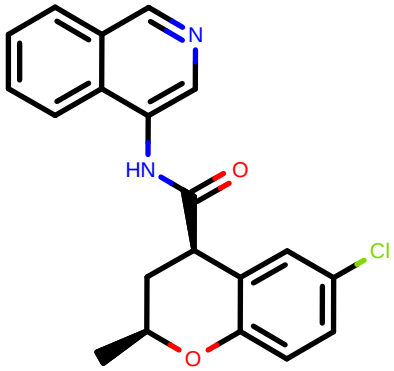
CID:	KAD-UNI-8a629cb0-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC56CC(C5)(CO6)C(=O)N
RUN:	RUN2085
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.38

ALP-POS-966f8da6-1_2



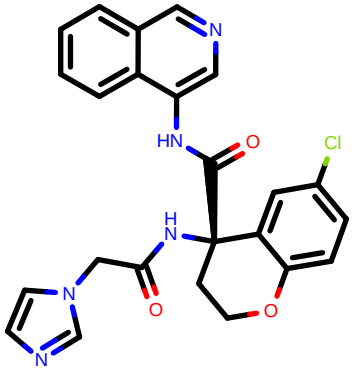
CID:	ALP-POS-966f8da6-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1219
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.26

DAR-DIA-0cde14eb-50_1



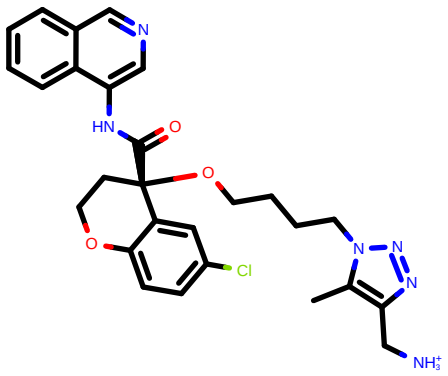
CID:	DAR-DIA-0cde14eb-50_1
SMILES:	CC1(CC1)c2cccc(c2)NC(=O)Nc3cncc4c3cccc4
RUN:	RUN15
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.21

MAK-UNK-919546f0-4_1



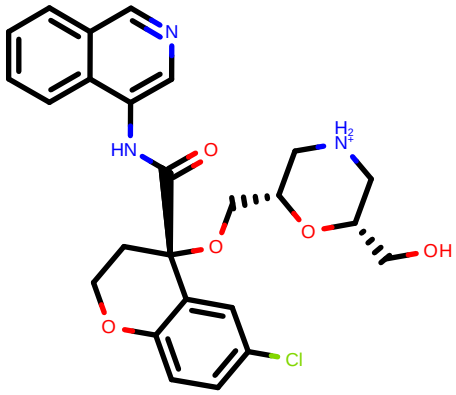
CID:	MAK-UNK-919546f0-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3ccccc3O
RUN:	RUN484
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.31

JAG-UCB-706446eb-1_1



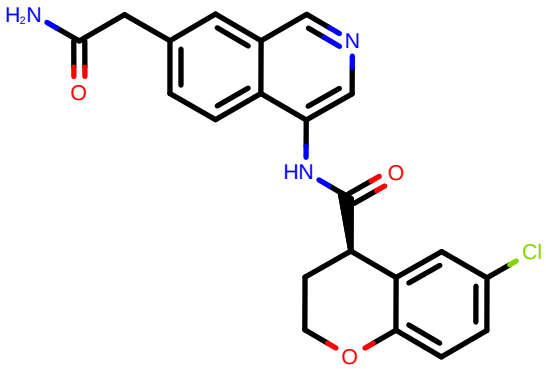
CID:	JAG-UCB-706446eb-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)NCC(F)(F)F
RUN:	RUN621
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.39

MAR-UCB-f313ec4d-3_1



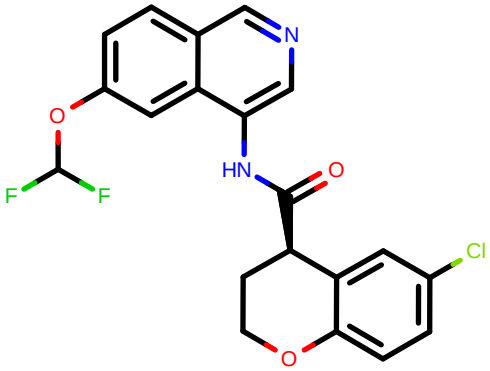
CID:	MAR-UCB-f313ec4d-3_1
SMILES:	COc1ccccc1OCCC(=O)Nc2cncc3c2cccc3
RUN:	RUN331
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.31

ERI-UCB-ce40166b-6_2



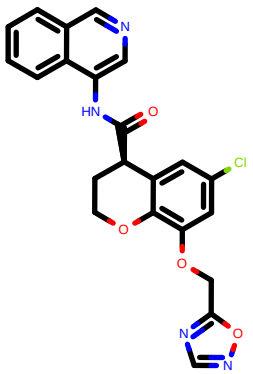
CID:	ERI-UCB-ce40166b-6_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Cl)O[C@H]4CCC(=O)N4
RUN:	RUN43
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.20

LON-WEI-4d77710c-7_1



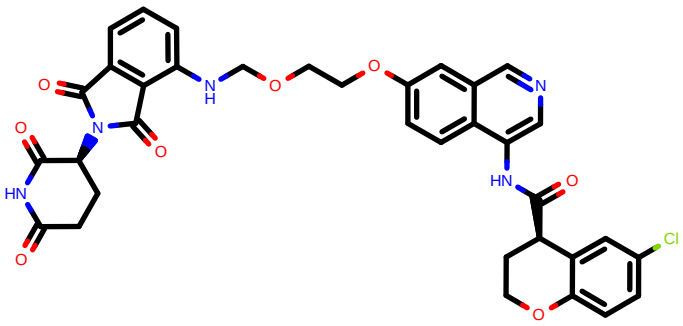
CID:	LON-WEI-4d77710c-7_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCC[N@@H+]3CCc4ccccc4C3
RUN:	RUN197
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.24

MAT-POS-e69ad64a-1_2



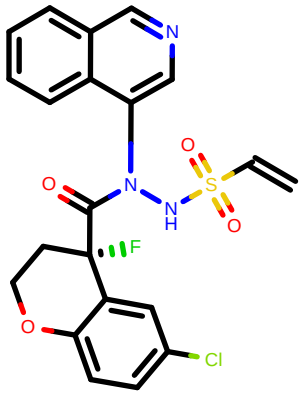
CID:	MAT-POS-e69ad64a-1_2
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN2331
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.36

MIC-UNK-9582b2c5-2_1



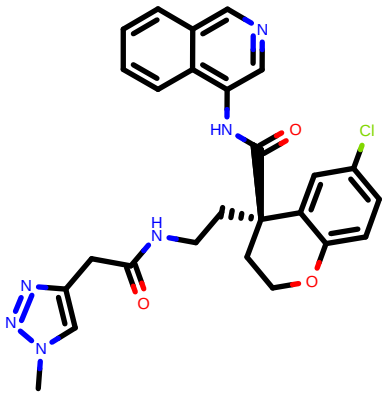
CID:	MIC-UNK-9582b2c5-2_1
SMILES:	CC(=O)N1CC[C@@H]2[C@@H](C1)C[C@@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN262
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.55

MAK-UNK-c749d764-15_3



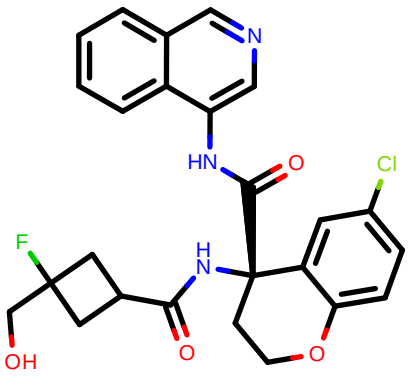
CID:	MAK-UNK-c749d764-15_3
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN958
DDG (kcal/mol):	-2.70
dDDG (kcal/mol):	0.23

RAL-THA-e002e396-1_1



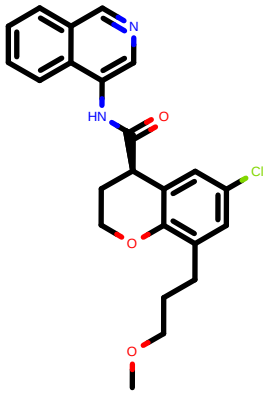
CID:	RAL-THA-e002e396-1_1
SMILES:	CS(=O)(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3451
DDG (kcal/mol):	-2.69
dDDG (kcal/mol):	0.19

EDJ-MED-28ec730d-3_1



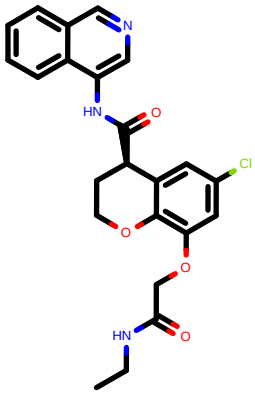
CID:	EDJ-MED-28ec730d-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5CCOCC5
RUN:	RUN652
DDG (kcal/mol):	-2.69
dDDG (kcal/mol):	0.26

VLA-UCB-05e51b3f-1_1



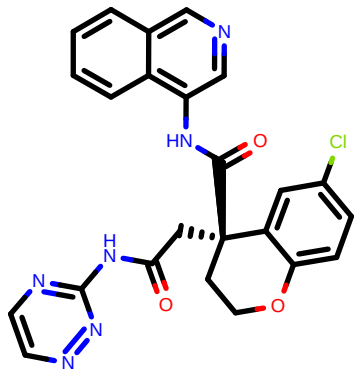
CID:	VLA-UCB-05e51b3f-1_1
SMILES:	CC(=O)N1CC[NH+](CC1)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN315
DDG (kcal/mol):	-2.69
dDDG (kcal/mol):	0.27

ALP-POS-2da19ca7-3_1



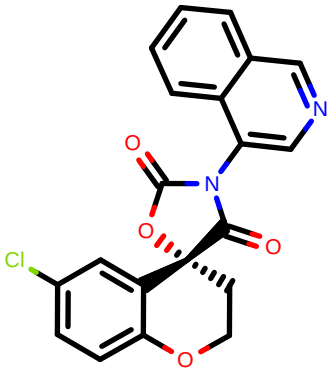
CID:	ALP-POS-2da19ca7-3_1
SMILES:	Cn1cnc2c(c1=O)CCN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2377
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.31

KAD-UNI-cb0f2bbc-22_1



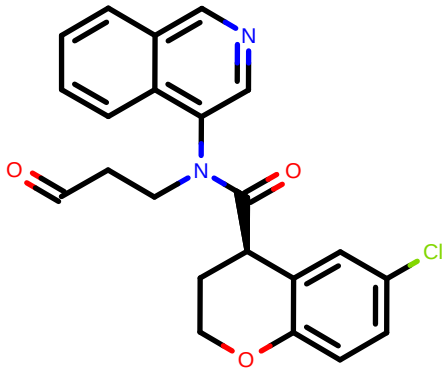
CID:	KAD-UNI-cb0f2bbc-22_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]CCN5C(=O)c6ccccc6C5=O
RUN:	RUN3711
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.12

LAU-MED-88a3970a-8_1



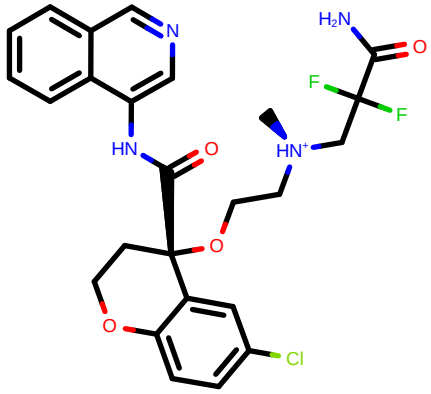
CID:	LAU-MED-88a3970a-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4CCCCO)Cl
RUN:	RUN1504
DDG (kcal/mol):	-2.68
dDDG (kcal/mol):	0.18

MAT-POS-e6dd326d-4_2



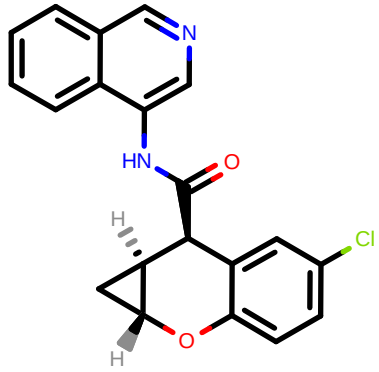
CID:	MAT-POS-e6dd326d-4_2
SMILES:	CS(=O)(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3944
DDG (kcal/mol):	-2.67
dDDG (kcal/mol):	0.15

EDJ-MED-50011917-3_1



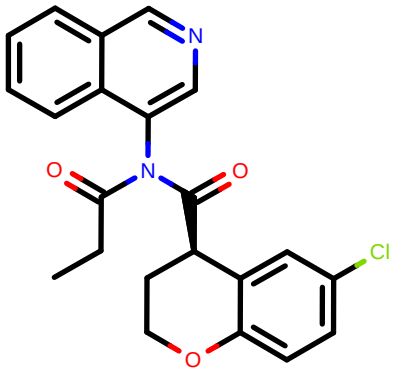
CID:	EDJ-MED-50011917-3_1
SMILES:	COc1c(cc(cc1CC(=O)Nc2cncc3c2cccc3)Cl)C[C@@H]4CC(=O)N4
RUN:	RUN377
DDG (kcal/mol):	-2.66
dDDG (kcal/mol):	0.30

NIR-WEI-f9286bb6-4_2



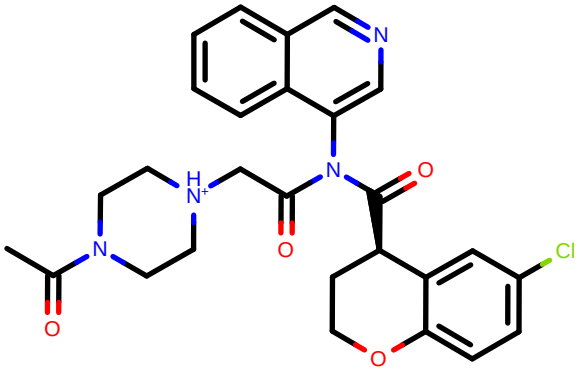
CID:	NIR-WEI-f9286bb6-4_2
SMILES:	CC(C)(C)NC(=O)[C@H](c1cncc2c1cccc2)N(Cc3ccccc3Cl)C(=O)C=C
RUN:	RUN142
DDG (kcal/mol):	-2.65
dDDG (kcal/mol):	0.14

LON-WEI-4d77710c-47_1



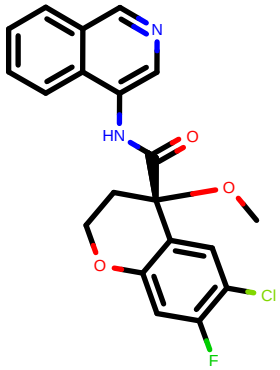
CID:	LON-WEI-4d77710c-47_1
SMILES:	CCc1ccccc1N(CC)C(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN236
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.29

LON-WEI-4d77710c-13_1



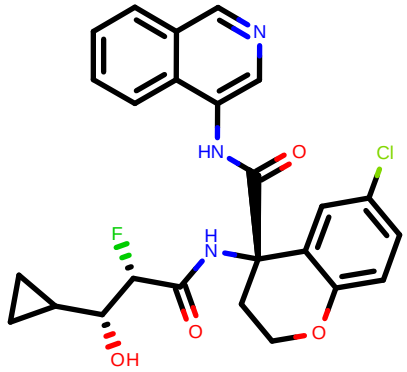
CID:	LON-WEI-4d77710c-13_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NC[C@@H]3CCCO3
RUN:	RUN201
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.44

DAR-DIA-5ff57136-11_1



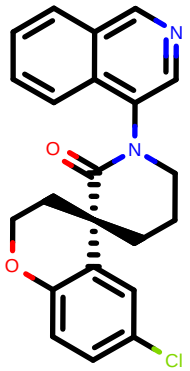
CID:	DAR-DIA-5ff57136-11_1
SMILES:	C=C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1379
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.19

MIC-UNK-cdc2493e-21_3



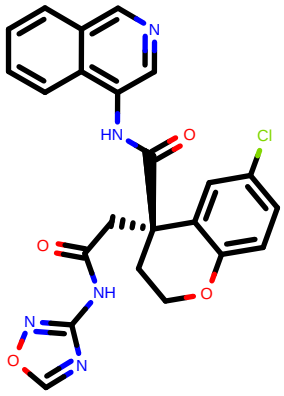
CID:	MIC-UNK-cdc2493e-21_3
SMILES:	CC(=O)N(C)[C@@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN571
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.27

EDG-MED-ba1ac7b9-26_2



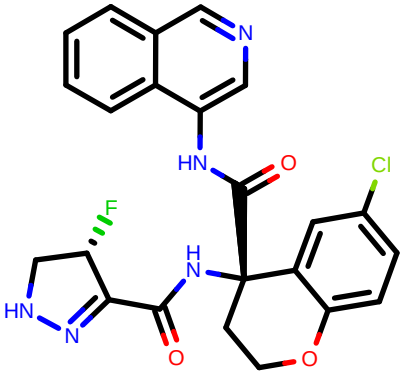
CID:	EDG-MED-ba1ac7b9-26_2
SMILES:	C[C@@H]1C[N@H+][C@H](CN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C)CCO
RUN:	RUN2721
DDG (kcal/mol):	-2.64
dDDG (kcal/mol):	0.18

KAD-UNI-cb0f2bbc-13_1



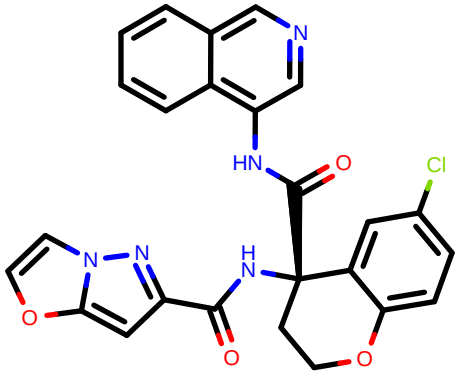
CID:	KAD-UNI-cb0f2bbc-13_1
SMILES:	Cn1c(nc2c1c(=O)[nH]c(=O)n2C)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3694
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.12

MAK-UNK-919546f0-2_2



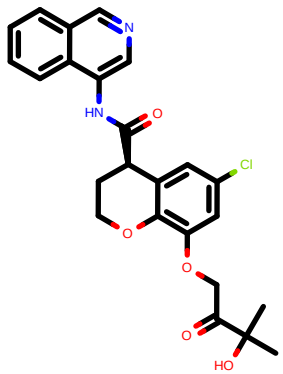
CID:	MAK-UNK-919546f0-2_2
SMILES:	c1ccc(cc1)[C@H](C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN483
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.23

EDJ-MED-841e0cf0-6_1



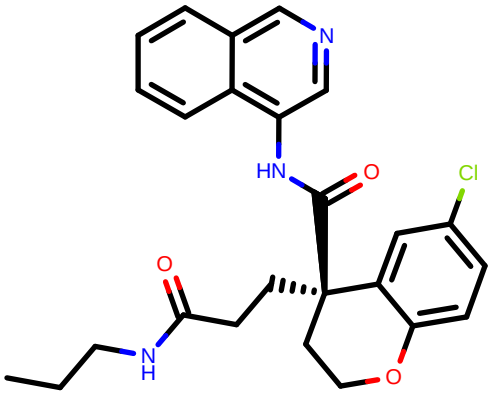
CID:	EDJ-MED-841e0cf0-6_1
SMILES:	CN(C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl
RUN:	RUN3840
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.13

ALP-POS-5bb456a5-2_6



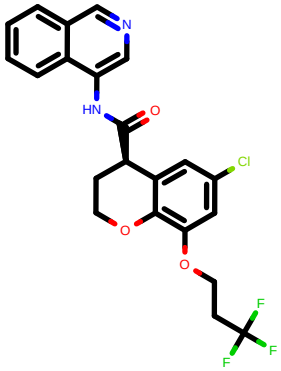
CID:	ALP-POS-5bb456a5-2_6
SMILES:	C[C@H]1C[N@@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2427
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.42

ALF-EVA-ced740bd-4_1



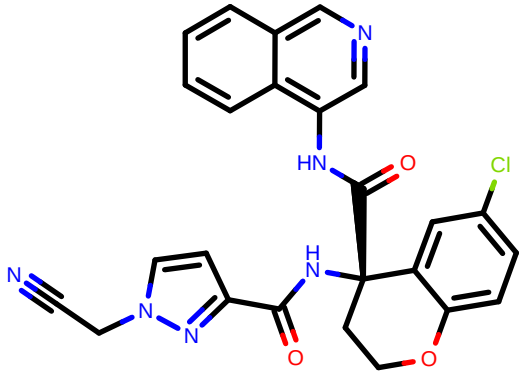
CID:	ALF-EVA-ced740bd-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3COc4c3cc(cc4)F
RUN:	RUN2795
DDG (kcal/mol):	-2.63
dDDG (kcal/mol):	0.13

ED_-GRI-5b13fbe2-35_1



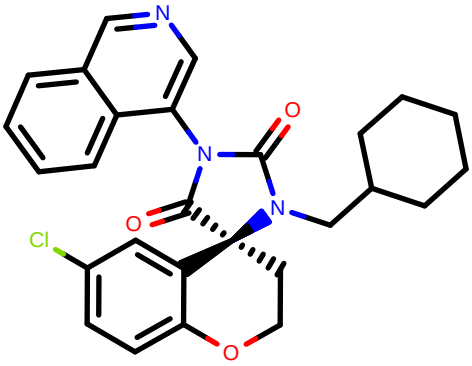
CID:	ED_-GRI-5b13fbe2-35_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5c(c(cn5)C6=CC[NH2+]CC6)N
RUN:	RUN1566
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.35

PET-UNK-5d7c542f-5_1



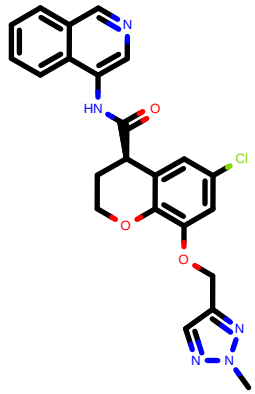
CID:	PET-UNK-5d7c542f-5_1
SMILES:	C=CS(=O)(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3858
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.14

DAR-DIA-0d514e7d-32_13



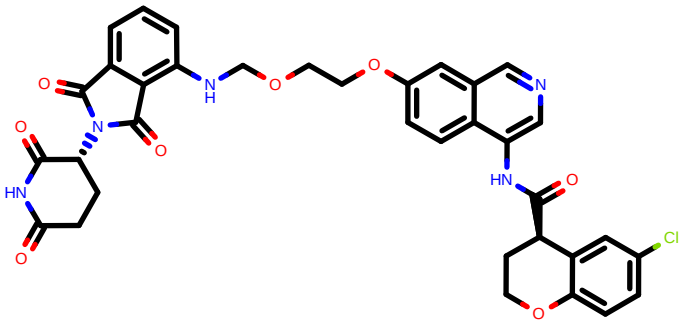
CID:	DAR-DIA-0d514e7d-32_13
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H]4C[C@H]4CO[C@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN862
DDG (kcal/mol):	-2.62
dDDG (kcal/mol):	0.23

ALF-EVA-5b152d2f-2_1



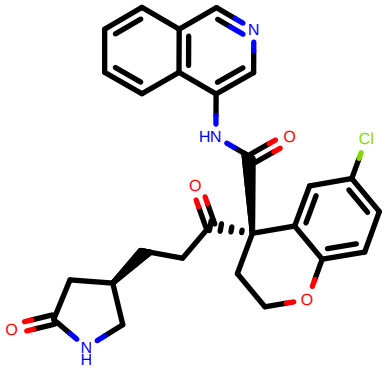
CID:	ALF-EVA-5b152d2f-2_1
SMILES:	Cc1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2357
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.30

LON-WEI-4d77710c-60_1



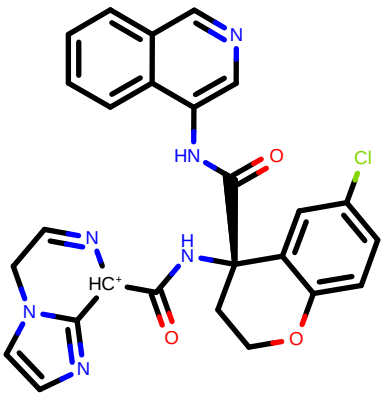
CID:	LON-WEI-4d77710c-60_1
SMILES:	CC1CC[NH+](CC1)CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN260
DDG (kcal/mol):	-2.60
dDDG (kcal/mol):	0.46

ALP-UNI-8e43a71e-2_6



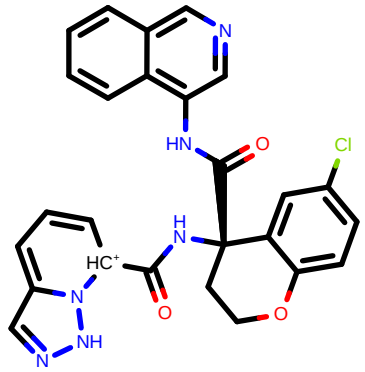
CID:	ALP-UNI-8e43a71e-2_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6[C@H]5CCC[N@@H+]6CCO
RUN:	RUN2927
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.21

MAK-UNK-c749d764-31_8



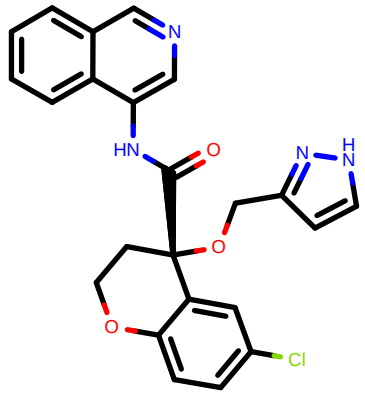
CID:	MAK-UNK-c749d764-31_8
SMILES:	CC/C=C(/c1cncc2c1cccc2)\C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1077
DDG (kcal/mol):	-2.58
dDDG (kcal/mol):	0.27

EDJ-MED-841e0cf0-4_2



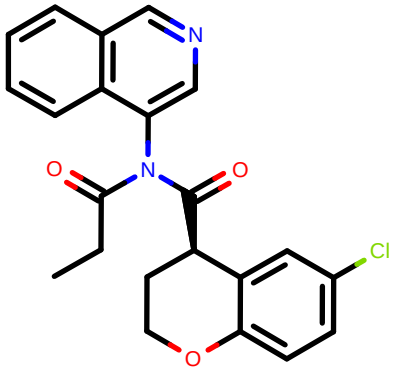
CID:	EDJ-MED-841e0cf0-4_2
SMILES:	C[C@@]1(C[N@](Cc2c1cc(cc2)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cc(cc4)S(=O)(=O)C
RUN:	RUN3834
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.17

RAL-THA-1d44ff04-2_1



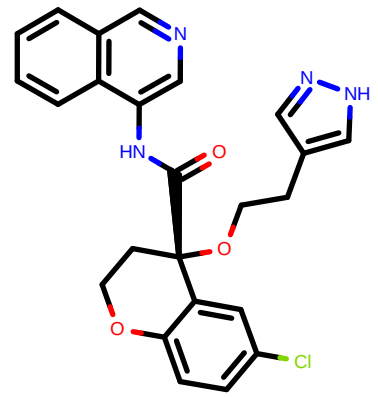
CID:	RAL-THA-1d44ff04-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCc4[nH]ncn4
RUN:	RUN436
DDG (kcal/mol):	-2.57
dDDG (kcal/mol):	0.22

MIC-UNK-5a93dd5f-3_11



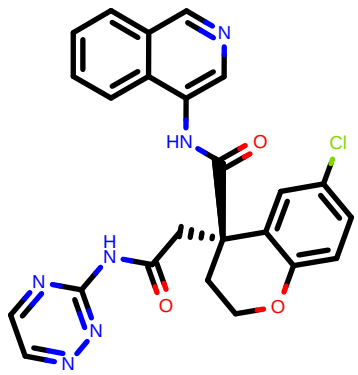
CID:	MIC-UNK-5a93dd5f-3_11
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@H+]4CC[C@@H]5CCCC[C@H]5C4
RUN:	RUN750
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.24

DAR-DIA-f6ee7aeb-4_1



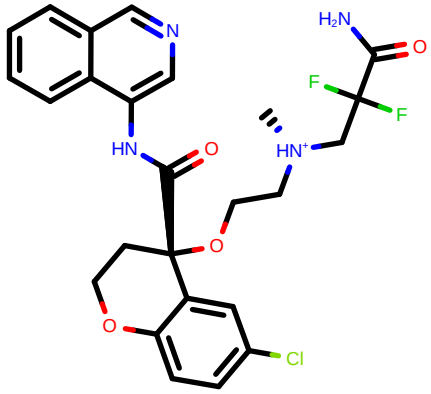
CID:	DAR-DIA-f6ee7aeb-4_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@H]([C@@H](CC3=O)c4cc(cc(c4)Cl)OCCC(F)(F)F)c5c[nH]c(=O)[nH]c5=O
RUN:	RUN3411
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-26_5



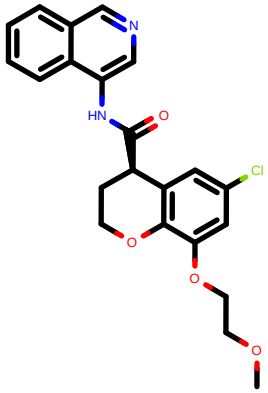
CID:	MAK-UNK-c749d764-26_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCCC[C@@H]([C@H]3O)Cl
RUN:	RUN1050
DDG (kcal/mol):	-2.56
dDDG (kcal/mol):	0.30

MIC-UNK-cdc2493e-10_2



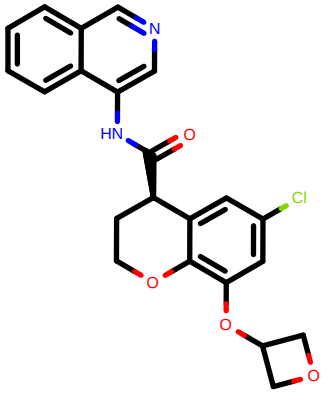
CID:	MIC-UNK-cdc2493e-10_2
SMILES:	CC(=O)N[C@H]1CC[C@@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN546
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.34

MAT-POS-1f3f1a6f-1_2



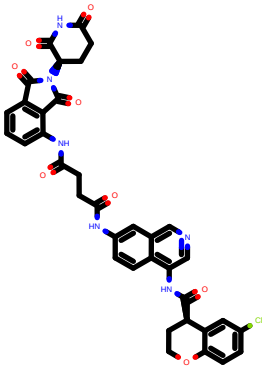
CID:	MAT-POS-1f3f1a6f-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)[NH3+]
RUN:	RUN2275
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.33

PET-UNK-c9c1e0d8-4_2



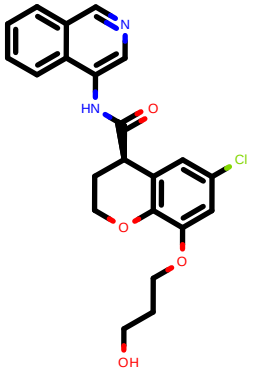
CID:	PET-UNK-c9c1e0d8-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN123
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.30

ALP-UNI-8e43a71e-5_10



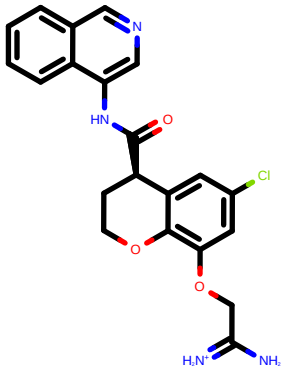
CID:	ALP-UNI-8e43a71e-5_10
SMILES:	C[C@H]1C[N@@]([CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2956
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.25

PET-UNK-c5865d42-2_2



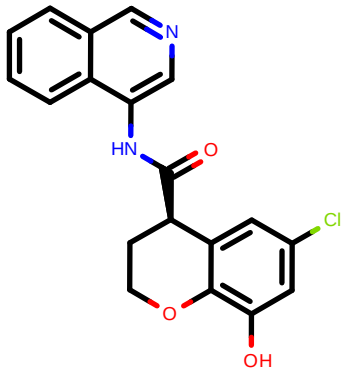
CID:	PET-UNK-c5865d42-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C([C@H]4CCN4)(F)F
RUN:	RUN429
DDG (kcal/mol):	-2.54
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-4_2



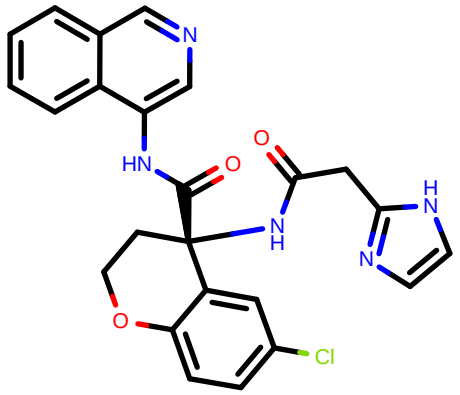
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NC6
RUN:	RUN2314
DDG (kcal/mol):	-2.53
dDDG (kcal/mol):	0.36

MIC-UNK-9582b2c5-2_5



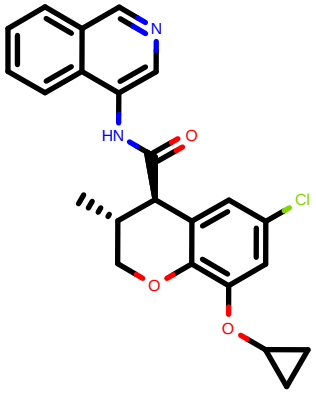
CID:	MIC-UNK-9582b2c5-2_5
SMILES:	CC(=O)N1CC[C@@H]2[C@@H](C1)C[C@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN266
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.29

MIC-UNK-bcd487e9-9_1



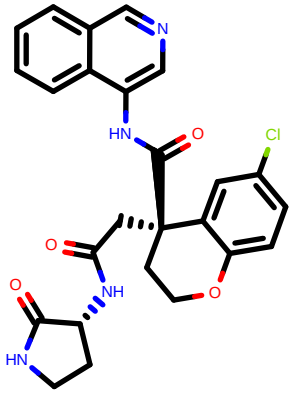
CID:	MIC-UNK-bcd487e9-9_1
SMILES:	Cn1cc(nn1)CN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN597
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.22

EDJ-MED-c314995a-1_1



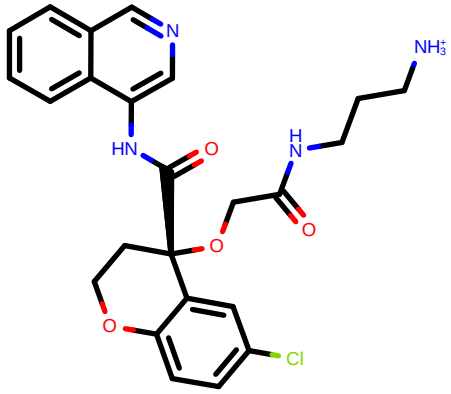
CID:	EDJ-MED-c314995a-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN126
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.25

ERI-UCB-d6de1f3c-5_1



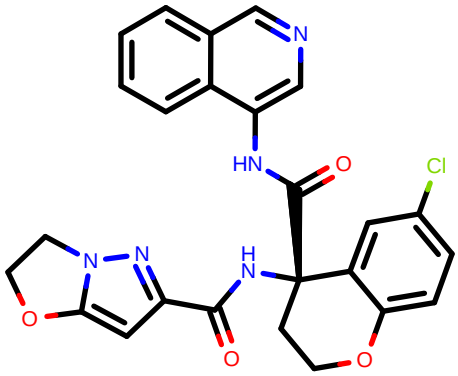
CID:	ERI-UCB-d6de1f3c-5_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N3C[C@@H](N(C(=O)C3)c4cccc(c4)Cl)CC5CCCCC5
RUN:	RUN1095
DDG (kcal/mol):	-2.51
dDDG (kcal/mol):	0.28

JAG-UCB-7b680c2b-1_1



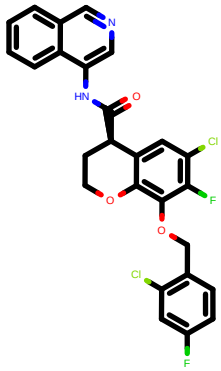
CID:	JAG-UCB-7b680c2b-1_1
SMILES:	CC(C)(C)OC(=O)NCc1cccc(c1)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN654
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.29

RAL-THA-8416115c-4_3



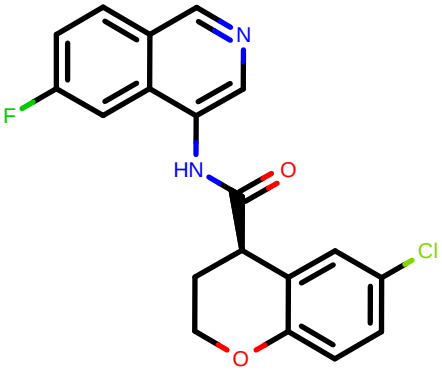
CID:	RAL-THA-8416115c-4_3
SMILES:	CCCN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1261
DDG (kcal/mol):	-2.50
dDDG (kcal/mol):	0.22

ALP-POS-ce760d3f-6_1



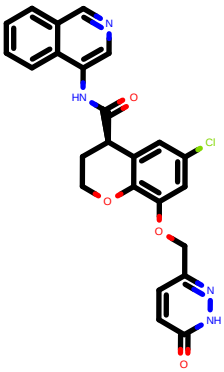
CID:	ALP-POS-ce760d3f-6_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)C3=CCOc4c3cc(cc4)Cl
RUN:	RUN1458
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.33

EDJ-MED-e4b030d8-6_1



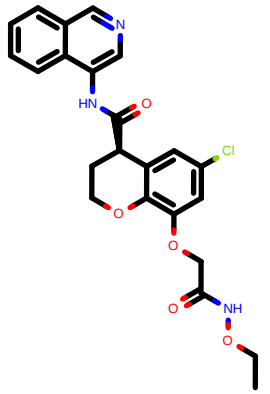
CID:	EDJ-MED-e4b030d8-6_1
SMILES:	CCC[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN288
DDG (kcal/mol):	-2.49
dDDG (kcal/mol):	0.18

EDG-MED-ba1ac7b9-13_2



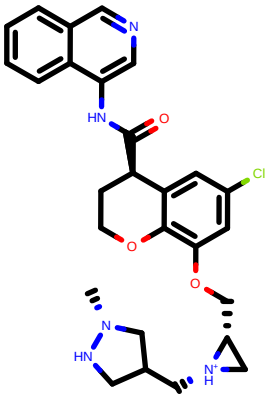
CID:	EDG-MED-ba1ac7b9-13_2
SMILES:	C[N@H+]1C[C@@H]2C[C@H]1CN2C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2663
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.31

ALP-POS-2da19ca7-6_1



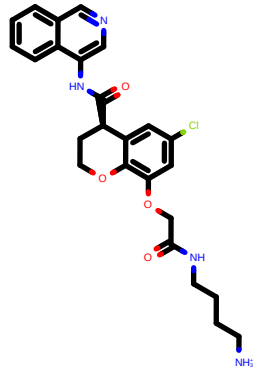
CID:	ALP-POS-2da19ca7-6_1
SMILES:	Cn1c(nnn1)C2=CCN(CC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2380
DDG (kcal/mol):	-2.48
dDDG (kcal/mol):	0.34

EDG-MED-ba1ac7b9-13_4



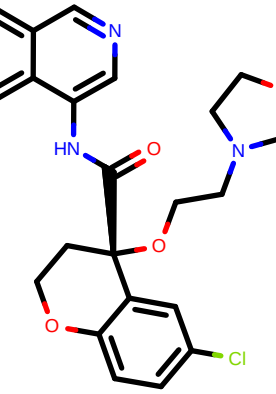
CID:	EDG-MED-ba1ac7b9-13_4
SMILES:	C[N@H+]1C[C@@H]2C[C@H]1CN2C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2665
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.50

ALP-UNI-3496895b-6_1



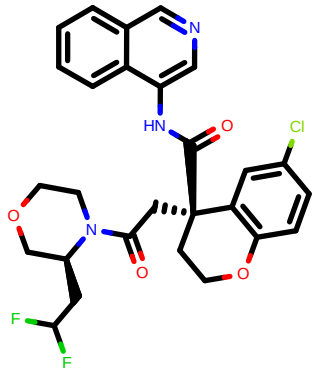
CID:	ALP-UNI-3496895b-6_1
SMILES:	CCN1CC[NH+](CC1)C2CN(C2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2520
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.40

ALP-POS-02c6a514-32_1



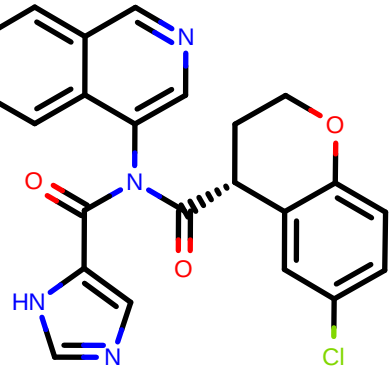
CID:	ALP-POS-02c6a514-32_1
SMILES:	CC(C)(C)c1ccc(cc1)N([C@@H](c2cncc3c2cccc3)C(=O)NCCc4cccc(c4)F)C(=O)c5ccco5
RUN:	RUN644
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.32

RAL-THA-4aa06b95-3_1



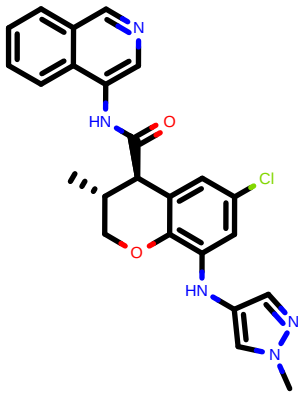
CID:	RAL-THA-4aa06b95-3_1
SMILES:	CNC(=O)N1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1232
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.29

MAT-POS-3b92565d-8_1



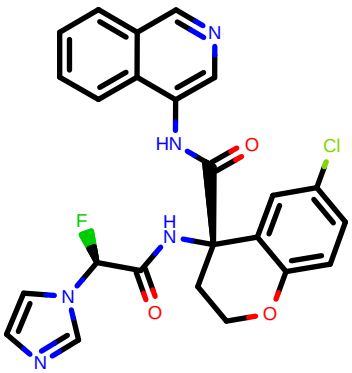
CID:	MAT-POS-3b92565d-8_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Cc3cc(cc(c3)Cl)OC
RUN:	RUN115
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.36

MIC-UNK-c66144cb-2_2



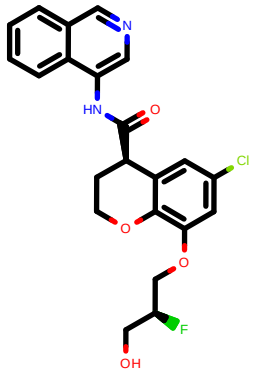
CID:	MIC-UNK-c66144cb-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3ccc(cc3)F)c4cccc(c4)Cl
RUN:	RUN131
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.30

MAK-UNK-8be7dca9-8_1



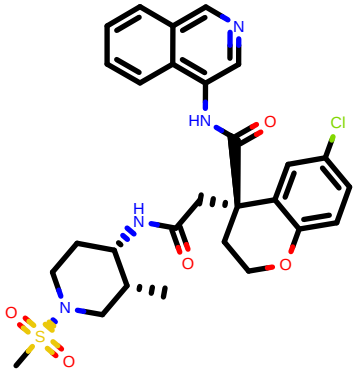
CID:	MAK-UNK-8be7dca9-8_1
SMILES:	c1cc2cncc(c2cc1CC(=O)[O-])NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN507
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.27

ALP-UNI-0676e700-10_1



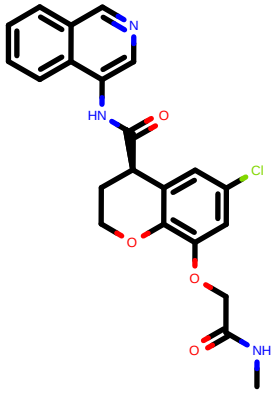
CID:	ALP-UNI-0676e700-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc6nnnn6c5
RUN:	RUN2453
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.40

MAK-UNK-c749d764-2_8



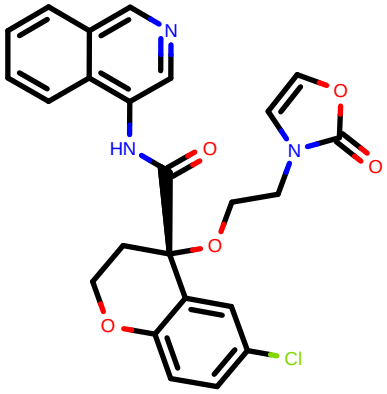
CID:	MAK-UNK-c749d764-2_8
SMILES:	CC[C@H]1CCC[C@H]([C@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN904
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.44

KAD-UNI-80f122c8-3_5



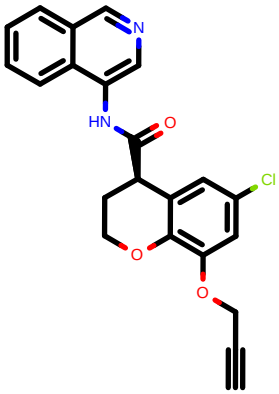
CID:	KAD-UNI-80f122c8-3_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6CS(=O)(=O)C[C@H]6C5
RUN:	RUN2293
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.28

NIR-THE-af15c15d-1_1



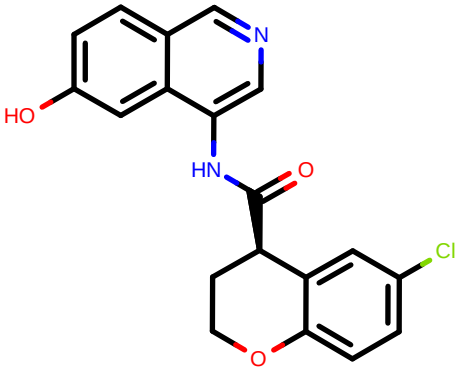
CID:	NIR-THE-af15c15d-1_1
SMILES:	CC#CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN3319
DDG (kcal/mol):	-2.46
dDDG (kcal/mol):	0.16

MAT-POS-e9e99895-3_1



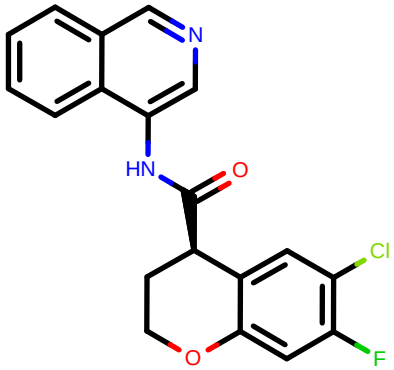
CID:	MAT-POS-e9e99895-3_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CCC(=O)NC4
RUN:	RUN2243
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.28

MAT-POS-f7918075-1_2



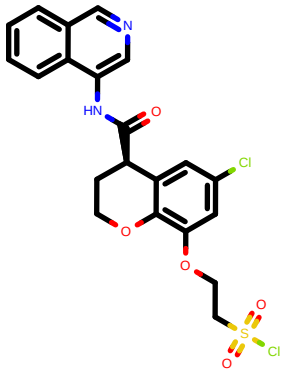
CID:	MAT-POS-f7918075-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN190
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.20

ED_-GRI-5b13fbe2-16_2



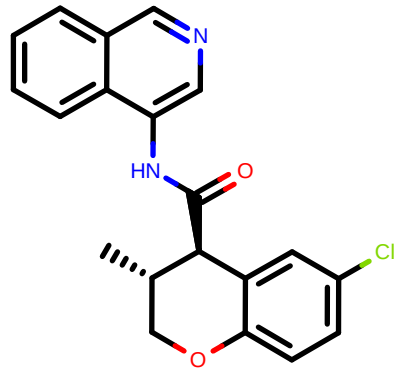
CID:	ED_-GRI-5b13fbe2-16_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5cn(nn5)CC6CC6)[NH3+]
RUN:	RUN1546
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.19

KAD-UNI-80f122c8-3_3



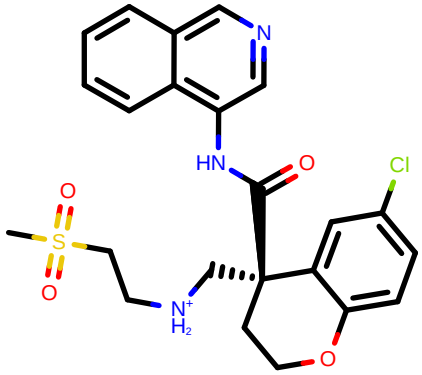
CID:	KAD-UNI-80f122c8-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN2289
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.37

DAR-DIA-0cde14eb-47_1



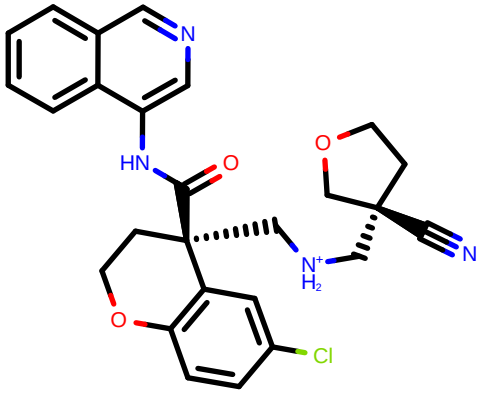
CID:	DAR-DIA-0cde14eb-47_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)C4(CC4)Cl
RUN:	RUN11
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.20

RAL-THA-b00e3cbf-1_1



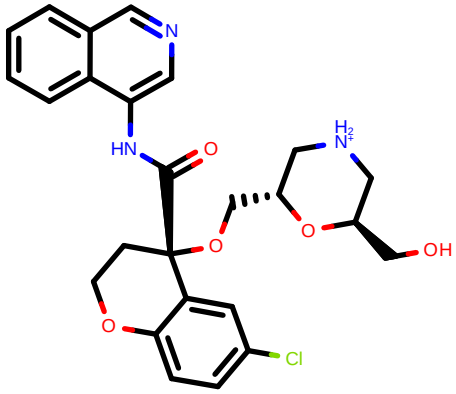
CID:	RAL-THA-b00e3cbf-1_1
SMILES:	c1ccc2c(c1)c(cnc2C#N)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN4177
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.21

DAR-DIA-076fb6ea-3_1



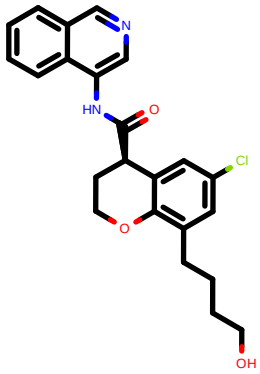
CID:	DAR-DIA-076fb6ea-3_1
SMILES:	COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1403
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.22

DAR-DIA-6a508060-3_1



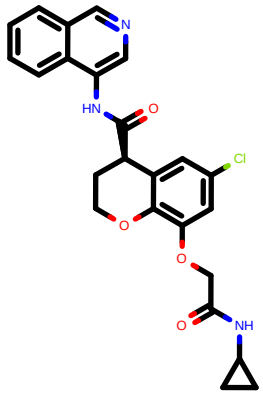
CID:	DAR-DIA-6a508060-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C#N
RUN:	RUN336
DDG (kcal/mol):	-2.45
dDDG (kcal/mol):	0.32

MAT-POS-afd4d4fd-3_1



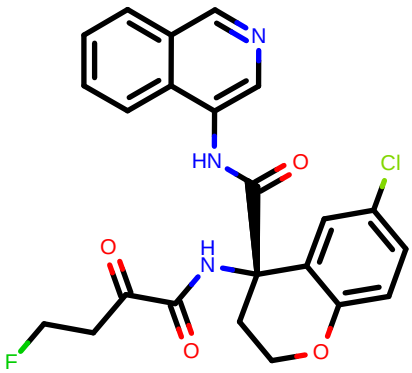
CID:	MAT-POS-afd4d4fd-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3Cl)Cl
RUN:	RUN305
DDG (kcal/mol):	-2.44
dDDG (kcal/mol):	0.33

ALP-POS-2da19ca7-7_8



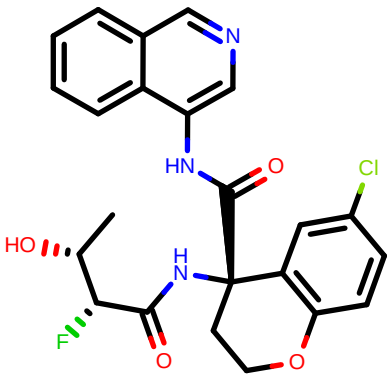
CID:	ALP-POS-2da19ca7-7_8
SMILES:	C[C@H]1C[N@](CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2392
DDG (kcal/mol):	-2.44
dDDG (kcal/mol):	0.34

MIC-UNK-cdc2493e-8_2



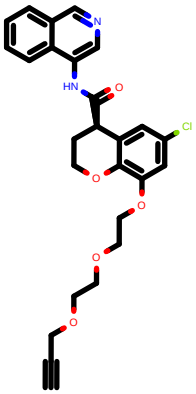
CID:	MIC-UNK-cdc2493e-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3Cl)[C@H]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN538
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.27

MAK-UNK-8be7dca9-7_1



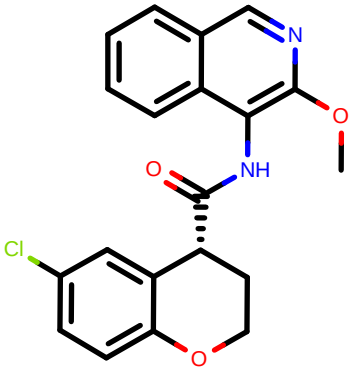
CID:	MAK-UNK-8be7dca9-7_1
SMILES:	c1cc2cncc(c2cc1C(=O)[O-])NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN503
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.24

ALP-UNI-3496895b-1_1



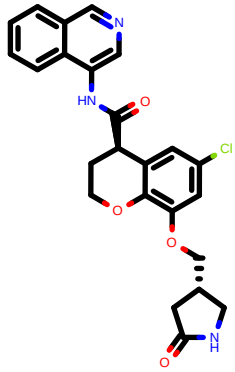
CID:	ALP-UNI-3496895b-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)(=O)N[C@@]6[C@@H]5CCCC6
RUN:	RUN2499
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.49

LON-WEI-4d77710c-15_1



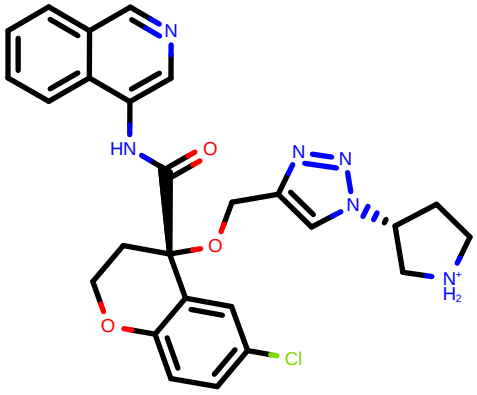
CID:	LON-WEI-4d77710c-15_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCCN3CCCC3=O
RUN:	RUN206
DDG (kcal/mol):	-2.43
dDDG (kcal/mol):	0.25

MAT-POS-fce787c2-8_2



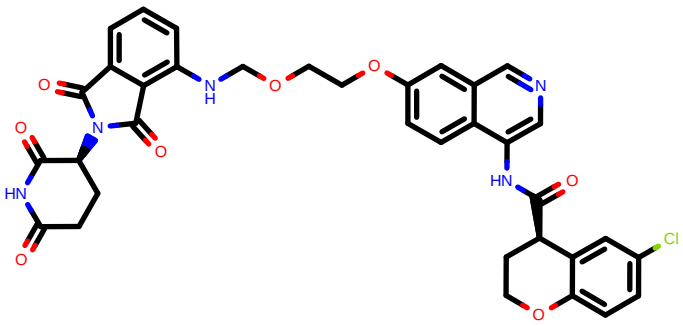
CID:	MAT-POS-fce787c2-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](C#N)c3ccc(c(c3)Cl)Cl
RUN:	RUN2155
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.35

MIC-UNK-cdc2493e-8_4



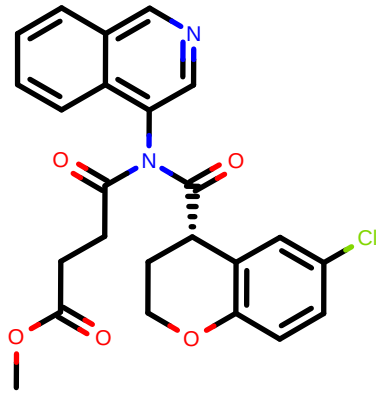
CID:	MIC-UNK-cdc2493e-8_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@H]4CC[C@H]5CCCC[C@@H]5C4
RUN:	RUN537
DDG (kcal/mol):	-2.42
dDDG (kcal/mol):	0.29

PET-UNK-1901c25b-1_1



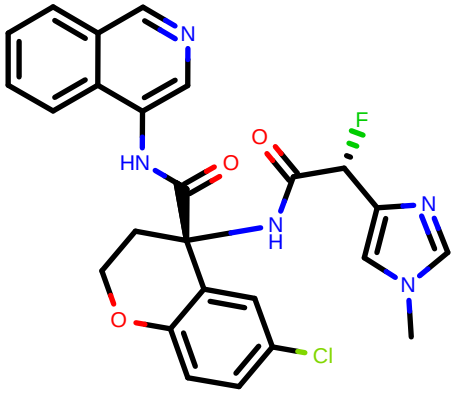
CID:	PET-UNK-1901c25b-1_1
SMILES:	CN(C)c1ccc(cc1)N(Cc2ccsc2)C(=O)Cc3cncc4c3cccc4
RUN:	RUN302
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.46

MAT-POS-96f51285-5_1



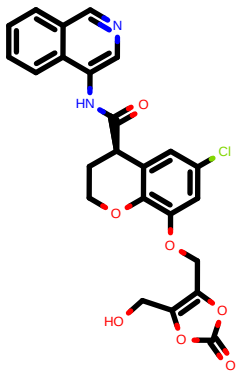
CID:	MAT-POS-96f51285-5_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(c(c4)F)Cl
RUN:	RUN3931
DDG (kcal/mol):	-2.41
dDDG (kcal/mol):	0.29

MAK-UNK-8be7dca9-2_1



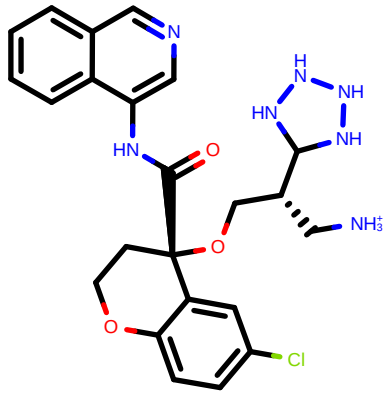
CID:	MAK-UNK-8be7dca9-2_1
SMILES:	c1cc2c(cc1CC(=O)N)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN492
DDG (kcal/mol):	-2.40
dDDG (kcal/mol):	0.28

EDJ-MED-d203f206-16_1



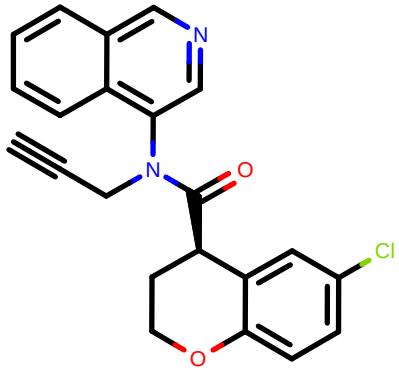
CID:	EDJ-MED-d203f206-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5c6n[n-]nn6
RUN:	RUN2578
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.31

ALP-UNI-8e43a71e-15_24



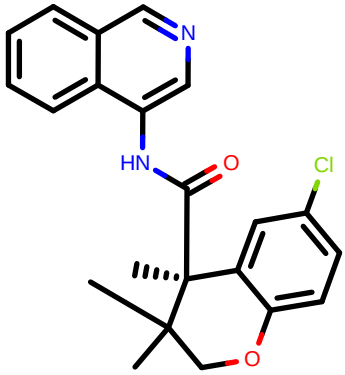
CID:	ALP-UNI-8e43a71e-15_24
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN3005
DDG (kcal/mol):	-2.39
dDDG (kcal/mol):	0.19

DAR-DIA-ecdbc7dd-12_1



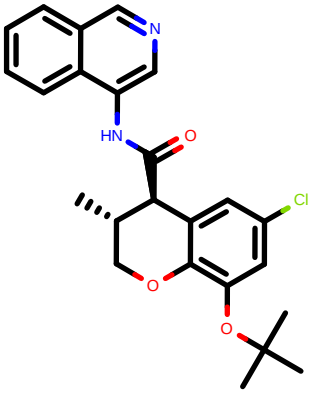
CID:	DAR-DIA-ecdbc7dd-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCNc4c3cc(cc4)Cl)C[NH+]5CCCCC5
RUN:	RUN2894
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.10

DAR-DIA-53551c05-6_1



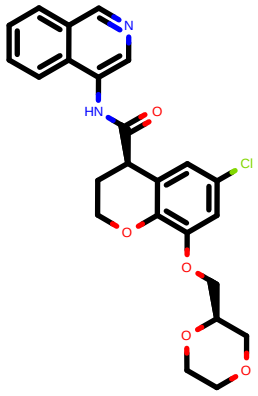
CID:	DAR-DIA-53551c05-6_1
SMILES:	c1ccc2c(c1)cncc2CN3c4ccccc4C(=O)C3=O
RUN:	RUN140
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.21

NIR-WEI-f9286bb6-1_2



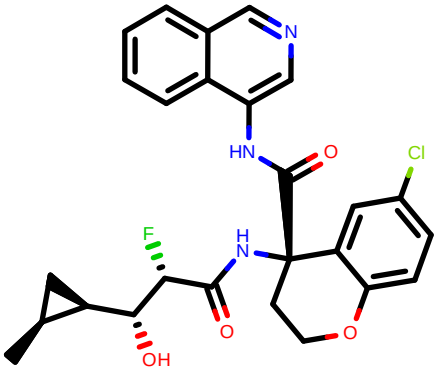
CID:	NIR-WEI-f9286bb6-1_2
SMILES:	CNC(=O)[C@H](c1cncc2c1cccc2)N(Cc3ccccc3Cl)C(=O)C=C
RUN:	RUN137
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.31

KAD-UNI-8a629cb0-20_1



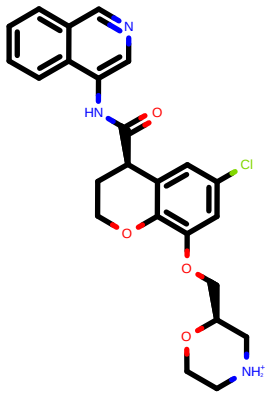
CID:	KAD-UNI-8a629cb0-20_1
SMILES:	C[C@@H](C(=O)N1CCC(CC1)C(=O)N)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2103
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.42

MAK-UNK-ffc90da7-2_2



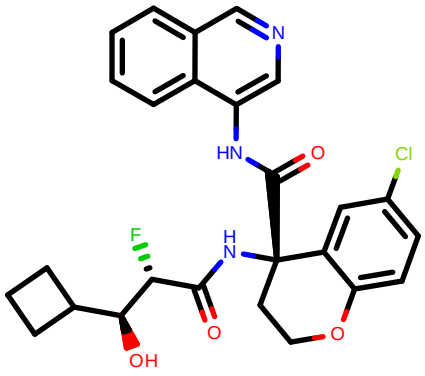
CID:	MAK-UNK-ffc90da7-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@@H]([C@@H]3O)Cl
RUN:	RUN682
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.29

DAR-DIA-6be260fc-1_1



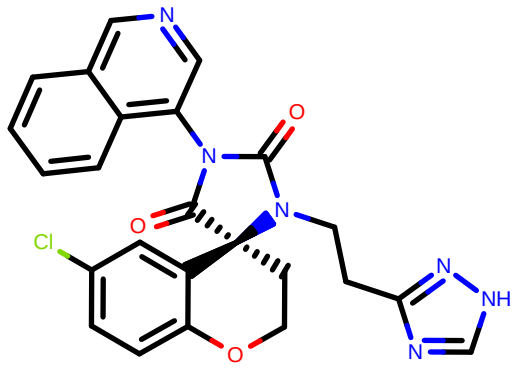
CID:	DAR-DIA-6be260fc-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNc5c4cc(cc5)Cl
RUN:	RUN2127
DDG (kcal/mol):	-2.37
dDDG (kcal/mol):	0.35

VLA-UCB-34f3ed0c-1_1



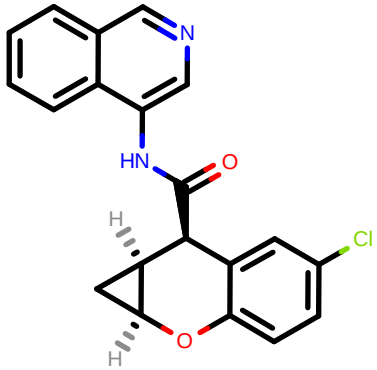
CID:	VLA-UCB-34f3ed0c-1_1
SMILES:	C=C(C#N)C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN627
DDG (kcal/mol):	-2.37
dDDG (kcal/mol):	0.29

MIC-UNK-0a05c952-3_1



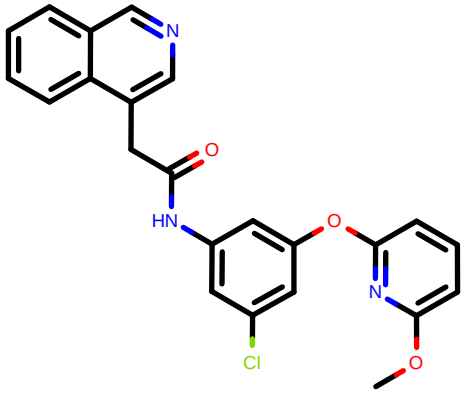
CID:	MIC-UNK-0a05c952-3_1
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](C[C@@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@@H]5CO5
RUN:	RUN3513
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.17

PET-UNK-8df914d1-1_1



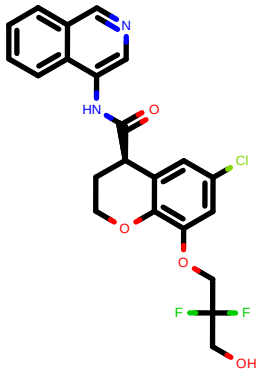
CID:	PET-UNK-8df914d1-1_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN139
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.14

ERI-UCB-fbdd3ea1-27_2



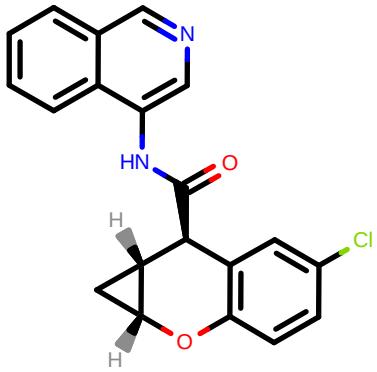
CID:	ERI-UCB-fbdd3ea1-27_2
SMILES:	CC(C)(C)c1cc(no1)N([C@H](c2cncc3c2cccc3)C(=O)NC(C)(C)C)C(=O)C=C
RUN:	RUN6
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.32

VLA-UNK-83c3754c-1_1



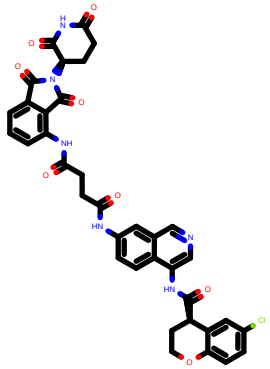
CID:	VLA-UNK-83c3754c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(COc5c4cc(cc5)Cl)NC3=O
RUN:	RUN2320
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.37

LON-WEI-4d77710c-59_1



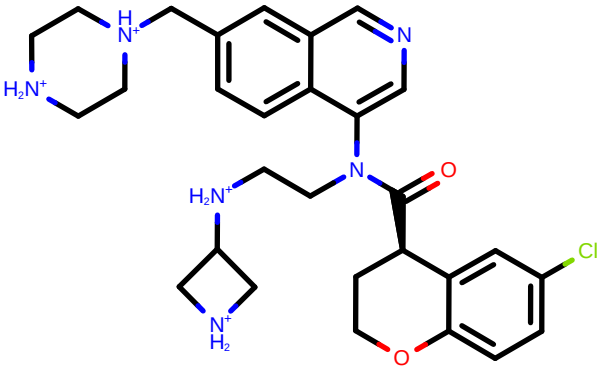
CID:	LON-WEI-4d77710c-59_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N(Cc3ccco3)C[C@@H]4CCCO4
RUN:	RUN251
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.13

ALP-POS-477dc5b7-1_1



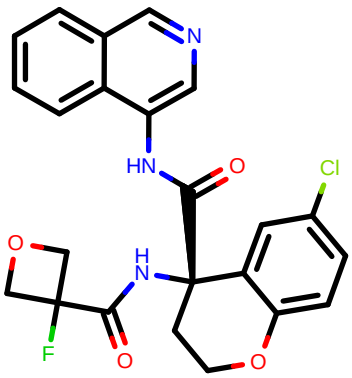
CID:	ALP-POS-477dc5b7-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCCc4c3cc(cc4)Cl
RUN:	RUN294
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.49

ALP-UNI-b33a865d-1_1



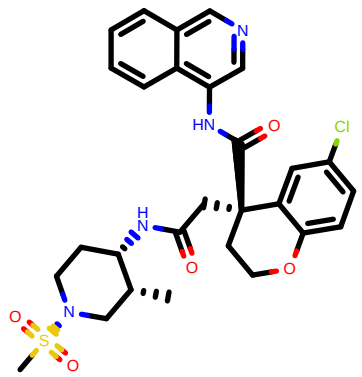
CID:	ALP-UNI-b33a865d-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN354
DDG (kcal/mol):	-2.36
dDDG (kcal/mol):	0.56

MIC-UNK-cdc2493e-14_1



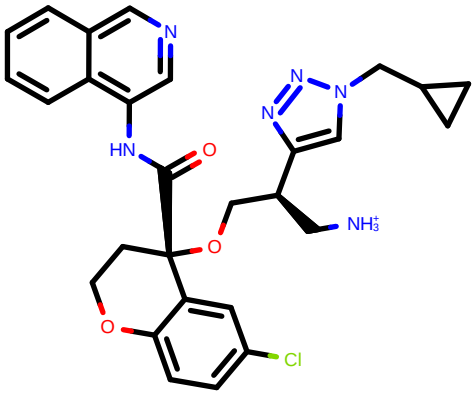
CID:	MIC-UNK-cdc2493e-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@@H](C4)[NH+]5CCCCC5
RUN:	RUN554
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.26

ALP-POS-a0a4abd7-3_2



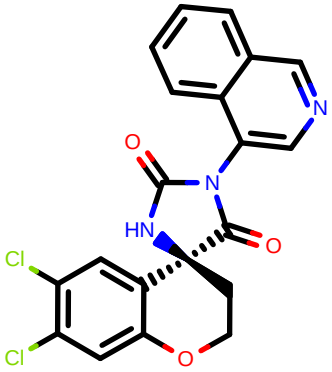
CID:	ALP-POS-a0a4abd7-3_2
SMILES:	Cn1c(=O)c(c[nH]c1=O)NC[C@]2(CCOc3c2ccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3570
DDG (kcal/mol):	-2.34
dDDG (kcal/mol):	0.25

MIC-UNK-cdc2493e-2_1



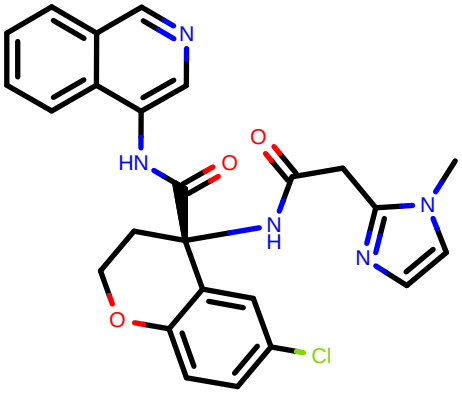
CID:	MIC-UNK-cdc2493e-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CC[C@@H]3CCCO3)c4cccc(c4)Cl
RUN:	RUN522
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-4_1



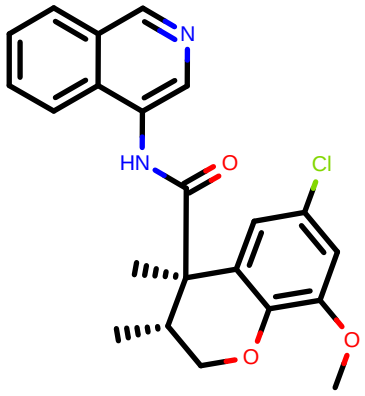
CID:	DAR-DIA-0d514e7d-4_1
SMILES:	C[C@H]1COc2c(cc(cc2OC3CCCC3)Cl)[C@@H]1C(=O)Nc4cncc5c4cccc5
RUN:	RUN808
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.23

MAK-UNK-8be7dca9-4_1



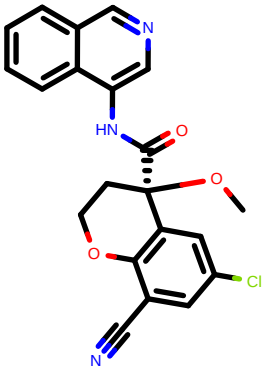
CID:	MAK-UNK-8be7dca9-4_1
SMILES:	c1cc2cncc(c2cc1N3CC[NH2+]CC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN502
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.22

VLA-UCB-1dbca3b4-18_1



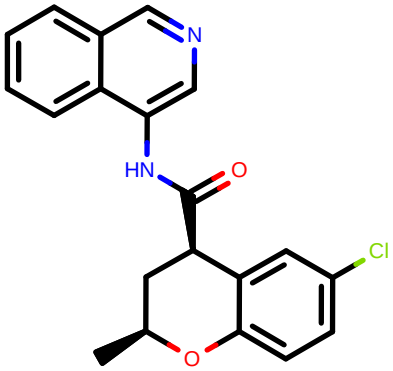
CID:	VLA-UCB-1dbca3b4-18_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@H](CNC3=O)c4cccc(c4)Cl
RUN:	RUN174
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.22

VLA-UCB-29506327-1_1



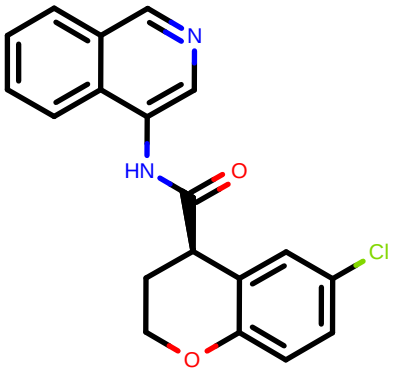
CID:	VLA-UCB-29506327-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1404
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.09

MIC-UNK-d36ab305-1_2



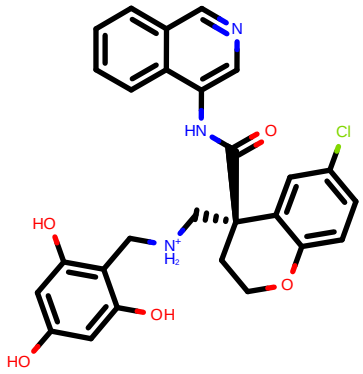
CID:	MIC-UNK-d36ab305-1_2
SMILES:	CC(=O)Nc1ccc(cc1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN152
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.18

ERI-UCB-ce40166b-9_1



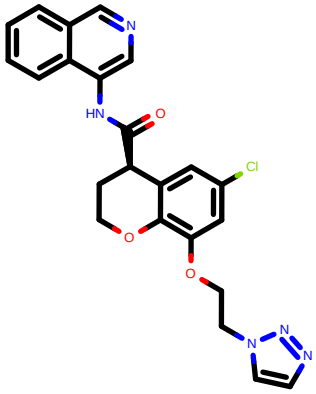
CID:	ERI-UCB-ce40166b-9_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)O[C@@H]4CC(=O)N4)C#N
RUN:	RUN45
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.19

EDG-MED-90036822-79_1



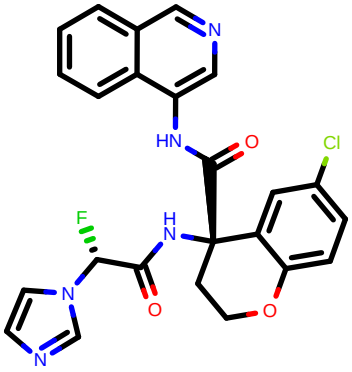
CID:	EDG-MED-90036822-79_1
SMILES:	Cc1c(c(n[nH]1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F
RUN:	RUN1776
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.37

ALF-EVA-5b152d2f-6_1



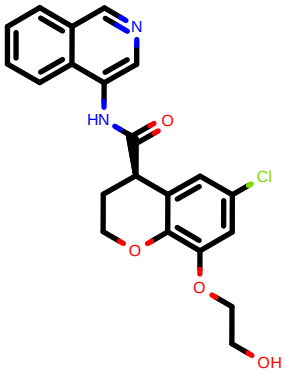
CID:	ALF-EVA-5b152d2f-6_1
SMILES:	C[C@H]1CCOc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN2359
DDG (kcal/mol):	-2.31
dDDG (kcal/mol):	0.35

MIC-UNK-cdc2493e-10_4



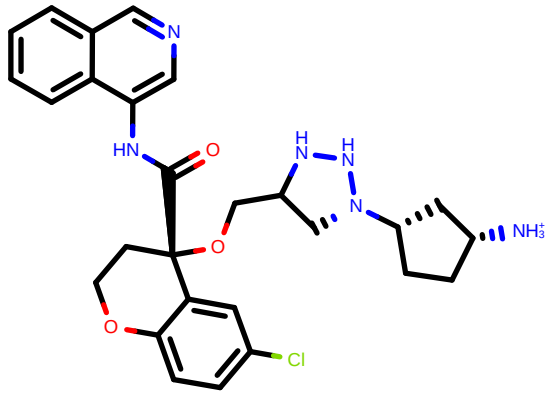
CID:	MIC-UNK-cdc2493e-10_4
SMILES:	CC(=O)N[C@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN548
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.27

MAT-POS-e9e99895-2_7



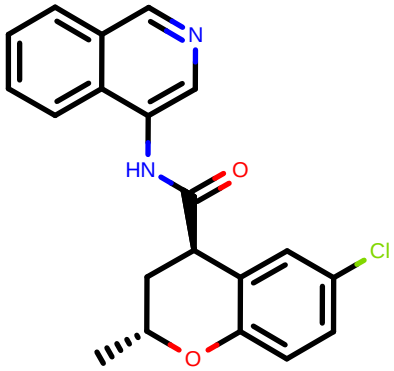
CID:	MAT-POS-e9e99895-2_7
SMILES:	CC(C)[N@@H+]1CCO[C@H](C1)C(=O)N[C@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2241
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.40

MIC-UNK-91acba05-5_2



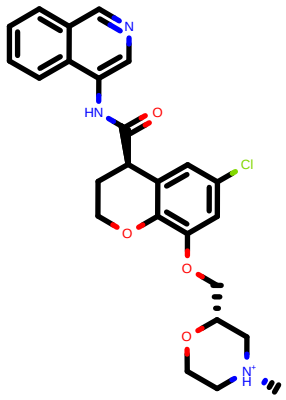
CID:	MIC-UNK-91acba05-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN477
DDG (kcal/mol):	-2.30
dDDG (kcal/mol):	0.35

VLA-UCB-1dbca3b4-3_1



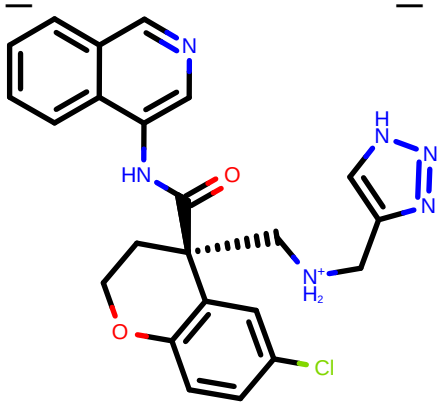
CID:	VLA-UCB-1dbca3b4-3_1
SMILES:	c1ccc2c(c1)cncc2n3c(cn(c3=O)c4cccc(c4)Cl)[O-]
RUN:	RUN153
DDG (kcal/mol):	-2.29
dDDG (kcal/mol):	0.20

LEE-CAM-7ab9b158-1_1



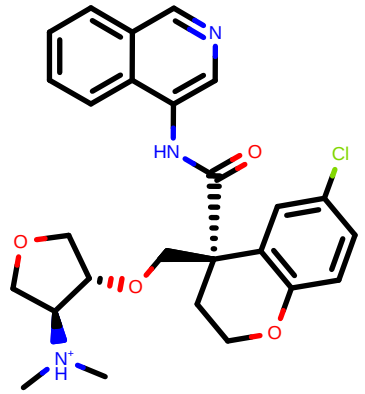
CID:	LEE-CAM-7ab9b158-1_1
SMILES:	C[NH+](C)[C@@H]1COC[C@@H]1OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2199
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.35

ED_-GRI-5b13fbe2-74_1



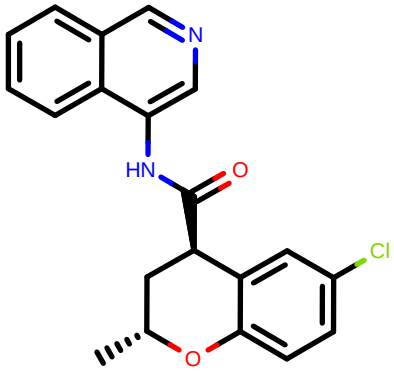
CID:	ED_-GRI-5b13fbe2-74_1
SMILES:	C[N@@H+]1CCO[C@@H](C1)c2nccc(n2)CO[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN1631
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.43

DAR-DIA-0d514e7d-31_10



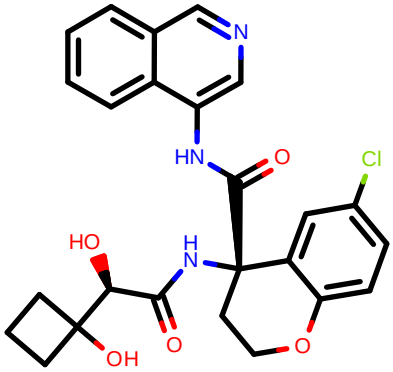
CID:	DAR-DIA-0d514e7d-31_10
SMILES:	C[C@H]1CCO[C@@H]2C=CC(=C[C@@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN842
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.23

ADA-UCB-6c2cb422-1_1



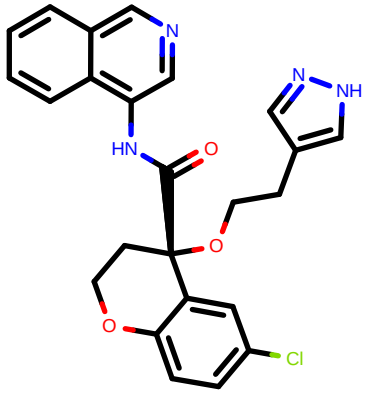
CID:	ADA-UCB-6c2cb422-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN53
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-29_7



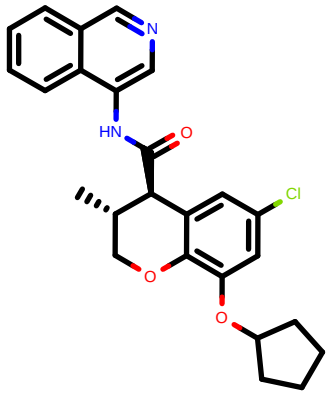
CID:	MAK-UNK-c749d764-29_7
SMILES:	c1ccc2c(c1)cncc2N(C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F)C(=O)ON
RUN:	RUN1071
DDG (kcal/mol):	-2.28
dDDG (kcal/mol):	0.27

EDJ-MED-ee07cf00-11_4



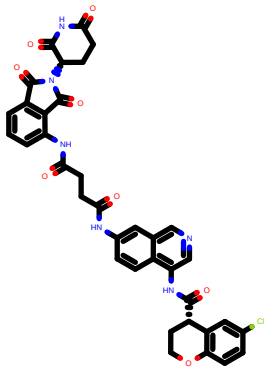
CID:	EDJ-MED-ee07cf00-11_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN2828
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.18

PET-UNK-c9c1e0d8-1_1



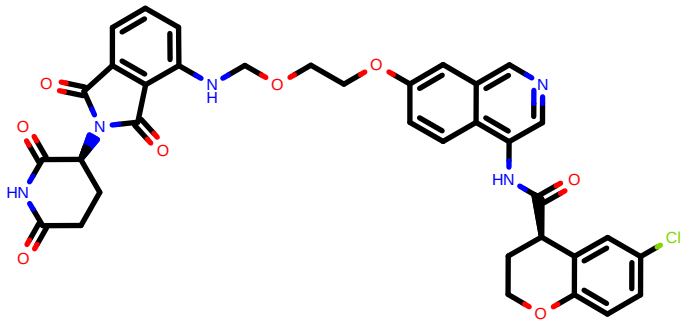
CID:	PET-UNK-c9c1e0d8-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Br
RUN:	RUN119
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.29

ALP-UNI-8e43a71e-7_2



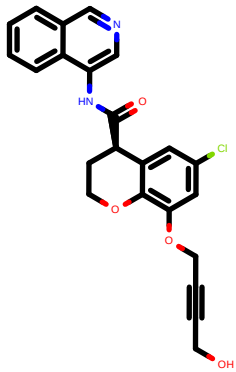
CID:	ALP-UNI-8e43a71e-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)CCC#N
RUN:	RUN2963
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.40

MAK-UNK-f481d203-4_1



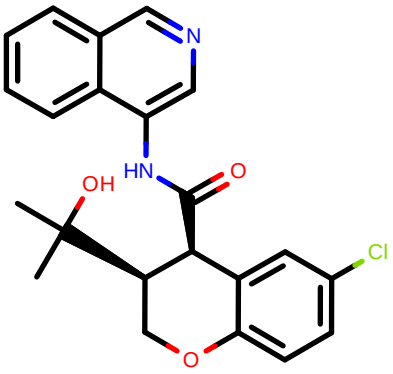
CID:	MAK-UNK-f481d203-4_1
SMILES:	c1ccc(cc1)[C@@H](C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN488
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.39

JOH-UNI-ea72002d-4_4



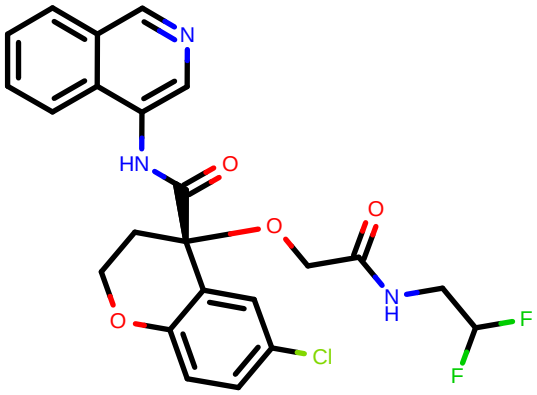
CID:	JOH-UNI-ea72002d-4_4
SMILES:	c1ccc2c(c1)cncc2[C@](C(=O)[C@H]3CCOc4c3cc(cc4)Cl)(N5C(=O)C=CC5=O)F
RUN:	RUN2491
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.35

VLA-UCB-1dbca3b4-18_2



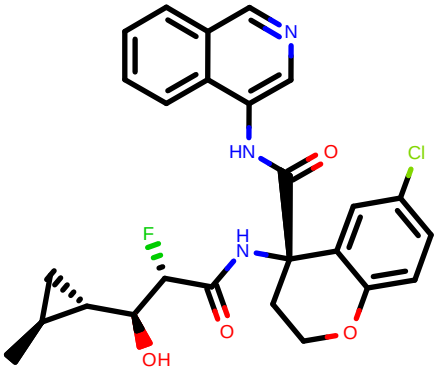
CID:	VLA-UCB-1dbca3b4-18_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@H](CNC3=O)c4cccc(c4)Cl
RUN:	RUN175
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.14

MAK-UNK-ffc90da7-9_2



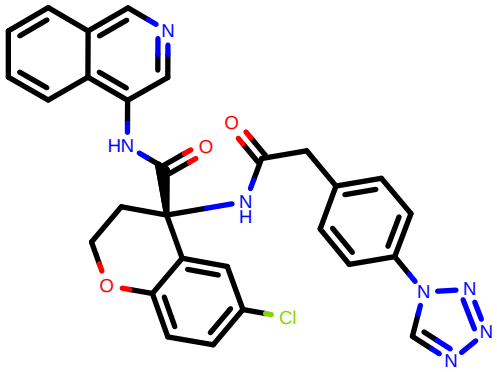
CID:	MAK-UNK-ffc90da7-9_2
SMILES:	C[C@H]1[C@@H](CCO1)SC[C@@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN710
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.27

DAR-DIA-0d514e7d-32_32



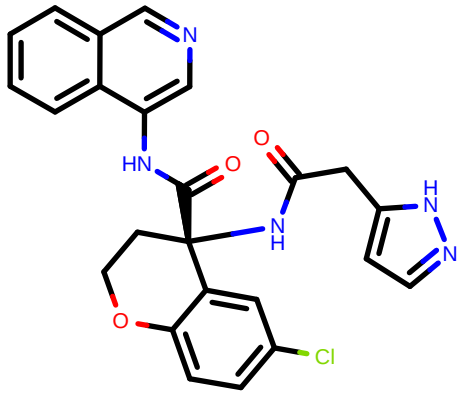
CID:	DAR-DIA-0d514e7d-32_32
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@H]4C[C@H]4CO[C@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN882
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.25

RAL-THA-8416115c-7_4



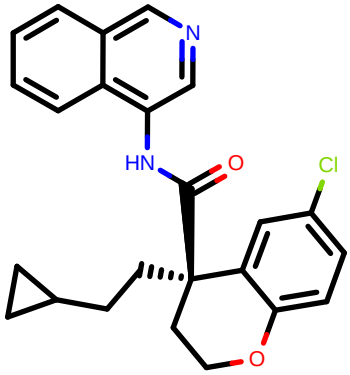
CID:	RAL-THA-8416115c-7_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)CC(=O)[O-]
RUN:	RUN1274
DDG (kcal/mol):	-2.26
dDDG (kcal/mol):	0.40

EDJ-MED-e4b030d8-7_1



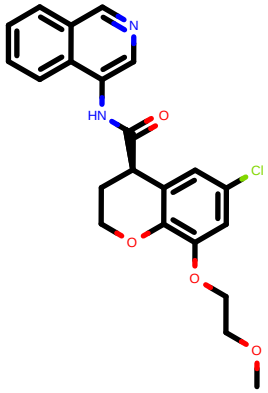
CID:	EDJ-MED-e4b030d8-7_1
SMILES:	COc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN289
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.31

EDG-MED-ba1ac7b9-22_2



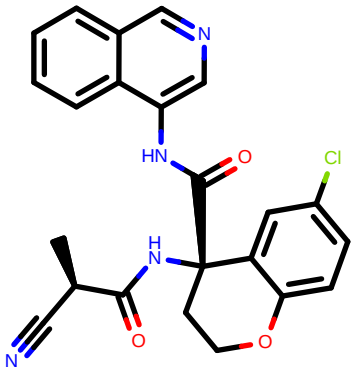
CID:	EDG-MED-ba1ac7b9-22_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5Cc6c(nc[nH]6)C[C@@H]5C(=O)N
RUN:	RUN2703
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.10

DAR-DIA-9e4459de-15_6



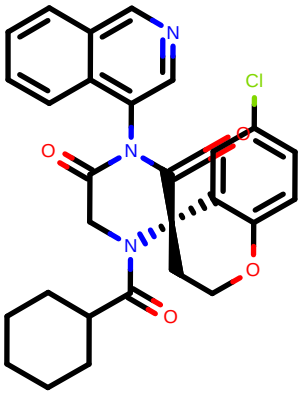
CID:	DAR-DIA-9e4459de-15_6
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1448
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.37

ADA-UCB-dc2b944c-13_1



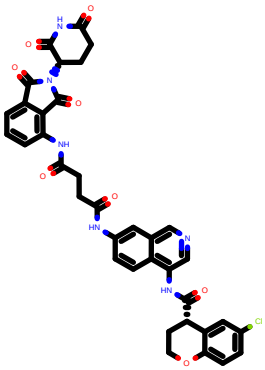
CID:	ADA-UCB-dc2b944c-13_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN611
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.28

EDJ-MED-ee07cf00-3_1



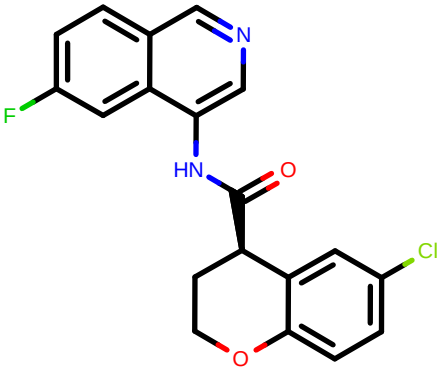
CID:	EDJ-MED-ee07cf00-3_1
SMILES:	Cn1c2c(cn1)c(=O)n(cn2)CC(=O)N[C@@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2805
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.23

ALP-POS-fe871b40-14_1



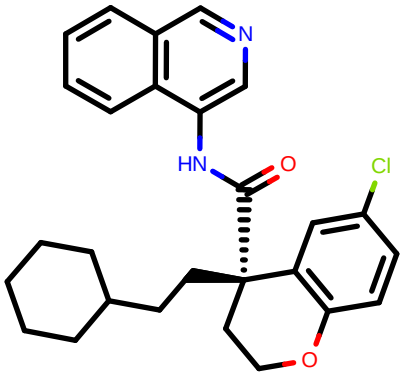
CID:	ALP-POS-fe871b40-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cn4)Cl
RUN:	RUN3133
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.49

PET-UNK-431b3bfb-1_1



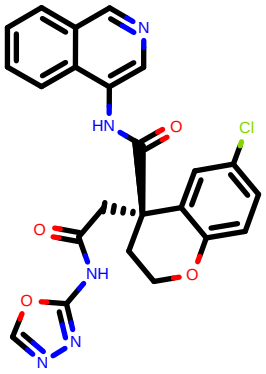
CID:	PET-UNK-431b3bfb-1_1
SMILES:	c1ccc2c(c1)cncc2N3CCO[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN271
DDG (kcal/mol):	-2.25
dDDG (kcal/mol):	0.19

LON-WEI-4d77710c-42_1



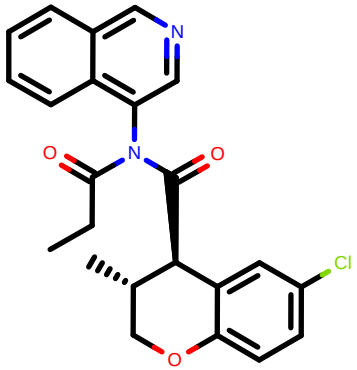
CID:	LON-WEI-4d77710c-42_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N[C@@H]3CCCc4c3cccc4
RUN:	RUN229
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.22

MAK-UNK-c749d764-22_3



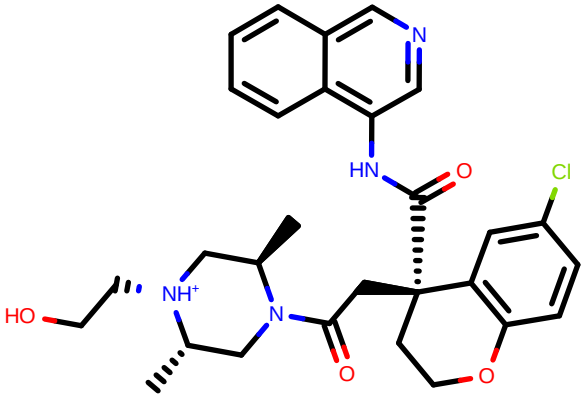
CID:	MAK-UNK-c749d764-22_3
SMILES:	C[C@@H](C[NH2+]C[C@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1024
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.30

LON-WEI-4d77710c-31_1



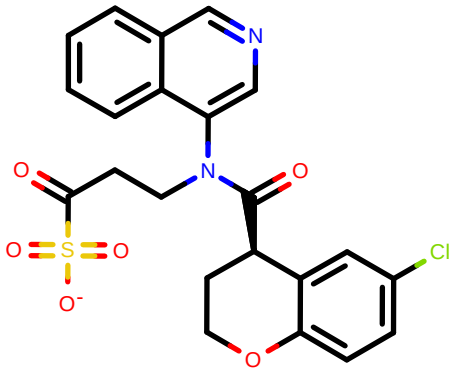
CID:	LON-WEI-4d77710c-31_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccsc3
RUN:	RUN212
DDG (kcal/mol):	-2.23
dDDG (kcal/mol):	0.24

EDJ-MED-670ad2ee-1_2



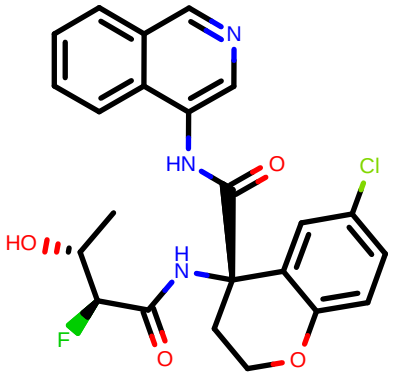
CID:	EDJ-MED-670ad2ee-1_2
SMILES:	CO[C@]1(C[N@](Cc2c1cc(c(c2)Cl)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3860
DDG (kcal/mol):	-2.22
dDDG (kcal/mol):	0.33

DAR-DIA-5ff57136-15_1



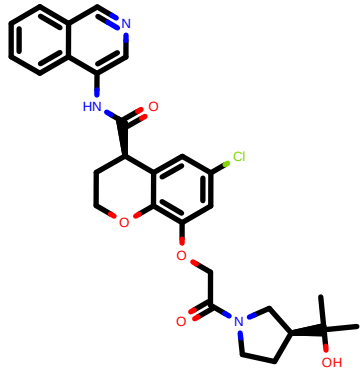
CID:	DAR-DIA-5ff57136-15_1
SMILES:	C#CC1(CC1)N(c2cncc3c2cccc3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN1384
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.45

VLA-UCB-34f3ed0c-14_1



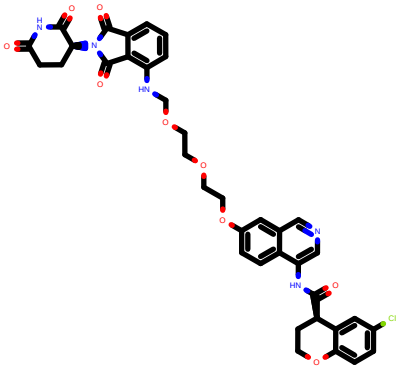
CID:	VLA-UCB-34f3ed0c-14_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN636
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.27

ALP-POS-5bb456a5-2_5



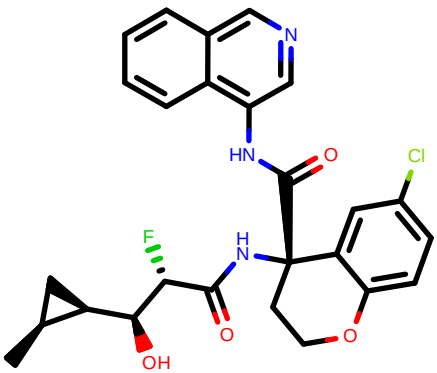
CID:	ALP-POS-5bb456a5-2_5
SMILES:	C[C@@H]1C[N@@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2426
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.40

VLA-UCB-50c39ae8-9_1



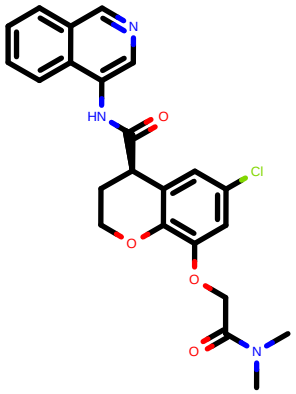
CID:	VLA-UCB-50c39ae8-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN395
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.59

PET-UNK-824b5c6a-1_1



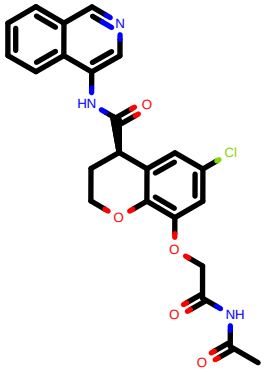
CID:	PET-UNK-824b5c6a-1_1
SMILES:	CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3287
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.15

KAD-UNI-8a629cb0-10_1



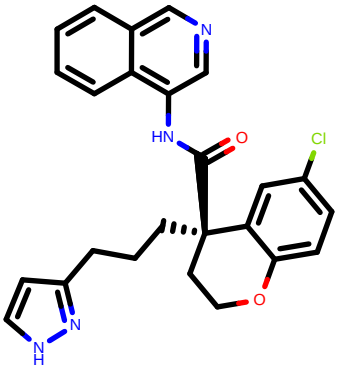
CID:	KAD-UNI-8a629cb0-10_1
SMILES:	CC(=O)N1C[C@@H]2C[C@H]1CN2C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2090
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.26

ALP-UNI-0676e700-27_1



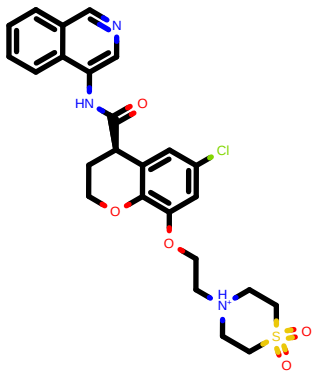
CID:	ALP-UNI-0676e700-27_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6cncn6c(=O)[nH]5
RUN:	RUN2475
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.30

DAR-DIA-ecdbc7dd-4_1



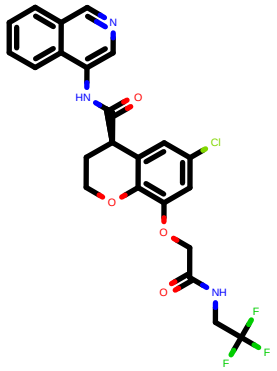
CID:	DAR-DIA-ecdbc7dd-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH+]5CCC5
RUN:	RUN2881
DDG (kcal/mol):	-2.20
dDDG (kcal/mol):	0.14

EDG-MED-ba1ac7b9-14_4



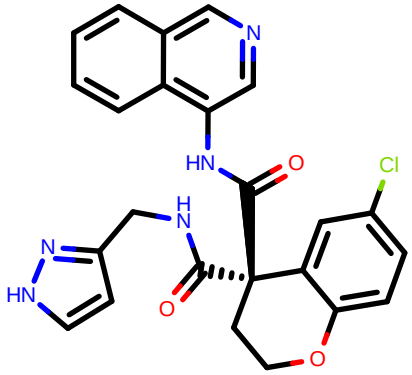
CID:	EDG-MED-ba1ac7b9-14_4
SMILES:	C[N@]1CCN(C[C@H]1C#N)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2669
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.56

ALP-UNI-3496895b-15_6



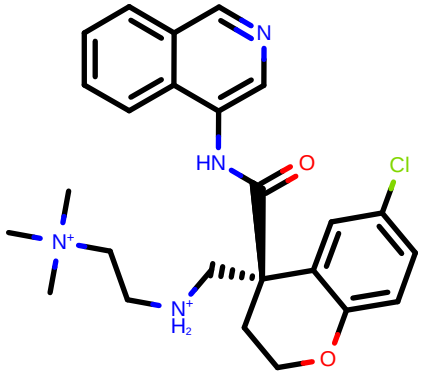
CID:	ALP-UNI-3496895b-15_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@@H]6[C@H]5C[C@H](C6)C(=O)N
RUN:	RUN2535
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.35

ALF-EVA-650655fc-3_2



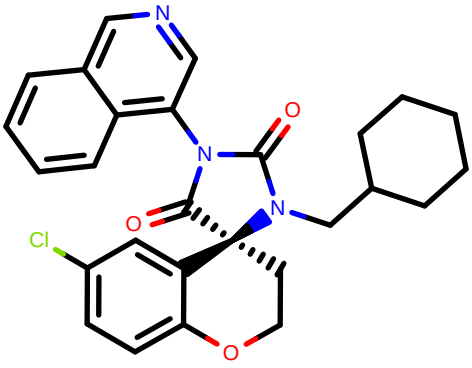
CID:	ALF-EVA-650655fc-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCC3)c4cc(cc(c4)Cl)O[C@H]5CC(=O)N5
RUN:	RUN2856
DDG (kcal/mol):	-2.19
dDDG (kcal/mol):	0.16

EDG-MED-90036822-30_1



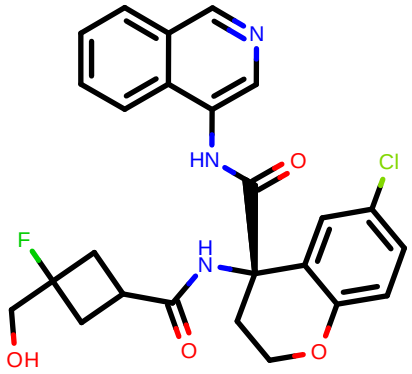
CID:	EDG-MED-90036822-30_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CNC5COC5)(F)F
RUN:	RUN1706
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.25

MIC-UNK-0a05c952-1_3



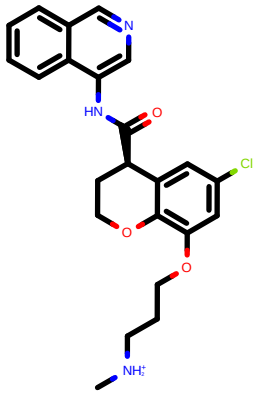
CID:	MIC-UNK-0a05c952-1_3
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](C[C@H](C3=O)c4cccc(c4)Cl)[C@@H]5CO5
RUN:	RUN3498
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.20

JAG-UCB-706446eb-6_1



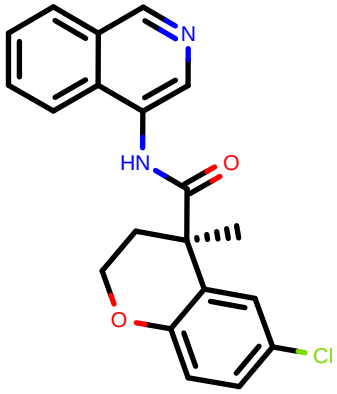
CID:	JAG-UCB-706446eb-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ccn[nH]5
RUN:	RUN618
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.26

RAL-THA-05e671eb-36_2



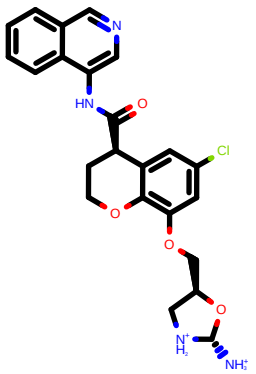
CID:	RAL-THA-05e671eb-36_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3c(ccc4)C#N
RUN:	RUN2077
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.43

MAT-POS-2492181e-8_1



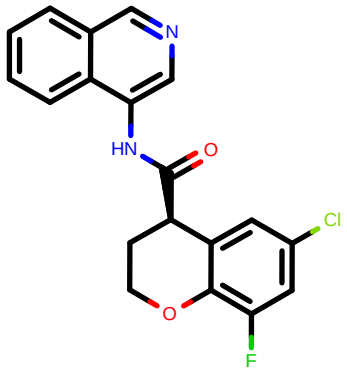
CID:	MAT-POS-2492181e-8_1
SMILES:	CC1CCN(CC1)c2ccc(cc2)NC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN98
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.22

KAD-UNI-8a629cb0-44_1



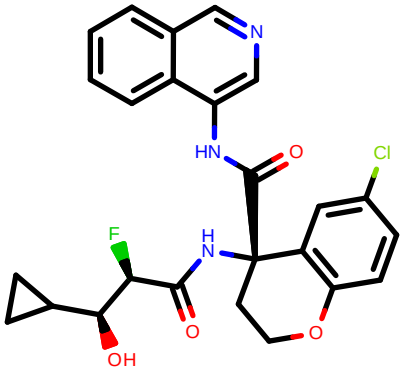
CID:	KAD-UNI-8a629cb0-44_1
SMILES:	CS(=O)(=O)[N@@]1CC[C@@H](C1)OCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2129
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.44

MAK-UNK-ffc90da7-4_2



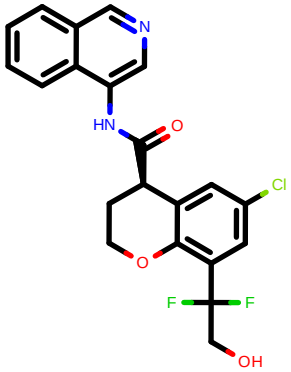
CID:	MAK-UNK-ffc90da7-4_2
SMILES:	C[C@H](C[NH2+]C[C@@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN694
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.18

MIC-UNK-cdc2493e-21_2



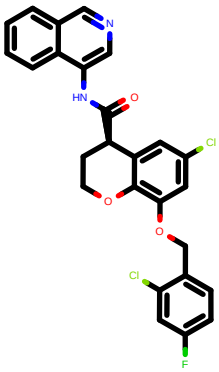
CID:	MIC-UNK-cdc2493e-21_2
SMILES:	CC(=O)N(C)[C@H]1CC[C@@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN568
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.28

EDJ-MED-50011917-1_1



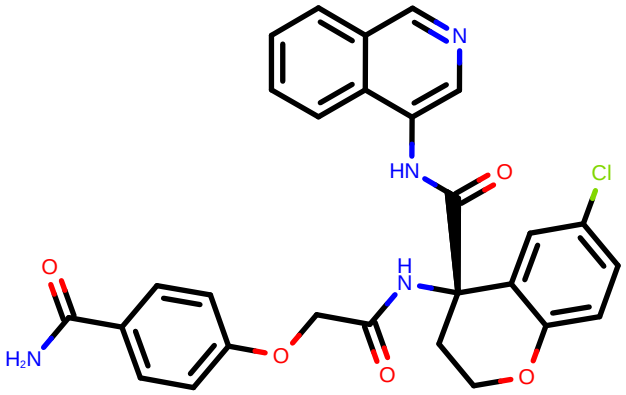
CID:	EDJ-MED-50011917-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@@H]4CC(=O)N4
RUN:	RUN370
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.26

ALP-POS-ce760d3f-5_1



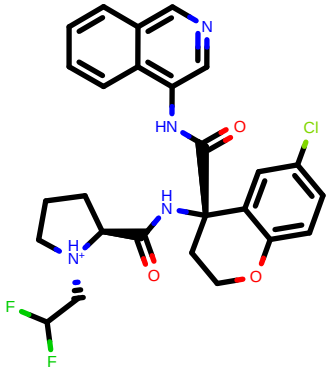
CID:	ALP-POS-ce760d3f-5_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)C3=CCOc4c3cc(cc4)Cl
RUN:	RUN1459
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.37

ALP-POS-966f8da6-1_3



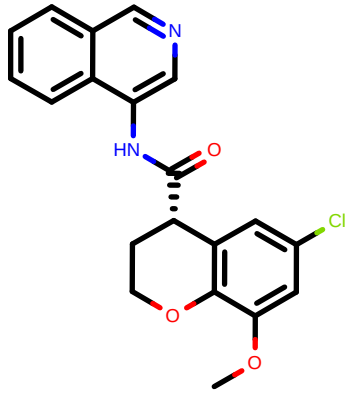
CID:	ALP-POS-966f8da6-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1220
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.30

DAR-DIA-f6ee7aeb-5_4



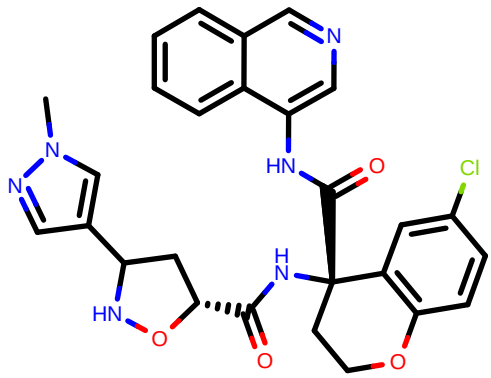
CID:	DAR-DIA-f6ee7aeb-5_4
SMILES:	CCCOc1cc(cc(c1)Cl)[C@H]2CC(=O)N(C[C@H]2c3c[nH]c(=O)[nH]c3=O)c4cncc5c4cccc5
RUN:	RUN3418
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.19

MAT-POS-b5746674-106_2



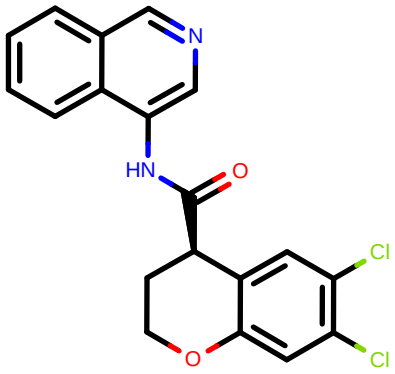
CID:	MAT-POS-b5746674-106_2
SMILES:	C[C@H](c1ccncc1)N(CCCOC)C(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN87
DDG (kcal/mol):	-2.17
dDDG (kcal/mol):	0.14

RAL-THA-4aa06b95-6_2



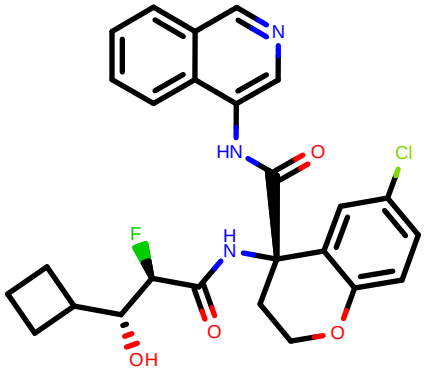
CID:	RAL-THA-4aa06b95-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)CCO
RUN:	RUN1241
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.27

MIC-UNK-50cce87d-3_1



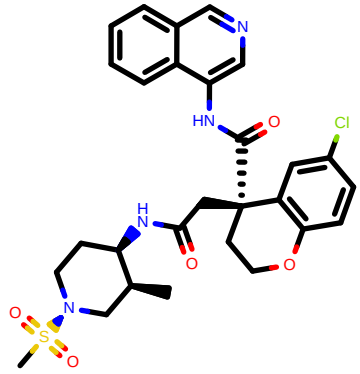
CID:	MIC-UNK-50cce87d-3_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN662
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.26

MIC-UNK-5a93dd5f-9_3



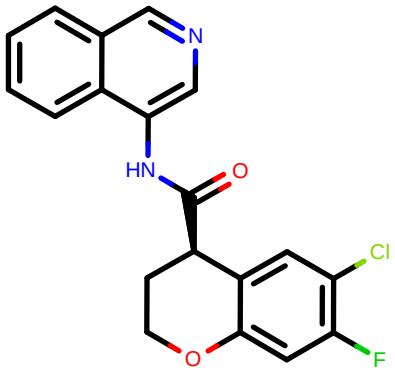
CID:	MIC-UNK-5a93dd5f-9_3
SMILES:	CN(C)[C@@H]1CC[N@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN780
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.27

MAK-UNK-c749d764-2_5



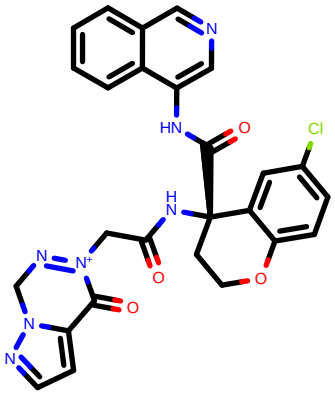
CID:	MAK-UNK-c749d764-2_5
SMILES:	CC[C@@H]1CCC[C@@H]([C@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN901
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.27

MIC-UNK-5a93dd5f-5_3



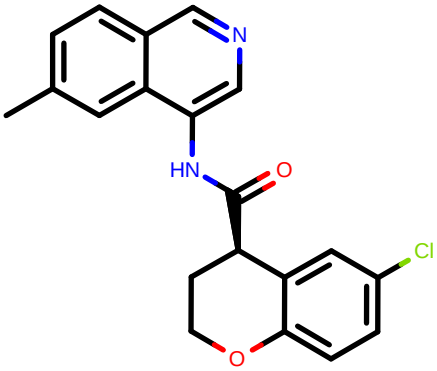
CID:	MIC-UNK-5a93dd5f-5_3
SMILES:	CC(=O)N[C@@H]1CC[N@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN760
DDG (kcal/mol):	-2.16
dDDG (kcal/mol):	0.20

MAK-UNK-c749d764-1_8



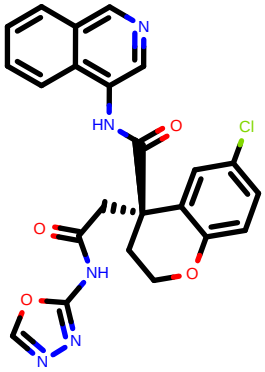
CID:	MAK-UNK-c749d764-1_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@H]([C@H]3O)C4CC4
RUN:	RUN896
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.30

DAR-DIA-0d514e7d-31_13



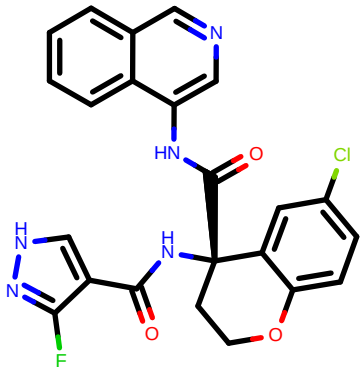
CID:	DAR-DIA-0d514e7d-31_13
SMILES:	C[C@@H]1CCO[C@@H]2C=CC(=C[C@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN846
DDG (kcal/mol):	-2.15
dDDG (kcal/mol):	0.19

KAD-UNI-b13decd3-8_1



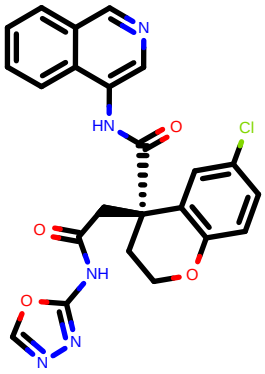
CID:	KAD-UNI-b13decd3-8_1
SMILES:	COC(=O)CCc1c(con1)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3790
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.11

ADA-UCB-dc2b944c-8_1



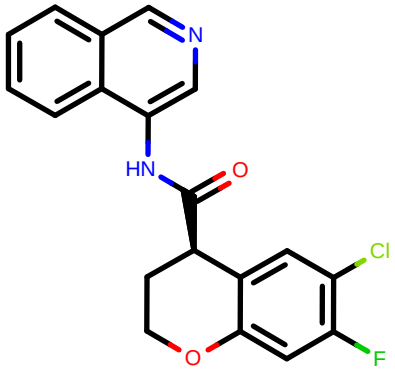
CID:	ADA-UCB-dc2b944c-8_1
SMILES:	c1cc2c(cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)c(c1)Cl
RUN:	RUN606
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.25

DAR-DIA-0d514e7d-32_2



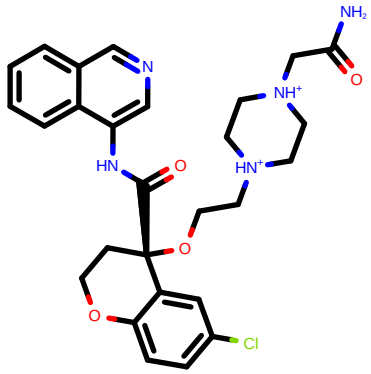
CID:	DAR-DIA-0d514e7d-32_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@@H]4C[C@@H]4CO[C@@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN851
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.19

ALP-POS-75715966-2_1



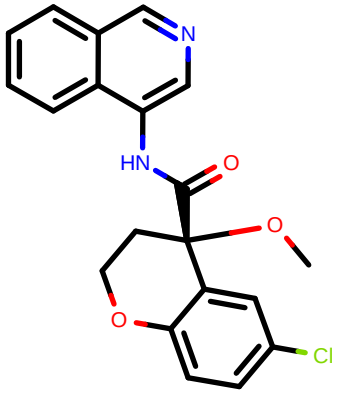
CID:	ALP-POS-75715966-2_1
SMILES:	CN(C)c1ccc(cc1)N(Cc2cccc(c2)Cl)C(=O)Cc3cncc4c3cccc4
RUN:	RUN1490
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.20

MIC-UNK-cdc2493e-17_1



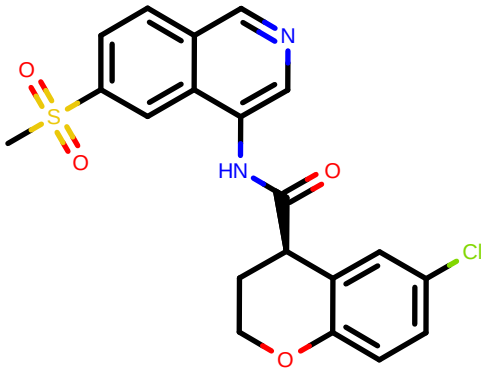
CID:	MIC-UNK-cdc2493e-17_1
SMILES:	CC(=O)N1CCC(CC1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN564
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.36

DAR-DIA-0d514e7d-31_7



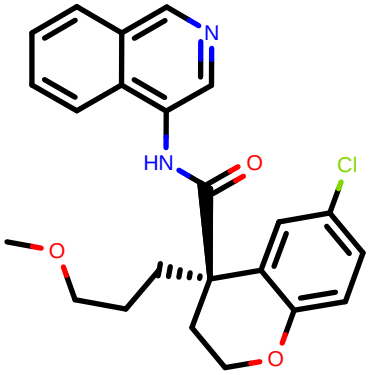
CID:	DAR-DIA-0d514e7d-31_7
SMILES:	C[C@@H]1CCO[C@H]2C=CC(=C[C@H]2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN840
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.22

EDJ-MED-e4b030d8-11_1



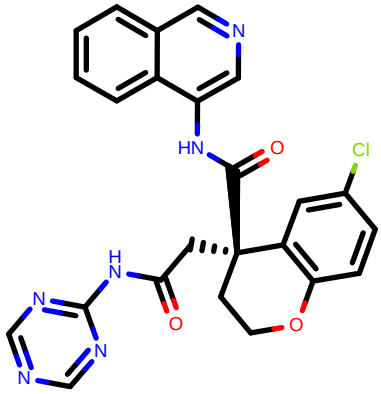
CID:	EDJ-MED-e4b030d8-11_1
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN295
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.26

ALP-UNI-dbbfd3db-16_1



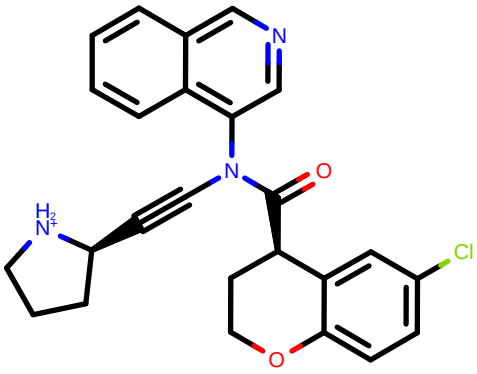
CID:	ALP-UNI-dbbfd3db-16_1
SMILES:	Cn1c2c(cn1)c(=O)n(cn2)CC(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2785
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.12

NAU-LAT-2fed8305-4_2



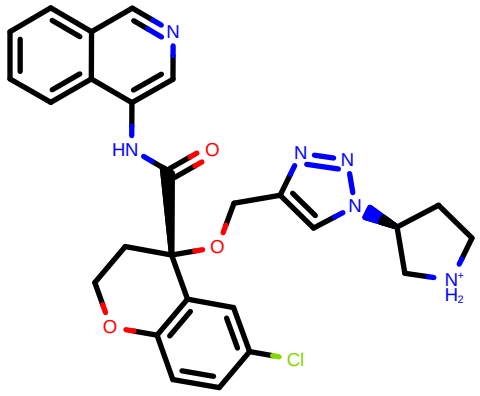
CID:	NAU-LAT-2fed8305-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[N@H+]3CCC=C(C3)F
RUN:	RUN1110
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.24

ALP-UNI-8e43a71e-7_1



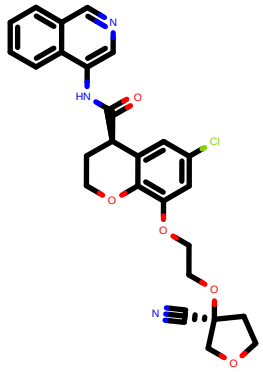
CID:	ALP-UNI-8e43a71e-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)CCC#N
RUN:	RUN2964
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.18

FRA-DIA-b66f7109-4_2



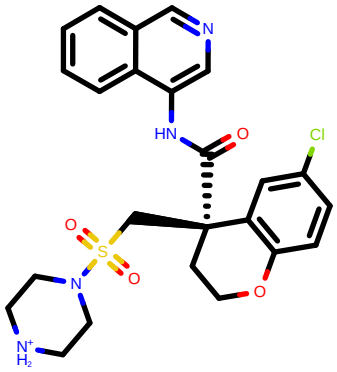
CID:	FRA-DIA-b66f7109-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4Cl)O[C@H]5CC(=O)N5
RUN:	RUN400
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.29

EDJ-MED-d203f206-30_1



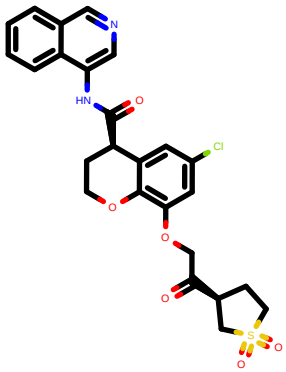
CID:	EDJ-MED-d203f206-30_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5C(=O)N
RUN:	RUN2590
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.42

EDG-MED-90036822-13_1



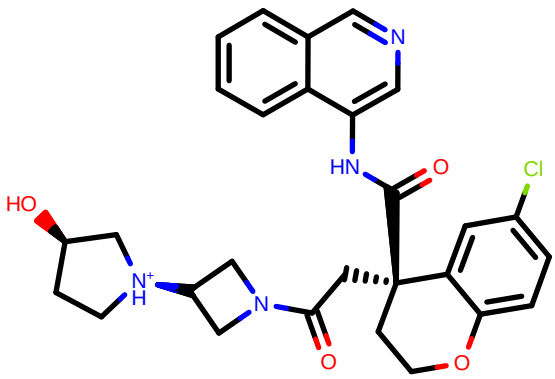
CID:	EDG-MED-90036822-13_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO
RUN:	RUN1670
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.20

EDG-MED-ba1ac7b9-12_3



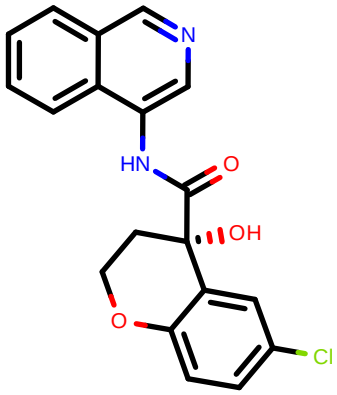
CID:	EDG-MED-ba1ac7b9-12_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5c6n[n-]nn6
RUN:	RUN2660
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.46

GIA-UNK-80c9bc96-1_1



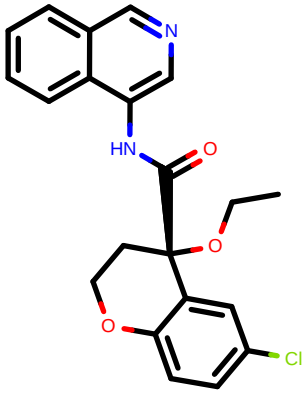
CID:	GIA-UNK-80c9bc96-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN1101
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.40

PET-UNK-c5865d42-1_1



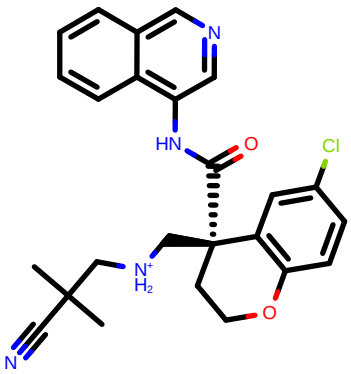
CID:	PET-UNK-c5865d42-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@@H]4CC[NH2+]4
RUN:	RUN423
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.21

DAR-DIA-9e4459de-11_14



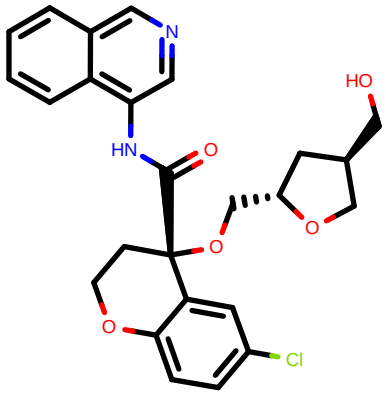
CID:	DAR-DIA-9e4459de-11_14
SMILES:	c1cc2c(c(c1)NCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1422
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.18

MAT-POS-4223bc15-29_4



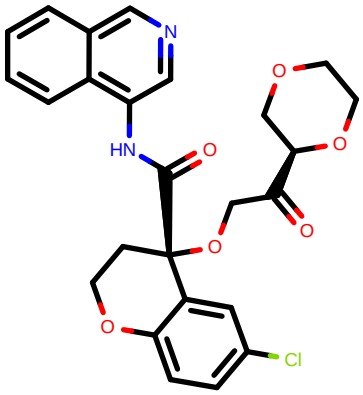
CID:	MAT-POS-4223bc15-29_4
SMILES:	CNC(=O)NS(=O)(=O)[N@]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4132
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.17

MAT-POS-dd3ad2b5-2_2



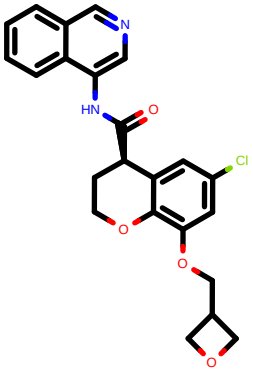
CID:	MAT-POS-dd3ad2b5-2_2
SMILES:	CC(=O)N1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3534
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.19

NIR-THE-2069301b-1_2



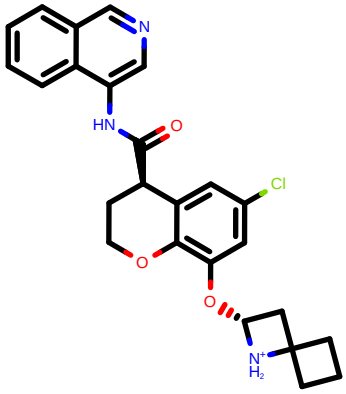
CID:	NIR-THE-2069301b-1_2
SMILES:	C=C(C(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl)F
RUN:	RUN3321
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.20

MAT-POS-1f3f1a6f-3_2



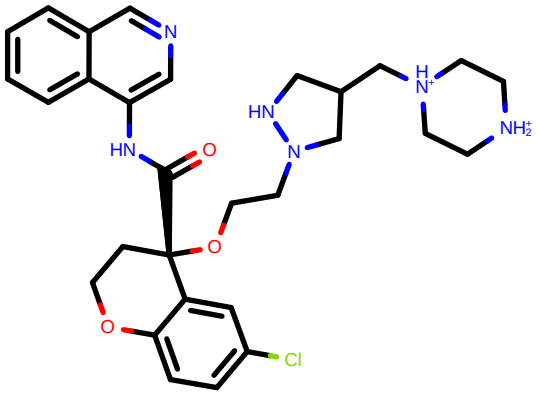
CID:	MAT-POS-1f3f1a6f-3_2
SMILES:	CC(=O)N[C@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2282
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.34

MAT-POS-b5746674-101_1



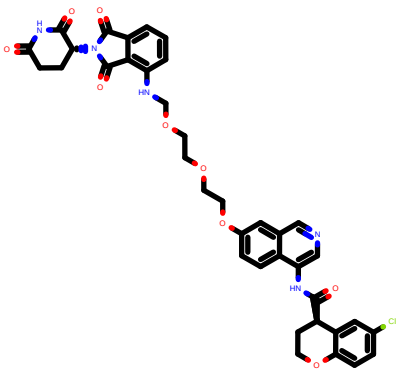
CID:	MAT-POS-b5746674-101_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CC[C@@H](C3)c4ccccc4
RUN:	RUN77
DDG (kcal/mol):	-2.11
dDDG (kcal/mol):	0.47

DAR-DIA-6a508060-11_3



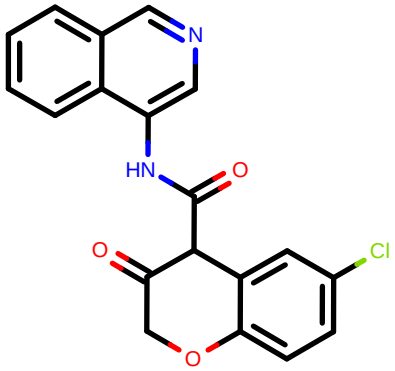
CID:	DAR-DIA-6a508060-11_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@@H]4C[C@H]4Cl
RUN:	RUN352
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.37

ALP-POS-477dc5b7-1_2



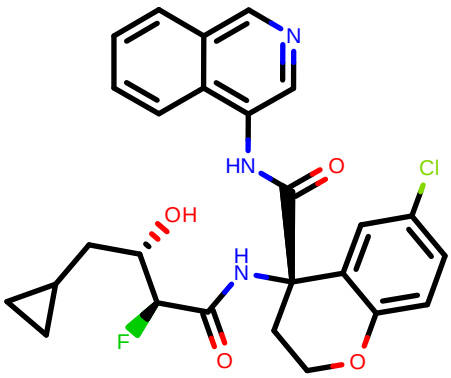
CID:	ALP-POS-477dc5b7-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCCc4c3cc(cc4)Cl
RUN:	RUN296
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.48

LON-WEI-adc59df6-52_1



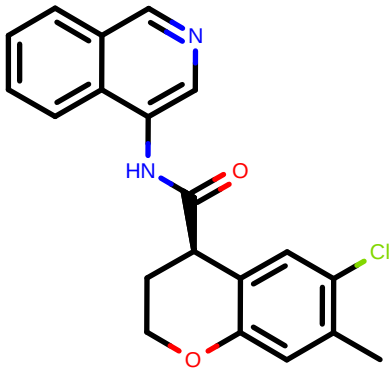
CID:	LON-WEI-adc59df6-52_1
SMILES:	CC(C)(C)c1ccc(cc1)N([C@@H](c2cncc3c2cccc3)C(=O)NC(C)(C)C)C(=O)C=C
RUN:	RUN4
DDG (kcal/mol):	-2.10
dDDG (kcal/mol):	0.21

MIC-UNK-0a05c952-1_6



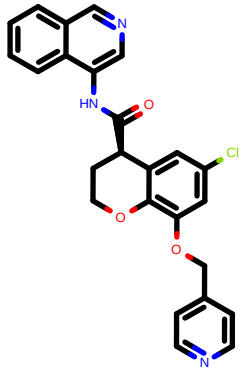
CID:	MIC-UNK-0a05c952-1_6
SMILES:	c1ccc2c(c1)cncc2N3[C@H](C[C@@H](C3=O)c4cccc(c4Cl)[C@H]5CO5
RUN:	RUN3502
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.19

DAR-DIA-0d514e7d-13_1



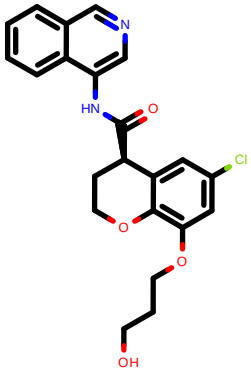
CID:	DAR-DIA-0d514e7d-13_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4Cl)c5ccc(cc5)F
RUN:	RUN815
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.25

ED_-GRI-5b13fbe2-36_1



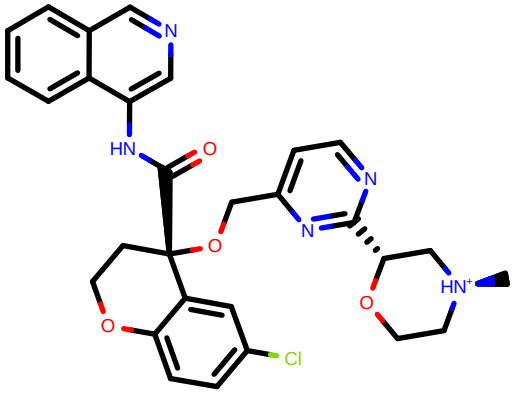
CID:	ED_-GRI-5b13fbe2-36_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3(CCOc4c3cc(cc4Cl)OCC[C@@H](c5cn(nn5)CC6CC6)[NH3+]
RUN:	RUN1569
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.37

MAT-POS-e9e99895-6_1



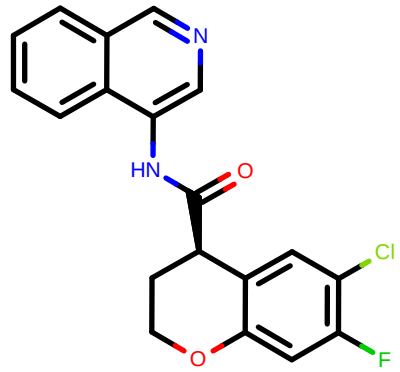
CID:	MAT-POS-e9e99895-6_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)CN4CCN(C4=O)C5CC5
RUN:	RUN2256
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.30

DAR-DIA-23e5a6a0-10_2



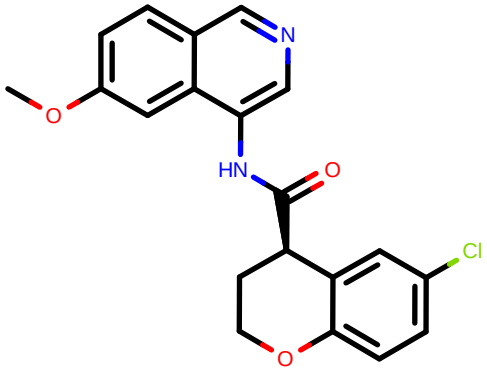
CID:	DAR-DIA-23e5a6a0-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC6([NH2+]5)CC6)Cl
RUN:	RUN421
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.33

MIC-UNK-50cce87d-8_1



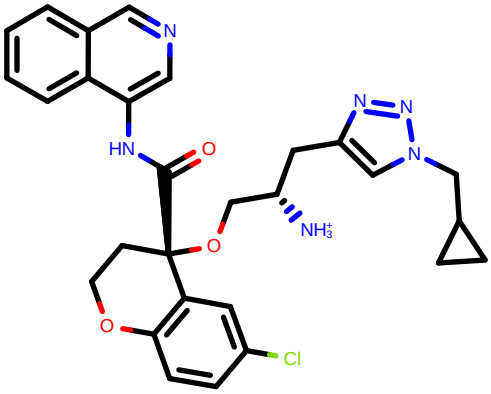
CID:	MIC-UNK-50cce87d-8_1
SMILES:	COc1cccc2c1c(cnc2)N3CC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN671
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.21

DAR-DIA-0d514e7d-32_15



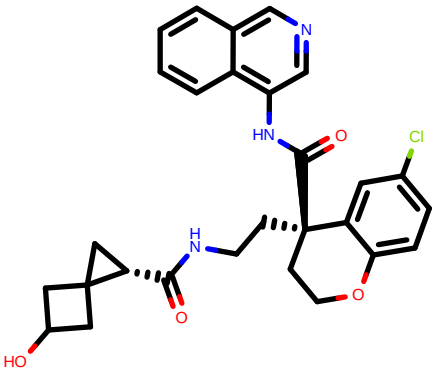
CID:	DAR-DIA-0d514e7d-32_15
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@H]4C[C@H]4CO[C@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN864
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.20

MIC-UNK-50cce87d-5_1



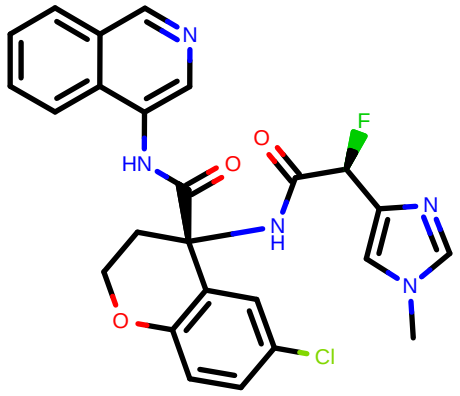
CID:	MIC-UNK-50cce87d-5_1
SMILES:	c1cc(cc(c1)Cl)[C@@H]2CCN(C2=O)c3cncc4c3c(ccc4)F
RUN:	RUN663
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.38

RAL-THA-e002e396-10_2



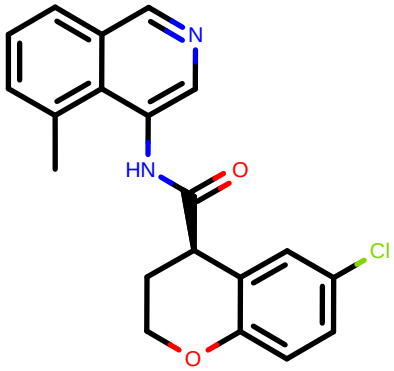
CID:	RAL-THA-e002e396-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CS(=O)(=O)N5CC[NH2+]CC5
RUN:	RUN3473
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.18

MIC-UNK-91acba05-6_1



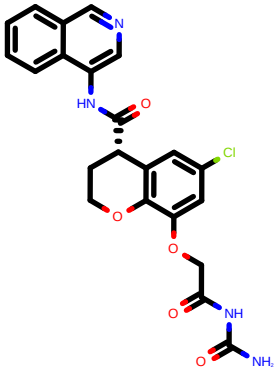
CID:	MIC-UNK-91acba05-6_1
SMILES:	CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN478
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.29

ALP-POS-477dc5b7-3_2



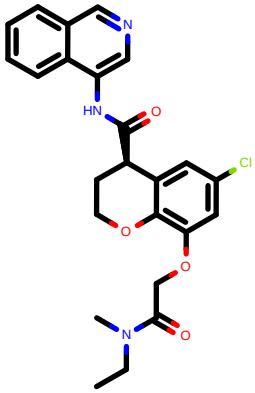
CID:	ALP-POS-477dc5b7-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CCC5CC5
RUN:	RUN307
DDG (kcal/mol):	-2.08
dDDG (kcal/mol):	0.18

KAD-UNI-8a629cb0-7_1



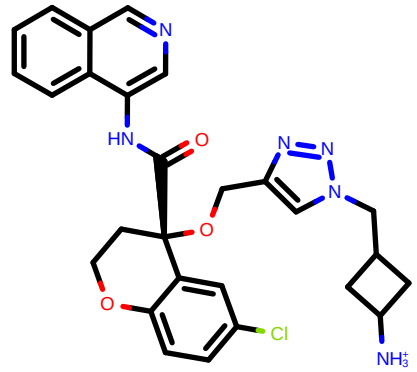
CID:	KAD-UNI-8a629cb0-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN2084
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.24

EDJ-MED-9e38fd34-6_1



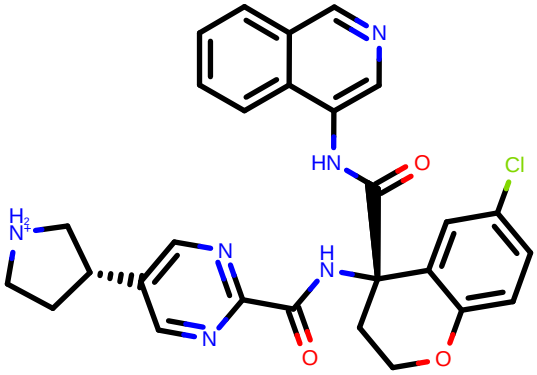
CID:	EDJ-MED-9e38fd34-6_1
SMILES:	C[C@@]1(c2cc(c(cc2NC1=O)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2352
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.31

DAR-DIA-6a508060-8_1



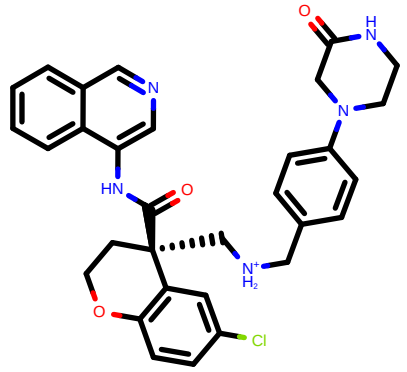
CID:	DAR-DIA-6a508060-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)C5CC5
RUN:	RUN344
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.34

MAK-UNK-c749d764-18_4



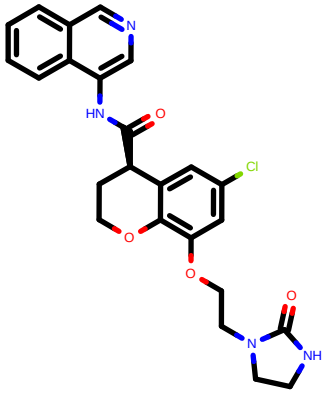
CID:	MAK-UNK-c749d764-18_4
SMILES:	CC(C)SCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN993
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.28

ED_-GRI-5b13fbe2-49_1



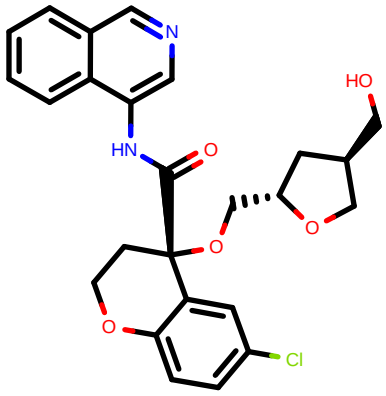
CID:	ED_-GRI-5b13fbe2-49_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](C[NH3+])c5cn(nn5)CC6CC6
RUN:	RUN1593
DDG (kcal/mol):	-2.07
dDDG (kcal/mol):	0.39

ALP-UNI-3496895b-9_1



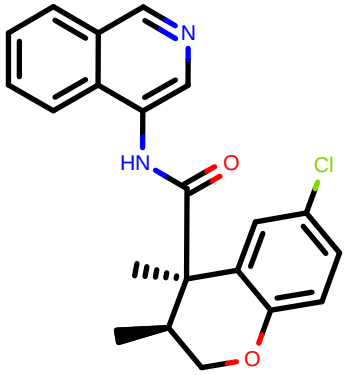
CID:	ALP-UNI-3496895b-9_1
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2522
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.30

MAK-UNK-ffc90da7-3_1



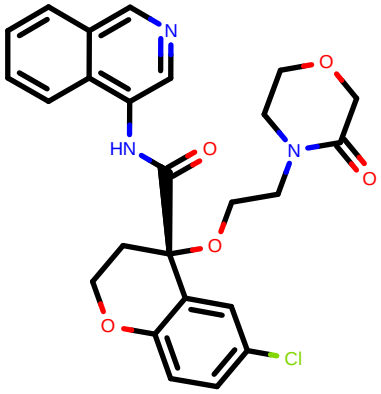
CID:	MAK-UNK-ffc90da7-3_1
SMILES:	CC(C)OC[C@@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C
RUN:	RUN695
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.30

LON-WEI-4d77710c-53_2



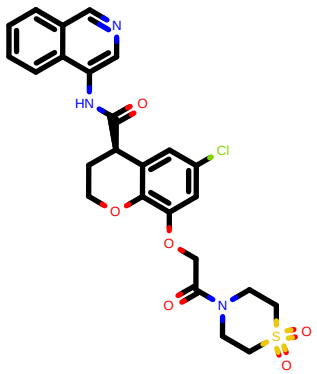
CID:	LON-WEI-4d77710c-53_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CCC[N@H+](C3)Cc4ccccc4F
RUN:	RUN245
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.19

DAR-DIA-0587064e-24_2



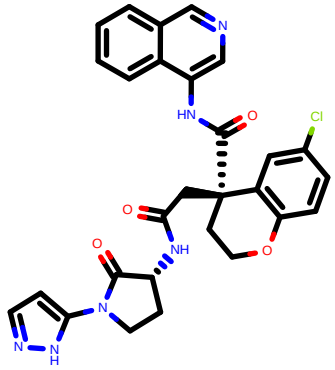
CID:	DAR-DIA-0587064e-24_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCc5ccc(cc5Cl)F)Cl
RUN:	RUN3386
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.16

EDG-MED-ba1ac7b9-14_1



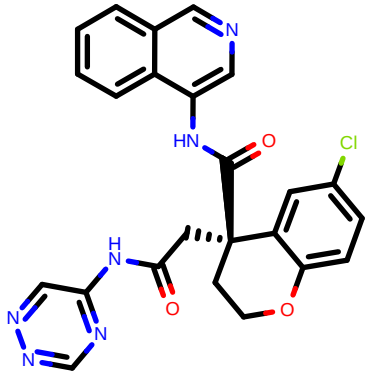
CID:	EDG-MED-ba1ac7b9-14_1
SMILES:	C[N@@]1CCN(C[C@@H]1C#N)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2666
DDG (kcal/mol):	-2.06
dDDG (kcal/mol):	0.39

ALP-POS-696356e4-1_1



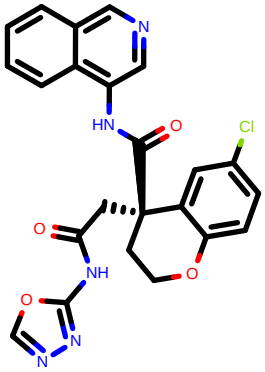
CID:	ALP-POS-696356e4-1_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1314
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-24_4



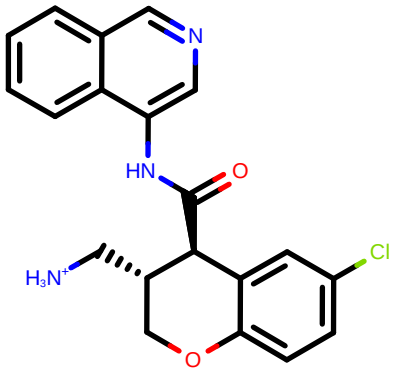
CID:	MAK-UNK-c749d764-24_4
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1033
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.25

MAT-POS-932d1078-1_4



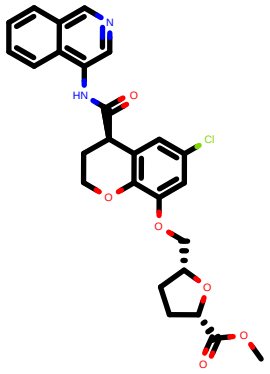
CID:	MAT-POS-932d1078-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCC[N@@]5CC(F)(F)F
RUN:	RUN3589
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.10

MAT-POS-3b92565d-9_1



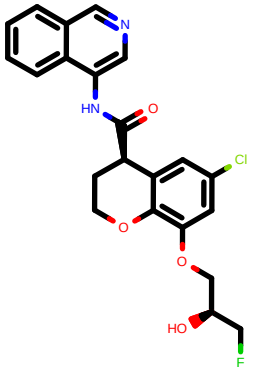
CID:	MAT-POS-3b92565d-9_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4
RUN:	RUN118
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.24

EDJ-MED-d203f206-6_1



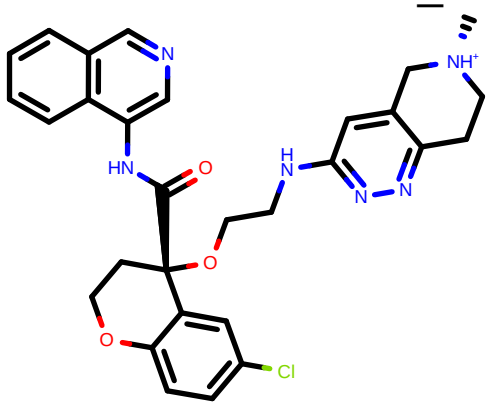
CID:	EDJ-MED-d203f206-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5C[C@H]6CS(=O)(=O)C[C@]6(C5)C#N
RUN:	RUN2568
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.37

MAT-POS-1f3f1a6f-5_2



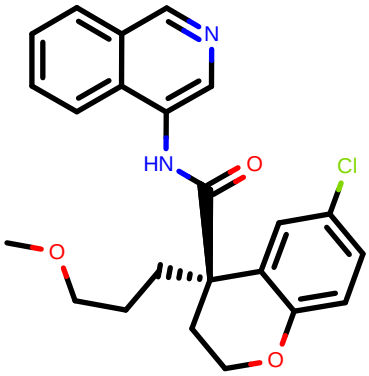
CID:	MAT-POS-1f3f1a6f-5_2
SMILES:	c1ccc2c(c1)cncc2n3c(c([nH]c3=O)c4ccc(c(c4)Cl)Cl)[O-]
RUN:	RUN2280
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.46

DAR-DIA-23e5a6a0-4_2



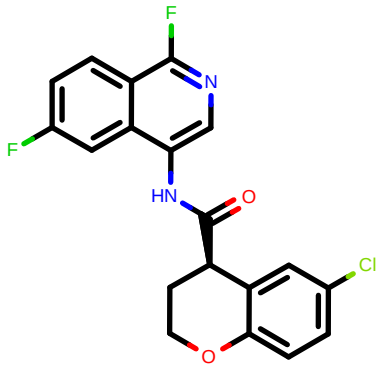
CID:	DAR-DIA-23e5a6a0-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6(CC6)C[NH2+]5)Cl
RUN:	RUN408
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.55

MIC-UNK-9582b2c5-1_2



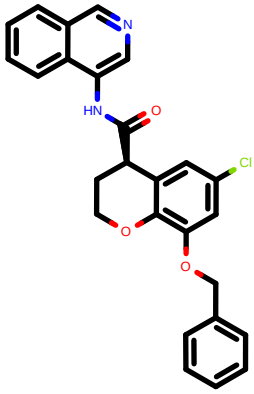
CID:	MIC-UNK-9582b2c5-1_2
SMILES:	CC(=O)N1CC[C@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN253
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.29

LON-WEI-4d77710c-45_1



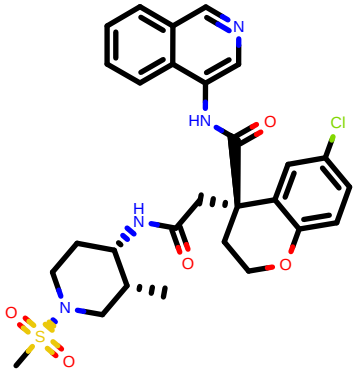
CID:	LON-WEI-4d77710c-45_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N3CCN(CC3)C(=O)c4ccco4
RUN:	RUN235
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.21

DAR-DIA-9e4459de-15_9



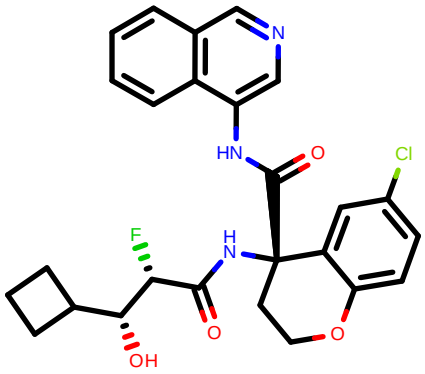
CID:	DAR-DIA-9e4459de-15_9
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1449
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.32

MAK-UNK-c749d764-12_7



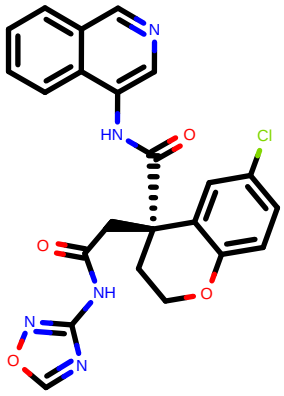
CID:	MAK-UNK-c749d764-12_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@H]([C@H]3O)Cl
RUN:	RUN956
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.39

MIC-UNK-5a93dd5f-12_6



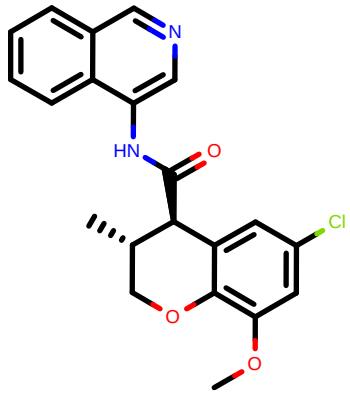
CID:	MIC-UNK-5a93dd5f-12_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@@]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN795
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.35

MIC-UNK-5a93dd5f-12_8



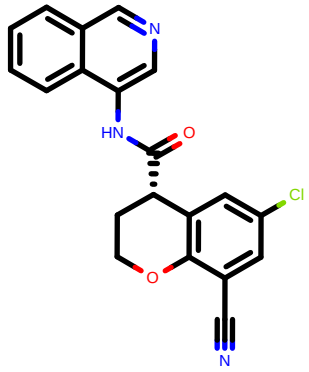
CID:	MIC-UNK-5a93dd5f-12_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3Cl)[N@]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN798
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.18

MAT-POS-3b92565d-2_1



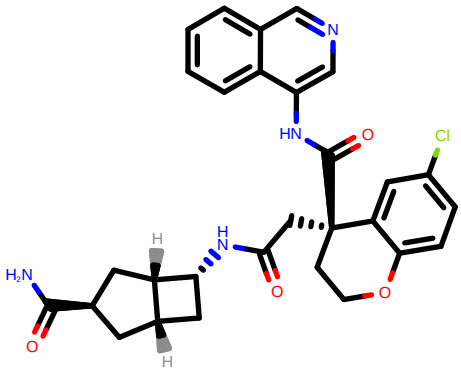
CID:	MAT-POS-3b92565d-2_1
SMILES:	COc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN109
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.19

DAR-DIA-5ff57136-2_1



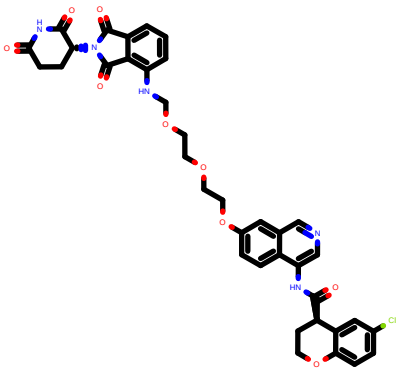
CID:	DAR-DIA-5ff57136-2_1
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl
RUN:	RUN1373
DDG (kcal/mol):	-2.02
dDDG (kcal/mol):	0.14

LON-WEI-5e7d1b3e-29_1



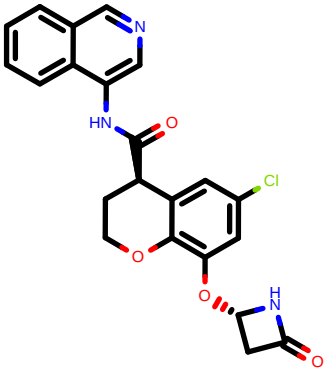
CID:	LON-WEI-5e7d1b3e-29_1
SMILES:	CCOC(=O)Cc1csc(n1)NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN1340
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.35

MAK-UNK-919546f0-2_1



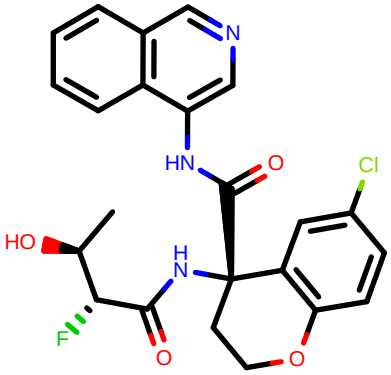
CID:	MAK-UNK-919546f0-2_1
SMILES:	c1ccc(cc1)[C@@H](C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN481
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.54

NIR-WEI-f9286bb6-4_1



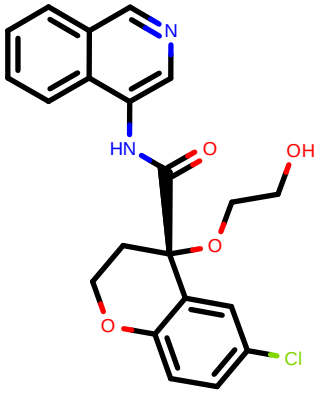
CID:	NIR-WEI-f9286bb6-4_1
SMILES:	CC(C)(C)NC(=O)[C@@H](c1cncc2c1cccc2)N(Cc3ccccc3Cl)C(=O)C=C
RUN:	RUN138
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.26

MAK-UNK-8be7dca9-5_1



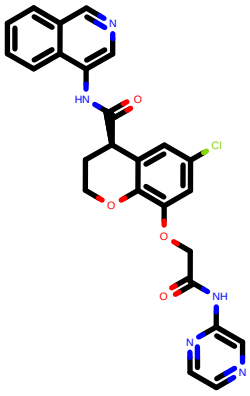
CID:	MAK-UNK-8be7dca9-5_1
SMILES:	c1cc2c(cc1C[NH3+])cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN499
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.23

DAR-DIA-23e5a6a0-3_2



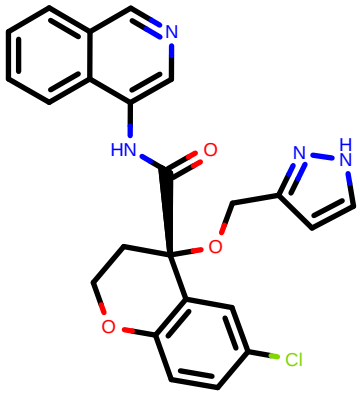
CID:	DAR-DIA-23e5a6a0-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6([NH2+]5)COC6)Cl
RUN:	RUN406
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.23

MAT-POS-e9e99895-8_3



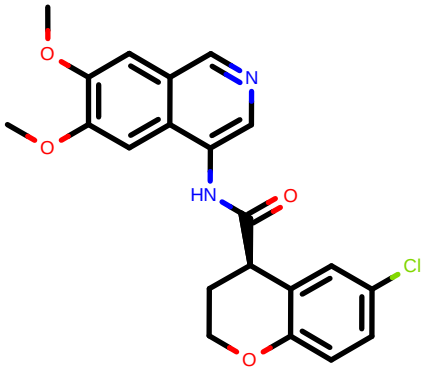
CID:	MAT-POS-e9e99895-8_3
SMILES:	Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@](C)(c3ccc(c(c3)Cl)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2255
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.29

FRA-DIA-13af2da5-1_1



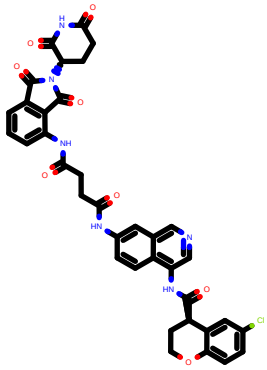
CID:	FRA-DIA-13af2da5-1_1
SMILES:	CN(C)c1ccc(cc1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN467
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.22

ED_-GRI-5b13fbe2-3_2



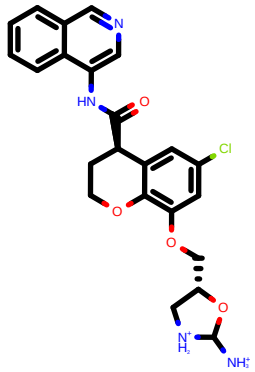
CID:	ED_-GRI-5b13fbe2-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5n[n-]nn5)[NH3+]
RUN:	RUN1524
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.26

MAR-UCB-6ab2ec87-2_1



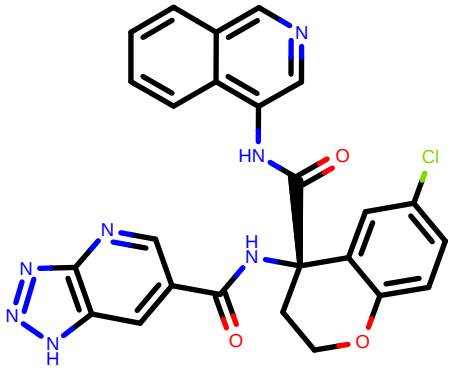
CID:	MAR-UCB-6ab2ec87-2_1
SMILES:	C[C@@H]1[C@H](c2cc(ccc2N1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3022
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.25

KAD-UNI-8a629cb0-33_1



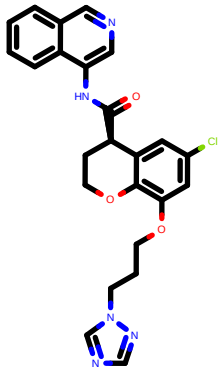
CID:	KAD-UNI-8a629cb0-33_1
SMILES:	CC[C@H](C[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)O
RUN:	RUN2120
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.42

KAD-UNI-877d7bed-17_1



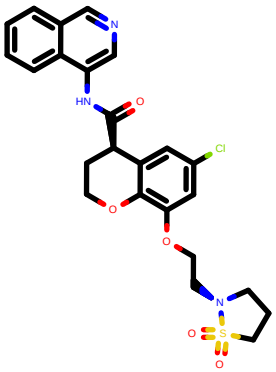
CID:	KAD-UNI-877d7bed-17_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCC(=O)NC5(CCC5)C#N)Cl
RUN:	RUN3763
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.16

EDG-MED-ba1ac7b9-13_1



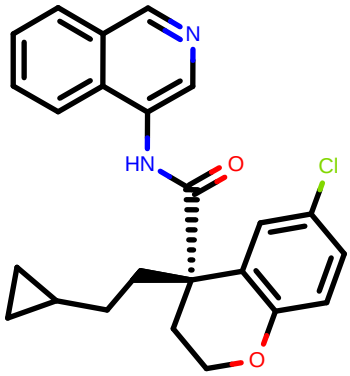
CID:	EDG-MED-ba1ac7b9-13_1
SMILES:	C[N@@H+]1C[C@@H]2C[C@H]1CN2C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2661
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.40

ALP-POS-5bb456a5-1_7



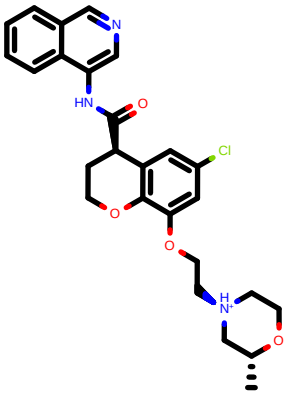
CID:	ALP-POS-5bb456a5-1_7
SMILES:	C[C@@H]1C[N@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2412
DDG (kcal/mol):	-2.01
dDDG (kcal/mol):	0.33

MAT-POS-b5746674-108_4



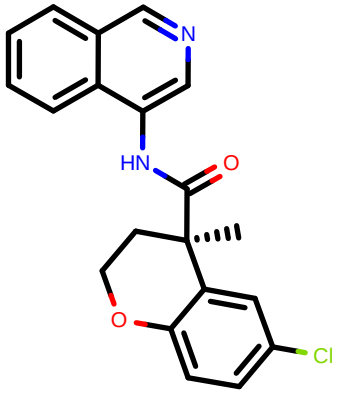
CID:	MAT-POS-b5746674-108_4
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN95
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.16

EDJ-MED-d203f206-2_1



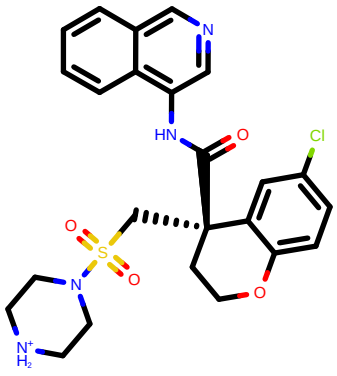
CID:	EDJ-MED-d203f206-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncon5
RUN:	RUN2563
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.54

DAR-DIA-0cde14eb-48_1



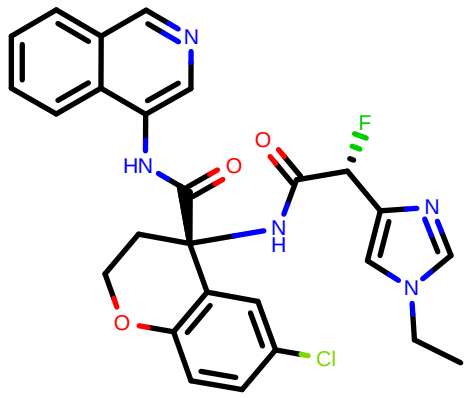
CID:	DAR-DIA-0cde14eb-48_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)C4(CC4)F
RUN:	RUN12
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.21

LAU-MED-88a3970a-13_1



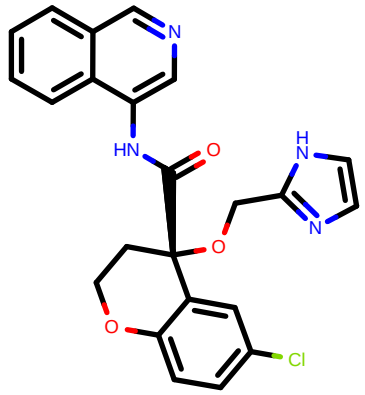
CID:	LAU-MED-88a3970a-13_1
SMILES:	COCCCc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1509
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.40

MIC-UNK-5a93dd5f-6_2



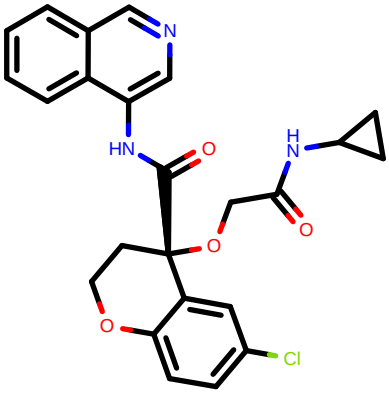
CID:	MIC-UNK-5a93dd5f-6_2
SMILES:	CC(=O)N(C)C1CC[NH+](CC1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN767
DDG (kcal/mol):	-2.00
dDDG (kcal/mol):	0.35

MAK-UNK-8be7dca9-3_4



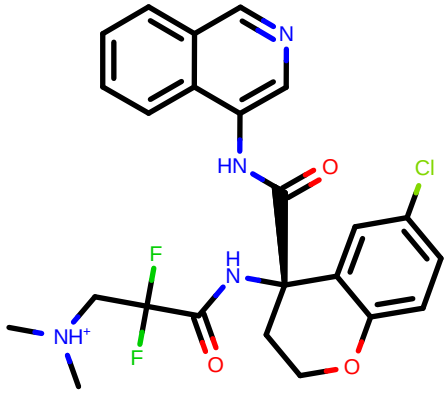
CID:	MAK-UNK-8be7dca9-3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4OC[C@H]3C[NH3+])Cl
RUN:	RUN498
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.21

DAR-DIA-0d514e7d-14_1



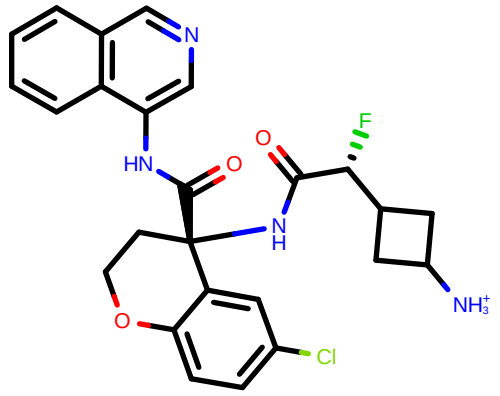
CID:	DAR-DIA-0d514e7d-14_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5cccc(c5F)F
RUN:	RUN817
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.23

JAG-UCB-706446eb-5_1



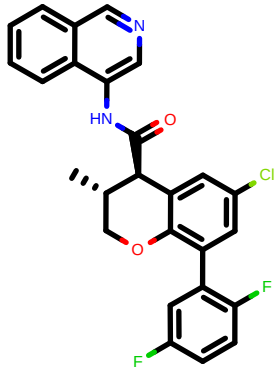
CID:	JAG-UCB-706446eb-5_1
SMILES:	COCCN([C@@H]1CCCOC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN623
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.28

MAK-UNK-8be7dca9-3_3



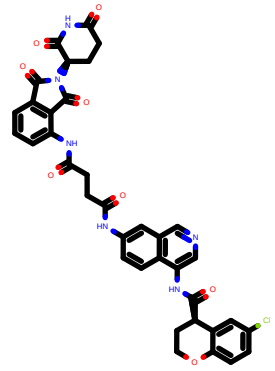
CID:	MAK-UNK-8be7dca9-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4OC[C@H]3C[NH3+])Cl
RUN:	RUN497
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.28

MAT-POS-4211dce8-1_1



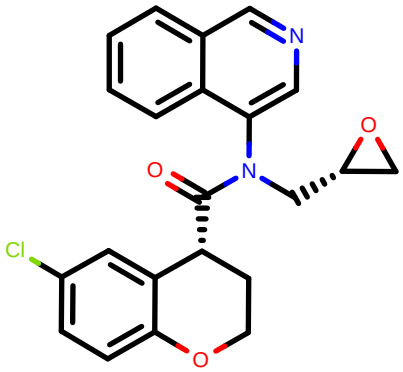
CID:	MAT-POS-4211dce8-1_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN180
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.33

ALP-UNI-8e43a71e-2_11



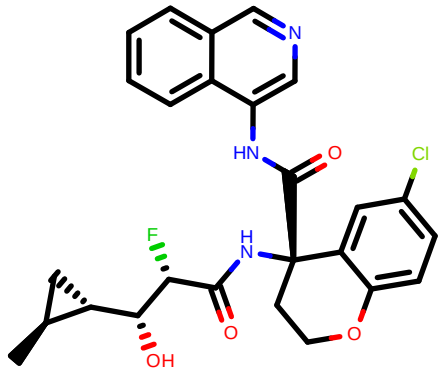
CID:	ALP-UNI-8e43a71e-2_11
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@@H]5CCC[N@H+]6CCO
RUN:	RUN2934
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.21

DAR-DIA-5ff57136-1_1



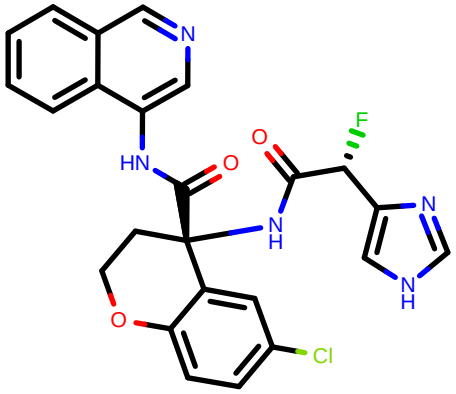
CID:	DAR-DIA-5ff57136-1_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@@H]1C(=O)N(c3cncc4c3cccc4)C(=O)C=C)Cl
RUN:	RUN1371
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.22

NAU-LAT-0543f7f2-9_1



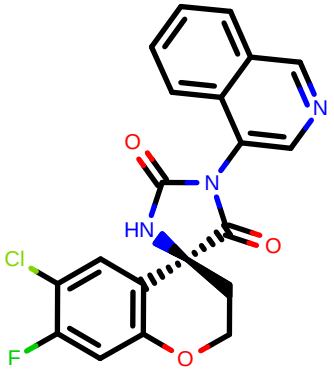
CID:	NAU-LAT-0543f7f2-9_1
SMILES:	CC(=O)NCCOc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN656
DDG (kcal/mol):	-1.98
dDDG (kcal/mol):	0.29

MIC-UNK-91acba05-2_1



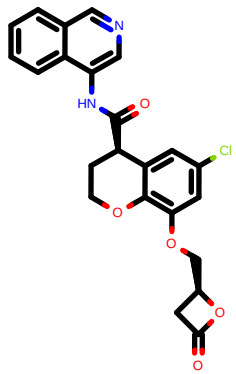
CID:	MIC-UNK-91acba05-2_1
SMILES:	CN1C[C@@H](c2cc(ccc2C1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN469
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.29

DAR-DIA-9e4459de-15_8



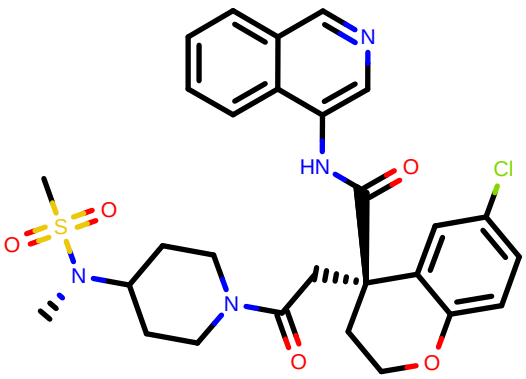
CID:	DAR-DIA-9e4459de-15_8
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1445
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.20

MAT-POS-5d65ec79-1_1



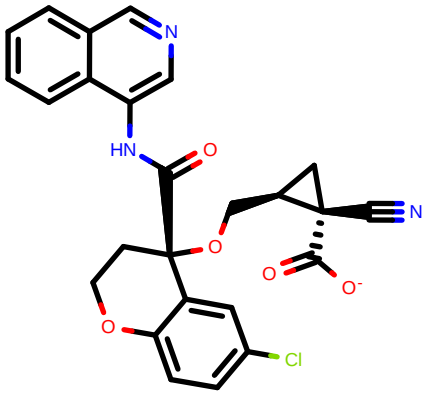
CID:	MAT-POS-5d65ec79-1_1
SMILES:	CN(C)C(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2080
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.41

MAK-UNK-c749d764-16_16



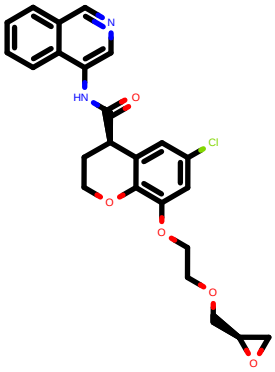
CID:	MAK-UNK-c749d764-16_16
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F)O
RUN:	RUN989
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.26

VLA-UCB-50c39ae8-6_1



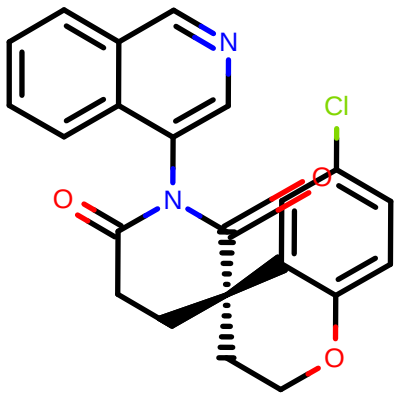
CID:	VLA-UCB-50c39ae8-6_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN385
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.30

MAT-POS-f9802937-7_1



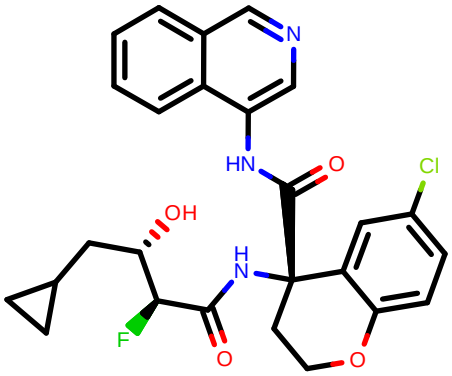
CID:	MAT-POS-f9802937-7_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2398
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.42

BAR-COM-0f94fc3d-47_1



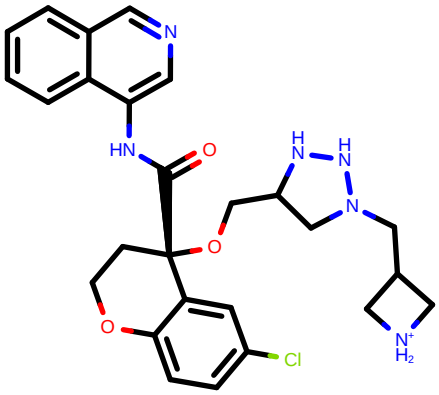
CID:	BAR-COM-0f94fc3d-47_1
SMILES:	Cc1ccc2c(c1)c(co2)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN8
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-3_15



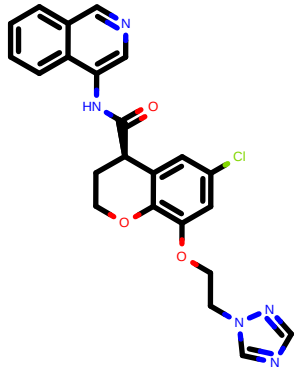
CID:	MIC-UNK-5a93dd5f-3_15
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@H+]4CC[C@H]5CCCC[C@H]5C4
RUN:	RUN755
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.33

VLA-UCB-50c39ae8-8_1



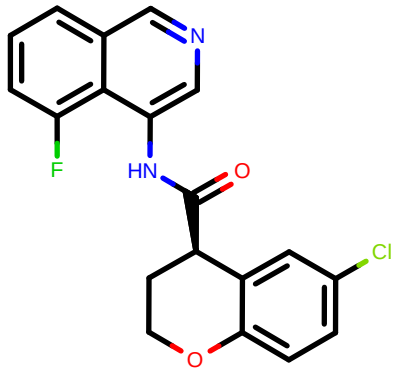
CID:	VLA-UCB-50c39ae8-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl
RUN:	RUN388
DDG (kcal/mol):	-1.96
dDDG (kcal/mol):	0.24

ALP-POS-5bb456a5-1_10



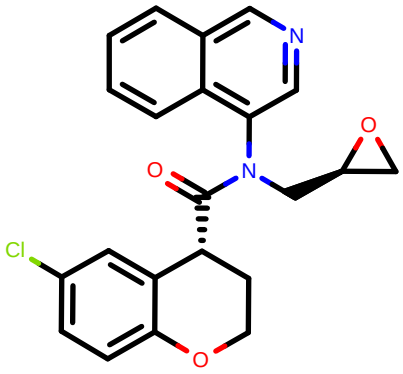
CID:	ALP-POS-5bb456a5-1_10
SMILES:	C[C@H]1C[N@@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2416
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.37

VLA-UCB-05e51b3f-10_1



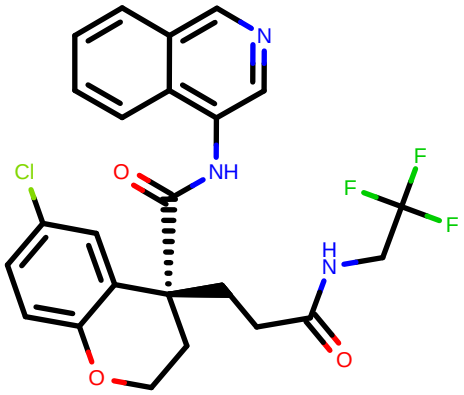
CID:	VLA-UCB-05e51b3f-10_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN318
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.21

MAT-POS-4223bc15-11_16



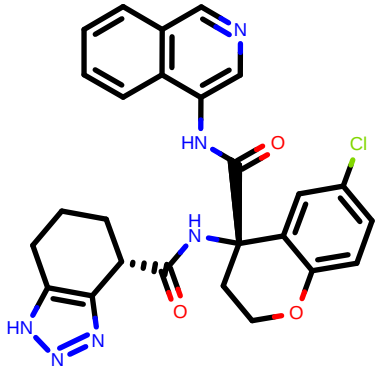
CID:	MAT-POS-4223bc15-11_16
SMILES:	C[C@H]1CC[N@](C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4043
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.13

ALP-UNI-dbbfd3db-4_1



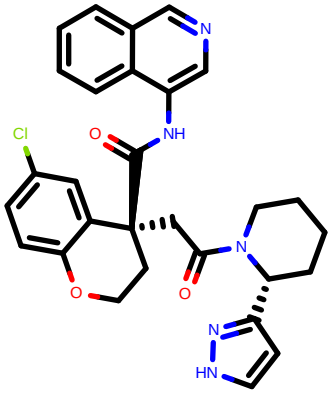
CID:	ALP-UNI-dbbfd3db-4_1
SMILES:	Cc1nc2n(n1)C[C@@H](CC2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2767
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.13

EDJ-MED-009f762b-5_2



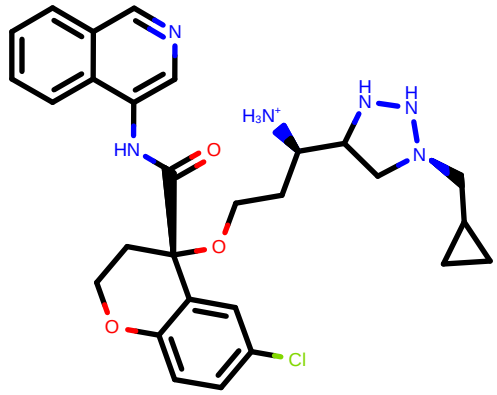
CID:	EDJ-MED-009f762b-5_2
SMILES:	CN(C)C(=O)C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl
RUN:	RUN3915
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.14

BEN-BAS-c2bc0d80-6_1



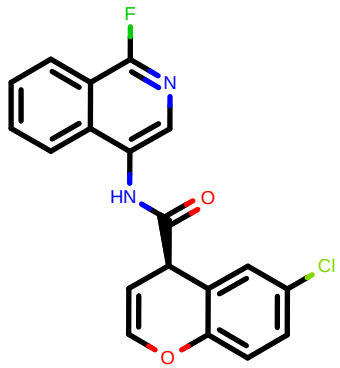
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1137
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.22

RAL-THA-1d44ff04-13_1



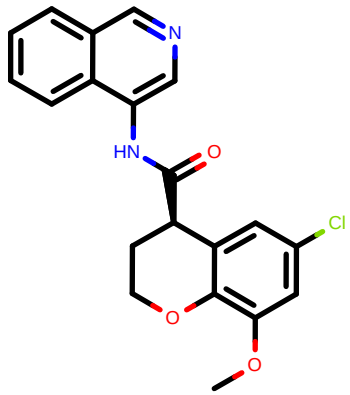
CID:	RAL-THA-1d44ff04-13_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(=O)NO
RUN:	RUN448
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.48

LON-WEI-4d77710c-30_1



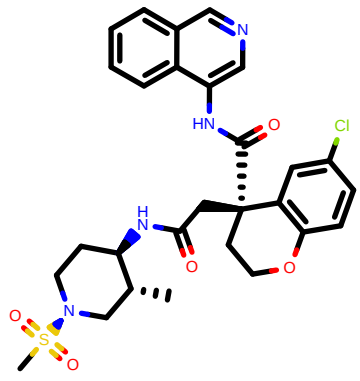
CID:	LON-WEI-4d77710c-30_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)Nc3nc4ccccc4s3
RUN:	RUN213
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.19

DAR-DIA-0cde14eb-52_1



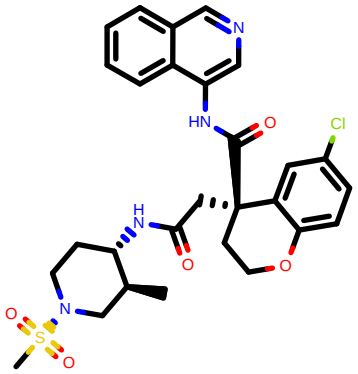
CID:	DAR-DIA-0cde14eb-52_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Nc3cccc(c3)C4(CC4)F
RUN:	RUN18
DDG (kcal/mol):	-1.95
dDDG (kcal/mol):	0.23

LON-WEI-5e7d1b3e-6_1



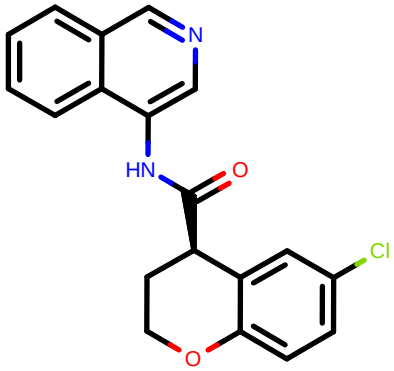
CID:	LON-WEI-5e7d1b3e-6_1
SMILES:	CC(=O)c1cccc(c1)NC(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN1312
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.26

ED_-GRI-5b13fbe2-58_1



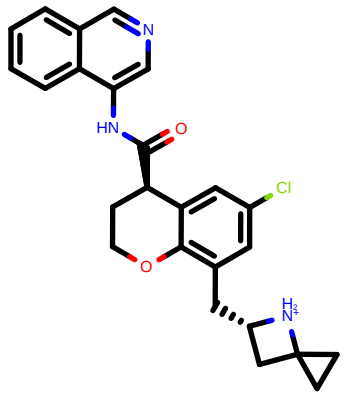
CID:	ED_-GRI-5b13fbe2-58_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cc(nn5)[C@@H]6CCC[NH2+]6
RUN:	RUN1605
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.41

DAR-DIA-0cde14eb-53_1



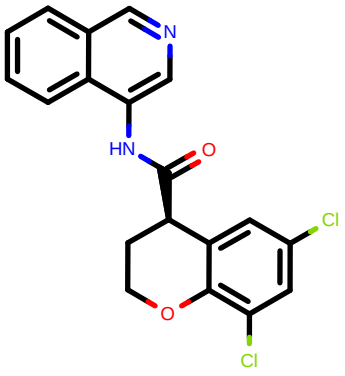
CID:	DAR-DIA-0cde14eb-53_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Nc3cccc(c3)C4(CC4)I
RUN:	RUN20
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.21

VLA-UCB-1dbca3b4-6_1



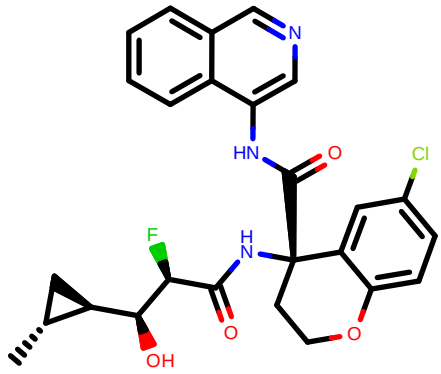
CID:	VLA-UCB-1dbca3b4-6_1
SMILES:	c1ccc2c(c1)cncc2n3c(cc(c3O)c4cccc(c4)Cl)O
RUN:	RUN156
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.40

MAK-UNK-ffc90da7-2_3



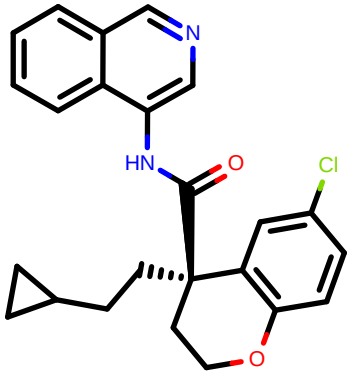
CID:	MAK-UNK-ffc90da7-2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@H]([C@@H]3O)Cl
RUN:	RUN683
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-5_8



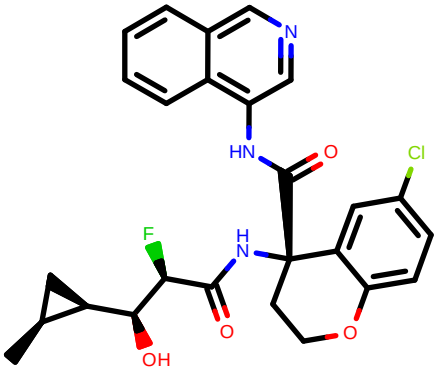
CID:	MAK-UNK-c749d764-5_8
SMILES:	c1ccc2c(c1)cncc2N(CO)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN928
DDG (kcal/mol):	-1.94
dDDG (kcal/mol):	0.32

MAR-TRE-04c86cea-39_1



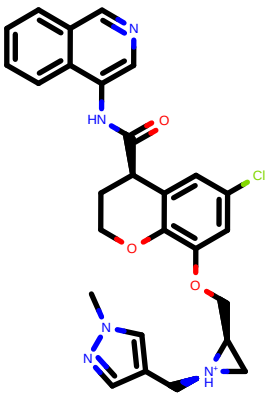
CID:	MAR-TRE-04c86cea-39_1
SMILES:	COc1ccccc1n2cc(c3ccccc3c2=O)C(=O)Nc4ccc(nc4)OC
RUN:	RUN52
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.24

EDJ-MED-6d9ff7d0-7_1



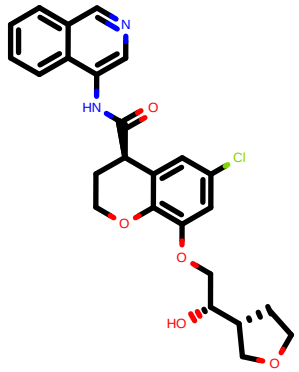
CID:	EDJ-MED-6d9ff7d0-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)[NH2+]CC[C@@H]5CCC(=O)N5
RUN:	RUN3431
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.14

EDG-MED-ba1ac7b9-14_7



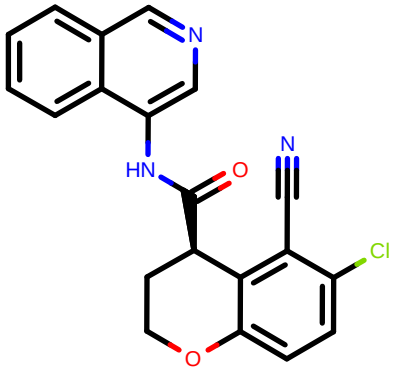
CID:	EDG-MED-ba1ac7b9-14_7
SMILES:	C[N@@]1CCN(C[C@H]1C#N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2672
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.50

ALP-UNI-0676e700-25_1



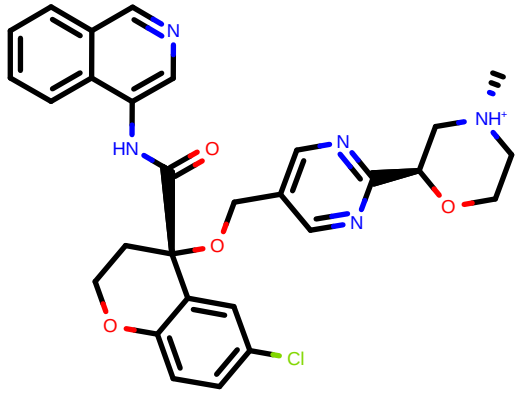
CID:	ALP-UNI-0676e700-25_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cc6nccn6c(=O)[nH]5
RUN:	RUN2470
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.41

MAK-UNK-ffc90da7-2_7



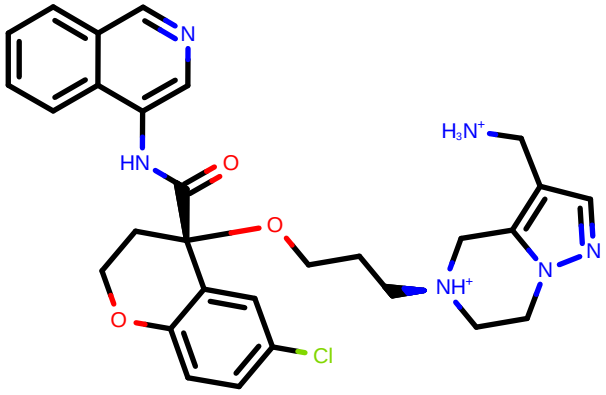
CID:	MAK-UNK-ffc90da7-2_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@H]([C@H]3O)Cl
RUN:	RUN692
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.20

DAR-DIA-23e5a6a0-10_1



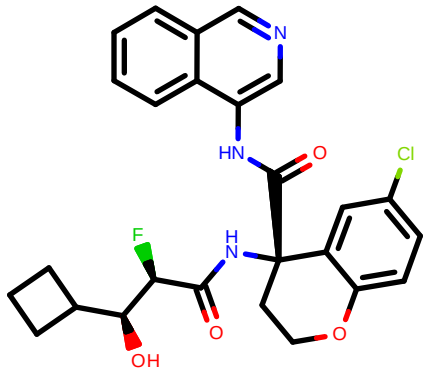
CID:	DAR-DIA-23e5a6a0-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6([NH2+]5)CC6)Cl
RUN:	RUN420
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.18

NAU-LAT-a5c7d7cb-2_1



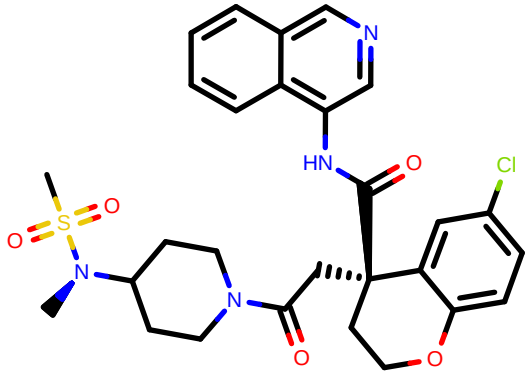
CID:	NAU-LAT-a5c7d7cb-2_1
SMILES:	CC(=O)N1CC[NH+](CC1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN581
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.44

VLA-UCB-34f3ed0c-5_1



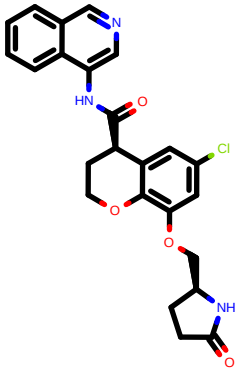
CID:	VLA-UCB-34f3ed0c-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C(=O)CCc4ccn[nH]4
RUN:	RUN635
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.27

MAT-POS-3ccb8ef6-1_1



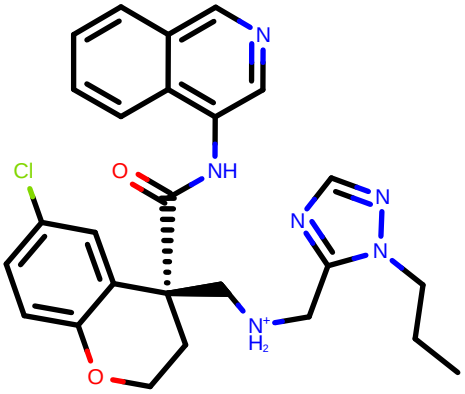
CID:	MAT-POS-3ccb8ef6-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[NH2+]Cc4c3cc(cc4)Cl
RUN:	RUN3625
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.16

EDG-MED-5d232de5-1_1



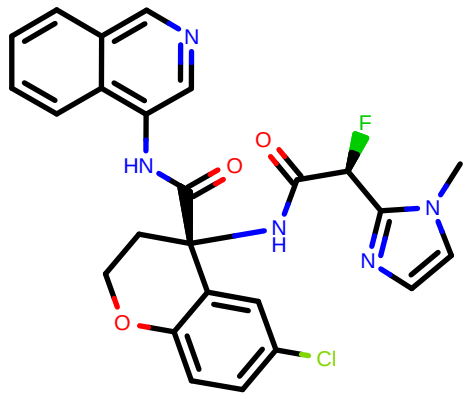
CID:	EDG-MED-5d232de5-1_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2363
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.39

EDJ-MED-1b5395f9-3_1



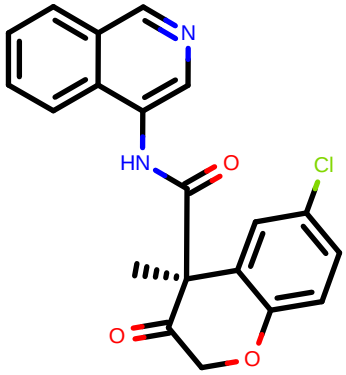
CID:	EDJ-MED-1b5395f9-3_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@H]3C[N@@](Cc4c3cc(c(c4)Cl)Cl)S(=O)(=O)C
RUN:	RUN4465
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.35

MIC-UNK-91acba05-1_1



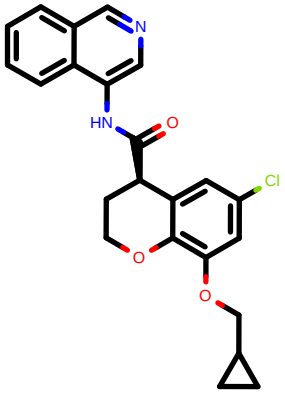
CID:	MIC-UNK-91acba05-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CNC(=O)c4c3cc(cc4)Cl
RUN:	RUN466
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.31

DAR-DIA-23aa0b97-19_1



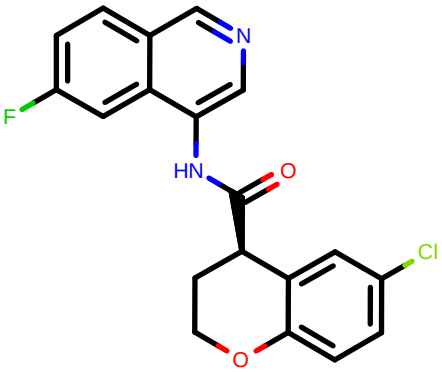
CID:	DAR-DIA-23aa0b97-19_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)C#N
RUN:	RUN1
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.22

ED_-GRI-5b13fbe2-11_1



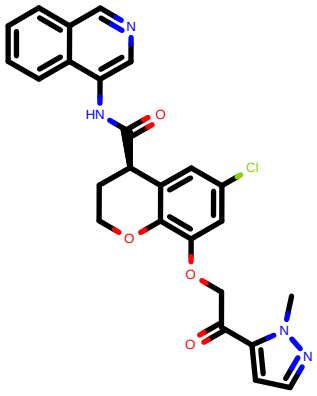
CID:	ED_-GRI-5b13fbe2-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CC[NH+](CC5)CC(=O)N
RUN:	RUN1541
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.29

DAR-DIA-0d514e7d-32_4



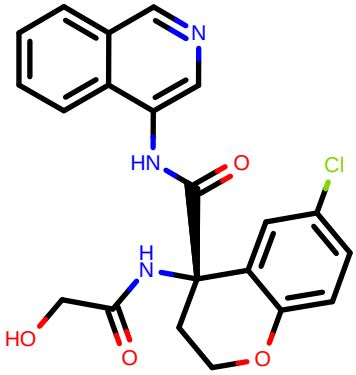
CID:	DAR-DIA-0d514e7d-32_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@H]4C[C@@H]4CO[C@@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN852
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.21

EDJ-MED-d203f206-37_1



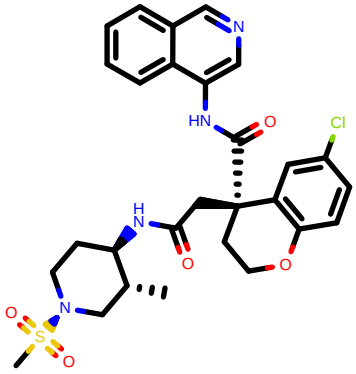
CID:	EDJ-MED-d203f206-37_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCS(=O)CC5
RUN:	RUN2599
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.31

MIC-UNK-cdc2493e-12_2



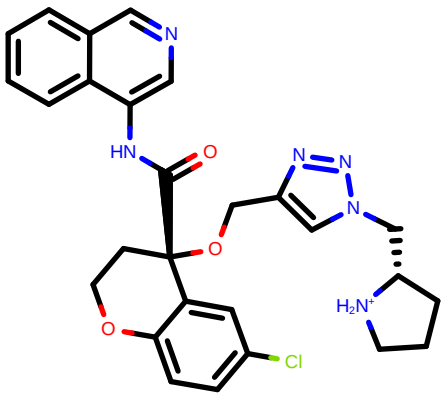
CID:	MIC-UNK-cdc2493e-12_2
SMILES:	C[NH+](C)[C@H]1CC[C@@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN549
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.25

DAR-DIA-56cf811e-1_1



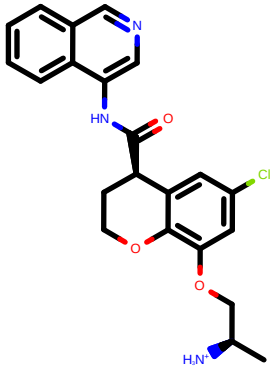
CID:	DAR-DIA-56cf811e-1_1
SMILES:	C#CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1518
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.30

FRA-DIA-b66f7109-3_2



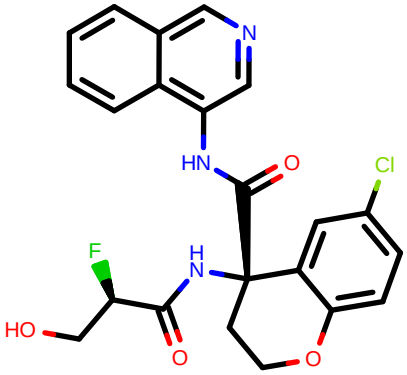
CID:	FRA-DIA-b66f7109-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4Cl)O[C@H]5CC(=O)N5
RUN:	RUN398
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.28

MAT-POS-e9e99895-9_2



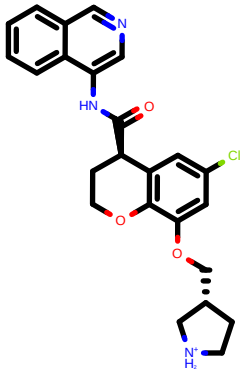
CID:	MAT-POS-e9e99895-9_2
SMILES:	C[C@](c1ccc(c(c1Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)COc4ccc(cc4)C(=O)N
RUN:	RUN2262
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.41

NIR-WEI-acbd6416-2_2



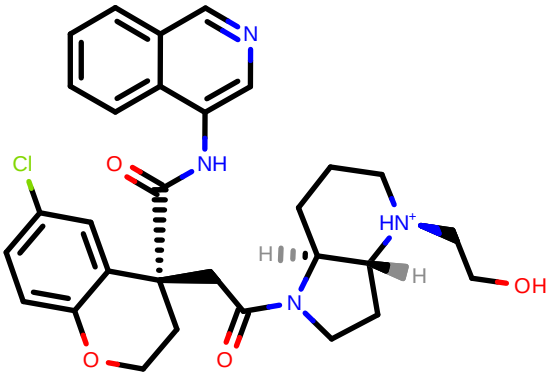
CID:	NIR-WEI-acbd6416-2_2
SMILES:	C=C(c1cncc2c1cccc2)C(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN460
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.25

KAD-UNI-8a629cb0-9_1



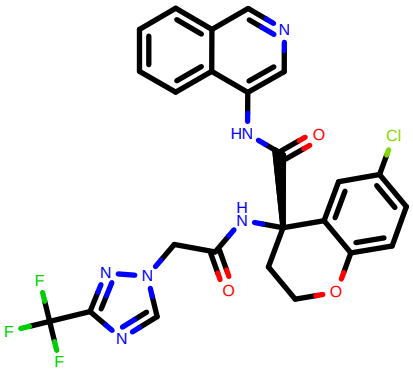
CID:	KAD-UNI-8a629cb0-9_1
SMILES:	C[C@@H](C(=O)N1CCN(CC1)C(=O)C)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2091
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.48

RAL-THA-8416115c-11_2



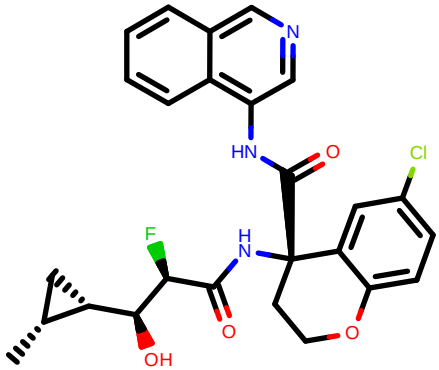
CID:	RAL-THA-8416115c-11_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1288
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.55

RAL-THA-8416115c-1_2



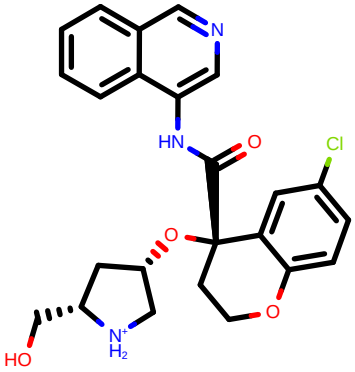
CID:	RAL-THA-8416115c-1_2
SMILES:	c1ccc(cc1)CN2CC[C@@H](c3c2ccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1248
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.34

MIK-ENA-fc9ceda2-1_1



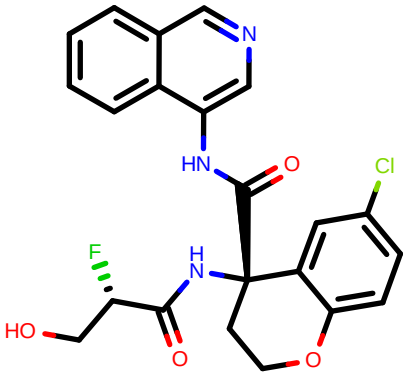
CID:	MIK-ENA-fc9ceda2-1_1
SMILES:	CO[C@@]1(CCOc2c1cc(cc2)Cl)CNc3cncc4c3cccc4
RUN:	RUN3292
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.14

MIC-UNK-91acba05-2_2



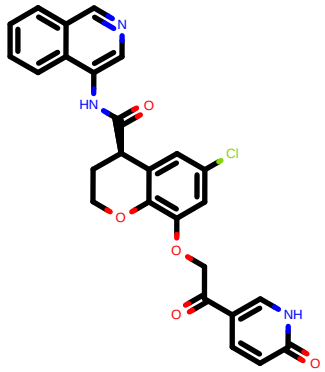
CID:	MIC-UNK-91acba05-2_2
SMILES:	CN1C[C@H](c2cc(ccc2C1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN470
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.36

ALP-UNI-44c99a80-3_1



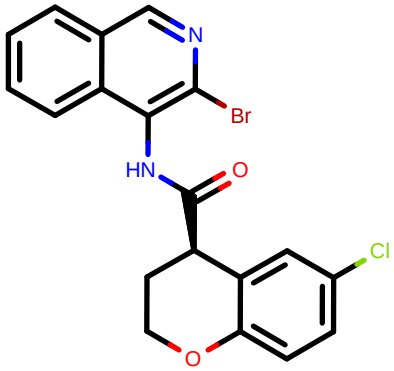
CID:	ALP-UNI-44c99a80-3_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnco3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN461
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.30

LEE-CAM-7ab9b158-4_1



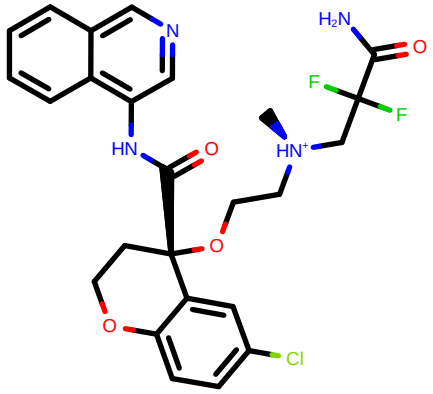
CID:	LEE-CAM-7ab9b158-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@@H]5CN6C[C@H](O5)CCC6=O
RUN:	RUN2209
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.35

LON-WEI-4d77710c-13_2



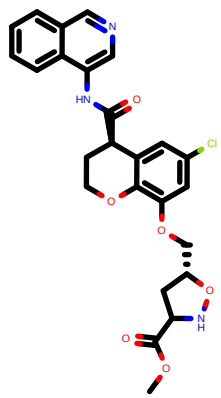
CID:	LON-WEI-4d77710c-13_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NC[C@H]3CCCO3
RUN:	RUN202
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.25

ERI-UCB-b3e6b0c2-18_1



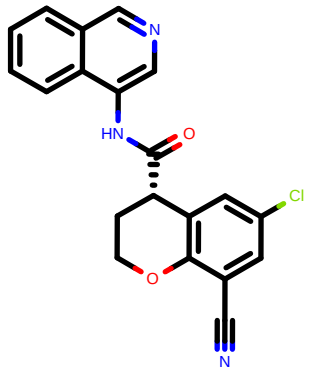
CID:	ERI-UCB-b3e6b0c2-18_1
SMILES:	c1cc2c(cc1CN3CC[NH2+]CC3)cncc2N4CC[C@@]5(C4=O)COc6c5cc(cc6)Cl
RUN:	RUN3052
DDG (kcal/mol):	-1.89
dDDG (kcal/mol):	0.28

EDJ-MED-40433386-1_1



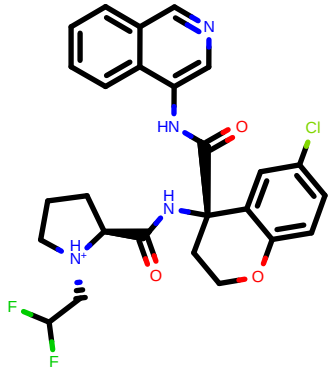
CID:	EDJ-MED-40433386-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCC[N@@]5CC(F)(F)F
RUN:	RUN2554
DDG (kcal/mol):	-1.88
dDDG (kcal/mol):	0.37

MIC-UNK-50cce87d-12_2



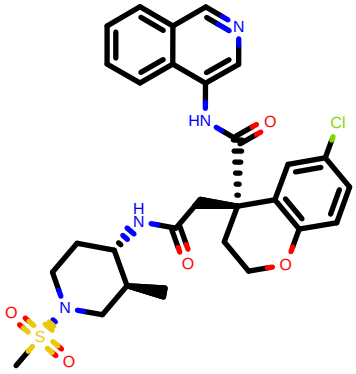
CID:	MIC-UNK-50cce87d-12_2
SMILES:	COc1cccc2c1c(cnc2)N3CCC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN680
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.13

JAG-UCB-706446eb-7_1



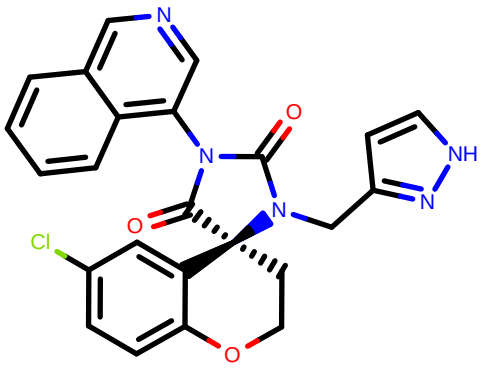
CID:	JAG-UCB-706446eb-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCCOC5
RUN:	RUN622
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.31

DAR-DIA-0d514e7d-32_31



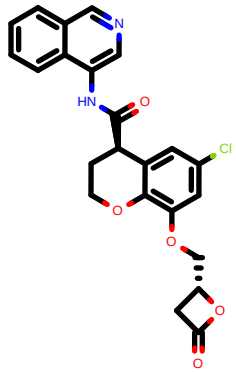
CID:	DAR-DIA-0d514e7d-32_31
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@H]4C[C@H]4CO[C@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN881
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.35

MAT-POS-a13804f0-4_2



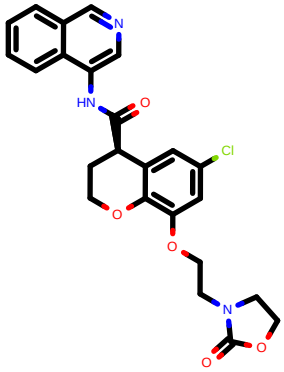
CID:	MAT-POS-a13804f0-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN3491
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.18

LEE-CAM-7ab9b158-2_1



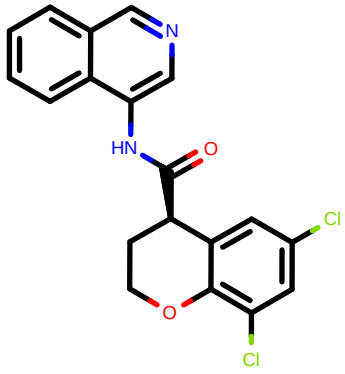
CID:	LEE-CAM-7ab9b158-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COCc5[nH]c(=O)c6c(n5)CCOC6
RUN:	RUN2207
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.37

ALP-POS-5bb456a5-2_2



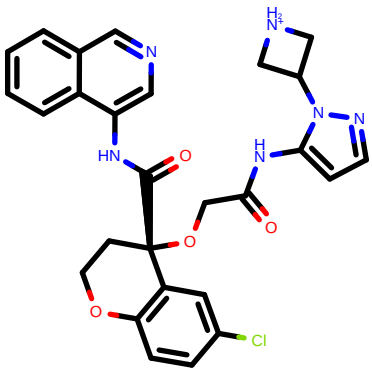
CID:	ALP-POS-5bb456a5-2_2
SMILES:	C[C@H]1C[N@@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2424
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.41

MIC-UNK-5a93dd5f-12_5



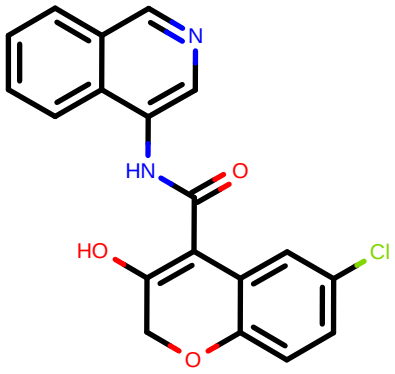
CID:	MIC-UNK-5a93dd5f-12_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@@]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN794
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.20

MIC-UNK-644c43c7-4_1



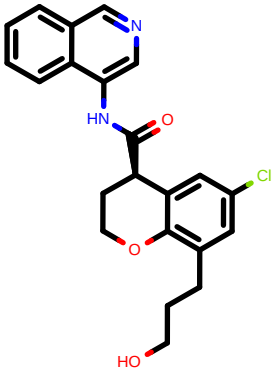
CID:	MIC-UNK-644c43c7-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CNC(C(F)(F)F)C(F)(F)F
RUN:	RUN439
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.36

MAT-POS-b5746674-35_1



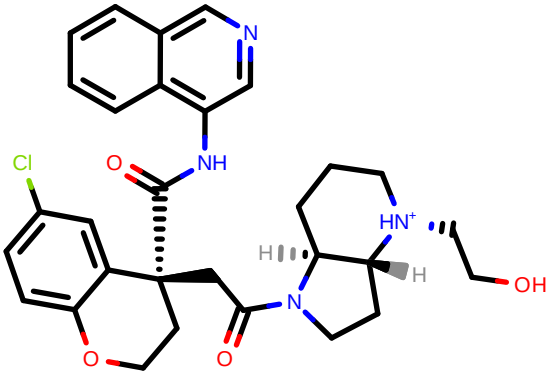
CID:	MAT-POS-b5746674-35_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCC[N@@H+](Cc3ccco3)C4CCCC4
RUN:	RUN69
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.24

MAT-POS-8a69d52e-4_4



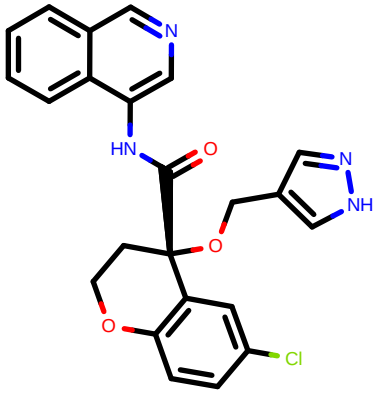
CID:	MAT-POS-8a69d52e-4_4
SMILES:	C[C@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN369
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.30

MAT-POS-e6dd326d-7_2



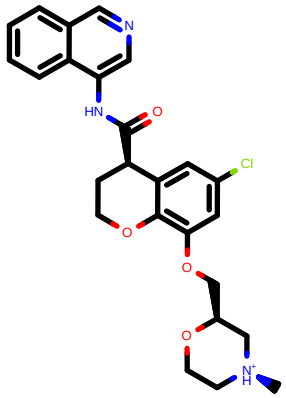
CID:	MAT-POS-e6dd326d-7_2
SMILES:	CCOC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3952
DDG (kcal/mol):	-1.86
dDDG (kcal/mol):	0.36

MAT-POS-8a69d52e-7_1



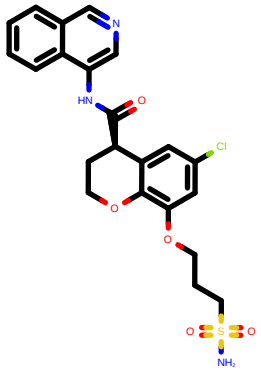
CID:	MAT-POS-8a69d52e-7_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN375
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.25

MAT-POS-fce787c2-9_1



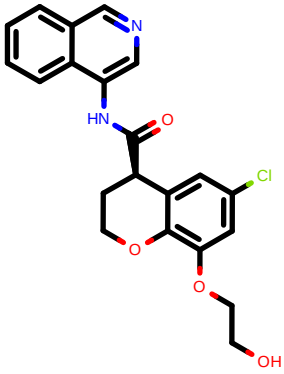
CID:	MAT-POS-fce787c2-9_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)[NH2+]C
RUN:	RUN2156
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.44

EDJ-MED-d08626de-1_1



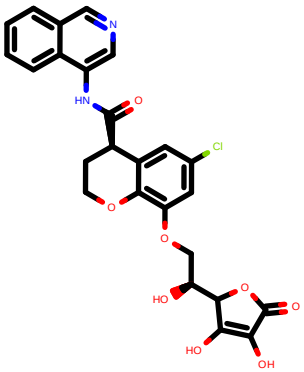
CID:	EDJ-MED-d08626de-1_1
SMILES:	CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2340
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.37

MAT-POS-afd4d4fd-2_1



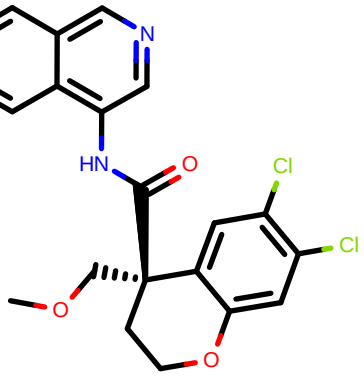
CID:	MAT-POS-afd4d4fd-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(n3)Cl
RUN:	RUN304
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.28

EDJ-MED-d203f206-32_1



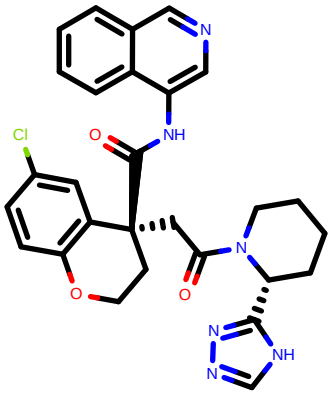
CID:	EDJ-MED-d203f206-32_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6COCCN6C(=O)C5
RUN:	RUN2593
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.45

MIC-UNK-5d22d78d-1_1



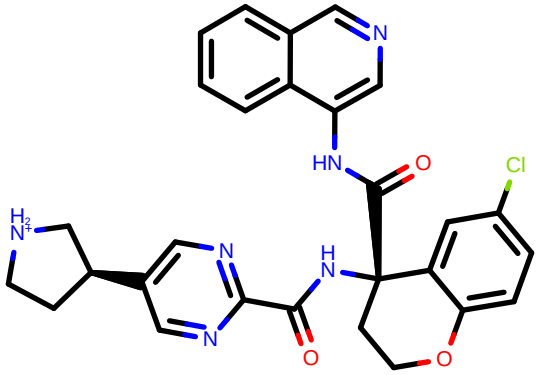
CID:	MIC-UNK-5d22d78d-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5CC5
RUN:	RUN4200
DDG (kcal/mol):	-1.84
dDDG (kcal/mol):	0.09

NAU-LAT-2fed8305-9_1



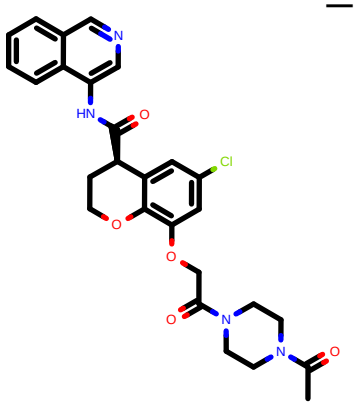
CID:	NAU-LAT-2fed8305-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(co3)Cl
RUN:	RUN1115
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.23

MAK-UNK-ffc90da7-4_4



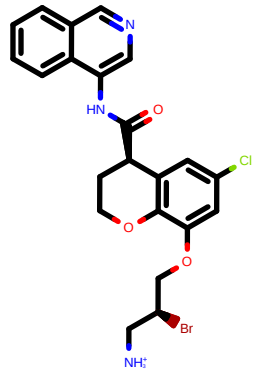
CID:	MAK-UNK-ffc90da7-4_4
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN697
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.28

MAT-POS-1f3f1a6f-2_1



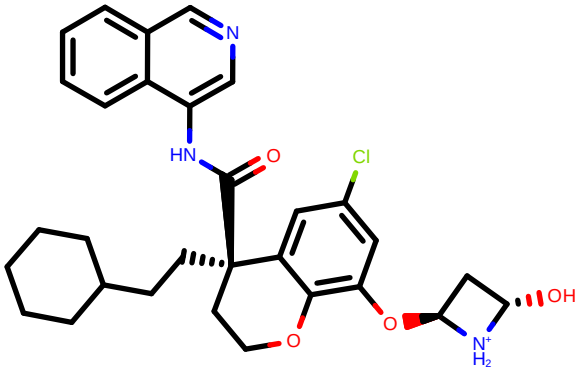
CID:	MAT-POS-1f3f1a6f-2_1
SMILES:	C[NH+](C)[C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2277
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.38

MAT-POS-e9e99895-5_2



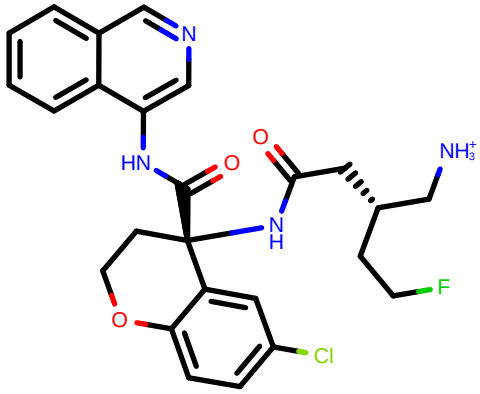
CID:	MAT-POS-e9e99895-5_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)c4cc5n(n4)CCO5
RUN:	RUN2250
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.44

ERI-UCB-ce40166b-7_1



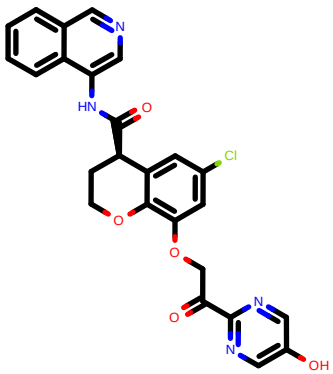
CID:	ERI-UCB-ce40166b-7_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Cl)Oc4cccc(=O)[nH]4
RUN:	RUN44
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.32

ADA-UCB-dc2b944c-4_1



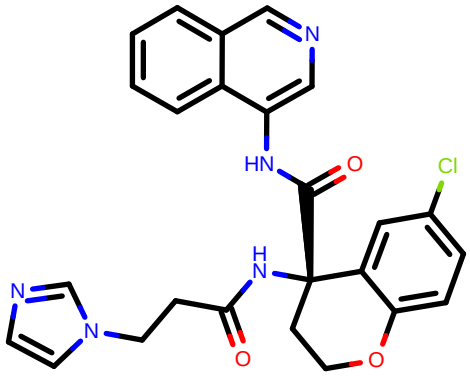
CID:	ADA-UCB-dc2b944c-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]34C[C@H]3COc5c4cc(cc5)Cl
RUN:	RUN600
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.36

EDJ-MED-6864a934-2_1



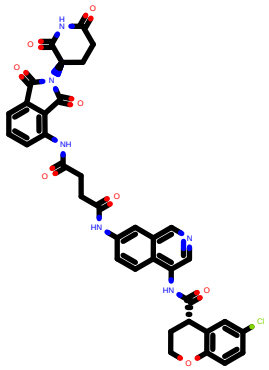
CID:	EDJ-MED-6864a934-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6n(n5)CCO6
RUN:	RUN2606
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.39

NAU-LAT-a5c7d7cb-5_2



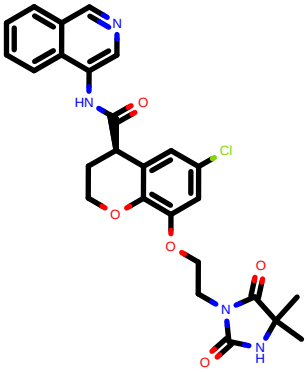
CID:	NAU-LAT-a5c7d7cb-5_2
SMILES:	CC(=O)N1CC[NH+](CC1)[C@H](c2ccc(cc2)N(C)C)C(=O)Cc3cncc4c3cccc4
RUN:	RUN580
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.24

VLA-UNK-9a7dc93f-5_1



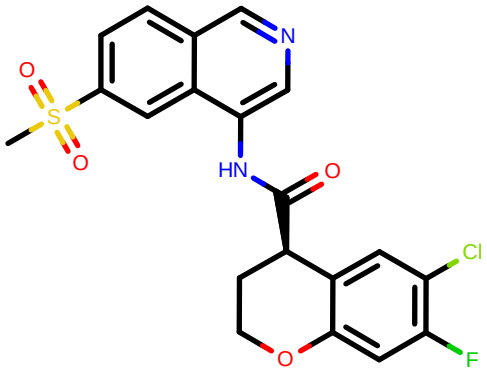
CID:	VLA-UNK-9a7dc93f-5_1
SMILES:	CO[C@@H](c1cc(c(c(c1)Cl)F)F)C(=O)Nc2cncc3c2cccc3
RUN:	RUN3085
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.45

MAT-POS-e9e99895-8_2



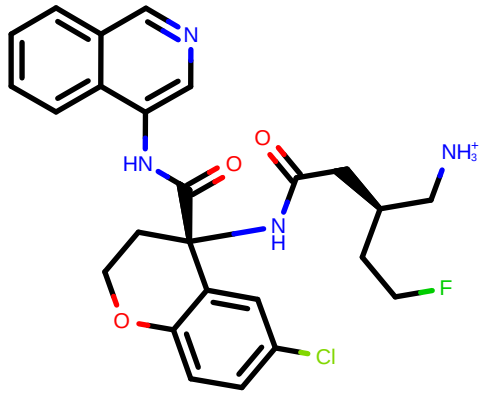
CID:	MAT-POS-e9e99895-8_2
SMILES:	Cc1nc2n(n1)C[C@H](CC2)C(=O)N[C@@](C)(c3ccc(c(c3)Cl)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2252
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.37

LAU-MED-88a3970a-12_1



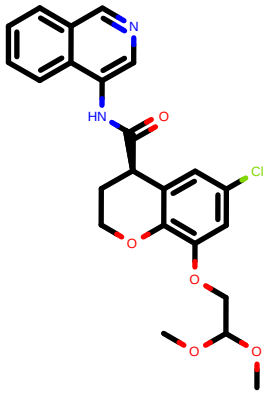
CID:	LAU-MED-88a3970a-12_1
SMILES:	C[NH2+]CCCc1cc(cc2c1OCC[C@@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1508
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.23

ADA-UCB-dc2b944c-17_1



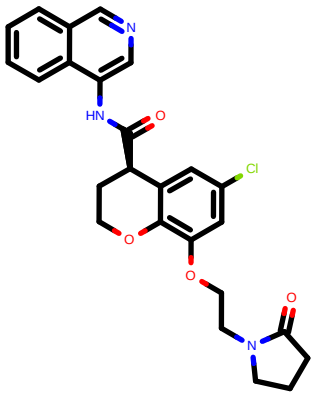
CID:	ADA-UCB-dc2b944c-17_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cc(ccc4Cl)Cl
RUN:	RUN615
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.28

ALP-POS-e0fe77e5-10_1



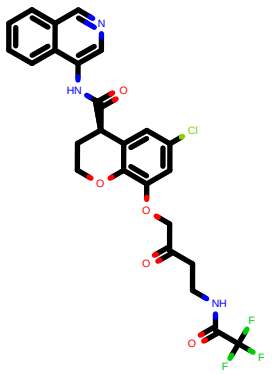
CID:	ALP-POS-e0fe77e5-10_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@@]4(C3=O)CCNc5c4cc(c(c5)Cl)Cl
RUN:	RUN2326
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.40

ALP-UNI-0676e700-20_1



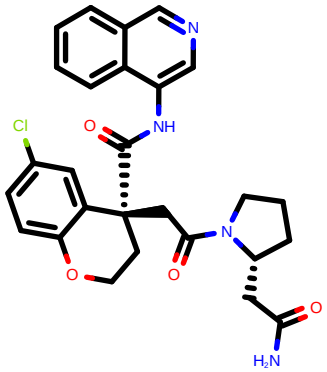
CID:	ALP-UNI-0676e700-20_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cn5)n6cnnn6
RUN:	RUN2467
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.42

KAD-UNI-80f122c8-2_2



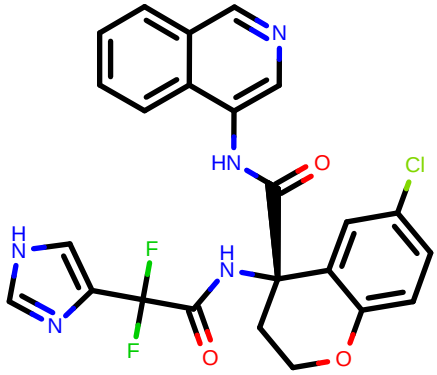
CID:	KAD-UNI-80f122c8-2_2
SMILES:	CC(=O)N1C[C@H]2C[C@@H]1CN2C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2286
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.31

NAU-LAT-2fed8305-5_1



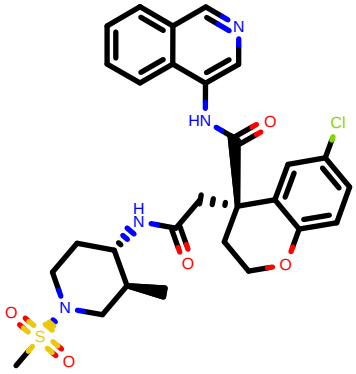
CID:	NAU-LAT-2fed8305-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cs3)Cl
RUN:	RUN1111
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.22

NAU-LAT-a5c7d7cb-2_2



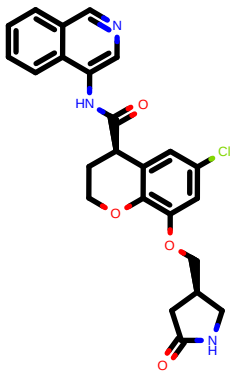
CID:	NAU-LAT-a5c7d7cb-2_2
SMILES:	CC(=O)N1CC[NH+](CC1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN582
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.33

MAK-UNK-c749d764-1_5



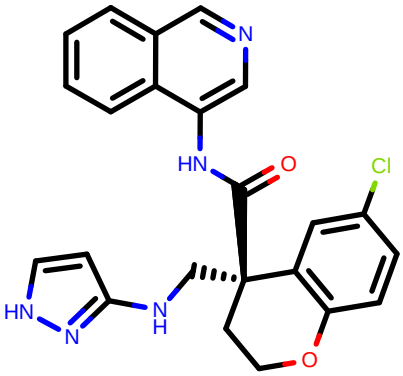
CID:	MAK-UNK-c749d764-1_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C4CC4
RUN:	RUN893
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.32

CHO-MSK-a31cca77-2_1



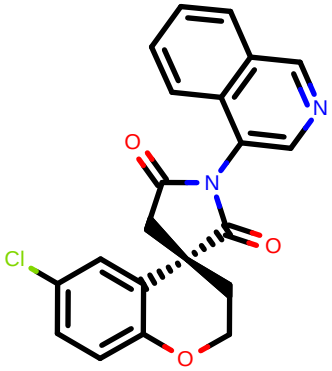
CID:	CHO-MSK-a31cca77-2_1
SMILES:	Cn1cnnc1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2193
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.32

ED_-GRI-5b13fbe2-21_1



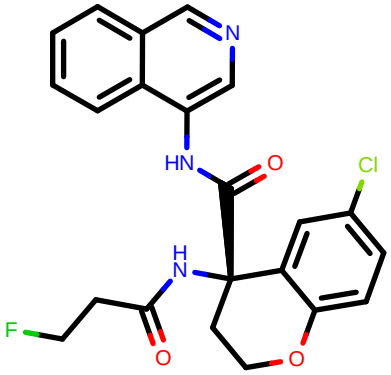
CID:	ED_-GRI-5b13fbe2-21_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[NH2+]C[C@@H](O5)CO
RUN:	RUN1550
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.14

EDG-MED-ba1ac7b9-17_1



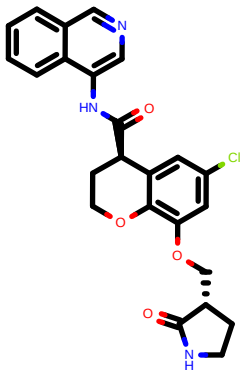
CID:	EDG-MED-ba1ac7b9-17_1
SMILES:	Cn1ccnc1CN(C2CC2)C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2688
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.15

MAK-UNK-ffc90da7-7_1



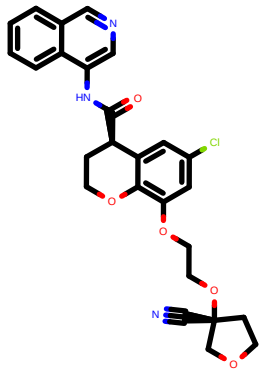
CID:	MAK-UNK-ffc90da7-7_1
SMILES:	CC(C)OC[C@@H]([C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)[NH2+]C
RUN:	RUN707
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.27

EDG-MED-5d232de5-5_1



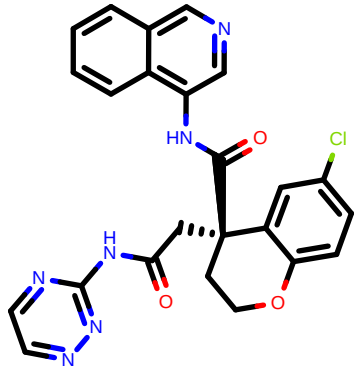
CID:	EDG-MED-5d232de5-5_1
SMILES:	CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2367
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.41

EDJ-MED-d203f206-4_1



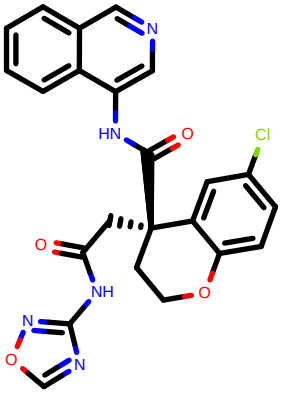
CID:	EDJ-MED-d203f206-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN2566
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.58

ALP-UNI-c3ef0aba-2_1



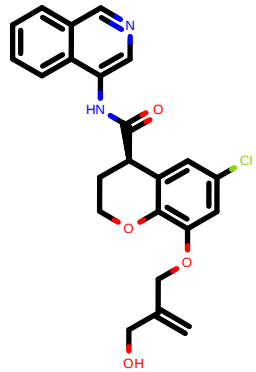
CID:	ALP-UNI-c3ef0aba-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3COCc4c3cc(cc4)Cl
RUN:	RUN3545
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.13

EDJ-MED-15e90dfc-6_2



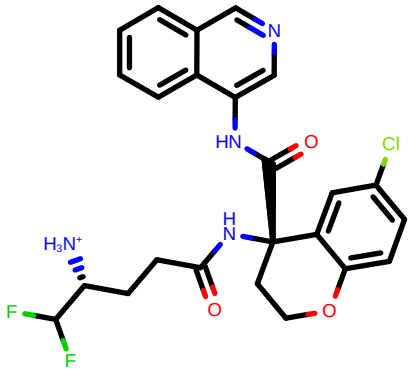
CID:	EDJ-MED-15e90dfc-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@@H]5CCC(=O)N5
RUN:	RUN3447
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.12

RAL-THA-05e671eb-35_1



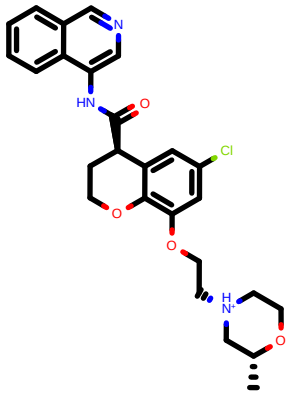
CID:	RAL-THA-05e671eb-35_1
SMILES:	COc1cccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2074
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.38

NAU-LAT-a5c7d7cb-5_1



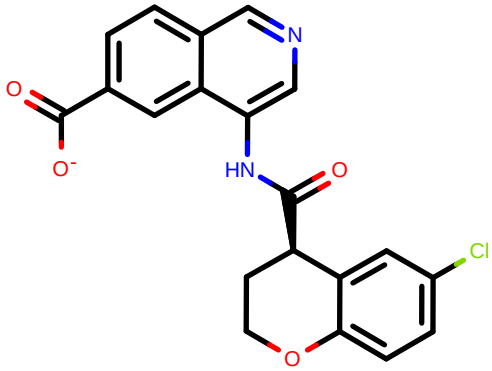
CID:	NAU-LAT-a5c7d7cb-5_1
SMILES:	CC(=O)N1CC[NH+](CC1)[C@@H](c2ccc(cc2)N(C)C)C(=O)Cc3cncc4c3cccc4
RUN:	RUN579
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.38

ALP-UNI-3496895b-15_4



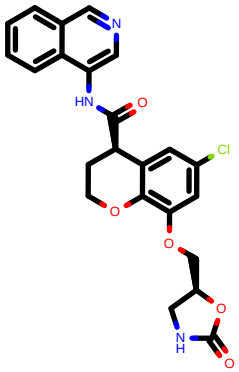
CID:	ALP-UNI-3496895b-15_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN2534
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.40

LON-WEI-4d77710c-58_1



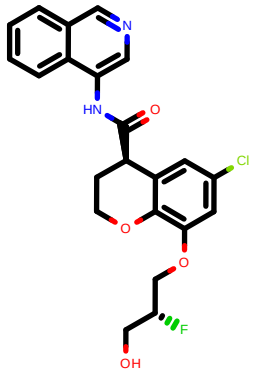
CID:	LON-WEI-4d77710c-58_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)Nc3nc4ccc(cc4s3)OC
RUN:	RUN250
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.19

EDJ-MED-d203f206-39_1



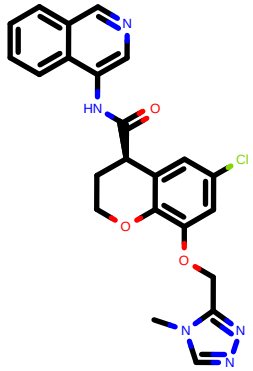
CID:	EDJ-MED-d203f206-39_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@](C5)(C(=O)N)O
RUN:	RUN2601
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.44

MAT-POS-1f3f1a6f-5_1



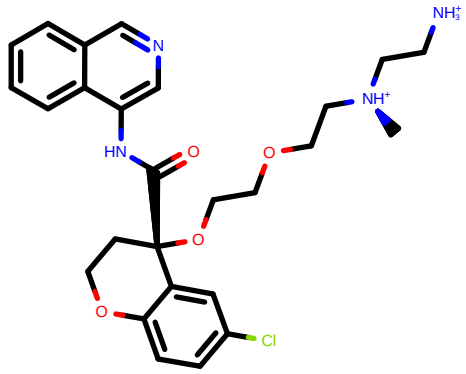
CID:	MAT-POS-1f3f1a6f-5_1
SMILES:	c1ccc2c(c1)cncc2n3c(c([nH]c3=O)c4ccc(c(c4)Cl)Cl)[O-]
RUN:	RUN2279
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.37

ALP-POS-5bb456a5-1_3



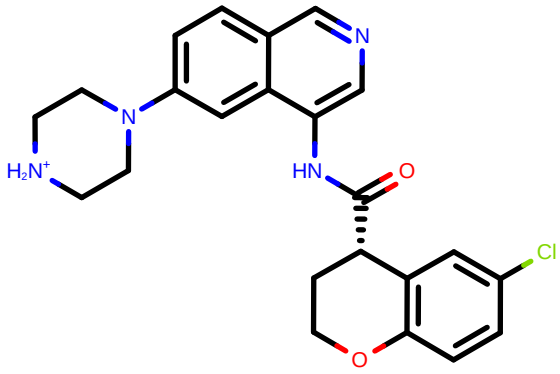
CID:	ALP-POS-5bb456a5-1_3
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2409
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.39

MAR-UCB-f313ec4d-6_1



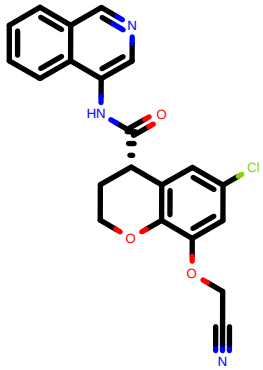
CID:	MAR-UCB-f313ec4d-6_1
SMILES:	c1ccc(cc1)N2CCN(CC2)C(=O)c3cncc4c3cccc4
RUN:	RUN330
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.46

MAT-POS-2492181e-7_1



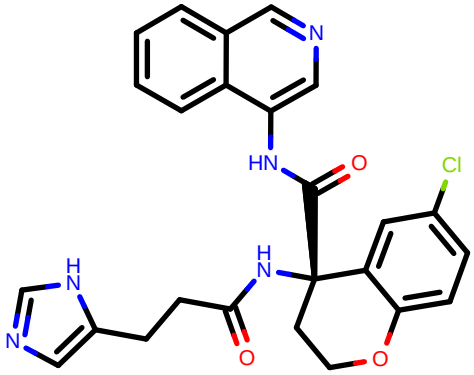
CID:	MAT-POS-2492181e-7_1
SMILES:	CC1CC[NH+](CC1)CCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN100
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.13

MAT-POS-e9e99895-2_4



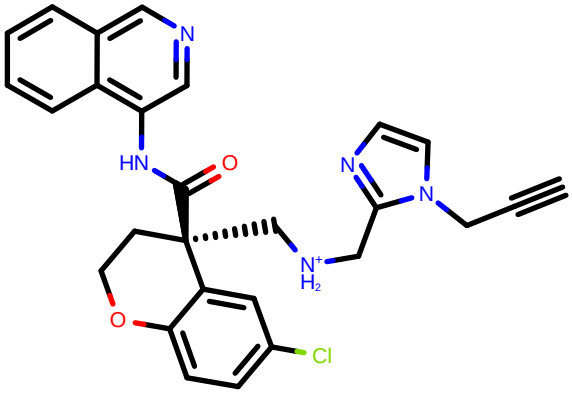
CID:	MAT-POS-e9e99895-2_4
SMILES:	CC(C)[N@H+]1CCO[C@H](C1)C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2237
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.19

MIC-UNK-bcd487e9-7_1



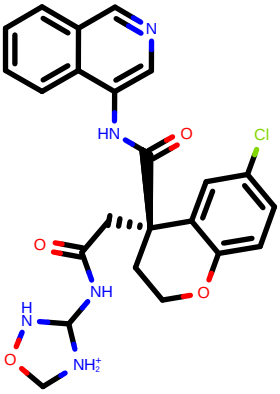
CID:	MIC-UNK-bcd487e9-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(Cc3cn[nH]n3)c4cccc(c4)Cl
RUN:	RUN595
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.27

EDJ-MED-1981ceba-5_3



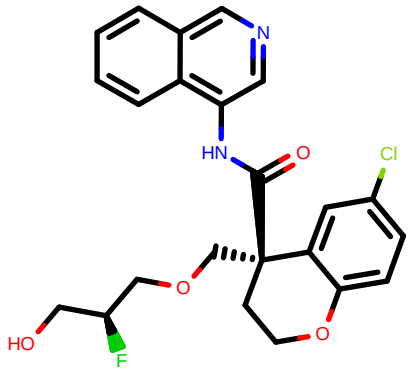
CID:	EDJ-MED-1981ceba-5_3
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4699
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.29

MAK-UNK-c749d764-22_5



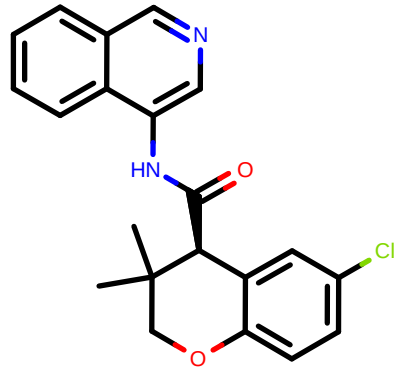
CID:	MAK-UNK-c749d764-22_5
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1026
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.27

KAD-UNI-cb0f2bbc-8_1



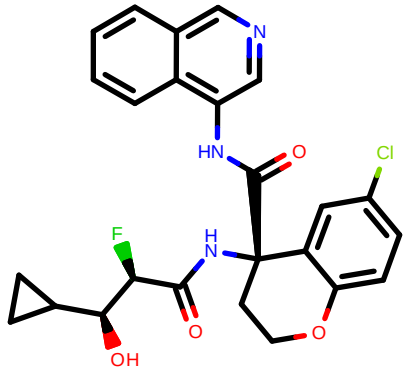
CID:	KAD-UNI-cb0f2bbc-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4cc(cc4)Cl)C[NH2+]Cc5c(nc6ccccn6c5=O)N7CCOCC7
RUN:	RUN3690
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.13

MAT-POS-3b92565d-1_1



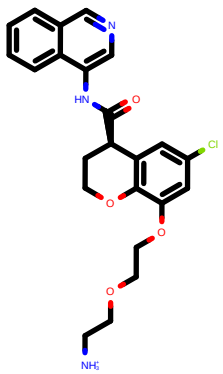
CID:	MAT-POS-3b92565d-1_1
SMILES:	COc1ccc(cc1CC(=O)Nc2cncc3c2cccc3)Cl
RUN:	RUN106
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.19

MIC-UNK-b9827f26-2_1



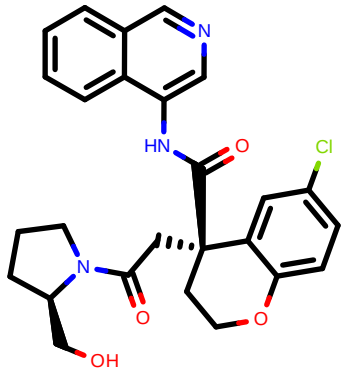
CID:	MIC-UNK-b9827f26-2_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N3CCN(C(=O)C3)c4cc(cc(c4)Cl)Cl
RUN:	RUN3247
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.12

EDJ-MED-2f867453-1_1



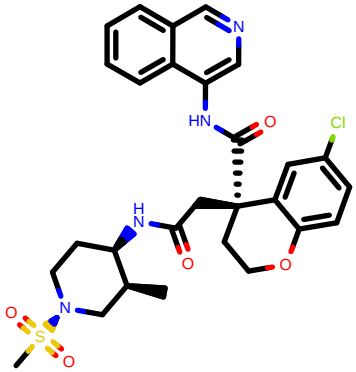
CID:	EDJ-MED-2f867453-1_1
SMILES:	C[C@@]1(CNc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2334
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.54

MAK-UNK-c749d764-33_5



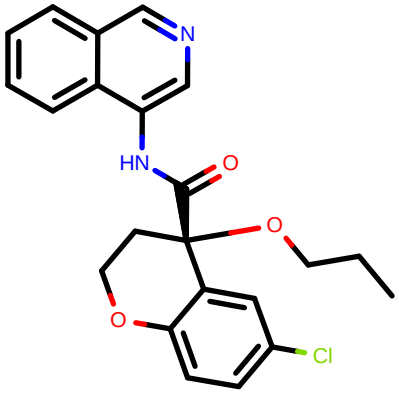
CID:	MAK-UNK-c749d764-33_5
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1084
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.29

MAK-UNK-c749d764-16_1



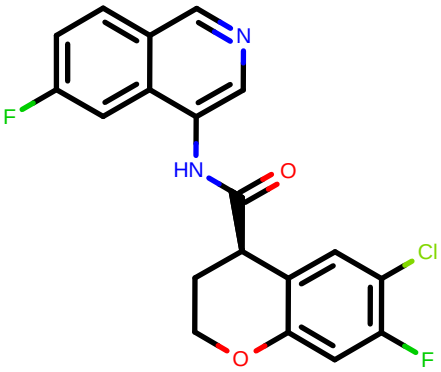
CID:	MAK-UNK-c749d764-16_1
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F)O
RUN:	RUN974
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.25

DAR-DIA-9e4459de-13_1



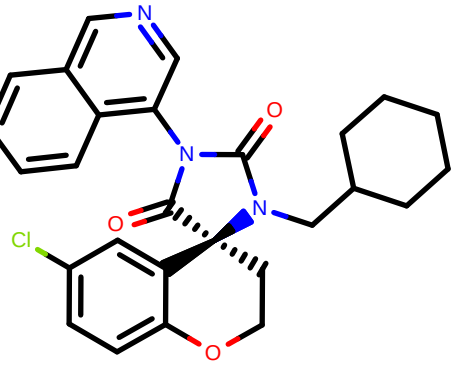
CID:	DAR-DIA-9e4459de-13_1
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1425
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.23

ED_-GRI-5b13fbe2-74_2



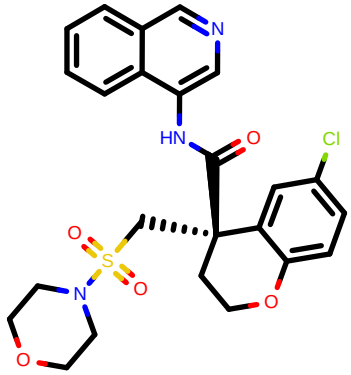
CID:	ED_-GRI-5b13fbe2-74_2
SMILES:	C[N@H+]1CCO[C@@H](C1)c2nccc(n2)CO[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN1632
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.21

ALF-EVA-0b412456-7_1



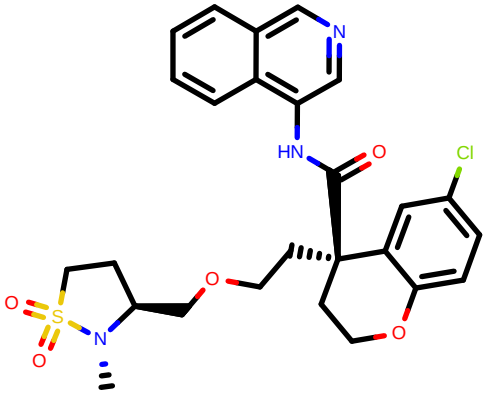
CID:	ALF-EVA-0b412456-7_1
SMILES:	c1cc2c(cc1OCC3CC3)cncc2NC(=O)Cc4cc(cc(c4)Cl)O[C@@H]5CC(=O)N5
RUN:	RUN2764
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.20

EDG-MED-90036822-7_2



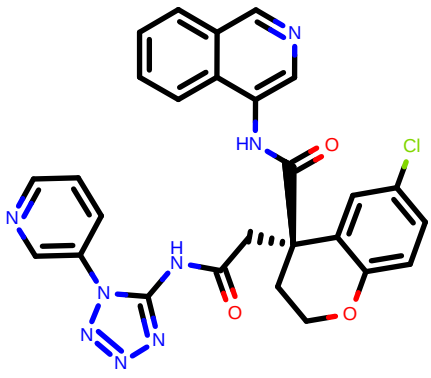
CID:	EDG-MED-90036822-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]5CC(=O)N(C5)CCC[NH3+]
RUN:	RUN1668
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.30

EDJ-MED-6d9ff7d0-1_1



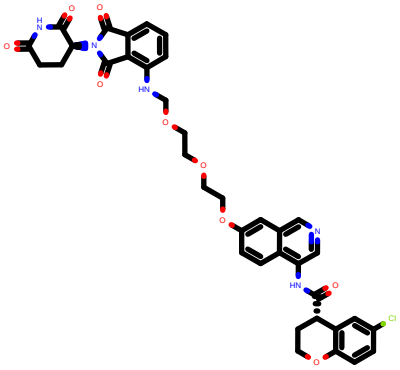
CID:	EDJ-MED-6d9ff7d0-1_1
SMILES:	COCCCC[NH2+][C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3427
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-25_4



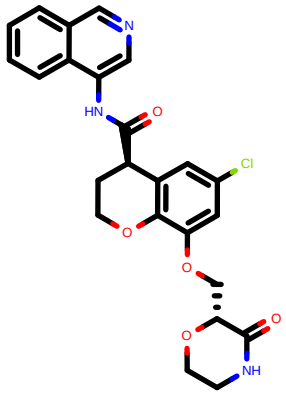
CID:	MAK-UNK-c749d764-25_4
SMILES:	COC(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1041
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.28

DAR-DIA-6a508060-1_2



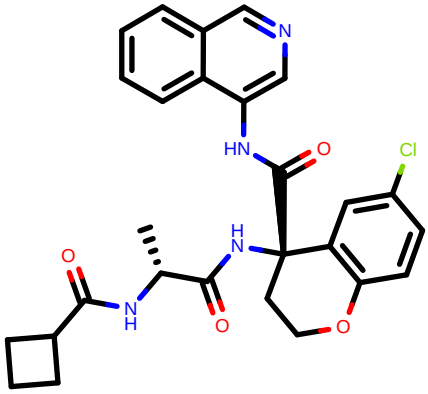
CID:	DAR-DIA-6a508060-1_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN333
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.51

ALP-POS-5bb456a5-2_1



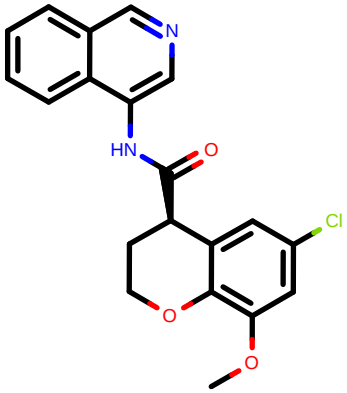
CID:	ALP-POS-5bb456a5-2_1
SMILES:	C[C@@H]1C[N@@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2422
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.41

RAL-THA-8416115c-12_1



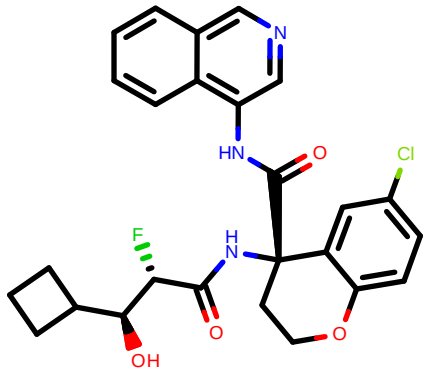
CID:	RAL-THA-8416115c-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5n[n-]nn5
RUN:	RUN1291
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.30

MAK-UNK-ffc90da7-7_2



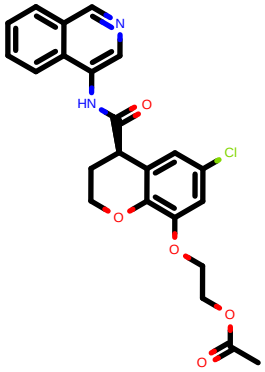
CID:	MAK-UNK-ffc90da7-7_2
SMILES:	CC(C)OC[C@H]([C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)[NH2+]C
RUN:	RUN708
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.21

ALF-EVA-b701bd13-6_2



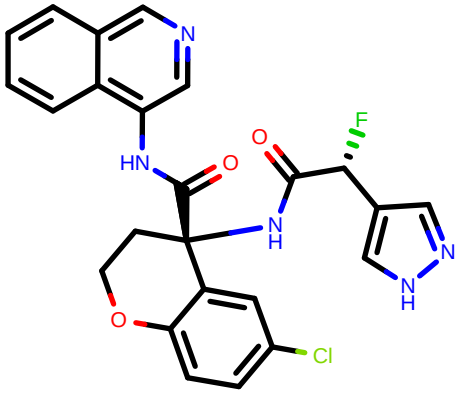
CID:	ALF-EVA-b701bd13-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCC(=O)Nc4c3cc(c(c4)Cl)Cl
RUN:	RUN3641
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.17

EDJ-MED-6864a934-1_1



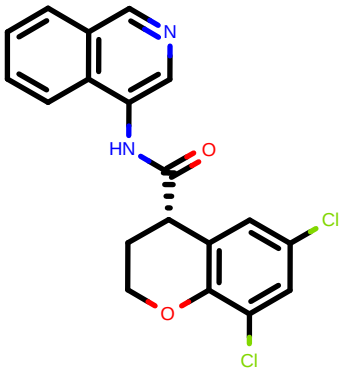
CID:	EDJ-MED-6864a934-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc(cc(c5)CO)CO
RUN:	RUN2605
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.36

EDJ-MED-f893e2a1-3_2



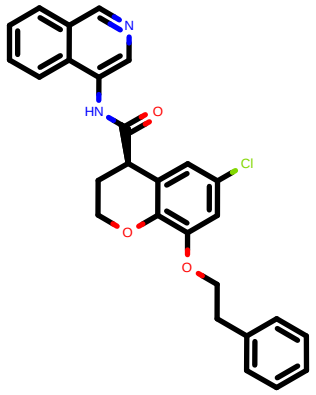
CID:	EDJ-MED-f893e2a1-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]CC5(CCC5)CO
RUN:	RUN3197
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.15

DAR-DIA-0d514e7d-1_1



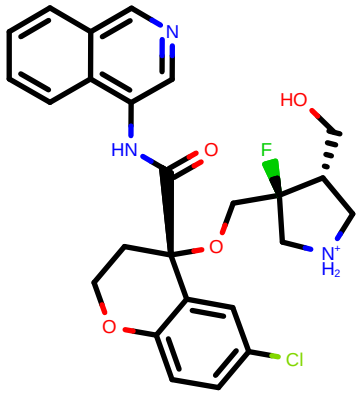
CID:	DAR-DIA-0d514e7d-1_1
SMILES:	C[C@H]1COc2c(cc(cc2OC)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4
RUN:	RUN804
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.11

ED_-GRI-5b13fbe2-50_1



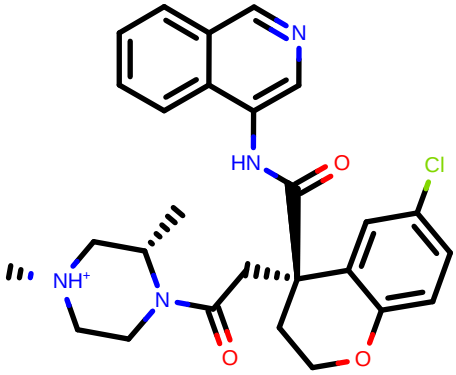
CID:	ED_-GRI-5b13fbe2-50_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5C[C@@]5(C#N)C(=O)[O-]
RUN:	RUN1587
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.50

VLA-UNK-4b5c0188-1_1



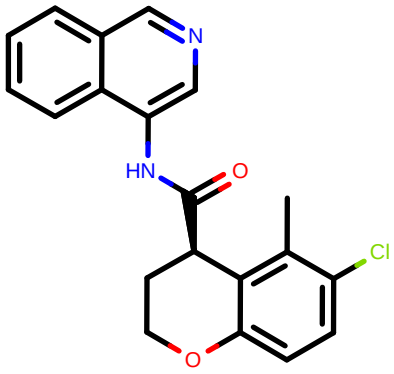
CID:	VLA-UNK-4b5c0188-1_1
SMILES:	c1ccc2c(c1)cncc2N(C[C@@H]3CO3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN3074
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.23

BEN-BAS-c2bc0d80-5_1



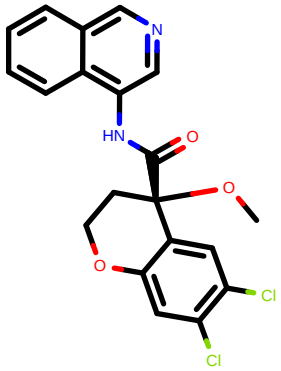
CID:	BEN-BAS-c2bc0d80-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3[nH]c(cc4=O)Cl
RUN:	RUN1140
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.30

MAK-UNK-ffc90da7-2_4



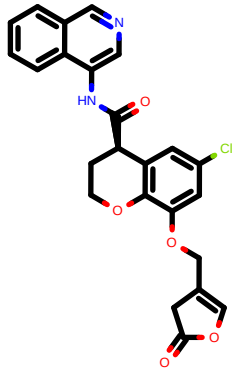
CID:	MAK-UNK-ffc90da7-2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@H]([C@@H]3O)Cl
RUN:	RUN684
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.17

MAT-POS-23a8a11a-1_1



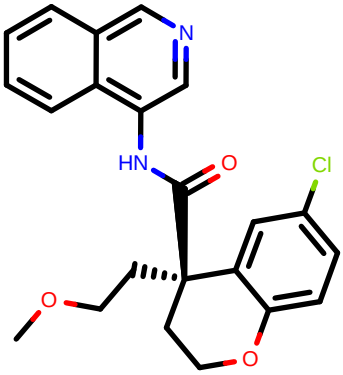
CID:	MAT-POS-23a8a11a-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3ccc(c(c3)Cl)Cl
RUN:	RUN1406
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.23

EDG-MED-5d232de5-6_1



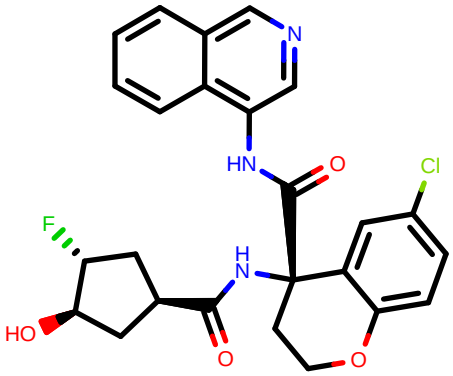
CID:	EDG-MED-5d232de5-6_1
SMILES:	CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2371
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.34

VLA-UNK-5c5a631c-1_2



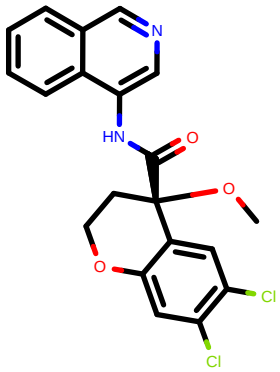
CID:	VLA-UNK-5c5a631c-1_2
SMILES:	c1ccc2c(c1)cncc2N(CC[C@H](O)S(=O)(=O)[O-])C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2916
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.08

MIC-UNK-02d7a284-2_1



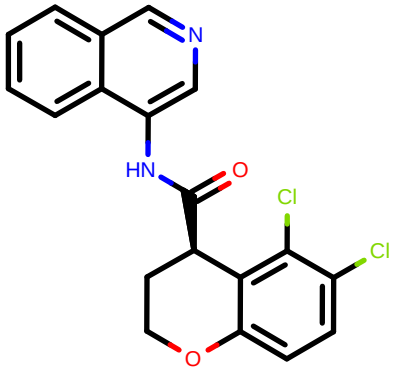
CID:	MIC-UNK-02d7a284-2_1
SMILES:	CCC(=O)N1CCC2(CC1)CN(CC(=O)N2c3cccc(c3)Cl)C(=O)c4cncc5c4cccc5
RUN:	RUN3261
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.13

DAR-DIA-9e4459de-11_13



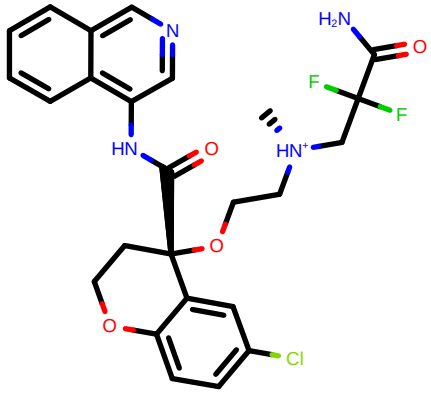
CID:	DAR-DIA-9e4459de-11_13
SMILES:	c1cc2c(c(c1)NCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1421
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.23

MAK-UNK-ffc90da7-2_1



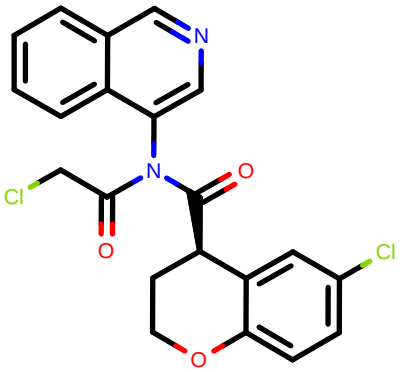
CID:	MAK-UNK-ffc90da7-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)Cl
RUN:	RUN681
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.18

ERI-UCB-b3e6b0c2-5_1



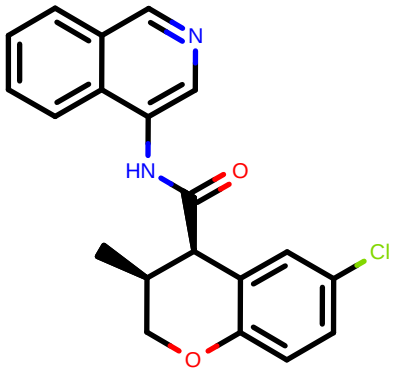
CID:	ERI-UCB-b3e6b0c2-5_1
SMILES:	c1cc2cncc(c2cc1CN3CC[NH2+]CC3)NC(=O)[C@@H]4CNc5c4cc(cc5)Cl
RUN:	RUN3037
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.21

PET-UNK-3e354a91-1_1



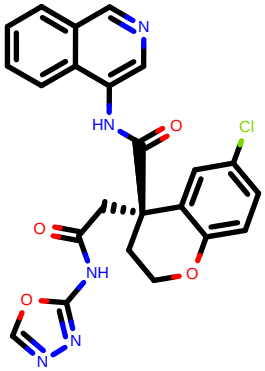
CID:	PET-UNK-3e354a91-1_1
SMILES:	c1ccc2c(c1)cncc2N3[C@H](CC[C@H](C3=O)c4cccc(c4)Cl)C#N
RUN:	RUN135
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.24

ERI-UCB-ce40166b-8_1



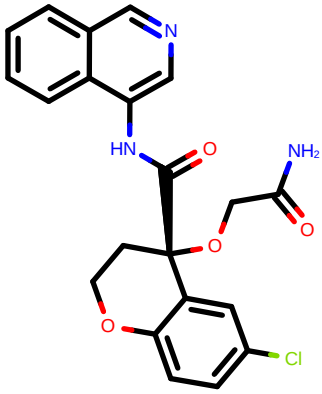
CID:	ERI-UCB-ce40166b-8_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Cl)Oc4cccnc4
RUN:	RUN46
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.18

MIC-UNK-5a93dd5f-7_4



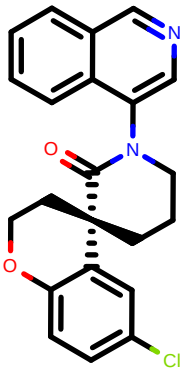
CID:	MIC-UNK-5a93dd5f-7_4
SMILES:	CC(=O)N(C)[C@H]1CC[N@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN771
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.33

RAL-THA-1d44ff04-1_1



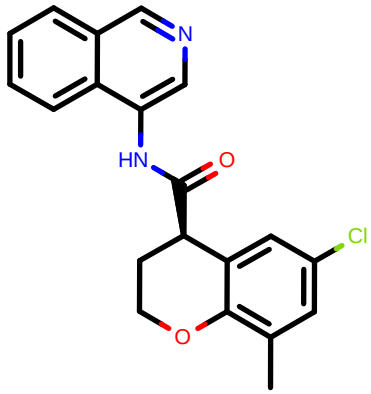
CID:	RAL-THA-1d44ff04-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCc4[nH]ccn4
RUN:	RUN434
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.20

DAR-DIA-0d514e7d-28_1



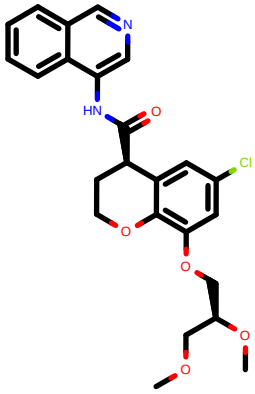
CID:	DAR-DIA-0d514e7d-28_1
SMILES:	C[C@H]1COc2ccc(cc2[C@]1(C)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN835
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.18

MIC-UNK-50cce87d-9_2



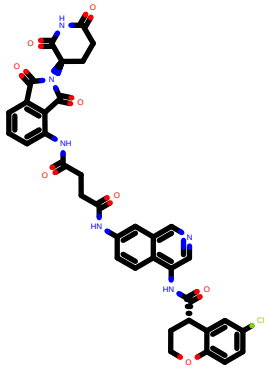
CID:	MIC-UNK-50cce87d-9_2
SMILES:	c1cc(cc(c1)Cl)[C@H]2CCCN(C2=O)c3cncc4c3c(ccc4)F
RUN:	RUN675
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.18

KAD-UNI-8a629cb0-8_1



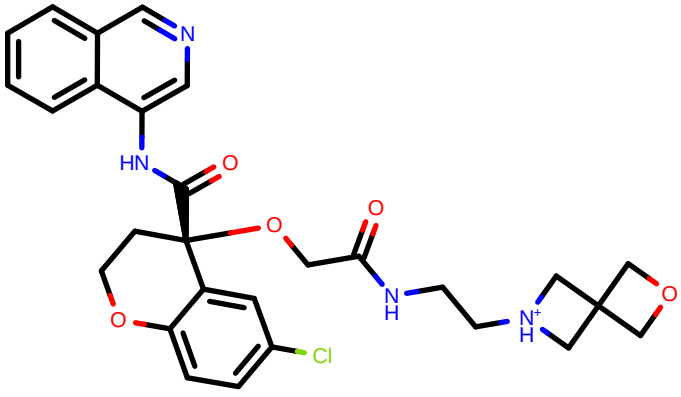
CID:	KAD-UNI-8a629cb0-8_1
SMILES:	C[C@@H](C(=O)N)[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2092
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.50

VLA-UNK-db5e3064-2_2



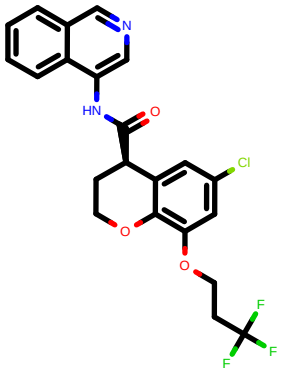
CID:	VLA-UNK-db5e3064-2_2
SMILES:	c1ccc2c(c1)cncc2n3c(c(oc3=O)c4cccc(c4)Cl)[O-]
RUN:	RUN3096
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.38

MIC-UNK-cdc2493e-2_2



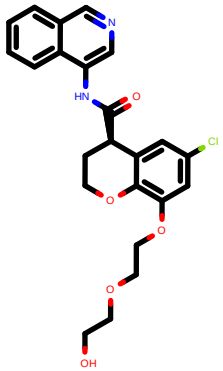
CID:	MIC-UNK-cdc2493e-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CC[C@H]3CCCO3)c4cccc(c4)Cl
RUN:	RUN525
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.38

DAR-DIA-9e4459de-15_13



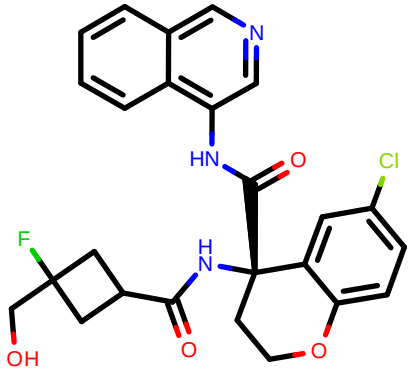
CID:	DAR-DIA-9e4459de-15_13
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1452
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.36

EDJ-MED-6864a934-10_1



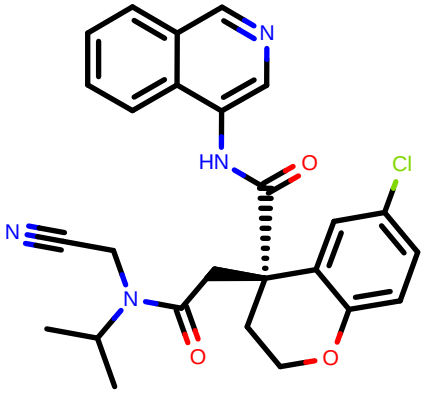
CID:	EDJ-MED-6864a934-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](C5(CCC5)O)O
RUN:	RUN2614
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.31

MAT-POS-78e1d523-2_2



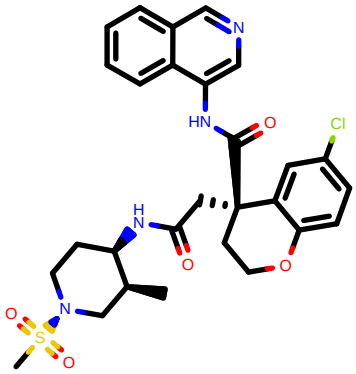
CID:	MAT-POS-78e1d523-2_2
SMILES:	CNC(=O)[C@]1(CCOc2c1cc(cc2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN3281
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.14

ALP-POS-d3acb8cc-4_1



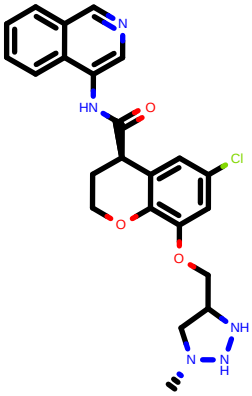
CID:	ALP-POS-d3acb8cc-4_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1098
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.20

MAK-UNK-c749d764-12_6



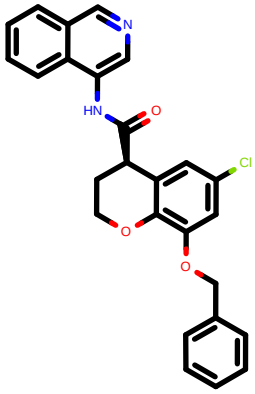
CID:	MAK-UNK-c749d764-12_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@@H]([C@H]3O)Cl
RUN:	RUN957
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.40

ALP-UNI-0676e700-24_1



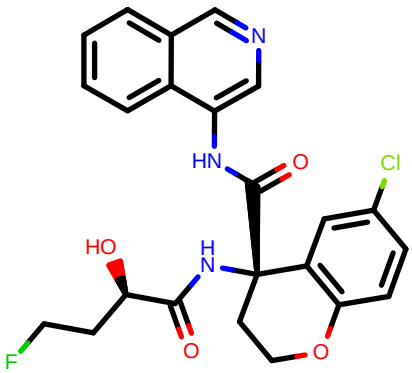
CID:	ALP-UNI-0676e700-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@H]5[C@H](CC(=O)N5)C(F)(F)F
RUN:	RUN2469
DDG (kcal/mol):	-1.73
dDDG (kcal/mol):	0.38

ED_-GRI-5b13fbe2-16_1



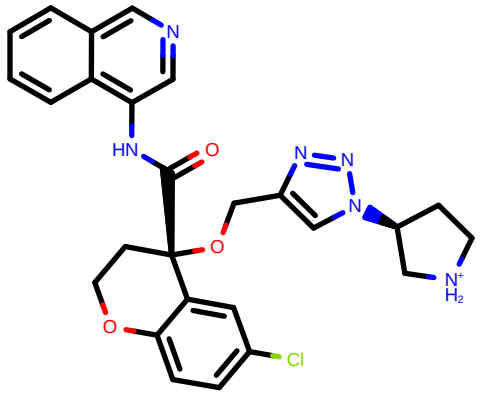
CID:	ED_-GRI-5b13fbe2-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]([C5cn(nn5)CC6CC6)[NH3+]
RUN:	RUN1543
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.35

MIC-UNK-cdc2493e-23_1



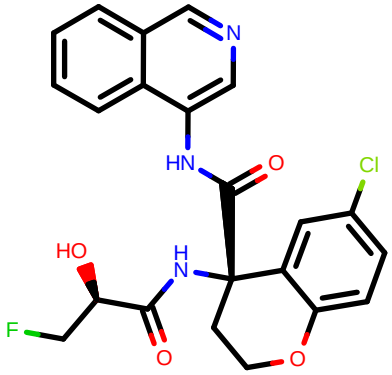
CID:	MIC-UNK-cdc2493e-23_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCn3cnnc3)c4cccc(c4)Cl
RUN:	RUN573
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.28

ROB-UNI-322e8f70-3_2



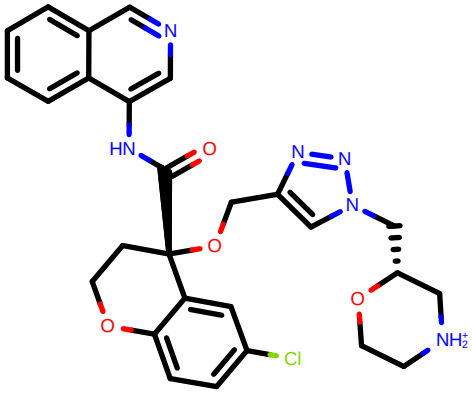
CID:	ROB-UNI-322e8f70-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CNC(=O)c4c3cc(cc4)Cl
RUN:	RUN3155
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.17

ADA-UCB-dc2b944c-15_1



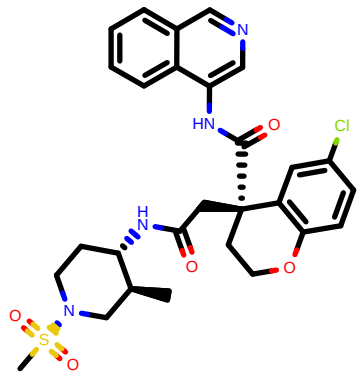
CID:	ADA-UCB-dc2b944c-15_1
SMILES:	CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C
RUN:	RUN613
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.25

DAR-DIA-23e5a6a0-2_2



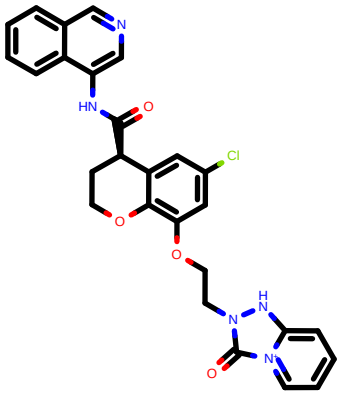
CID:	DAR-DIA-23e5a6a0-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC6([NH2+]5)CCC6)Cl
RUN:	RUN404
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.32

MAK-UNK-c749d764-4_7



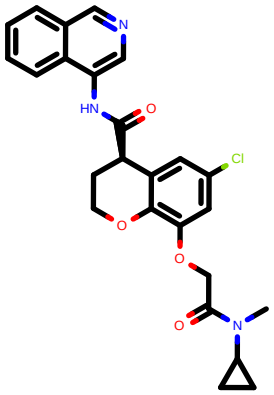
CID:	MAK-UNK-c749d764-4_7
SMILES:	CS[C@@H]1CCC[C@H]([C@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN919
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.25

EDG-MED-0e5afe9d-3_1



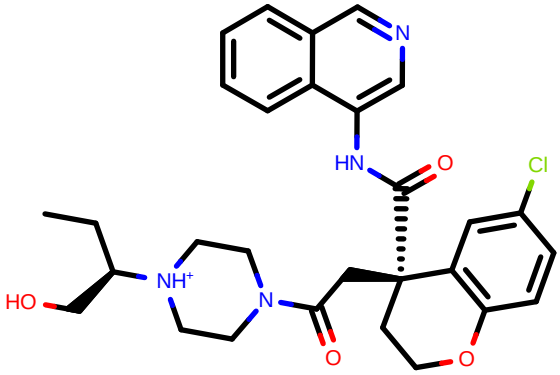
CID:	EDG-MED-0e5afe9d-3_1
SMILES:	CO[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2329
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.40

EDJ-MED-6864a934-9_1



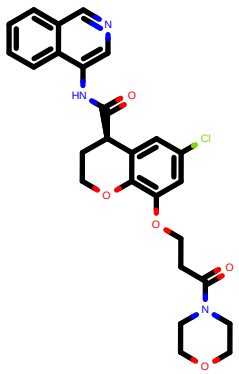
CID:	EDJ-MED-6864a934-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccn(n5)CC#N
RUN:	RUN2615
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.37

ALP-POS-b3306dea-1_1



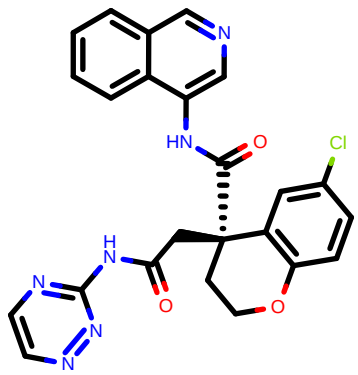
CID:	ALP-POS-b3306dea-1_1
SMILES:	Cc1nnc(s1)N(Cc2cccc(c2)Cl)C(=O)Cc3cncc4c3cccc4
RUN:	RUN1185
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.41

ALP-UNI-3496895b-14_1



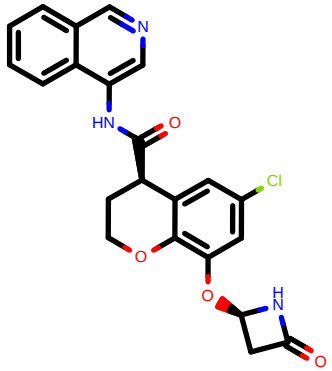
CID:	ALP-UNI-3496895b-14_1
SMILES:	Cc1cc(=O)n2c(n1)nc([nH]2)NC(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2529
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.44

MIC-UNK-5a93dd5f-9_2



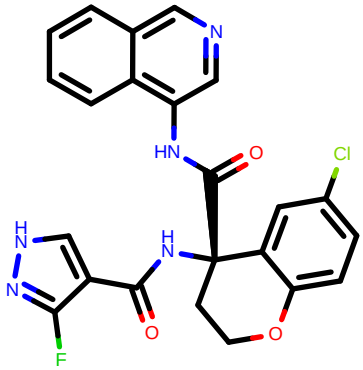
CID:	MIC-UNK-5a93dd5f-9_2
SMILES:	CN(C)[C@H]1CC[N@@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN779
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.20

MAT-POS-9ff17035-2_1



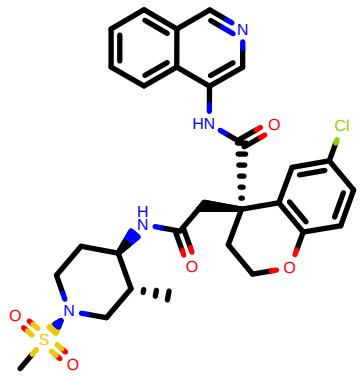
CID:	MAT-POS-9ff17035-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Oc4cccc(=O)[nH]4
RUN:	RUN147
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.28

DAR-DIA-0f2f46c9-7_2



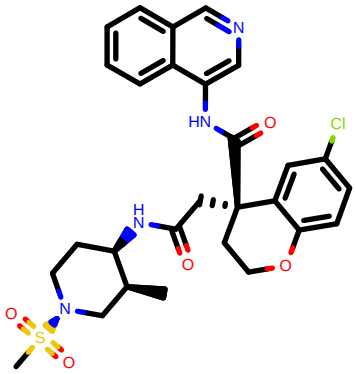
CID:	DAR-DIA-0f2f46c9-7_2
SMILES:	CNS(=O)(=O)[N@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3235
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.13

RAL-THA-4aa06b95-5_1



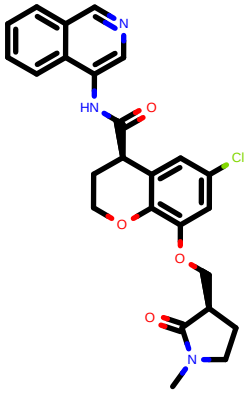
CID:	RAL-THA-4aa06b95-5_1
SMILES:	COCC(=O)N1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1237
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.24

ALP-POS-696356e4-1_2



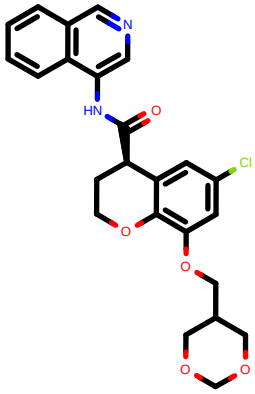
CID:	ALP-POS-696356e4-1_2
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1316
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.39

MAT-POS-fce787c2-7_2



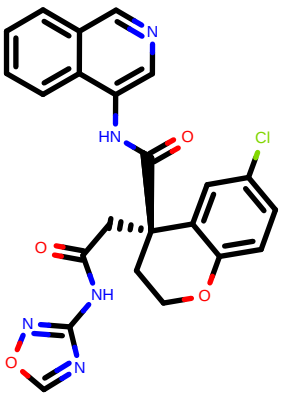
CID:	MAT-POS-fce787c2-7_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN2154
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.42

KAD-UNI-8a629cb0-16_1



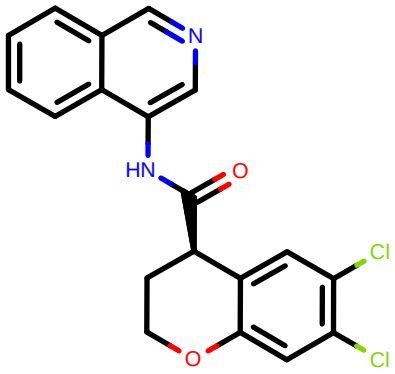
CID:	KAD-UNI-8a629cb0-16_1
SMILES:	CCN1CN(CC1=O)C(=O)CC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2098
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.36

MAK-UNK-3875bbc8-1_2



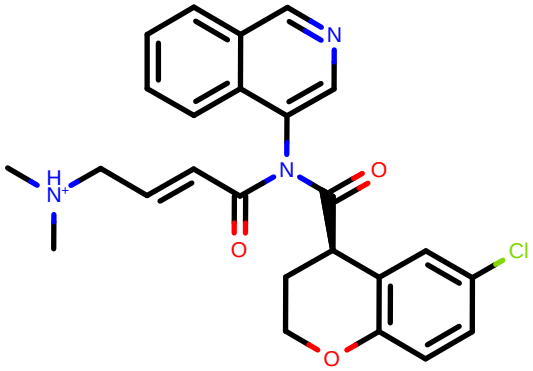
CID:	MAK-UNK-3875bbc8-1_2
SMILES:	Cc1ccc2c(c1)[C@H](CCO2)C(=O)N(C)c3cncc4c3cccc4
RUN:	RUN799
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.24

MIC-UNK-5a93dd5f-2_1



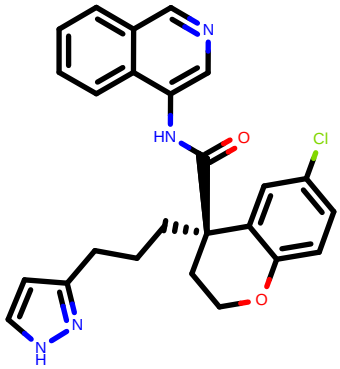
CID:	MIC-UNK-5a93dd5f-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCCC[C@H]5C4
RUN:	RUN731
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.25

MAT-POS-b3e365b9-1_1



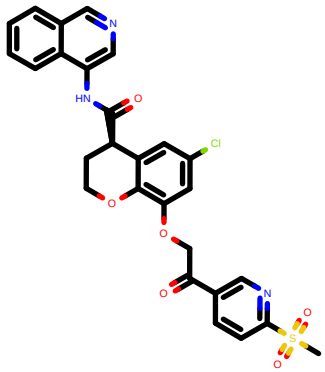
CID:	MAT-POS-b3e365b9-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN276
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.46

VLA-UCB-1dbca3b4-17_2



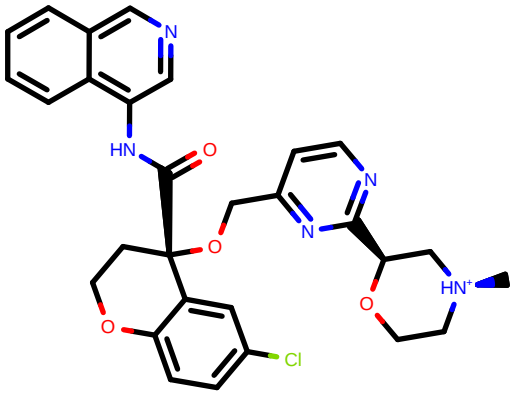
CID:	VLA-UCB-1dbca3b4-17_2
SMILES:	c1ccc2c(c1)cncc2n3c(c([nH]c3=O)c4cccc(c4)Cl)[O-]
RUN:	RUN167
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.26

EDG-MED-ba1ac7b9-11_4



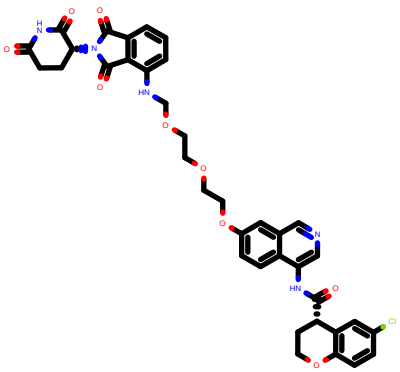
CID:	EDG-MED-ba1ac7b9-11_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5c6c[nH]nc6
RUN:	RUN2657
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.39

EDJ-MED-f893e2a1-5_1



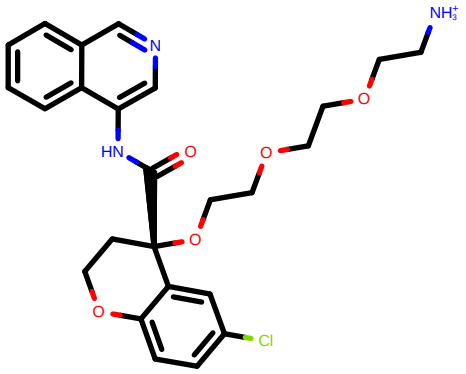
CID:	EDJ-MED-f893e2a1-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cc6nncn6nc5
RUN:	RUN3200
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.25

EDJ-MED-e4b030d8-3_1



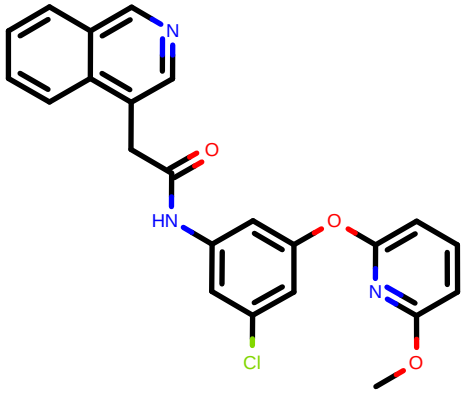
CID:	EDJ-MED-e4b030d8-3_1
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN285
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.40

DAR-DIA-6a508060-13_1



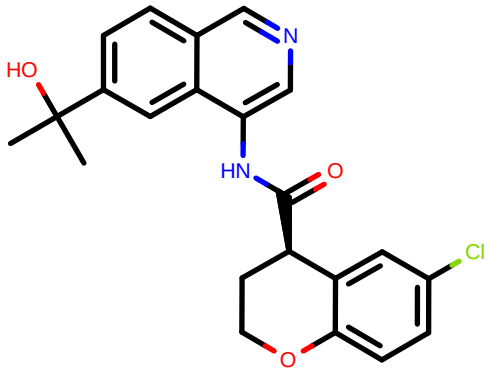
CID:	DAR-DIA-6a508060-13_1
SMILES:	CS(=O)(=O)NCC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN360
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.60

EDG-MED-ba1ac7b9-15_8



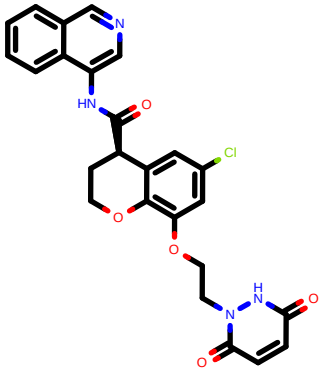
CID:	EDG-MED-ba1ac7b9-15_8
SMILES:	C[C@H]1C[N@H+](CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2681
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.33

NIR-THE-d08c3b48-1_1



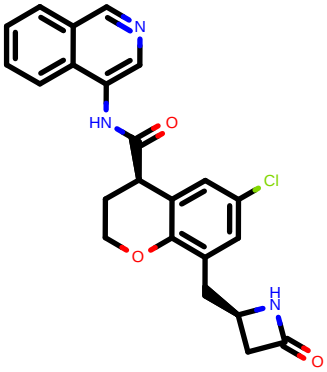
CID:	NIR-THE-d08c3b48-1_1
SMILES:	CC(=O)N1CC[NH+](CC1)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN189
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.25

EDG-MED-ba1ac7b9-7_2



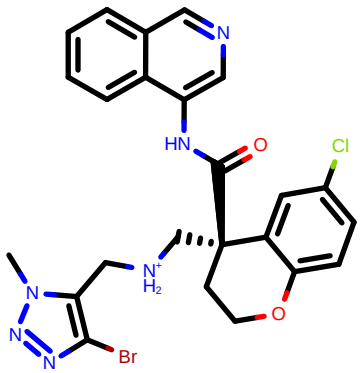
CID:	EDG-MED-ba1ac7b9-7_2
SMILES:	C[C@H]1N(CCO1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2640
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.44

ERI-UCB-ce40166b-1_2



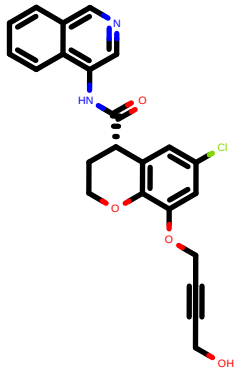
CID:	ERI-UCB-ce40166b-1_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)O[C@H]4CC(=O)N4
RUN:	RUN35
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.28

KAD-UNI-8a629cb0-21_1



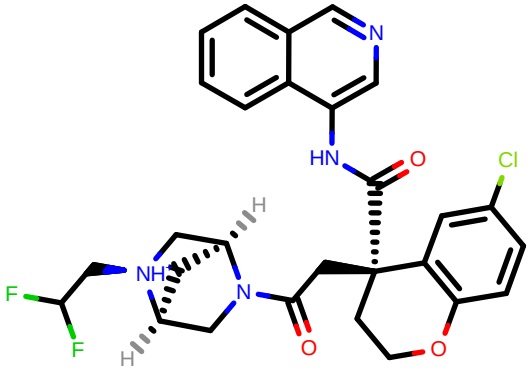
CID:	KAD-UNI-8a629cb0-21_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCN(CC5)CC(CO)(F)F
RUN:	RUN2111
DDG (kcal/mol):	-1.68
dDDG (kcal/mol):	0.42

ALF-EVA-a24cc7ce-6_1



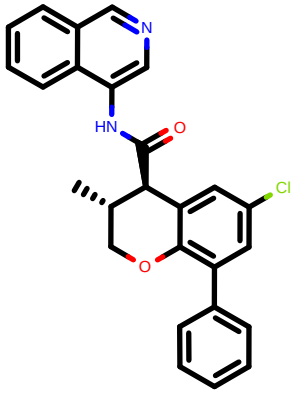
CID:	ALF-EVA-a24cc7ce-6_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN4958
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.24

WIL-UNI-0732ac76-2_1



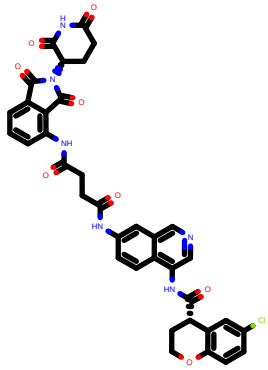
CID:	WIL-UNI-0732ac76-2_1
SMILES:	C[C@@](CN([C@@H](c1cncc2c1cccc2)C(=O)Nc3ccccc3)C(=O)c4ccncc4)(c5ccccc5F)C(=O)OC
RUN:	RUN1177
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.26

PET-UNK-c9c1e0d8-3_1



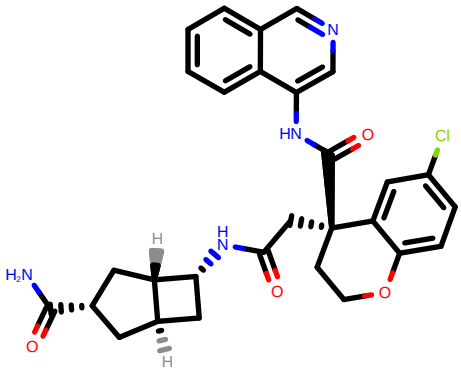
CID:	PET-UNK-c9c1e0d8-3_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN117
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.30

PET-UNK-4880b143-1_1



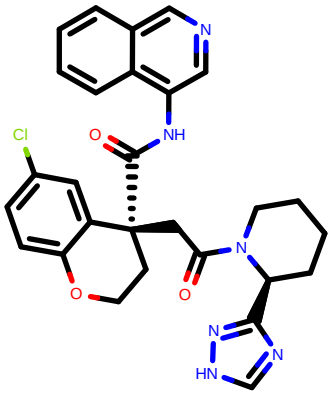
CID:	PET-UNK-4880b143-1_1
SMILES:	CS(=O)(=O)CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3294
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.43

DAR-DIA-0d514e7d-32_26



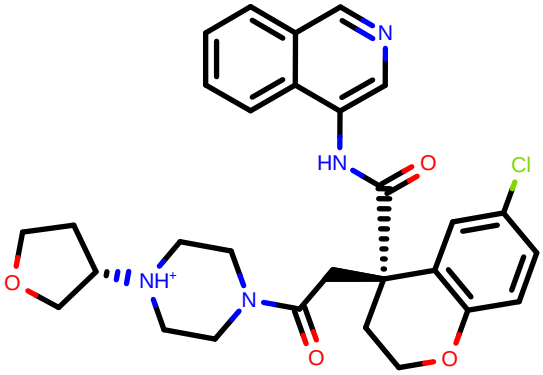
CID:	DAR-DIA-0d514e7d-32_26
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@@H]4C[C@@H]4CO[C@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN875
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.40

MAT-POS-96f51285-6_1



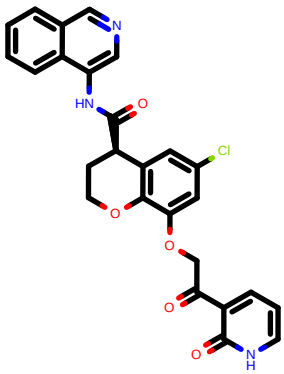
CID:	MAT-POS-96f51285-6_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN3935
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.21

MAK-UNK-c749d764-16_7



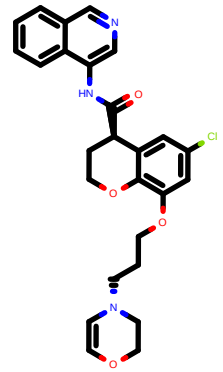
CID:	MAK-UNK-c749d764-16_7
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F)O
RUN:	RUN981
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.29

MAT-POS-e9e99895-13_5



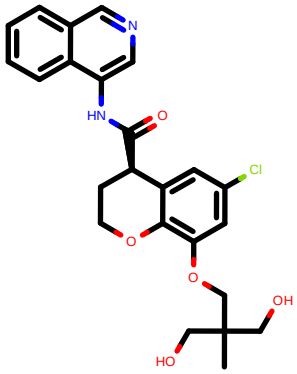
CID:	MAT-POS-e9e99895-13_5
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CC[N@H+](C4)C
RUN:	RUN2271
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.50

MAT-POS-2905de8c-3_1



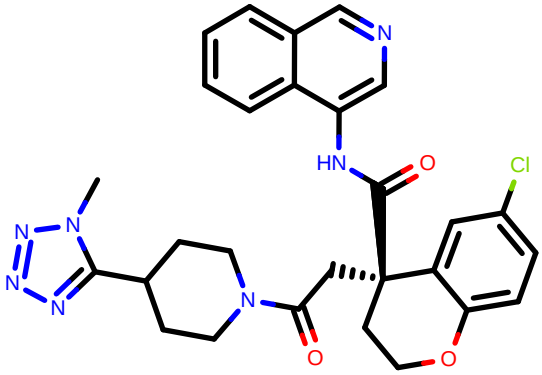
CID:	MAT-POS-2905de8c-3_1
SMILES:	C[NH+](C)[C@@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2231
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.35

MAT-POS-e9e99895-13_8



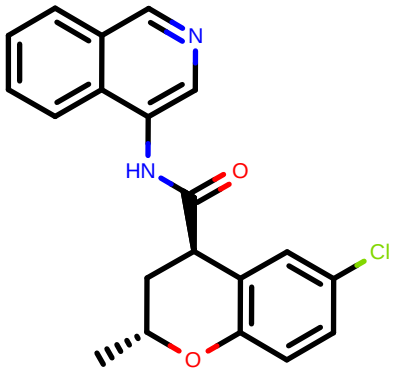
CID:	MAT-POS-e9e99895-13_8
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@H]4CC[N@H+](C4)C
RUN:	RUN2274
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.46

MIC-UNK-5a93dd5f-3_3



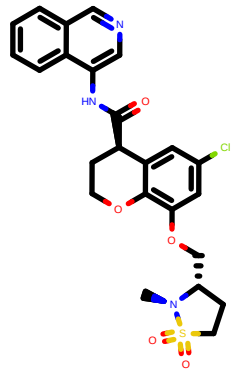
CID:	MIC-UNK-5a93dd5f-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[N@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN742
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.41

ERI-UCB-ce40166b-9_2



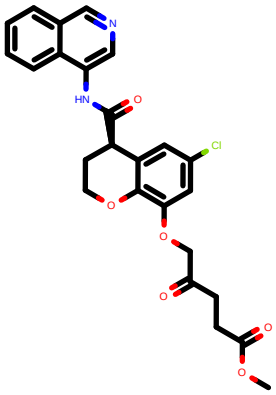
CID:	ERI-UCB-ce40166b-9_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)O[C@H]4CC(=O)N4)C#N
RUN:	RUN47
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.21

ALP-UNI-76695c4f-8_1



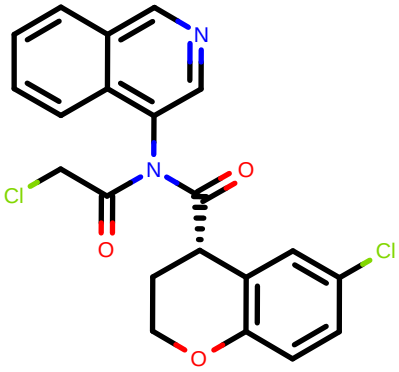
CID:	ALP-UNI-76695c4f-8_1
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@]2(CCOc3c2ccc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2177
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.40

JOH-UNI-ea72002d-5_2



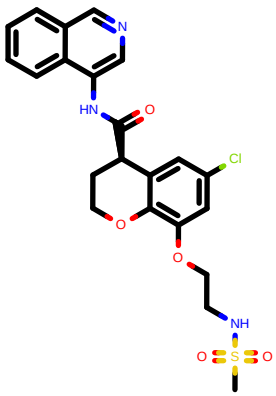
CID:	JOH-UNI-ea72002d-5_2
SMILES:	C=CS(=O)(=O)NN(c1cncc2c1cccc2)C(=O)[C@]3(CCOc4c3cc(cc4)Cl)F
RUN:	RUN2493
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.40

EDG-MED-ba1ac7b9-25_1



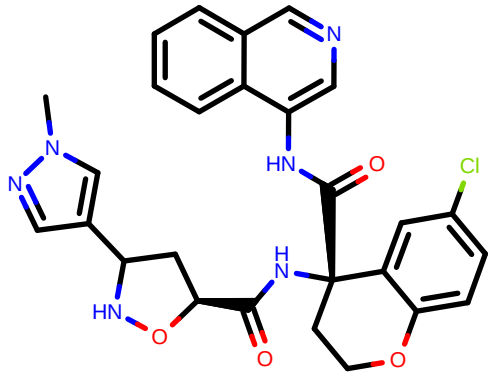
CID:	EDG-MED-ba1ac7b9-25_1
SMILES:	C[C@@H]1CN(CC[N@@H+]1CCO)C(=O)C[C@@]2(CCOc3c2ccc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2712
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.30

MAT-POS-e9e99895-11_1



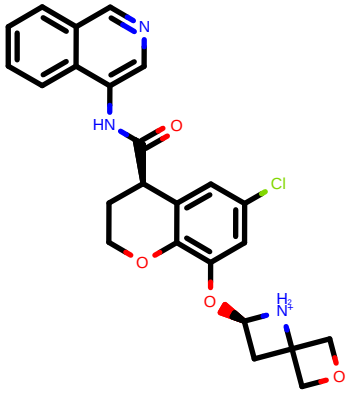
CID:	MAT-POS-e9e99895-11_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)COC
RUN:	RUN2263
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.45

ALP-POS-966f8da6-2_2



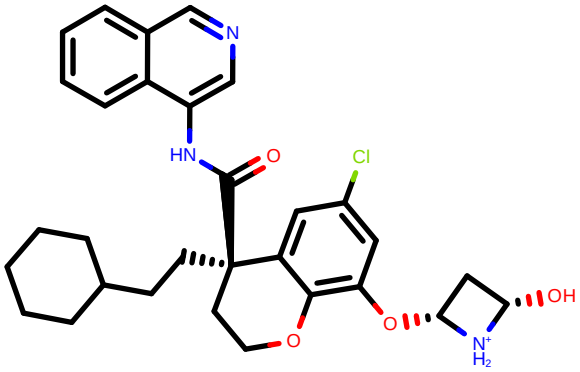
CID:	ALP-POS-966f8da6-2_2
SMILES:	CC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1226
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.30

MAT-POS-af71705c-1_1



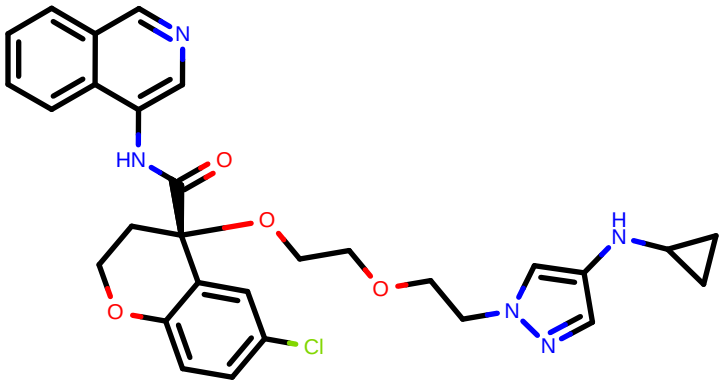
CID:	MAT-POS-af71705c-1_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccccn3
RUN:	RUN54
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.42

LON-WEI-4d77710c-22_1



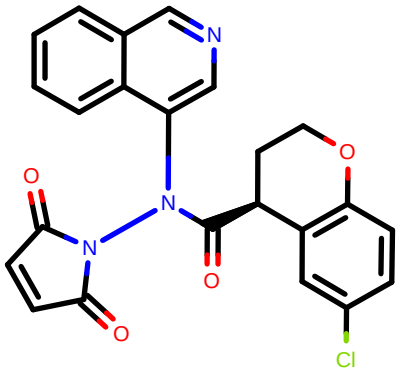
CID:	LON-WEI-4d77710c-22_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)Nc3cccnc3
RUN:	RUN209
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.32

MIC-UNK-cdc2493e-10_1



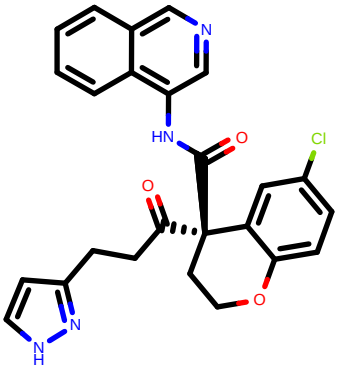
CID:	MIC-UNK-cdc2493e-10_1
SMILES:	CC(=O)N[C@@H]1CC[C@@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN545
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.37

MAK-UNK-c749d764-12_2



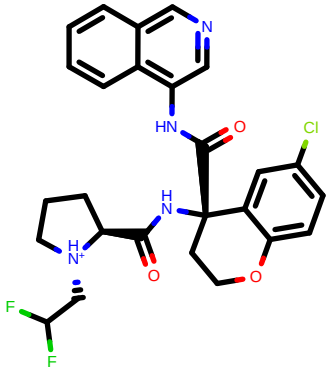
CID:	MAK-UNK-c749d764-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@@H]([C@@H]3O)Cl
RUN:	RUN951
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.36

ERI-UCB-b3e6b0c2-4_1



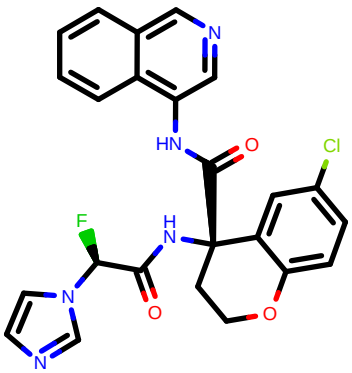
CID:	ERI-UCB-b3e6b0c2-4_1
SMILES:	C[N@@]1C[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cc(cc4)CN5CC[NH2+]CC5
RUN:	RUN3036
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.16

MIK-ENA-fc9ceda2-1_2



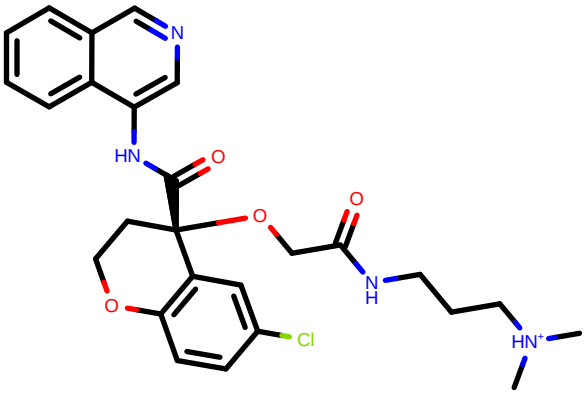
CID:	MIK-ENA-fc9ceda2-1_2
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)CNc3cncc4c3cccc4
RUN:	RUN3293
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.15

DAR-DIA-0f2f46c9-13_2



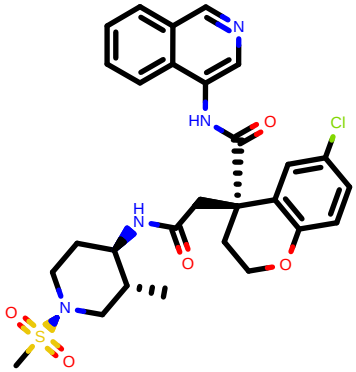
CID:	DAR-DIA-0f2f46c9-13_2
SMILES:	CN(C)S(=O)(=O)[N@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3248
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.12

RAL-THA-1d44ff04-10_1



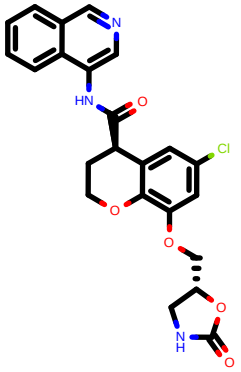
CID:	RAL-THA-1d44ff04-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)S(=O)(=O)N
RUN:	RUN445
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-36_1



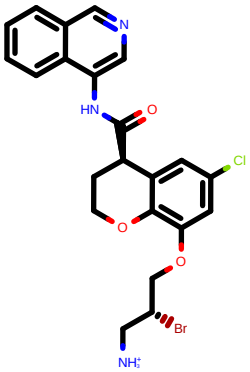
CID:	DAR-DIA-0d514e7d-36_1
SMILES:	CC1([C@@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C
RUN:	RUN888
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.26

MAT-POS-f9802937-2_2



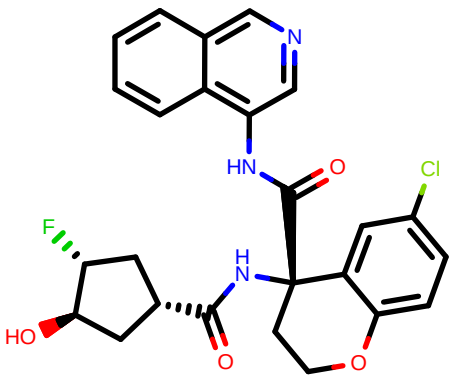
CID:	MAT-POS-f9802937-2_2
SMILES:	CN1c2ccc(cc2[C@](CC1=O)(C(=O)Nc3cncc4c3cccc4)O)Cl
RUN:	RUN2393
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.36

MAT-POS-fce787c2-10_1



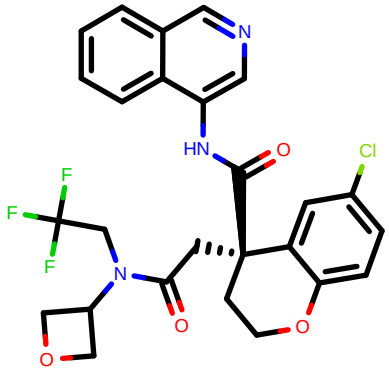
CID:	MAT-POS-fce787c2-10_1
SMILES:	CN(C)CC[NH2+][C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2160
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.38

MAT-POS-a9372f04-1_1



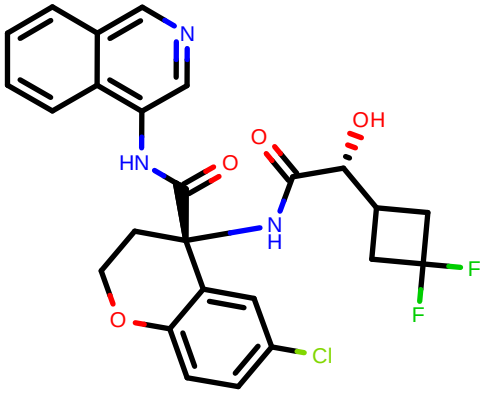
CID:	MAT-POS-a9372f04-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)c5cc(ccc5NC4=O)Cl
RUN:	RUN3309
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.14

FRA-DIA-a1f3a927-1_1



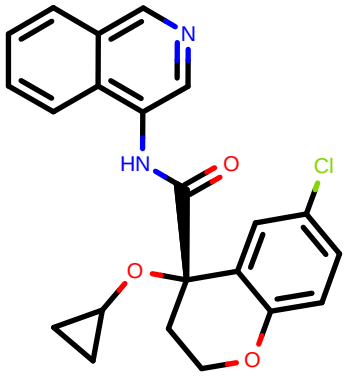
CID:	FRA-DIA-a1f3a927-1_1
SMILES:	C=C(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1176
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.26

ADA-UCB-dc2b944c-18_1



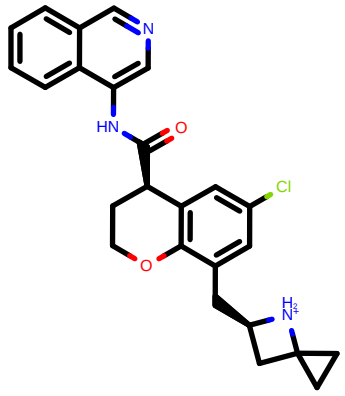
CID:	ADA-UCB-dc2b944c-18_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C(=O)CC4CCOCC4
RUN:	RUN616
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.28

JOH-UNI-a38a7bdd-5_1



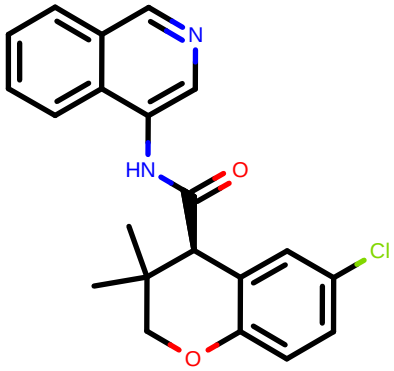
CID:	JOH-UNI-a38a7bdd-5_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@@H]4C[C@@H]4F
RUN:	RUN1485
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.19

MAT-POS-3b92565d-9_2



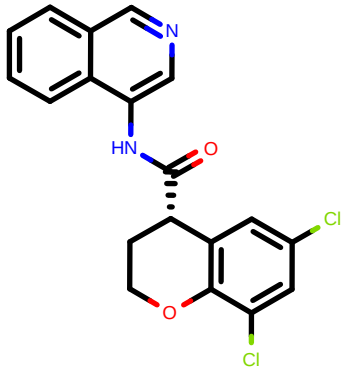
CID:	MAT-POS-3b92565d-9_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN120
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.37

MAT-POS-2492181e-12_1



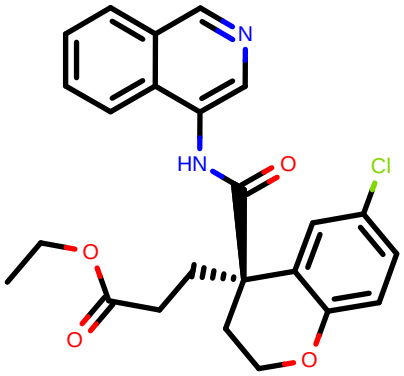
CID:	MAT-POS-2492181e-12_1
SMILES:	CCC[NH+](CCC)CCNC(=O)Nc1cn(c(=O)c2c1cccc2)CC(C)C
RUN:	RUN114
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.18

MAK-UNK-ffc90da7-9_6



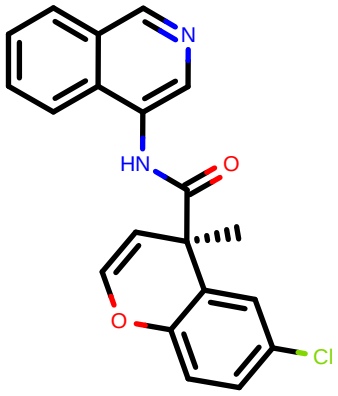
CID:	MAK-UNK-ffc90da7-9_6
SMILES:	C[C@H]1[C@@H](CCO1)SC[C@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN718
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.12

MAT-POS-2492181e-2_1



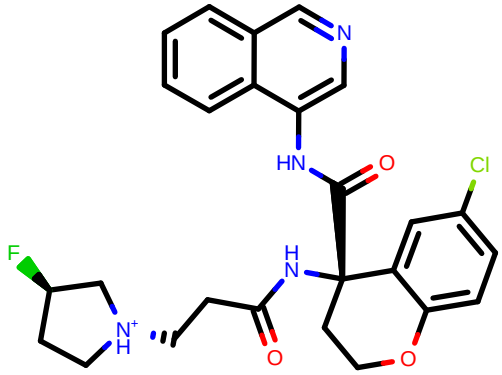
CID:	MAT-POS-2492181e-2_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCC[NH+]3CCCC3
RUN:	RUN94
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.24

MAT-POS-11b63608-1_2



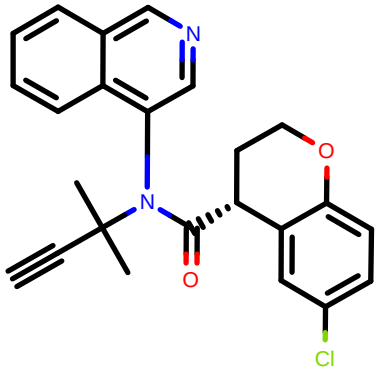
CID:	MAT-POS-11b63608-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Br
RUN:	RUN282
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.24

MIC-UNK-50cce87d-7_2



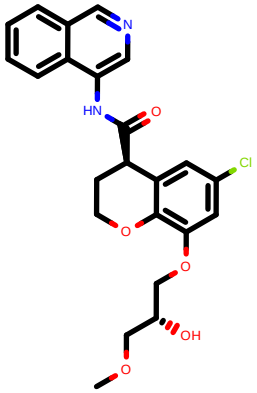
CID:	MIC-UNK-50cce87d-7_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN670
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.30

ALP-UNI-8e43a71e-5_11



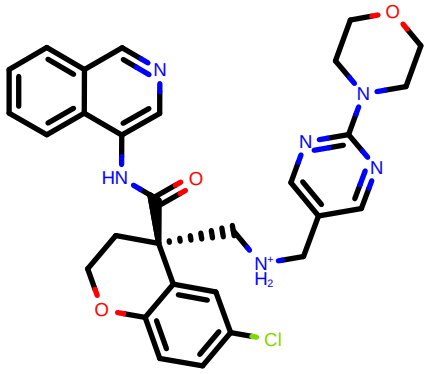
CID:	ALP-UNI-8e43a71e-5_11
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2954
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.14

MAT-POS-e69ad64a-2_2



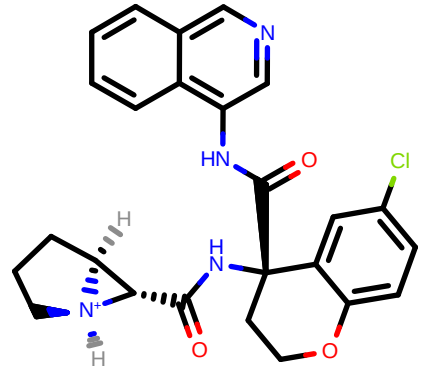
CID:	MAT-POS-e69ad64a-2_2
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN2333
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.42

EDG-MED-90036822-104_1



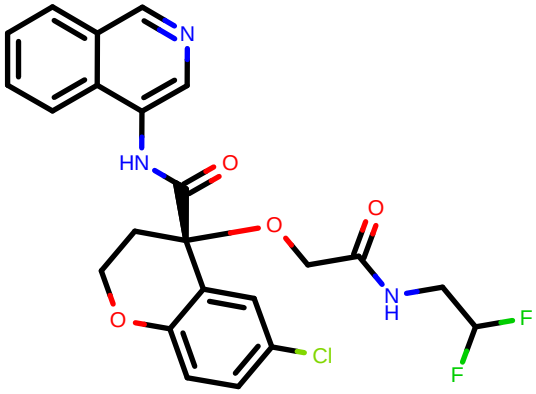
CID:	EDG-MED-90036822-104_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ncc(cn5)[C@@H]6CC[NH2+]C6
RUN:	RUN1837
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.46

MIC-UNK-02d7a284-1_1



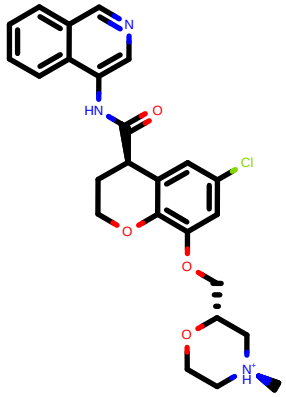
CID:	MIC-UNK-02d7a284-1_1
SMILES:	CC(=O)N1CCC2(CC1)CN(CC(=O)N2c3cccc(c3)Cl)C(=O)c4cncc5c4cccc5
RUN:	RUN3260
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.15

MIC-UNK-d854bf4c-7_2



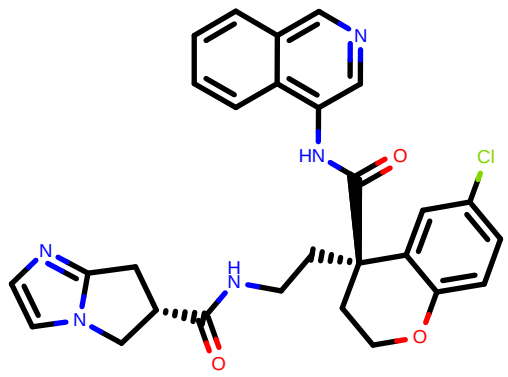
CID:	MIC-UNK-d854bf4c-7_2
SMILES:	CS(=O)(=O)N1CCC2(CC1)CCN(C(=O)[C@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN3342
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.15

KAD-UNI-80f122c8-1_1



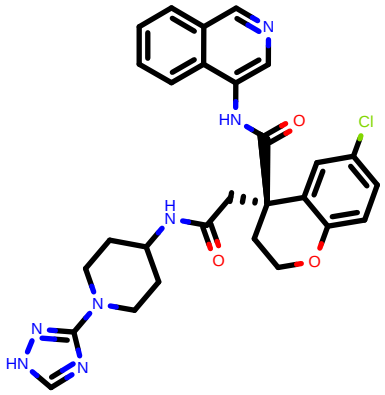
CID:	KAD-UNI-80f122c8-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)NCC56CC(C5)(CO6)C(=O)N
RUN:	RUN2291
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.43

DAR-DIA-0587064e-26_2



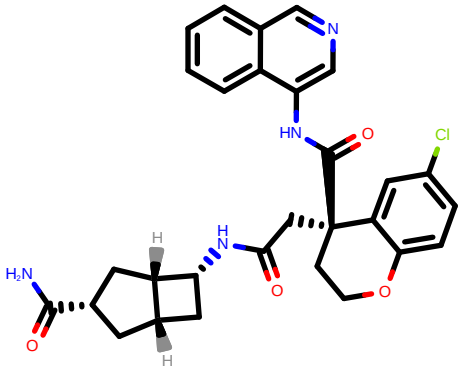
CID:	DAR-DIA-0587064e-26_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(c(c4OCc5ccc(cc5Cl)F)F)Cl
RUN:	RUN3389
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.22

MAK-UNK-c749d764-28_2



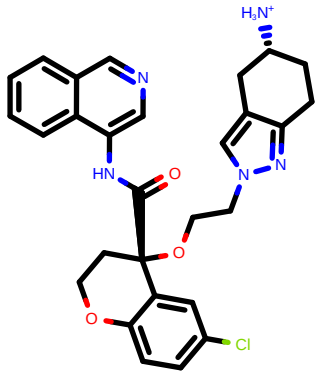
CID:	MAK-UNK-c749d764-28_2
SMILES:	c1ccc2c(c1)cncc2N(C=O)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1055
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.36

MAK-UNK-c749d764-26_3



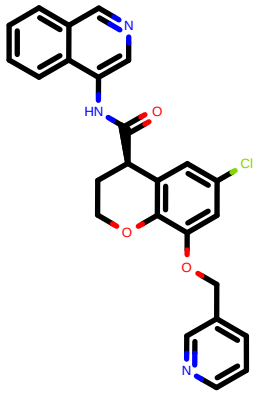
CID:	MAK-UNK-c749d764-26_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCCC[C@H]([C@@H]3O)Cl
RUN:	RUN1048
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.46

JAG-UCB-706446eb-2_1



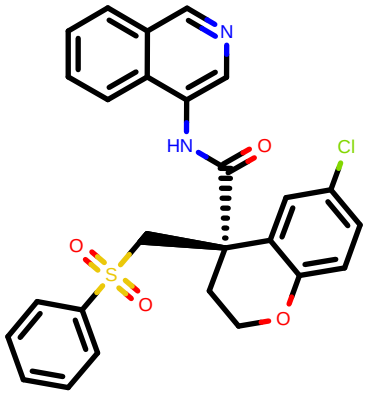
CID:	JAG-UCB-706446eb-2_1
SMILES:	CCCNC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN620
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.38

ED_-GRI-5b13fbe2-23_1



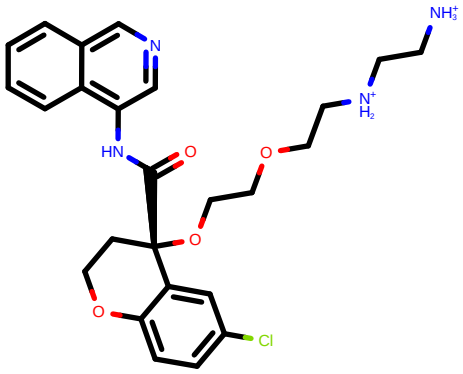
CID:	ED_-GRI-5b13fbe2-23_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@@H+]5CCn6c(c(cn6)C[NH3+])C5
RUN:	RUN1552
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.36

JOH-UNI-a38a7bdd-5_3



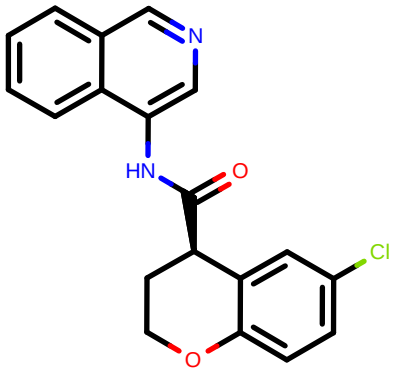
CID:	JOH-UNI-a38a7bdd-5_3
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@@H]4C[C@H]4F
RUN:	RUN1488
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.21

VLA-UCB-05e51b3f-12_1



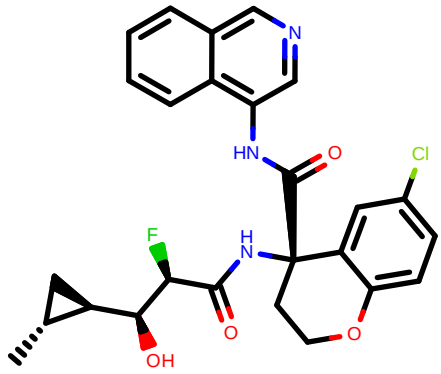
CID:	VLA-UCB-05e51b3f-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl)CCC6CCCCC6
RUN:	RUN323
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.56

DAR-DIA-eace69ff-19_1



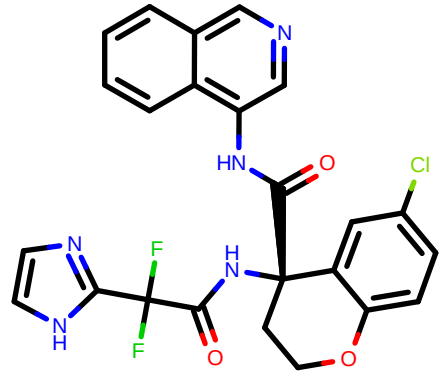
CID:	DAR-DIA-eace69ff-19_1
SMILES:	CCc1cc2c(cncc2c(c1)OC3CCCCC3)C[NH+](C)C
RUN:	RUN2
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.20

MAT-POS-3b97339c-1_1



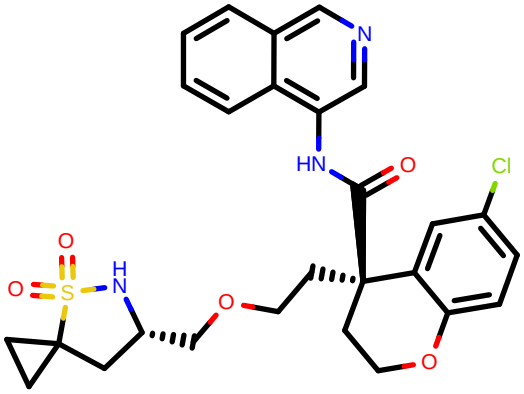
CID:	MAT-POS-3b97339c-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCSC5)O
RUN:	RUN3297
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.14

MAT-POS-dd3ad2b5-4_4



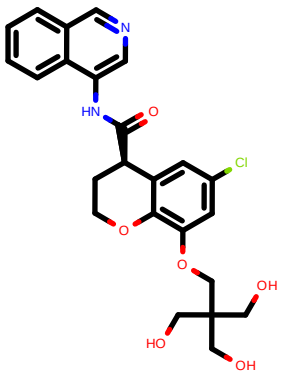
CID:	MAT-POS-dd3ad2b5-4_4
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3540
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.13

EDJ-MED-6d9ff7d0-9_1



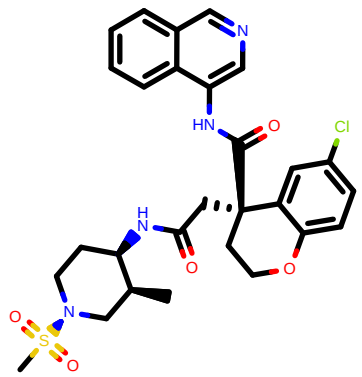
CID:	EDJ-MED-6d9ff7d0-9_1
SMILES:	CS(=O)(=O)CCN[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3436
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.20

EDG-MED-ba1ac7b9-9_3



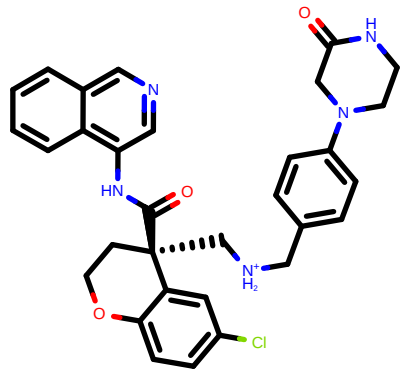
CID:	EDG-MED-ba1ac7b9-9_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5c6[nH]ncn6
RUN:	RUN2648
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.42

MAK-UNK-c749d764-19_1



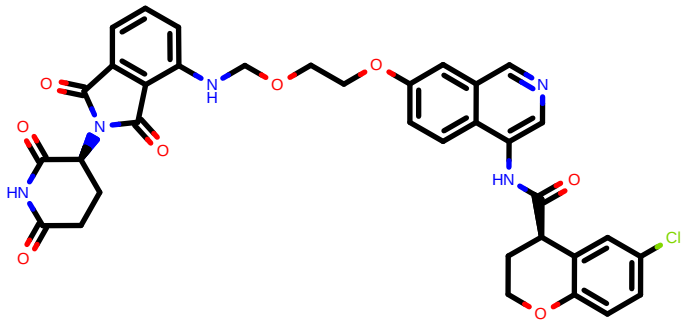
CID:	MAK-UNK-c749d764-19_1
SMILES:	c1ccc2c(c1)cncc2N(C[NH3+])C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN998
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.37

ALP-POS-347519b5-1_50



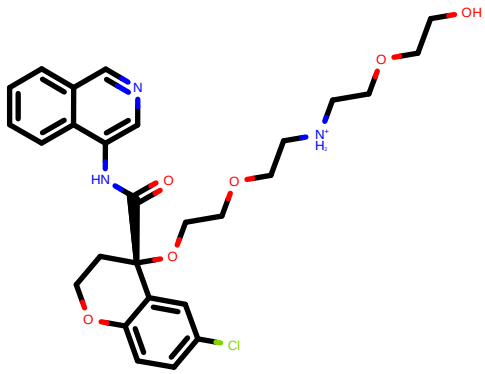
CID:	ALP-POS-347519b5-1_50
SMILES:	CS(=O)(=O)[N@]1C[C@@H]2[C@@H]3CC[C@@H](C3)[C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4257
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.27

DAR-DIA-6a508060-9_1



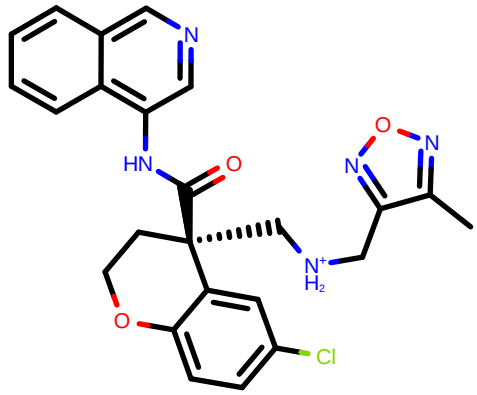
CID:	DAR-DIA-6a508060-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC5CCCCC5
RUN:	RUN348
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.48

MAT-POS-8a69d52e-1_4



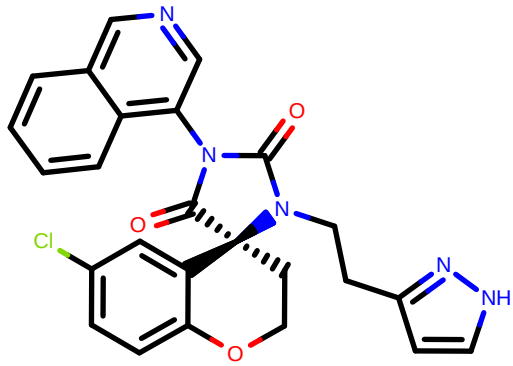
CID:	MAT-POS-8a69d52e-1_4
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN363
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.85

JOH-UNI-6e27fddc-4_1



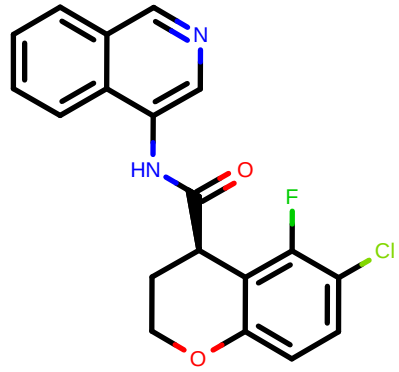
CID:	JOH-UNI-6e27fddc-4_1
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)/C(=C/c3cncc4c3cccc4)/F
RUN:	RUN4369
DDG (kcal/mol):	-1.58
dDDG (kcal/mol):	0.26

MAT-POS-dd3ad2b5-3_1



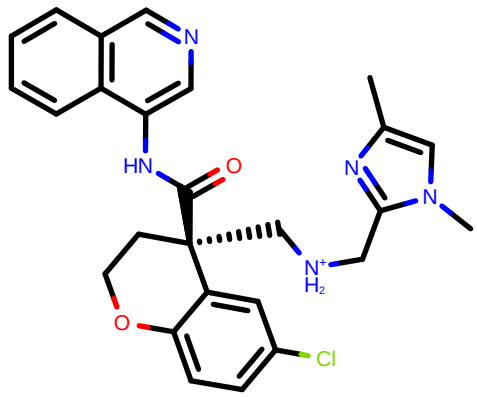
CID:	MAT-POS-dd3ad2b5-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CN(Cc4c3cc(cc4)Cl)C(=O)N
RUN:	RUN3535
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.19

MAK-UNK-ffc90da7-9_8



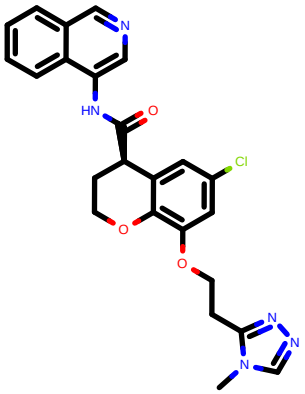
CID:	MAK-UNK-ffc90da7-9_8
SMILES:	C[C@H]1[C@H](CCO1)SC[C@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN719
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.20

ED_-GRI-5b13fbe2-66_2



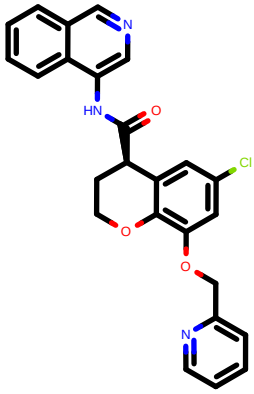
CID:	ED_-GRI-5b13fbe2-66_2
SMILES:	C[N@H+]1CCO[C@@H](C1)c2ncc(cn2)CO[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN1614
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.27

EDJ-MED-fcba3f31-9_1



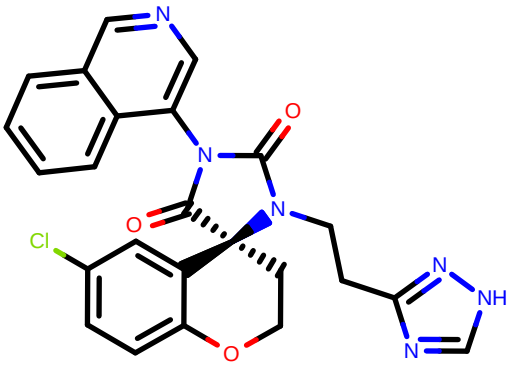
CID:	EDJ-MED-fcba3f31-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCC(=O)N5
RUN:	RUN2548
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.37

ED_-GRI-5b13fbe2-20_1



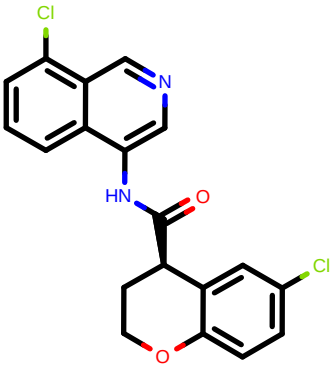
CID:	ED_-GRI-5b13fbe2-20_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H]5C[NH2+]C[C@@H](O5)CO
RUN:	RUN1547
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.35

DAR-DIA-0d514e7d-30_1



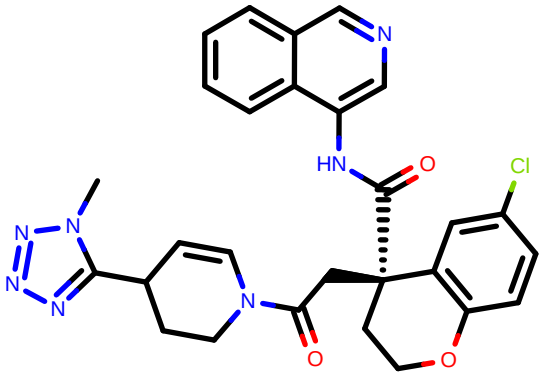
CID:	DAR-DIA-0d514e7d-30_1
SMILES:	C[C@@]1(c2cc(ccc2OCC1(C)C)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN837
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.20

MAT-POS-b5746674-106_1



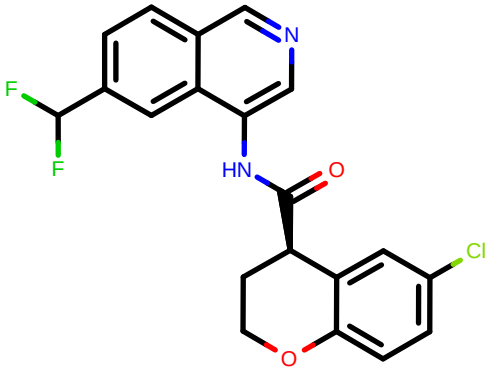
CID:	MAT-POS-b5746674-106_1
SMILES:	C[C@@H](c1ccncc1)N(CCCOC)C(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN86
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.18

MAK-UNK-c749d764-3_6



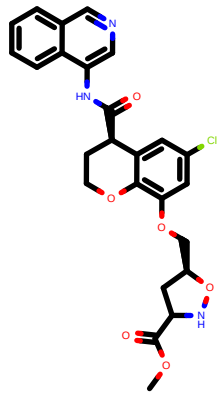
CID:	MAK-UNK-c749d764-3_6
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@H]4CCC[C@@H]([C@H]4O)C(F)F
RUN:	RUN910
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.27

LON-WEI-4d77710c-18_1



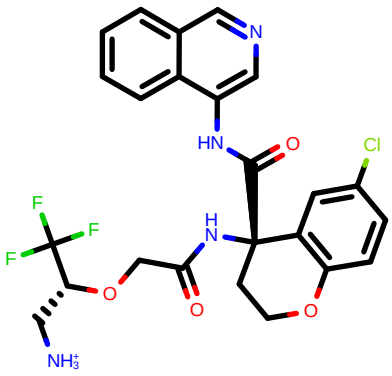
CID:	LON-WEI-4d77710c-18_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccc(cc3OC)OC
RUN:	RUN203
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.23

EDJ-MED-40433386-2_1



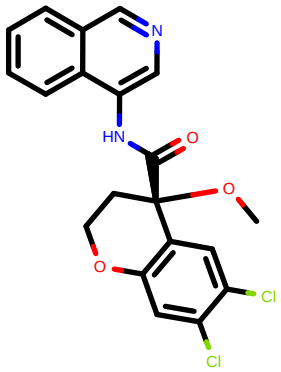
CID:	EDJ-MED-40433386-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]c5S(=O)(=O)N
RUN:	RUN2553
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.38

MAK-UNK-8be7dca9-6_2



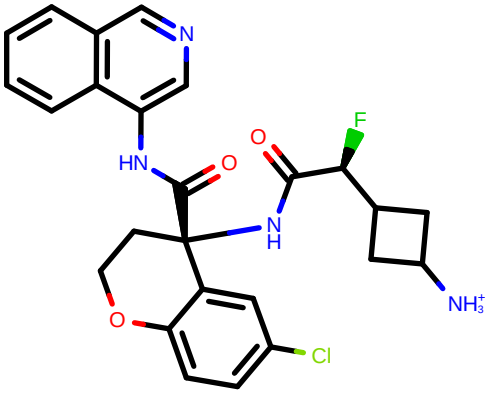
CID:	MAK-UNK-8be7dca9-6_2
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)C[NH3+]
RUN:	RUN504
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.49

DAR-DIA-0d514e7d-31_8



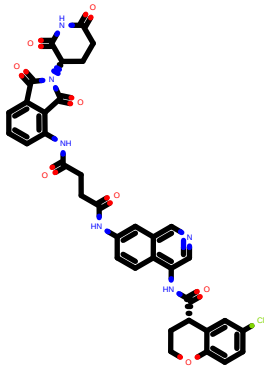
CID:	DAR-DIA-0d514e7d-31_8
SMILES:	C[C@H]1CCO[C@H]2C=CC(=C[C@H]2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN841
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.21

MAK-UNK-8be7dca9-1_1



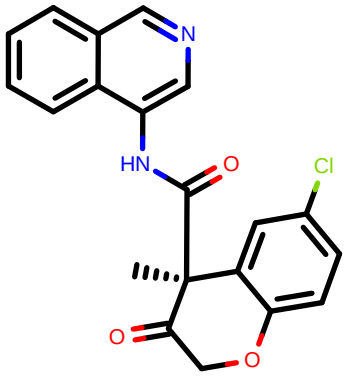
CID:	MAK-UNK-8be7dca9-1_1
SMILES:	c1cc2c(cc1CN3CC[NH2+]CC3)cncc2NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN491
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.27

JAG-UCB-f37eaa14-7_2



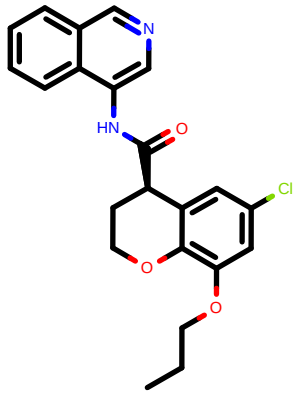
CID:	JAG-UCB-f37eaa14-7_2
SMILES:	CC[C@]1(C[C@@H](C1)[N@]2c3c(cc(cc3)Cl)[C@@]4(C2)C(=O)N(CC4)c5c6c(cnc5)cccc6)O)C
RUN:	RUN3067
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.51

MAT-POS-b5746674-102_2



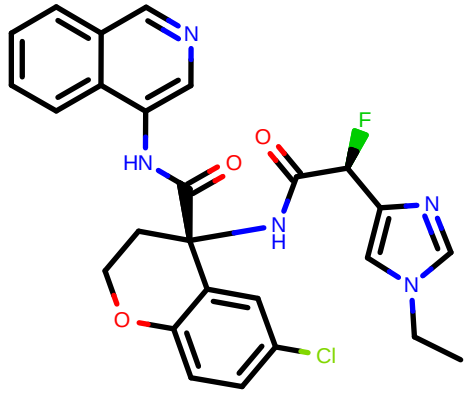
CID:	MAT-POS-b5746674-102_2
SMILES:	CCCCN(CCCNC(=O)Nc1cn(c(=O)c2c1cccc2)CC(C)C)c3ccccc3
RUN:	RUN84
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.20

ED_-GRI-5b13fbe2-27_1



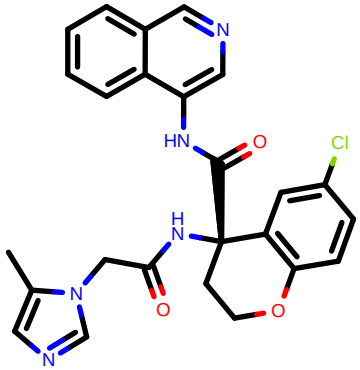
CID:	ED_-GRI-5b13fbe2-27_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cc(cn5)CN6CC[NH2+]CC6
RUN:	RUN1557
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.31

PET-UNK-a17c93d1-1_1



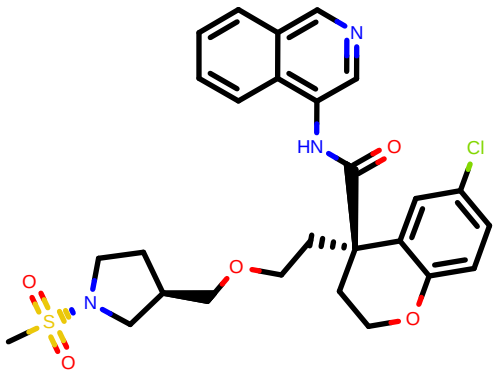
CID:	PET-UNK-a17c93d1-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)OCC4CCCCC4
RUN:	RUN520
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.27

VLA-UCB-34f3ed0c-18_1



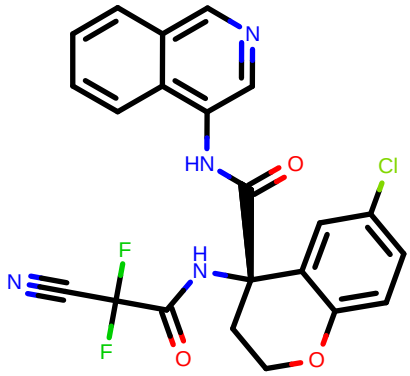
CID:	VLA-UCB-34f3ed0c-18_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CN([C@@]4(C3=O)CCOc5c4cc(cc5)Cl)C(=O)N6CC[NH2+]CC6
RUN:	RUN642
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.26

FRA-DIA-6238d354-2_3



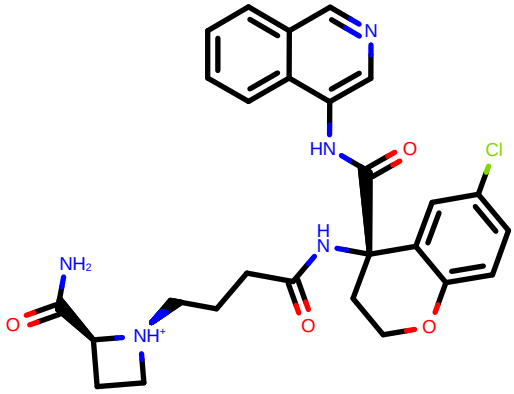
CID:	FRA-DIA-6238d354-2_3
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)C
RUN:	RUN3798
DDG (kcal/mol):	-1.56
dDDG (kcal/mol):	0.28

NIR-THE-47736cde-2_1



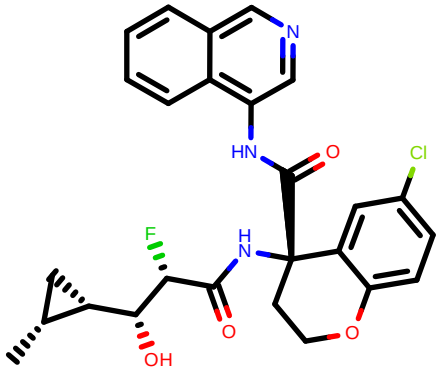
CID:	NIR-THE-47736cde-2_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN3328
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.10

MIC-UNK-91acba05-3_2



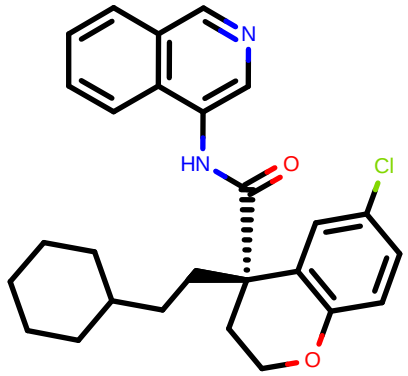
CID:	MIC-UNK-91acba05-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN473
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.33

VLA-UCB-34f3ed0c-8_1



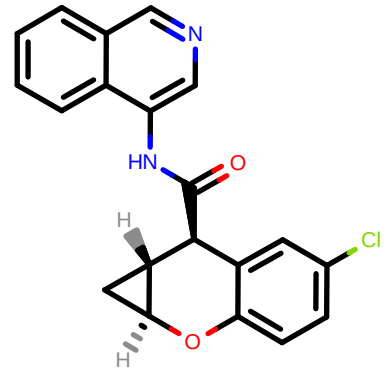
CID:	VLA-UCB-34f3ed0c-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CCc5ccn[nH]5
RUN:	RUN634
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.27

ALP-POS-3b848b35-2_2



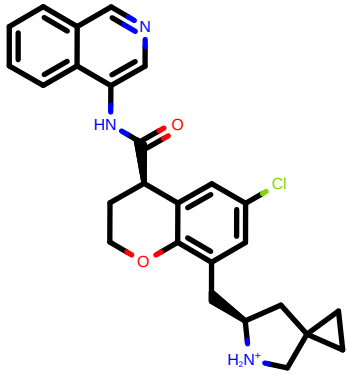
CID:	ALP-POS-3b848b35-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN60
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.21

LON-WEI-4d77710c-17_1



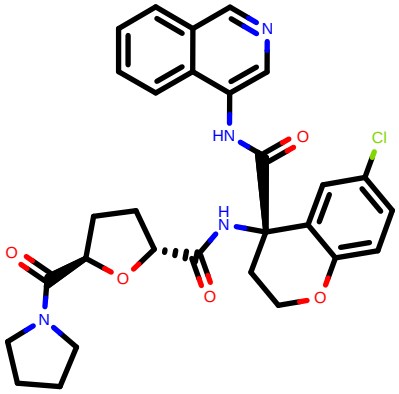
CID:	LON-WEI-4d77710c-17_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccc(cc3)Cl
RUN:	RUN205
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.13

DAR-DIA-0cde14eb-60_1



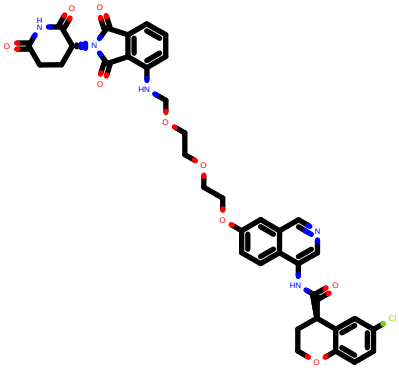
CID:	DAR-DIA-0cde14eb-60_1
SMILES:	C[C@@H](c1cccc(c1)C2(CC2)C#N)C(=O)Nc3cncc4c3cccc4
RUN:	RUN30
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.47

MIC-UNK-c5a20098-3_1



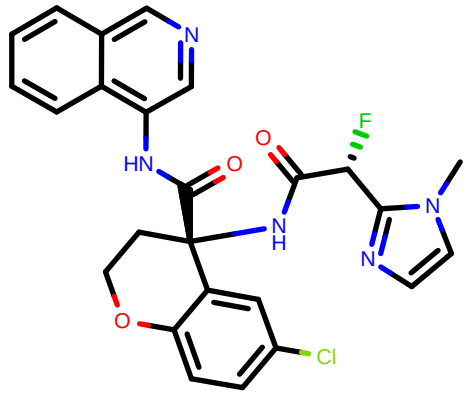
CID:	MIC-UNK-c5a20098-3_1
SMILES:	c1ccc2c(c1)cncc2C(=O)C(CC3CN(C3)c4cccc(c4)Cl)(F)F
RUN:	RUN1309
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.36

RAL-THA-1d44ff04-3_1



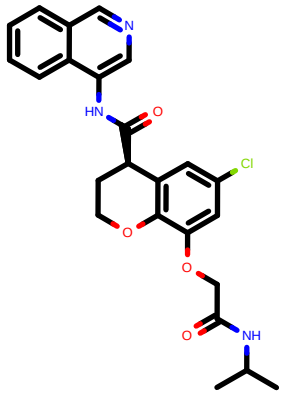
CID:	RAL-THA-1d44ff04-3_1
SMILES:	CC(=O)NCc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN437
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.57

EDJ-MED-37aac4bd-6_2



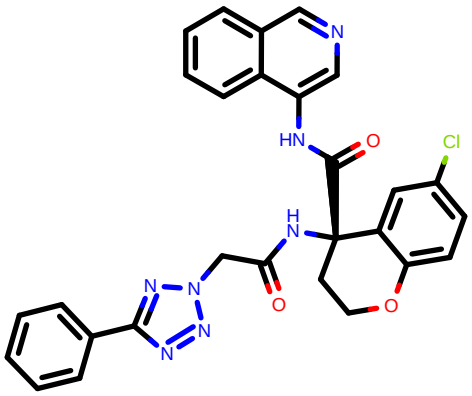
CID:	EDJ-MED-37aac4bd-6_2
SMILES:	COC[C@]1(CCOc2c1cc(cn2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3150
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.15

EDJ-MED-d08626de-5_1



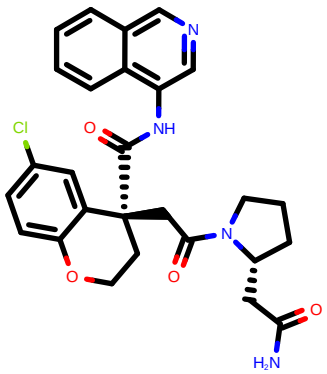
CID:	EDJ-MED-d08626de-5_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2345
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.29

MAT-POS-54c4bf04-2_1



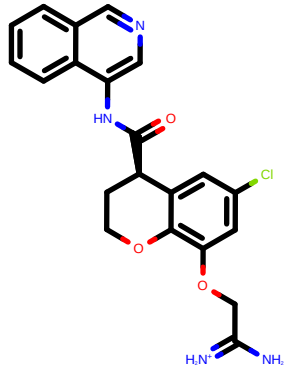
CID:	MAT-POS-54c4bf04-2_1
SMILES:	COc1ccc(cc1OCCNC(=O)c2cncc3c2cccc3)Cl
RUN:	RUN1222
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.39

KAD-UNI-877d7bed-10_2



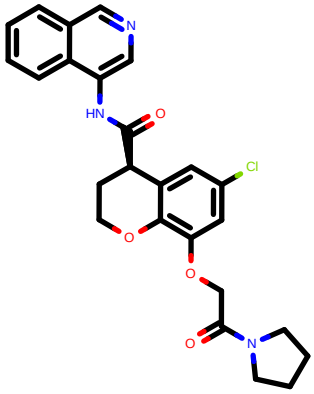
CID:	KAD-UNI-877d7bed-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCC(=O)N5CCOCC5)Cl
RUN:	RUN3746
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.12

ALP-POS-e0fe77e5-1_2



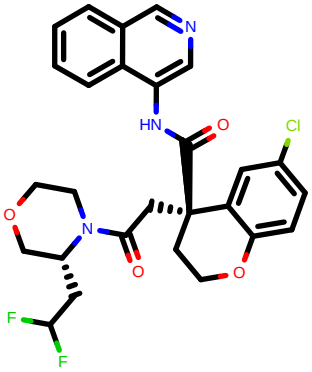
CID:	ALP-POS-e0fe77e5-1_2
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@H](C3=O)c4ccc(c(c4)Cl)Cl
RUN:	RUN2323
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.31

EDJ-MED-40433386-6_1



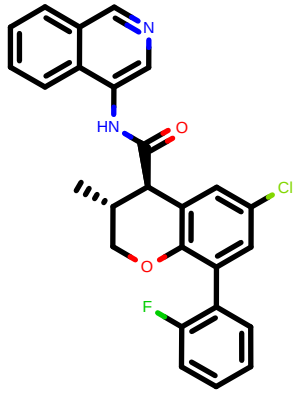
CID:	EDJ-MED-40433386-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]56CCO[C@H]5CCOC6
RUN:	RUN2557
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.32

PET-UNK-8922bd3c-1_1



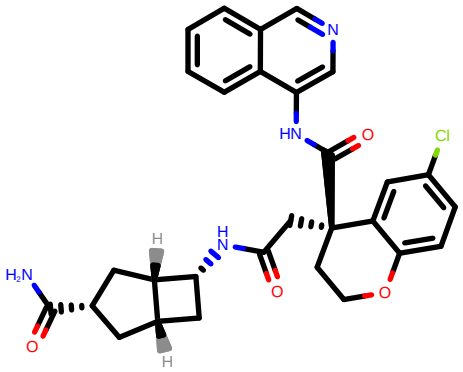
CID:	PET-UNK-8922bd3c-1_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)Cl
RUN:	RUN1168
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.24

MIC-UNK-c66144cb-3_1



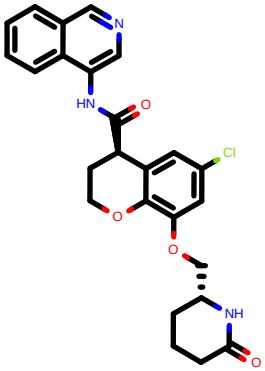
CID:	MIC-UNK-c66144cb-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN127
DDG (kcal/mol):	-1.54
dDDG (kcal/mol):	0.33

LON-WEI-5e7d1b3e-45_1



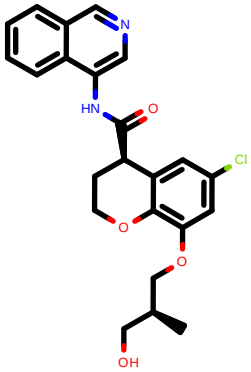
CID:	LON-WEI-5e7d1b3e-45_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N3CCN(CC3)C(=O)c4ccco4
RUN:	RUN1354
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.41

ALP-UNI-0676e700-2_2



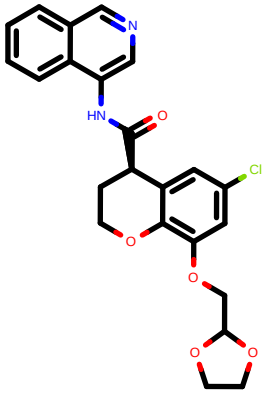
CID:	ALP-UNI-0676e700-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)CCNC(=O)[C@H]5CCCO5
RUN:	RUN2450
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.31

KAD-UNI-80f122c8-5_1



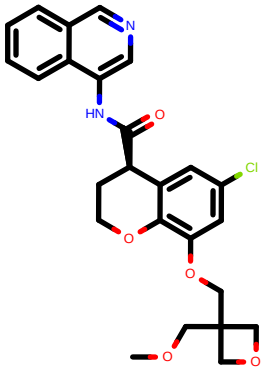
CID:	KAD-UNI-80f122c8-5_1
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2301
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.39

KAD-UNI-8a629cb0-25_1



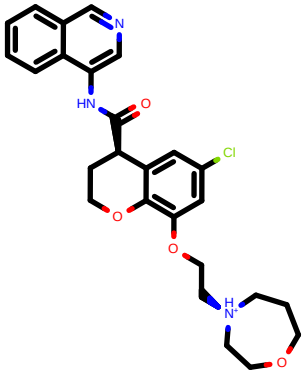
CID:	KAD-UNI-8a629cb0-25_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CCC(=O)NS(C[C@@H]6CCS(=O)(=O)C[C@H]6C5
RUN:	RUN2107
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.42

DAR-DIA-e7614d05-1_1



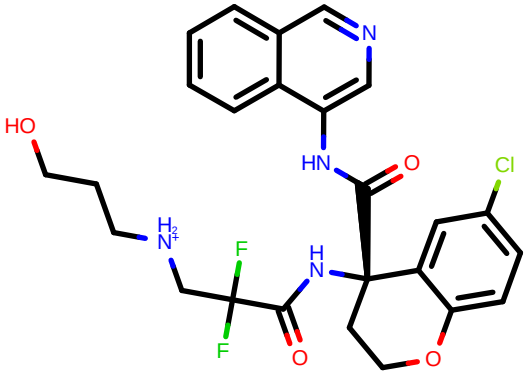
CID:	DAR-DIA-e7614d05-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC(F)(F)F
RUN:	RUN2477
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.35

EDG-MED-ba1ac7b9-5_4



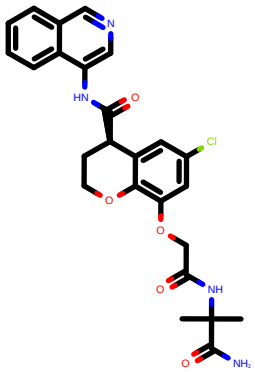
CID:	EDG-MED-ba1ac7b9-5_4
SMILES:	CC[C@H](CO)[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2641
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.60

ALP-POS-02c6a514-32_2



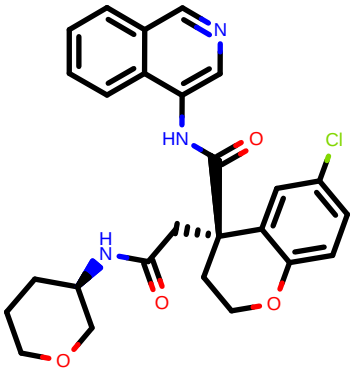
CID:	ALP-POS-02c6a514-32_2
SMILES:	CC(C)(C)c1ccc(cc1)N([C@H](c2cncc3c2cccc3)C(=O)NCCc4cccc(c4)F)C(=O)c5ccco5
RUN:	RUN645
DDG (kcal/mol):	-1.53
dDDG (kcal/mol):	0.43

ALP-UNI-3496895b-5_4



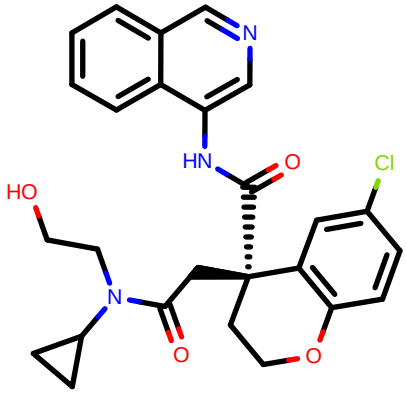
CID:	ALP-UNI-3496895b-5_4
SMILES:	C[C@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2515
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.44

LON-WEI-4d77710c-52_1



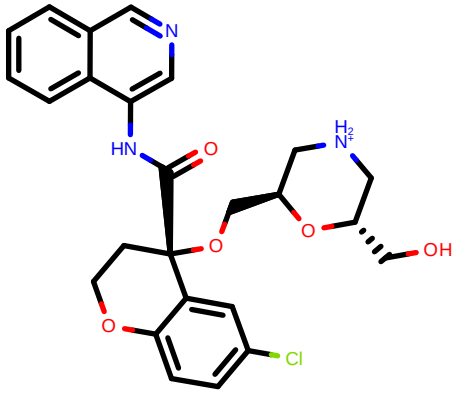
CID:	LON-WEI-4d77710c-52_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccc(cc3)Cl
RUN:	RUN239
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.32

JOH-SUS-a69c159d-1_2



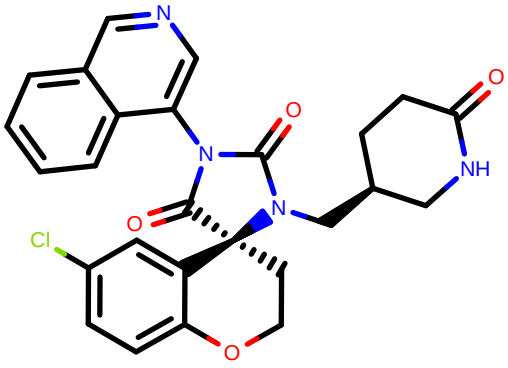
CID:	JOH-SUS-a69c159d-1_2
SMILES:	Cc1c2ccccc2c(cn1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1117
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.22

VLA-UCB-05e51b3f-16_1



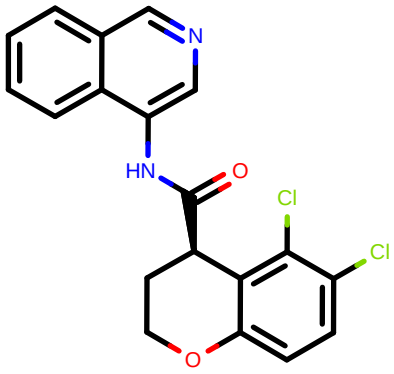
CID:	VLA-UCB-05e51b3f-16_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN328
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.45

MAK-UNK-c749d764-19_8



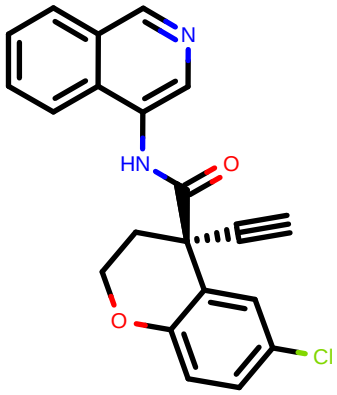
CID:	MAK-UNK-c749d764-19_8
SMILES:	c1ccc2c(c1)cncc2N(C[NH3+])C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1005
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.25

MAT-POS-b5746674-103_1



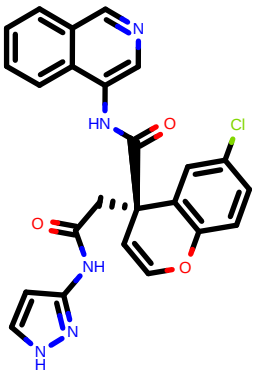
CID:	MAT-POS-b5746674-103_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CCN(CC3)c4ccccc4F
RUN:	RUN81
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.20

MAT-POS-2492181e-10_1



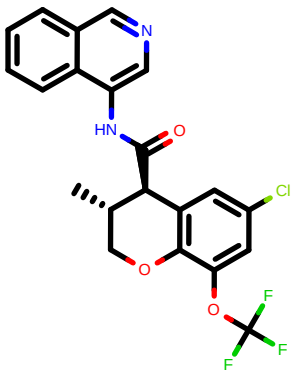
CID:	MAT-POS-2492181e-10_1
SMILES:	C[C@@H]1CCCC[N@@H+]1CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN104
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.20

LON-WEI-4d77710c-50_2



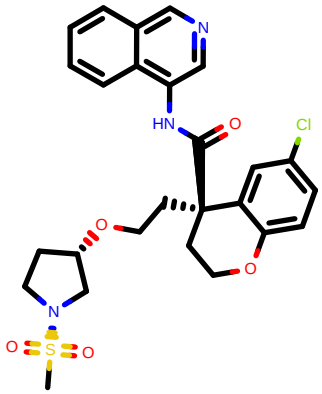
CID:	LON-WEI-4d77710c-50_2
SMILES:	CCCC[N@H+](CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C)Cc3ccco3
RUN:	RUN246
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.26

PET-UNK-7be94445-2_1



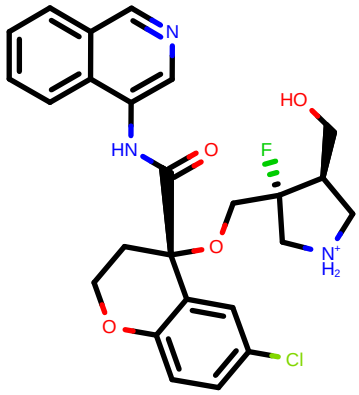
CID:	PET-UNK-7be94445-2_1
SMILES:	c1ccc2c(c1)cncc2N3CCN(C3=O)c4cccc(c4)Cl
RUN:	RUN133
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.25

RUB-POS-1325a9ea-2_1



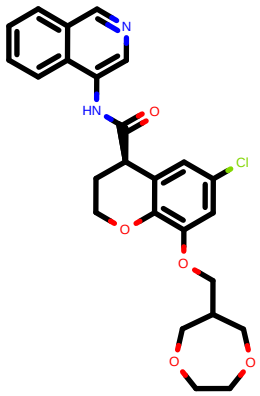
CID:	RUB-POS-1325a9ea-2_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2c(ccc3)F
RUN:	RUN3606
DDG (kcal/mol):	-1.51
dDDG (kcal/mol):	0.20

FRA-DIA-b66f7109-1_2



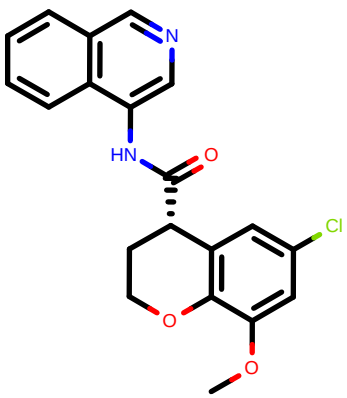
CID:	FRA-DIA-b66f7109-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CNc4c3cc(cc4Cl)O[C@H]5CC(=O)N5
RUN:	RUN392
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.32

JOH-UNI-ea72002d-4_1



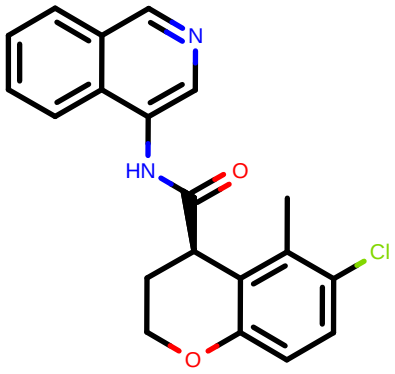
CID:	JOH-UNI-ea72002d-4_1
SMILES:	c1ccc2c(c1)cncc2[C@@](C(=O)[C@@H]3CCOc4c3cc(cc4Cl)(N5C(=O)C=CC5=O)F
RUN:	RUN2488
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.43

LON-WEI-4d77710c-21_1



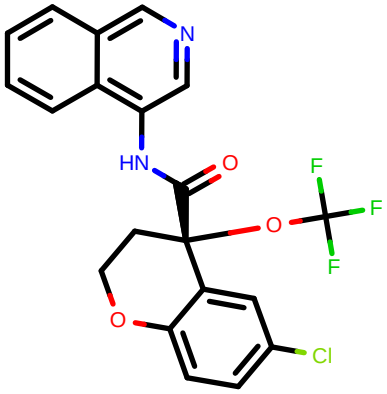
CID:	LON-WEI-4d77710c-21_1
SMILES:	Cc1cccnc1NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN207
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.13

DAR-DIA-0cde14eb-46_1



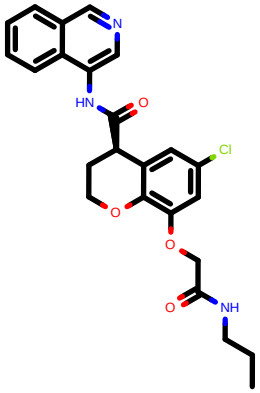
CID:	DAR-DIA-0cde14eb-46_1
SMILES:	CC1(CC1)c2cccc(c2)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN10
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.17

MAT-POS-5369c344-3_2



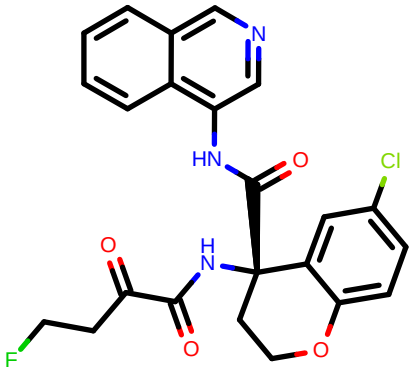
CID:	MAT-POS-5369c344-3_2
SMILES:	c1ccc(cc1)COc2cc(cc3c2OCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3619
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.08

EDJ-MED-9e38fd34-4_1



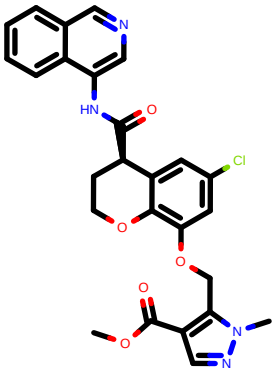
CID:	EDJ-MED-9e38fd34-4_1
SMILES:	C[C@@]1(c2cc(c(cc2NC1=O)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2349
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.34

DAR-DIA-0587064e-13_2



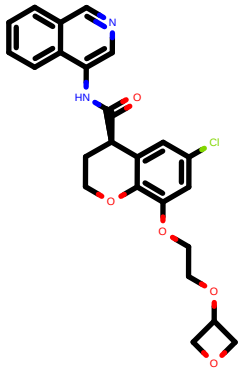
CID:	DAR-DIA-0587064e-13_2
SMILES:	CCCOc1cc(cc2c1NCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3361
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.12

EDJ-MED-d203f206-34_1



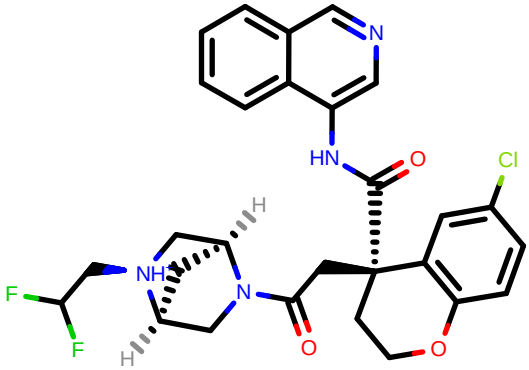
CID:	EDJ-MED-d203f206-34_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]5CO
RUN:	RUN2597
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.34

ALP-POS-2da19ca7-7_1



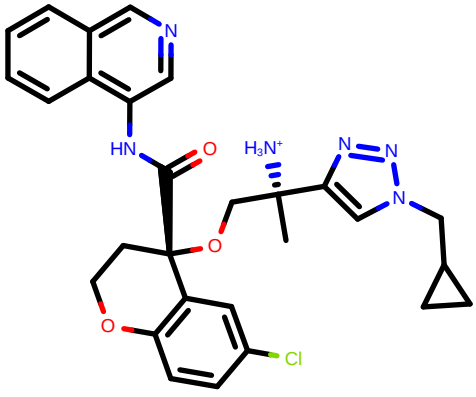
CID:	ALP-POS-2da19ca7-7_1
SMILES:	C[C@@H]1C[N@@]([CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2381
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.35

LON-WEI-5e7d1b3e-42_2



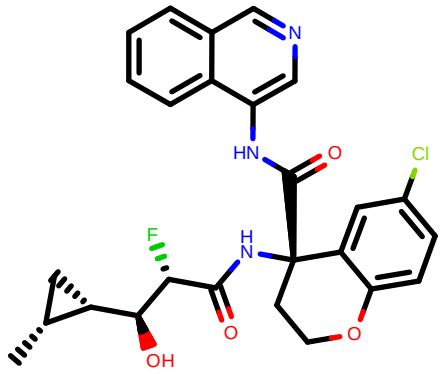
CID:	LON-WEI-5e7d1b3e-42_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N[C@H]3CCCc4c3cccc4
RUN:	RUN1349
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.26

RAL-THA-065e0743-2_1



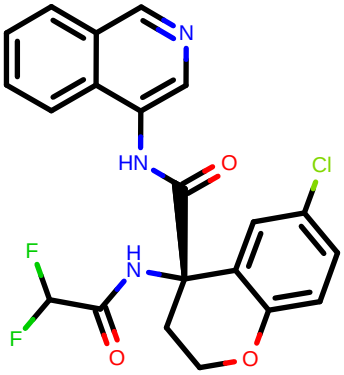
CID:	RAL-THA-065e0743-2_1
SMILES:	Cc1c(c2ccccc2cn1)NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4
RUN:	RUN450
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.49

ADA-UCB-dc2b944c-1_1



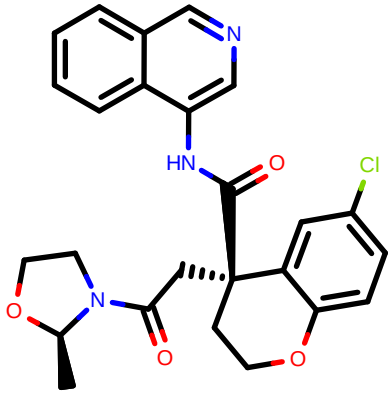
CID:	ADA-UCB-dc2b944c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[N@@H+][[C@@]4(C3=O)CCOc5c4cc(cc5)Cl)CC6CCCCC6
RUN:	RUN594
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.22

MIC-UNK-50cce87d-4_1



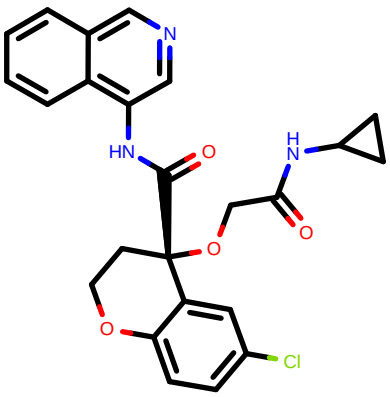
CID:	MIC-UNK-50cce87d-4_1
SMILES:	COc1cccc2c1c(cnc2)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN667
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.20

ALP-POS-d3acb8cc-1_1



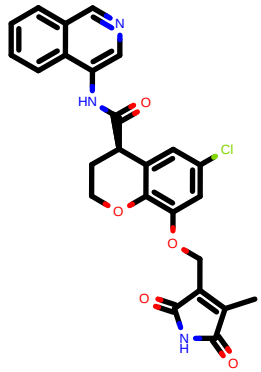
CID:	ALP-POS-d3acb8cc-1_1
SMILES:	C[C@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1092
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.26

MIC-UNK-d854bf4c-1_1



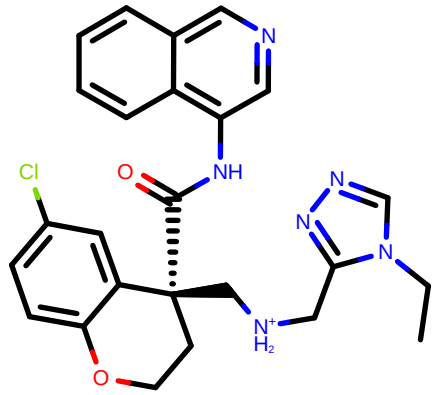
CID:	MIC-UNK-d854bf4c-1_1
SMILES:	CC(=O)N1CCC2(CC1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN3326
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.12

EDJ-MED-d203f206-41_1



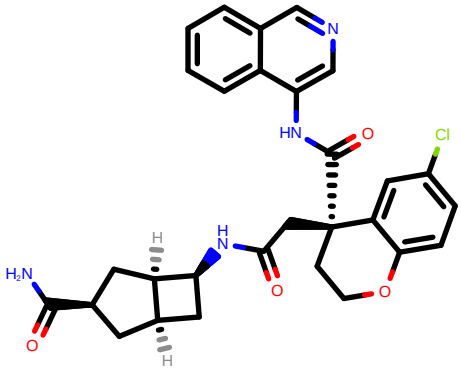
CID:	EDJ-MED-d203f206-41_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CO
RUN:	RUN2602
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.46

PET-UNK-9b23ef84-10_2



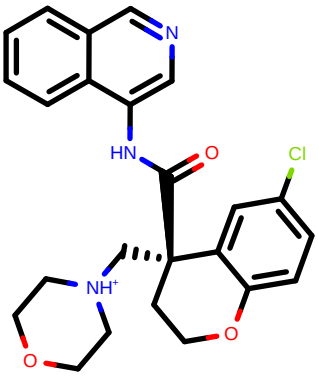
CID:	PET-UNK-9b23ef84-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(c(c4)F)Cl)c5ncno5
RUN:	RUN4440
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.26

DAR-DIA-9e4459de-15_12



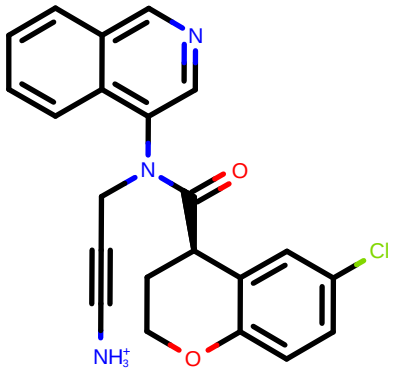
CID:	DAR-DIA-9e4459de-15_12
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1455
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.27

RAL-THA-8416115c-8_2



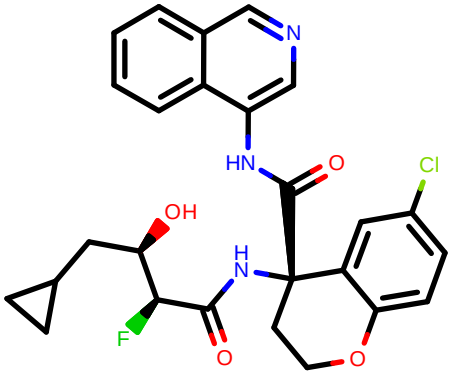
CID:	RAL-THA-8416115c-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)CC(=O)N
RUN:	RUN1276
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.25

DAR-DIA-ecdbc7dd-8_2



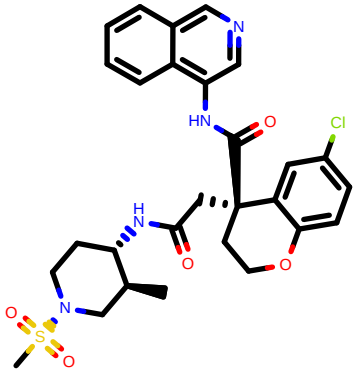
CID:	DAR-DIA-ecdbc7dd-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCNc4c3cc(cc4)Cl)C[NH+]5CCCC5
RUN:	RUN2888
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.13

DAR-DIA-0d514e7d-35_1



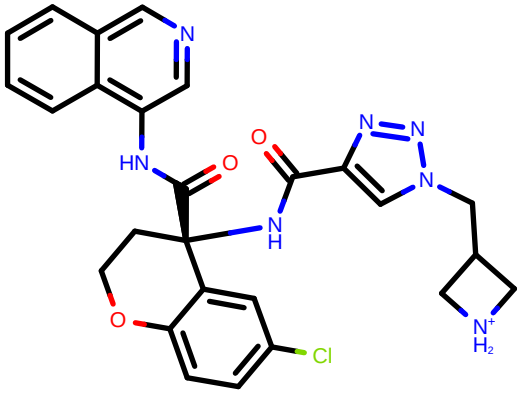
CID:	DAR-DIA-0d514e7d-35_1
SMILES:	C[C@H]1[C@@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN887
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.29

RAL-THA-8416115c-4_1



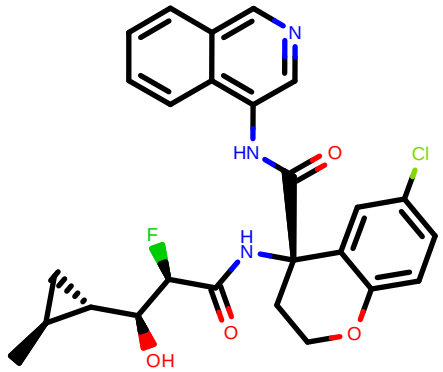
CID:	RAL-THA-8416115c-4_1
SMILES:	CCCN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1259
DDG (kcal/mol):	-1.48
dDDG (kcal/mol):	0.33

ALP-POS-fe871b40-14_2



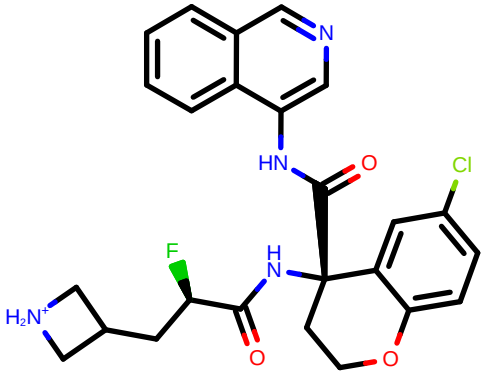
CID:	ALP-POS-fe871b40-14_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC(=O)Nc4c3cc(cn4)Cl
RUN:	RUN3134
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.15

EDJ-MED-15e90dfc-3_1



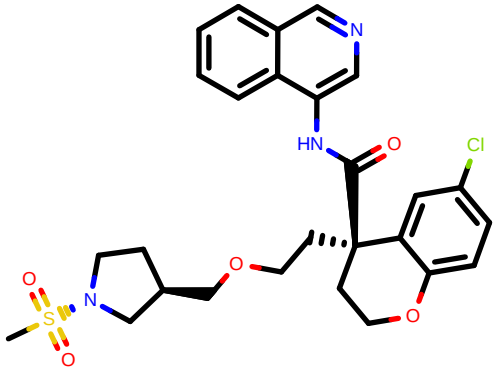
CID:	EDJ-MED-15e90dfc-3_1
SMILES:	COCC[NH2+]C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3441
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.14

MAK-UNK-c749d764-19_4



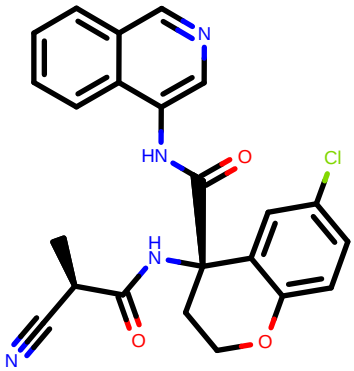
CID:	MAK-UNK-c749d764-19_4
SMILES:	c1ccc2c(c1)cncc2N(C[NH3+])C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1001
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.27

MAK-UNK-83e0a0b4-1_2



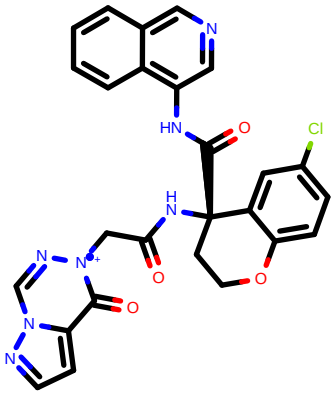
CID:	MAK-UNK-83e0a0b4-1_2
SMILES:	CCCCc1ccc2c(c1)[C@H](CCO2)C(=O)N(CCNC3C[NH2+]C3)c4cncc5c4ccc(c5)CN6CC[NH2+]CC6
RUN:	RUN733
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.37

ROB-UNI-611831f5-1_1



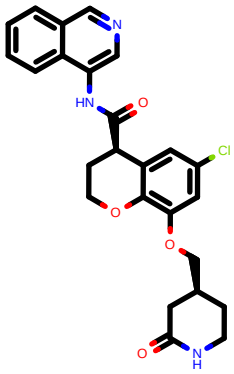
CID:	ROB-UNI-611831f5-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)Oc4cc(c(=O)[nH]c4)N
RUN:	RUN3323
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.12

RAL-THA-8416115c-1_4



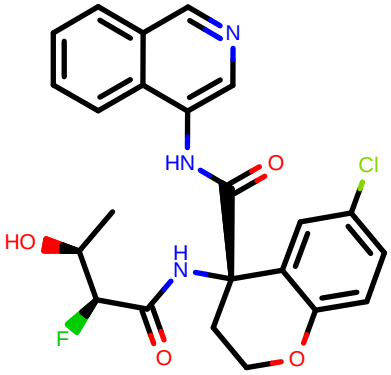
CID:	RAL-THA-8416115c-1_4
SMILES:	c1ccc(cc1)CN2CC[C@H](c3c2ccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1250
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.34

ALP-UNI-0676e700-14_1



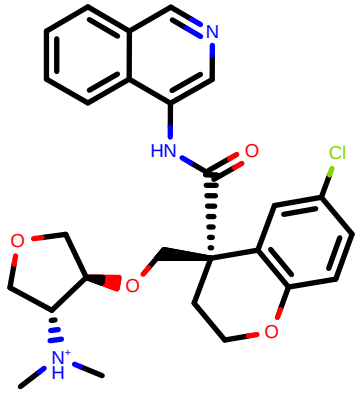
CID:	ALP-UNI-0676e700-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cnc6c(cnn6c5)C#N
RUN:	RUN2458
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.29

MIC-UNK-cdc2493e-8_7



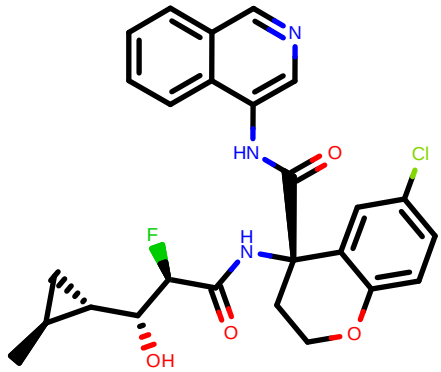
CID:	MIC-UNK-cdc2493e-8_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@H]5CCCC[C@H]5C4
RUN:	RUN542
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.24

MIC-UNK-5a93dd5f-10_2



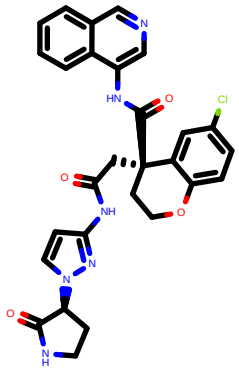
CID:	MIC-UNK-5a93dd5f-10_2
SMILES:	CC(=O)N1CC[NH+](CC1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN787
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.26

MIC-UNK-5a93dd5f-3_6



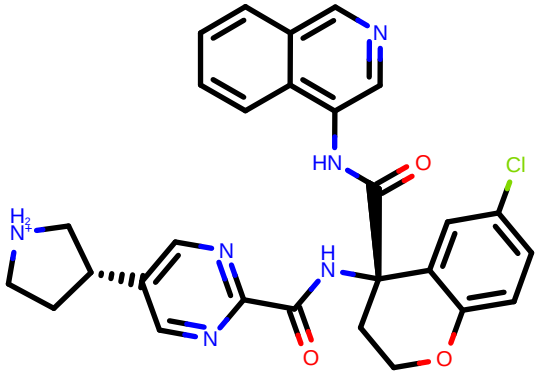
CID:	MIC-UNK-5a93dd5f-3_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@@H+]4CC[C@H]5CCCC[C@@H]5C4
RUN:	RUN745
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.28

DAR-DIA-9e4459de-11_3



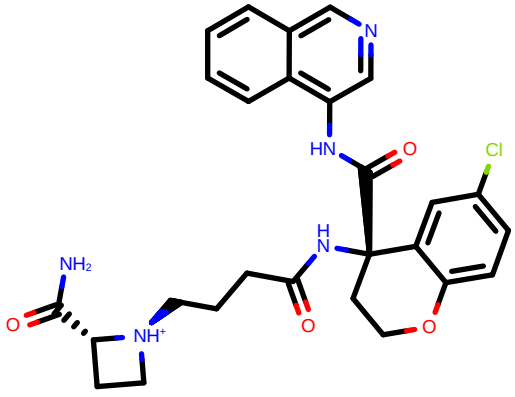
CID:	DAR-DIA-9e4459de-11_3
SMILES:	c1cc2c(c(c1)NCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1411
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.34

MIC-UNK-8758c41d-1_2



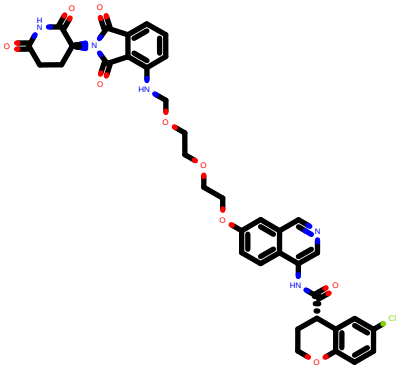
CID:	MIC-UNK-8758c41d-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCS(=O)(=O)c4c3cc(c(c4)Cl)Cl
RUN:	RUN3314
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.16

MAT-POS-0c8fa4a7-1_1



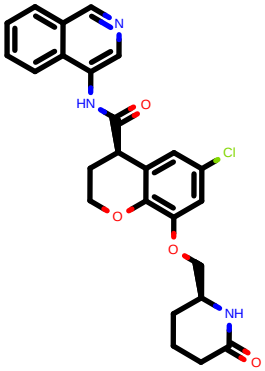
CID:	MAT-POS-0c8fa4a7-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3=CCCc4c3cc(cc4)Cl
RUN:	RUN517
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.37

MIC-UNK-9582b2c5-1_7



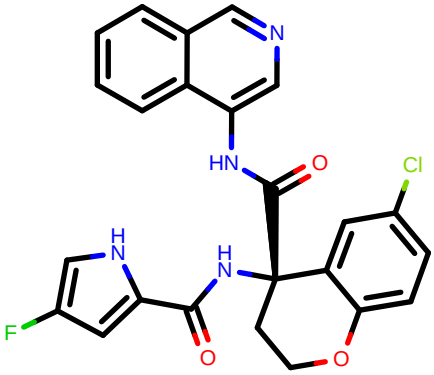
CID:	MIC-UNK-9582b2c5-1_7
SMILES:	CC(=O)N1CC[C@@H]2[C@H](C1)CN(C(=O)[C@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN259
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.44

ALP-UNI-0676e700-9_1



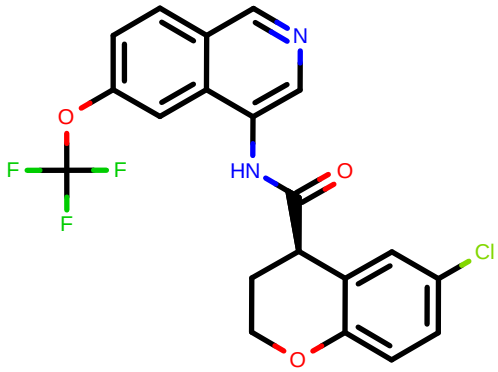
CID:	ALP-UNI-0676e700-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccn6c(c5)nnn6
RUN:	RUN2451
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.34

JAG-UCB-706446eb-5_2



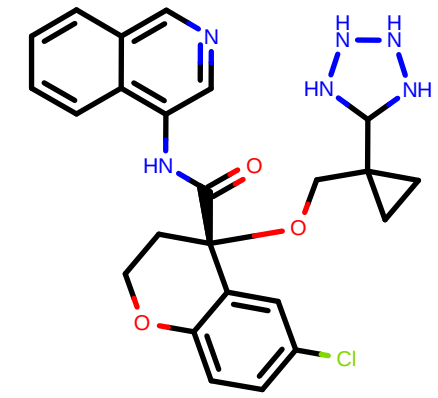
CID:	JAG-UCB-706446eb-5_2
SMILES:	COCCN([C@H]1CCCOC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN625
DDG (kcal/mol):	-1.46
dDDG (kcal/mol):	0.25

EDJ-MED-e4b030d8-12_1



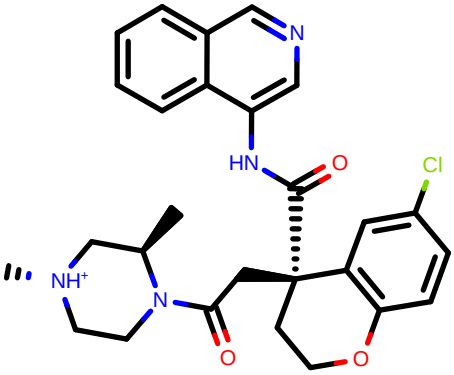
CID:	EDJ-MED-e4b030d8-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3Cc4cc(ccc4OC3)Cl
RUN:	RUN292
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.22

ALP-POS-fe871b40-10_1



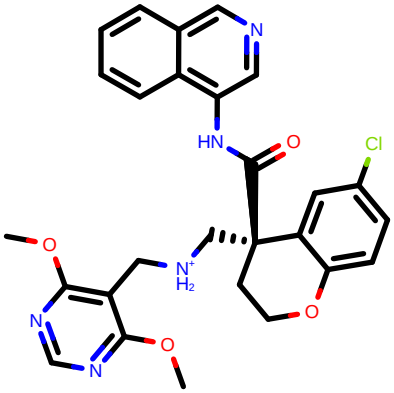
CID:	ALP-POS-fe871b40-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNc4c3cc(c(c4)F)Cl
RUN:	RUN3123
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.22

BEN-BAS-c2bc0d80-3_1



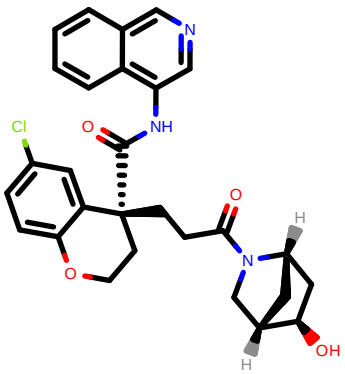
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3
RUN:	RUN1134
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.52

ALP-POS-347519b5-1_13



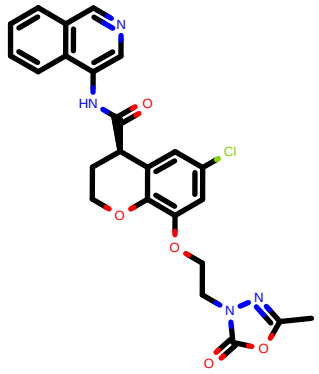
CID:	ALP-POS-347519b5-1_13
SMILES:	CS(=O)(=O)[N@@]1C[C@@H]2[C@H]3CC[C@H](C3)[C@@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4236
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.30

DAR-DIA-b4e9dd8d-6_2



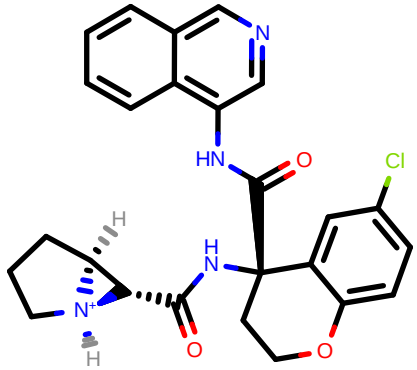
CID:	DAR-DIA-b4e9dd8d-6_2
SMILES:	COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN3399
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.16

ALP-UNI-3496895b-1_2



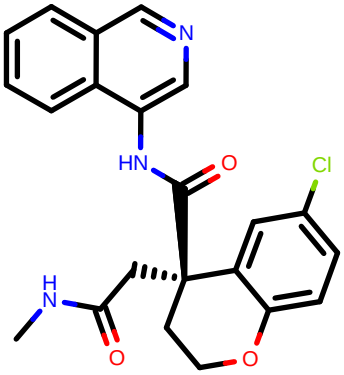
CID:	ALP-UNI-3496895b-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CCS(=O)(=O)N@]6[C@H]5CCCC6
RUN:	RUN2500
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.36

MIC-UNK-cdc2493e-11_1



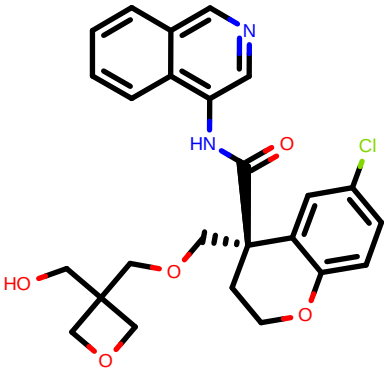
CID:	MIC-UNK-cdc2493e-11_1
SMILES:	C[NH+](C)C1CCC(CC1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN550
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-3_5



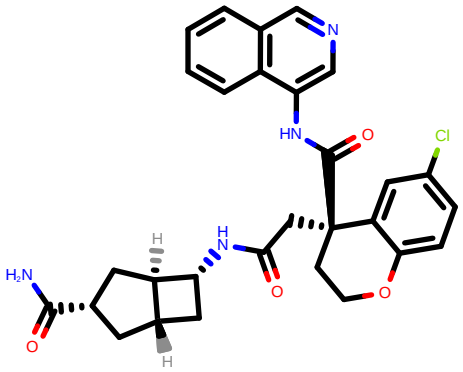
CID:	MAK-UNK-c749d764-3_5
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@@H]4CCC[C@@H]([C@H]4O)C(F)F
RUN:	RUN909
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.30

KAD-UNI-cb0f2bbc-2_1



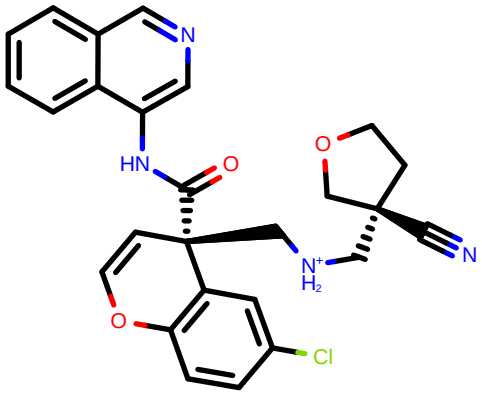
CID:	KAD-UNI-cb0f2bbc-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)C[NH2+]Cc5ccc(cc5)N6CC(=O)NC(=O)C6
RUN:	RUN3684
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.12

MAK-UNK-c749d764-19_7



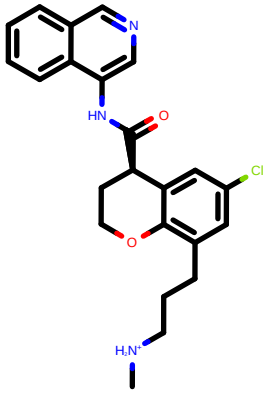
CID:	MAK-UNK-c749d764-19_7
SMILES:	c1ccc2c(c1)cncc2N(C[NH3+])C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1004
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.49

MIC-UNK-08fa0751-2_1



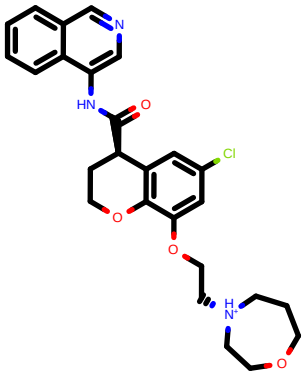
CID:	MIC-UNK-08fa0751-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C(CO)(F)F
RUN:	RUN1517
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.25

ALP-POS-477dc5b7-2_2



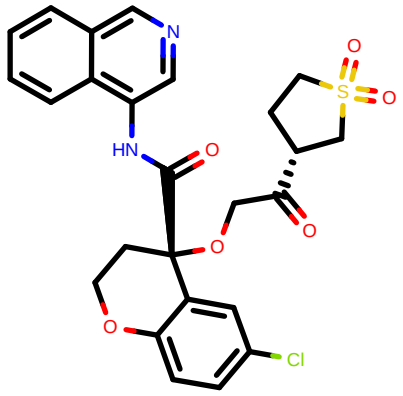
CID:	ALP-POS-477dc5b7-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN298
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.31

EDG-MED-ba1ac7b9-10_1



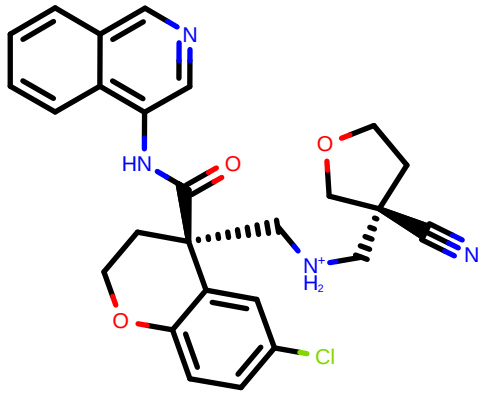
CID:	EDG-MED-ba1ac7b9-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@@H]5c6ccn[nH]6
RUN:	RUN2650
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.53

DAR-DIA-f6ee7aeb-5_2



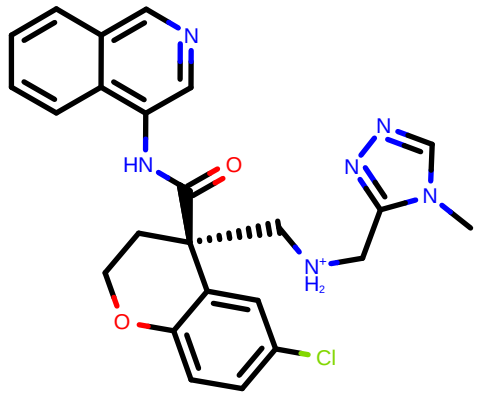
CID:	DAR-DIA-f6ee7aeb-5_2
SMILES:	CCCOc1cc(cc(c1)Cl)[C@H]2CC(=O)N(C[C@@H]2c3c[nH]c(=O)[nH]c3=O)c4cncc5c4cccc5
RUN:	RUN3415
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.20

MAT-POS-4223bc15-26_4



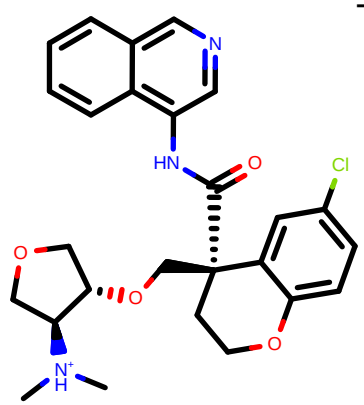
CID:	MAT-POS-4223bc15-26_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@](Cc4c3cc(cc4)Cl)CC(F)(F)F
RUN:	RUN4120
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.19

ALP-POS-347519b5-3_21



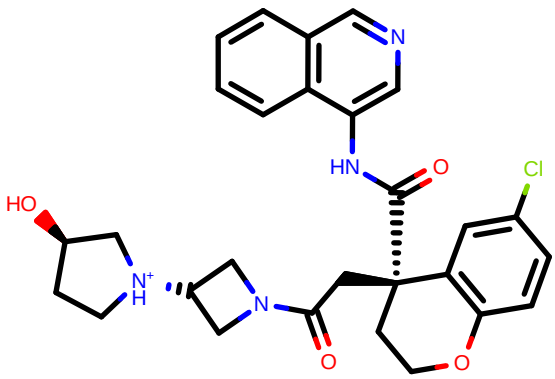
CID:	ALP-POS-347519b5-3_21
SMILES:	CS(=O)(=O)[N@@]1C[C@@H]2[C@H]3CC[C@@H]([C@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4304
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.20

EDJ-MED-15e90dfc-7_2



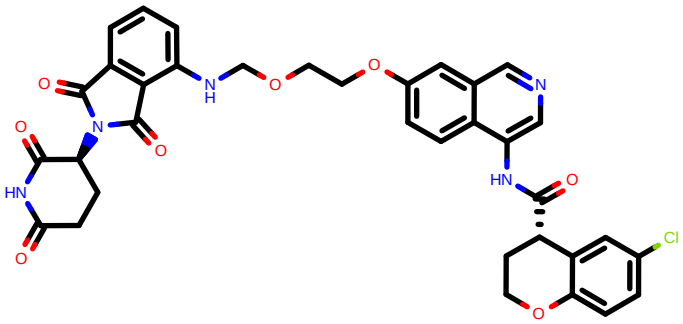
CID:	EDJ-MED-15e90dfc-7_2
SMILES:	CS(=O)(=O)CCNC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3458
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.35

LON-WEI-5e7d1b3e-34_2



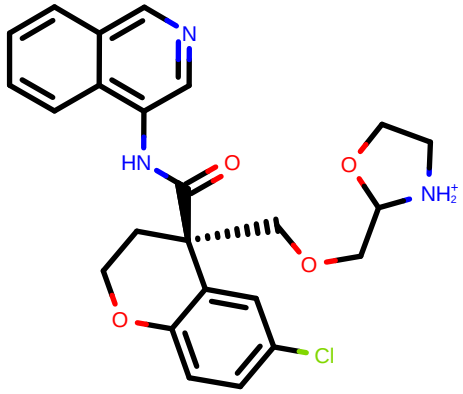
CID:	LON-WEI-5e7d1b3e-34_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CC[C@H](C3)c4ccccc4
RUN:	RUN1336
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.29

ALP-UNI-b33a865d-1_4



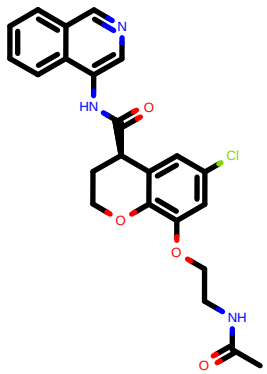
CID:	ALP-UNI-b33a865d-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN357
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.36

KAD-UNI-cb0f2bbc-1_2



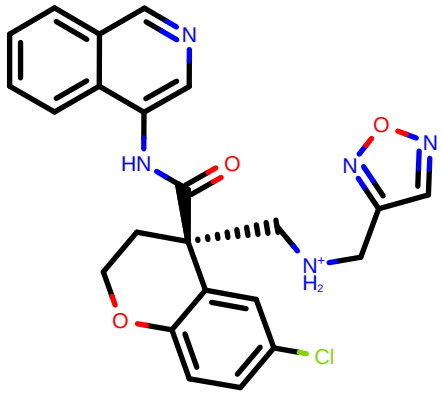
CID:	KAD-UNI-cb0f2bbc-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5ccc(cc5)N6CCNC(=O)C6
RUN:	RUN3682
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.11

ALP-POS-477dc5b7-4_1



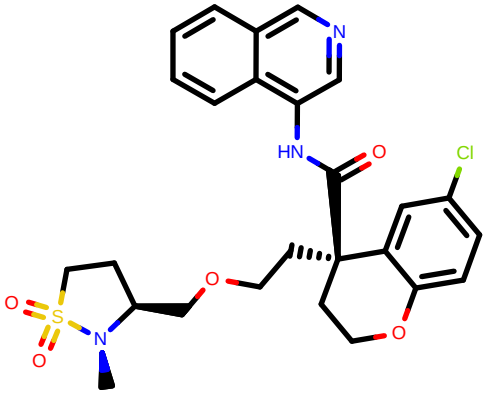
CID:	ALP-POS-477dc5b7-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN300
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.35

EDG-MED-90036822-94_2



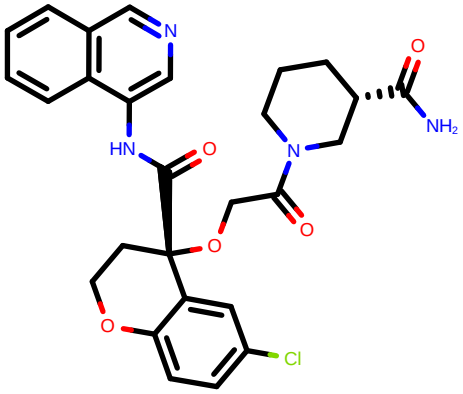
CID:	EDG-MED-90036822-94_2
SMILES:	C[C@H]1C[C@@H]1[C@@H]([C@@H](C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F)O
RUN:	RUN1805
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.41

EDJ-MED-6d9ff7d0-4_1



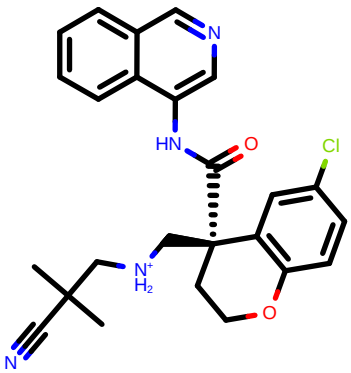
CID:	EDJ-MED-6d9ff7d0-4_1
SMILES:	COCCC[NH2+][C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3430
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.20

PET-UNK-29afea89-1_1



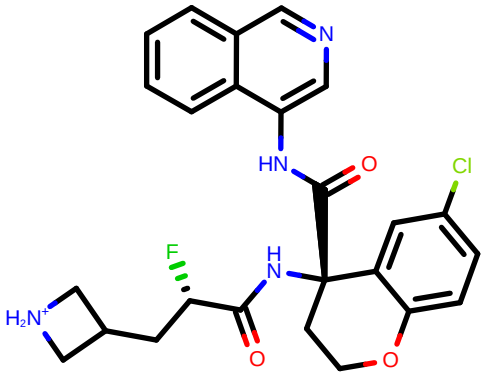
CID:	PET-UNK-29afea89-1_1
SMILES:	C#C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN657
DDG (kcal/mol):	-1.43
dDDG (kcal/mol):	0.34

DAR-DIA-9e4459de-13_6



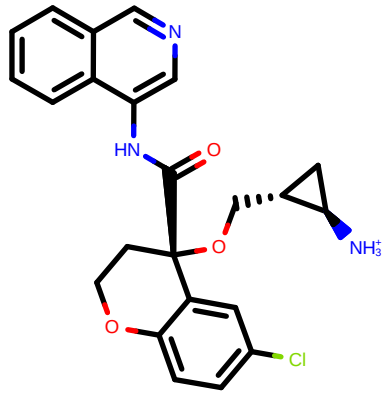
CID:	DAR-DIA-9e4459de-13_6
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1430
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.19

ADA-UCB-dc2b944c-12_1



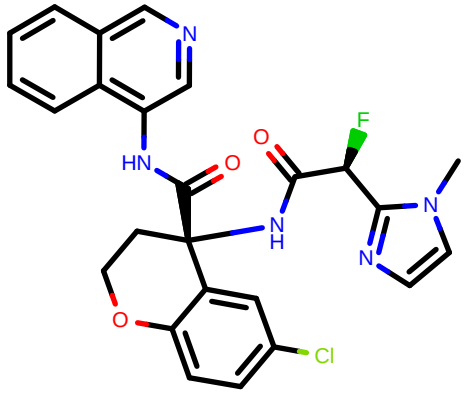
CID:	ADA-UCB-dc2b944c-12_1
SMILES:	Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN609
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.32

DAR-DIA-23e5a6a0-1_2



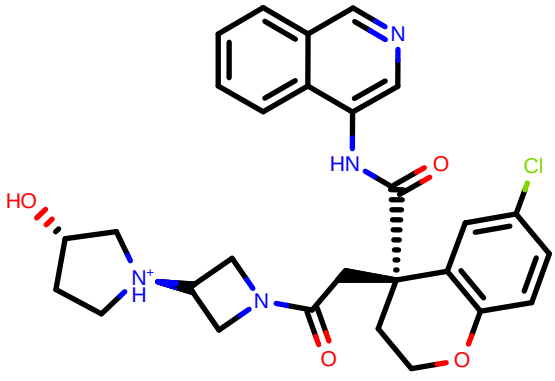
CID:	DAR-DIA-23e5a6a0-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CCC6([NH2+]5)CCC6)Cl
RUN:	RUN402
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.25

DAR-DIA-0587064e-17_1



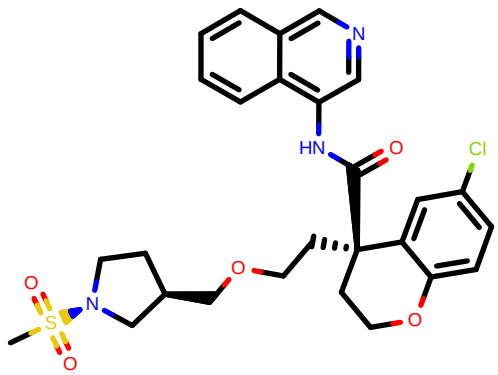
CID:	DAR-DIA-0587064e-17_1
SMILES:	COCCOc1cc(cc2c1OCC[C@@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3369
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.16

ERI-UCB-d6de1f3c-2_1



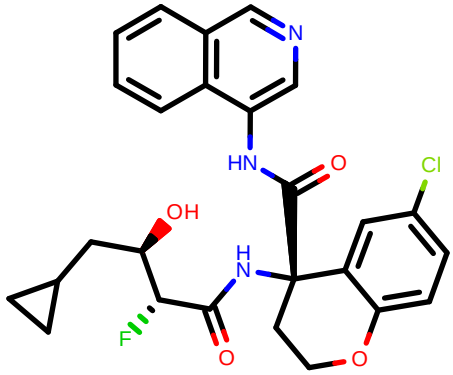
CID:	ERI-UCB-d6de1f3c-2_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N3CCN(C(=O)C3)c4cccc(c4)Cl
RUN:	RUN1091
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.33

ALP-POS-e4f7337d-1_3



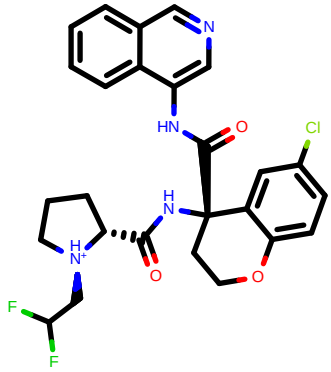
CID:	ALP-POS-e4f7337d-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[NH2+]C[C@@H]5CC[C@@H](O5)C(=O)N6CCCC6
RUN:	RUN3567
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.23

VLA-UCB-34f3ed0c-10_1



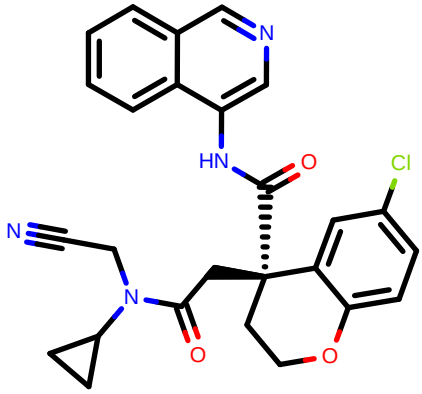
CID:	VLA-UCB-34f3ed0c-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCCc5ccn[nH]5
RUN:	RUN638
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.25

MAK-UNK-ffc90da7-5_1



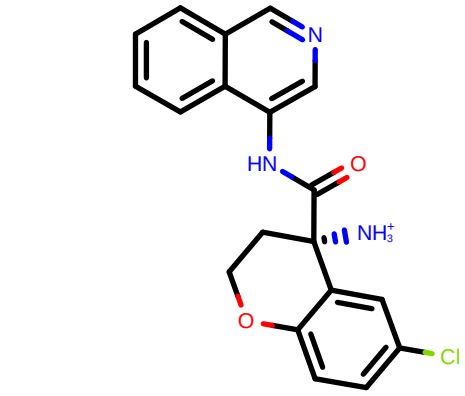
CID:	MAK-UNK-ffc90da7-5_1
SMILES:	C[C@@](CO)(c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C4CC4
RUN:	RUN702
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.35

DAR-DIA-5ff57136-12_1



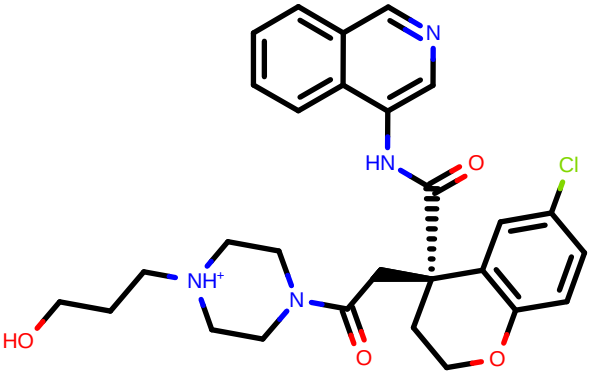
CID:	DAR-DIA-5ff57136-12_1
SMILES:	c1ccc2c(c1)cncc2N(C#C[C@@H]3CCC[NH2+]3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN1382
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.17

ALP-UNI-b33a865d-1_2



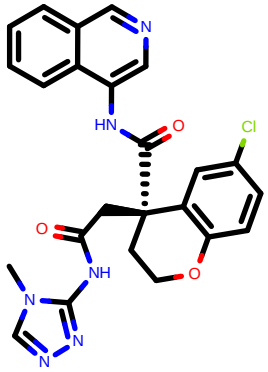
CID:	ALP-UNI-b33a865d-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN355
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.23

ED_-GRI-5b13fbe2-57_1



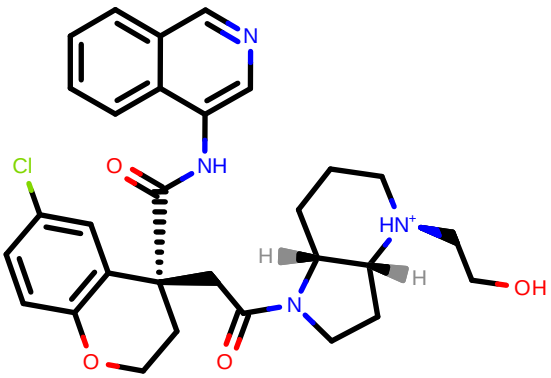
CID:	ED_-GRI-5b13fbe2-57_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5ccn[nH]5
RUN:	RUN1604
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.31

MIC-UNK-5a93dd5f-7_6



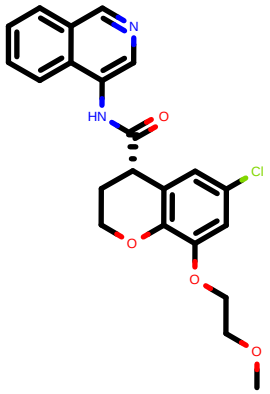
CID:	MIC-UNK-5a93dd5f-7_6
SMILES:	CC(=O)N(C)[C@H]1CC[N@@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN773
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.20

ED_-GRI-5b13fbe2-42_1



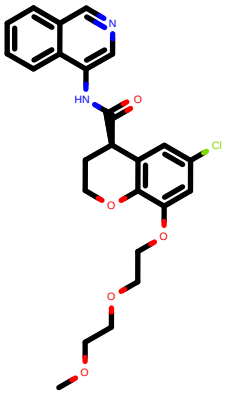
CID:	ED_-GRI-5b13fbe2-42_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](CF)[NH3+]
RUN:	RUN1576
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.60

EDJ-MED-d08626de-3_1



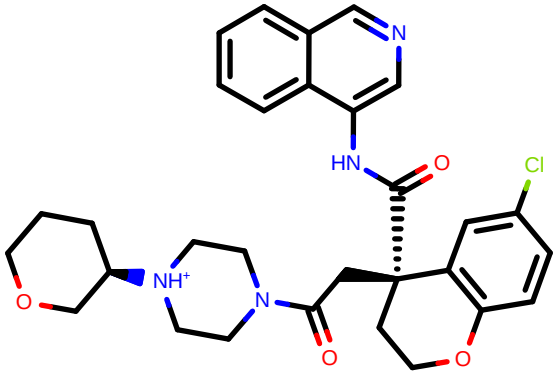
CID:	EDJ-MED-d08626de-3_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2341
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.24

KAD-UNI-8a629cb0-12_1



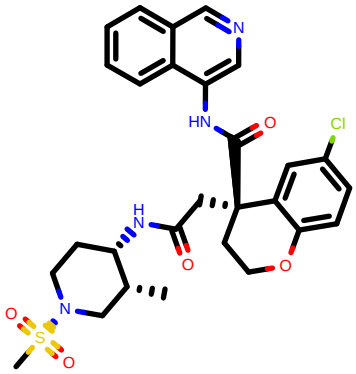
CID:	KAD-UNI-8a629cb0-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)[C@H]5Cc6[nH+]ccn6C5
RUN:	RUN2094
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.36

BEN-DND-f2e727cd-6_2



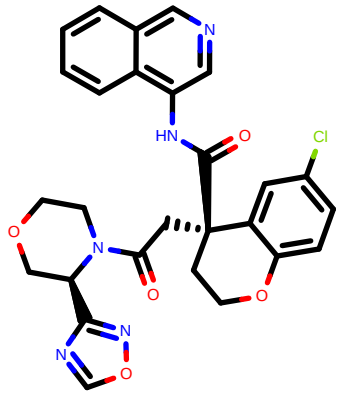
CID:	BEN-DND-f2e727cd-6_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1199
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.26

LON-WEI-5e7d1b3e-7_1



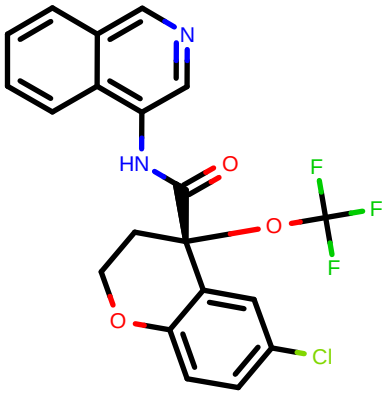
CID:	LON-WEI-5e7d1b3e-7_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCC[N@@H+]3CCc4ccccc4C3
RUN:	RUN1315
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.29

KAD-UNI-b13decd3-7_1



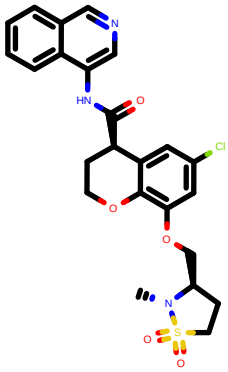
CID:	KAD-UNI-b13decd3-7_1
SMILES:	CC(=O)OCCn1cc(cn1)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3792
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.15

MAT-POS-5369c344-5_2



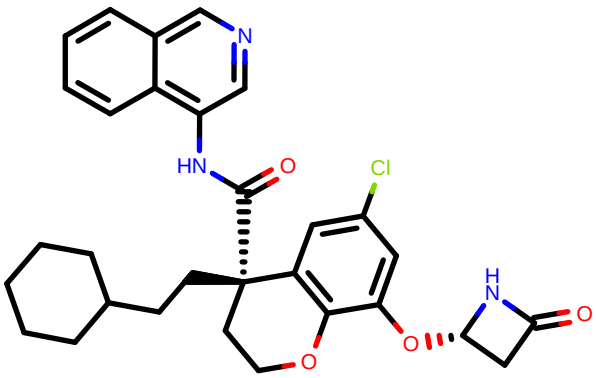
CID:	MAT-POS-5369c344-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCc5ccccn5)Cl
RUN:	RUN3623
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.07

ALP-UNI-76695c4f-8_2



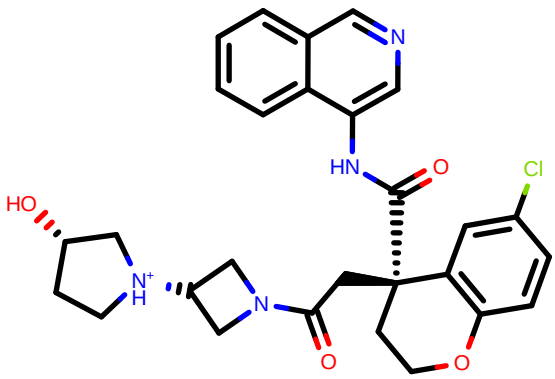
CID:	ALP-UNI-76695c4f-8_2
SMILES:	C[N@@]1(C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2179
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.43

DAR-DIA-ecdbc7dd-15_2



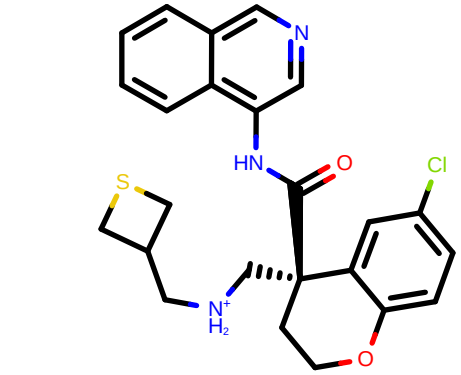
CID:	DAR-DIA-ecdbc7dd-15_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCNc4c3cc(cc4)Cl)C[NH3+]
RUN:	RUN2902
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.33

ERI-UCB-d6de1f3c-6_1



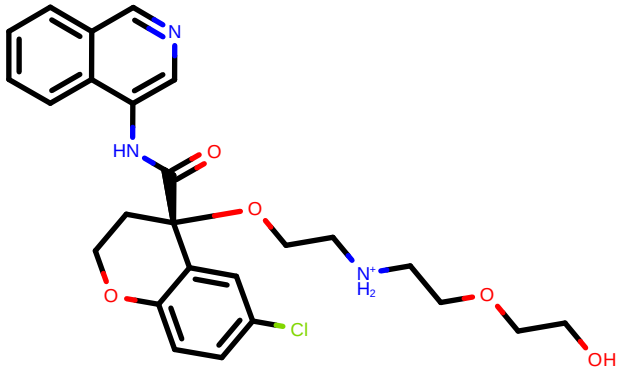
CID:	ERI-UCB-d6de1f3c-6_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N3C[C@@H](N(C(=O)C3)c4cccc(c4)Cl)C[NH+]5CCCCC5
RUN:	RUN1097
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.28

MIC-UNK-ea4eb352-4_2



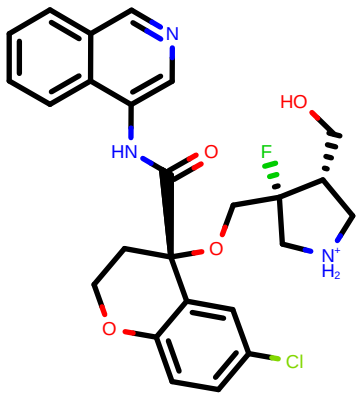
CID:	MIC-UNK-ea4eb352-4_2
SMILES:	CO[C@]1(CCSc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4641
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.18

DAR-DIA-2964957d-1_1



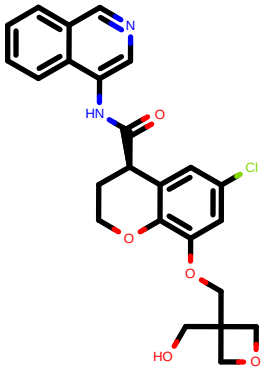
CID:	DAR-DIA-2964957d-1_1
SMILES:	c1ccc2c(c1)cncc2Nc3c(c(=O)c3=O)Nc4cccc(c4)Cl
RUN:	RUN515
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.63

FRA-DIA-b66f7109-4_1



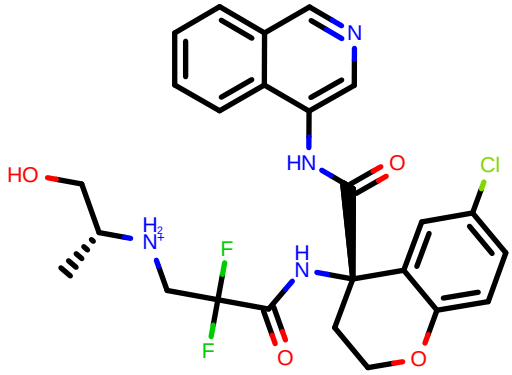
CID:	FRA-DIA-b66f7109-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4Cl)O[C@@H]5CC(=O)N5
RUN:	RUN399
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.35

KAD-UNI-8a629cb0-22_1



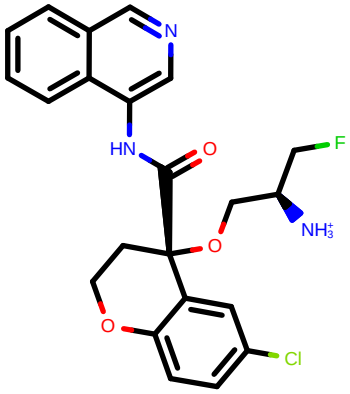
CID:	KAD-UNI-8a629cb0-22_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5cc6c([nH]c(=O)[nH]6)nc5
RUN:	RUN2104
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.41

MIC-UNK-cdc2493e-24_1



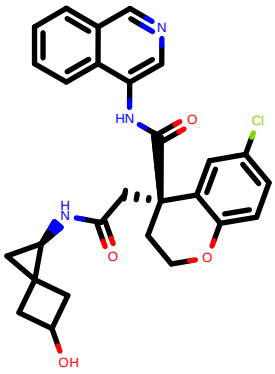
CID:	MIC-UNK-cdc2493e-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCn3cncn3)c4cccc(c4)Cl
RUN:	RUN575
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.43

MAT-POS-8a69d52e-5_1



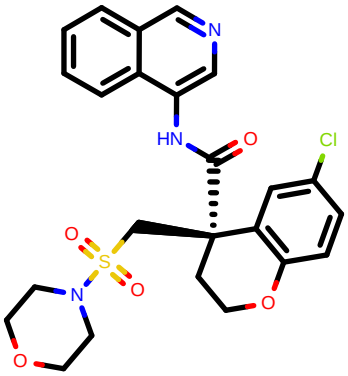
CID:	MAT-POS-8a69d52e-5_1
SMILES:	C[C@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN372
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.52

MAK-UNK-c749d764-24_1



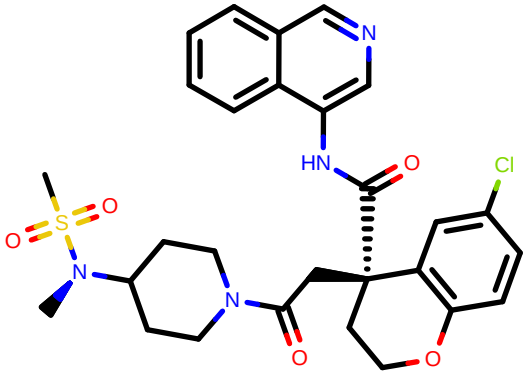
CID:	MAK-UNK-c749d764-24_1
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1030
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.32

LAU-MED-88a3970a-6_1



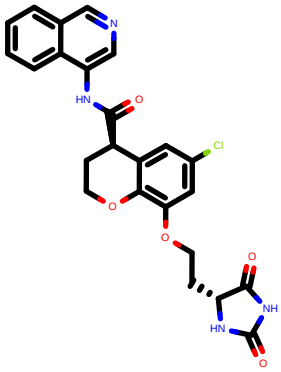
CID:	LAU-MED-88a3970a-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4CCCO)Cl
RUN:	RUN1500
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.18

MAK-UNK-c749d764-4_2



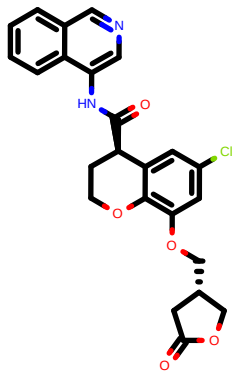
CID:	MAK-UNK-c749d764-4_2
SMILES:	CS[C@H]1CCC[C@@H]([C@@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN914
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.48

MAT-POS-e9e99895-2_6



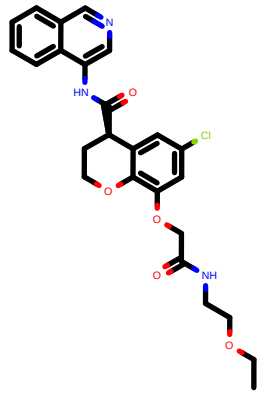
CID:	MAT-POS-e9e99895-2_6
SMILES:	CC(C)[N@H+]1CCO[C@@H](C1)C(=O)N[C@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2240
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.34

ALP-POS-2da19ca7-7_7



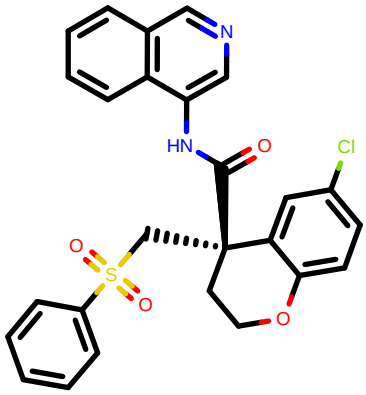
CID:	ALP-POS-2da19ca7-7_7
SMILES:	C[C@@H]1C[N@](CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2388
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.48

MAT-POS-fce787c2-6_1



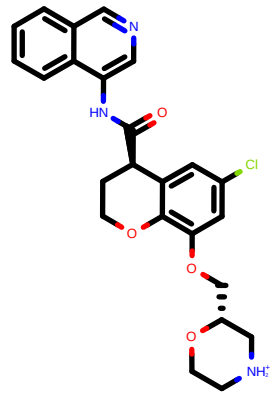
CID:	MAT-POS-fce787c2-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)C(c3ccc(c(c3)Cl)Cl)(F)F
RUN:	RUN2151
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.43

ED_-GRI-5b13fbe2-45_1



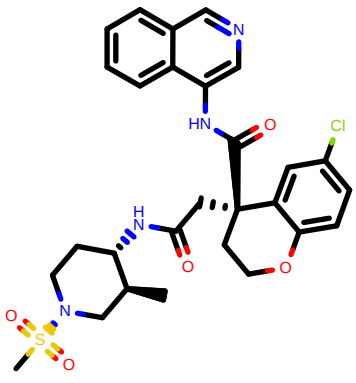
CID:	ED_-GRI-5b13fbe2-45_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](Cc5cn(nn5)CC6CC6)[NH3+]
RUN:	RUN1584
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.32

KAD-UNI-8a629cb0-39_1



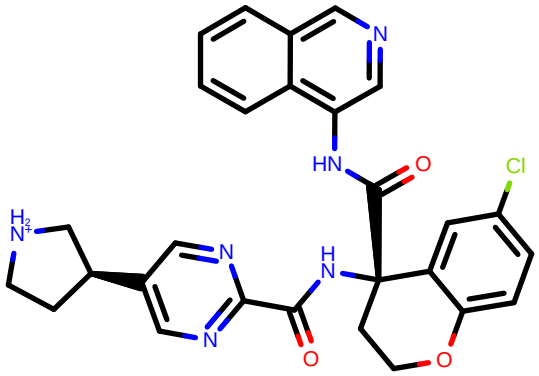
CID:	KAD-UNI-8a629cb0-39_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6(C5)COC6
RUN:	RUN2121
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.36

MAK-UNK-c749d764-2_1



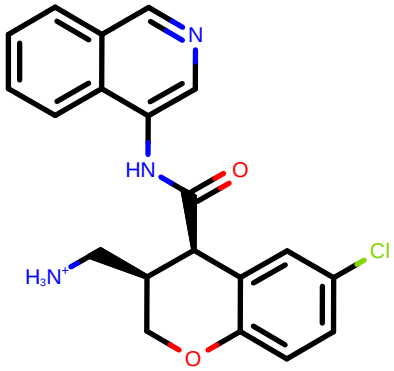
CID:	MAK-UNK-c749d764-2_1
SMILES:	CC[C@@H]1CCC[C@@H]([C@@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN897
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.49

PET-UNK-bb7ffe78-3_1



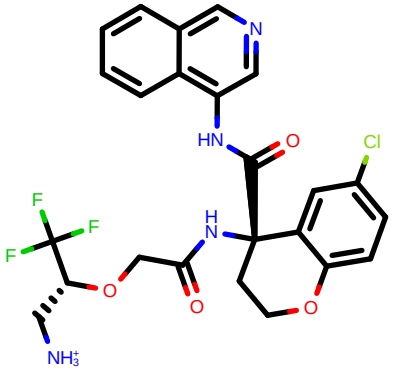
CID:	PET-UNK-bb7ffe78-3_1
SMILES:	CCCc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN3330
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.17

LON-WEI-4d77710c-34_2



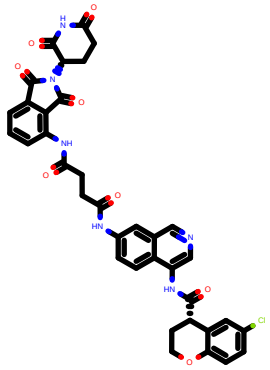
CID:	LON-WEI-4d77710c-34_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CC[C@H](C3)c4ccccc4
RUN:	RUN217
DDG (kcal/mol):	-1.38
dDDG (kcal/mol):	0.24

EDG-MED-70ae9412-2_2



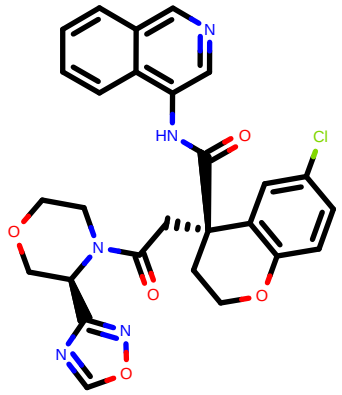
CID:	EDG-MED-70ae9412-2_2
SMILES:	C[NH+](C)CC(=O)NC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3168
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.39

EDJ-MED-50011917-1_2



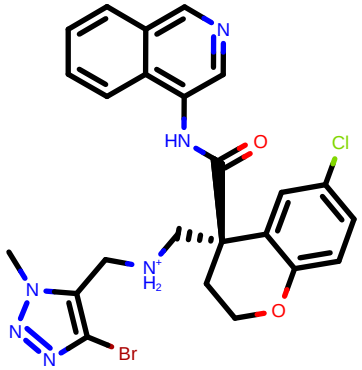
CID:	EDJ-MED-50011917-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@H]4CC(=O)N4
RUN:	RUN371
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.31

MAK-UNK-c749d764-24_5



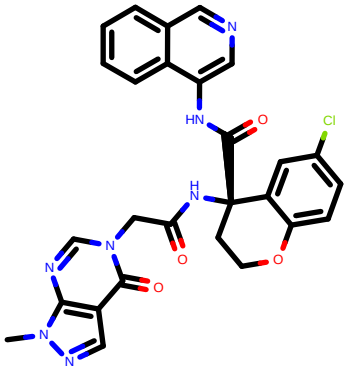
CID:	MAK-UNK-c749d764-24_5
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1034
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.36

PET-UNK-d61f3ea6-2_2



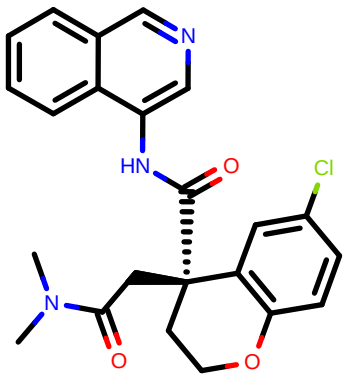
CID:	PET-UNK-d61f3ea6-2_2
SMILES:	CC(C)(C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4738
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.28

LON-WEI-5e7d1b3e-43_1



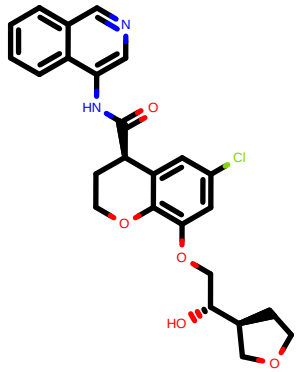
CID:	LON-WEI-5e7d1b3e-43_1
SMILES:	Cc1cc(c(cc1Cl)OC)NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN1350
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.28

DAR-DIA-0d514e7d-32_10



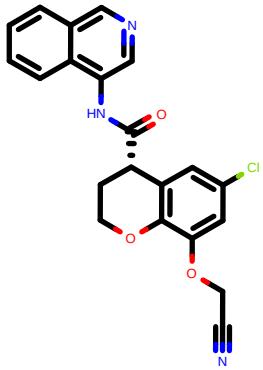
CID:	DAR-DIA-0d514e7d-32_10
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@@H]4C[C@@H]4CO[C@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN859
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.17

EDG-MED-ba1ac7b9-14_8



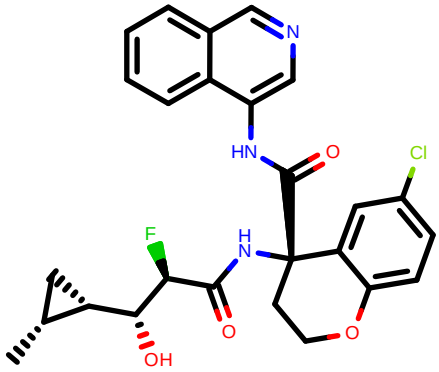
CID:	EDG-MED-ba1ac7b9-14_8
SMILES:	C[N@]1CCN(C[C@H]1C#N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2673
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.37

ALF-EVA-07677224-4_11



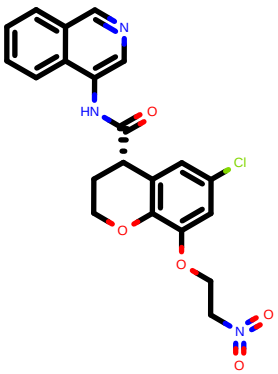
CID:	ALF-EVA-07677224-4_11
SMILES:	C[C@@H]1[C@H](CCO1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4918
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.29

ADA-UCB-dc2b944c-10_1



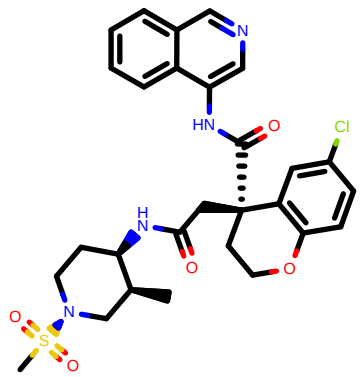
CID:	ADA-UCB-dc2b944c-10_1
SMILES:	Cc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN608
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.25

ALP-UNI-0676e700-19_1



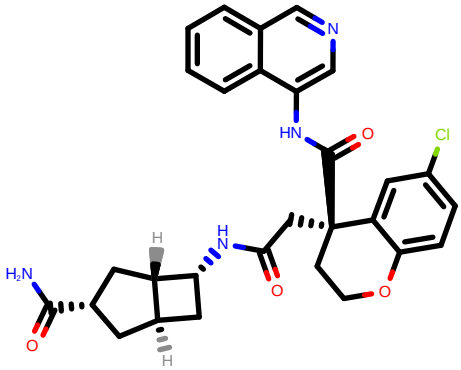
CID:	ALP-UNI-0676e700-19_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCS(=O)(=O)CC5)C#N
RUN:	RUN2465
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.26

LON-WEI-5e7d1b3e-4_1



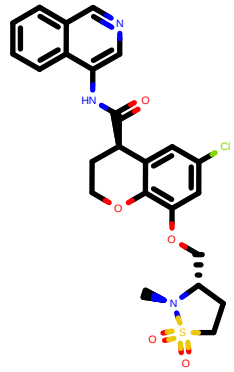
CID:	LON-WEI-5e7d1b3e-4_1
SMILES:	Cc1ccc(c(c1)Br)NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN1311
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.23

MAK-UNK-c749d764-18_5



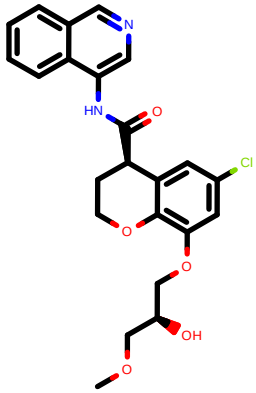
CID:	MAK-UNK-c749d764-18_5
SMILES:	CC(C)SCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN994
DDG (kcal/mol):	-1.36
dDDG (kcal/mol):	0.36

CHO-MSK-a31cca77-1_1



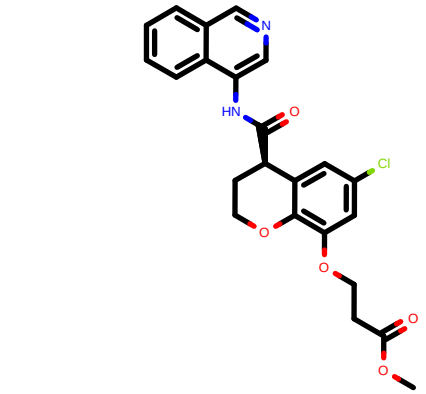
CID:	CHO-MSK-a31cca77-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5nnco5
RUN:	RUN2191
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.39

ALP-UNI-3496895b-2_4



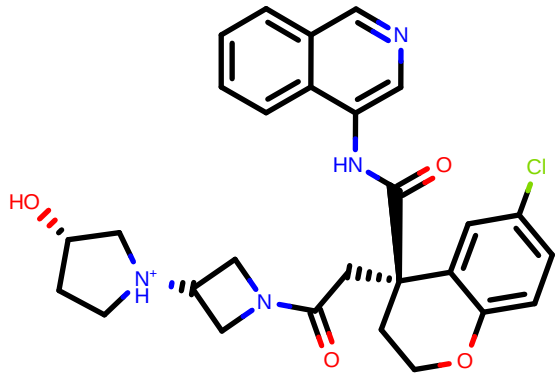
CID:	ALP-UNI-3496895b-2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@H]5CCC[N@@H+]6CCO
RUN:	RUN2504
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.45

EDJ-MED-40433386-8_1



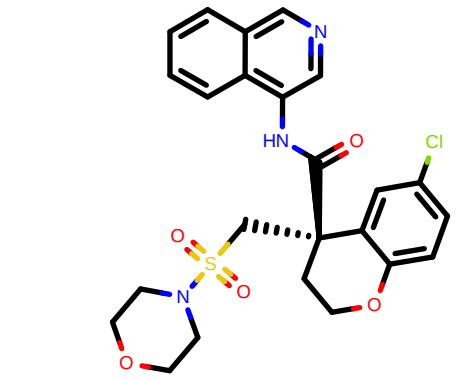
CID:	EDJ-MED-40433386-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCOC5)C#N
RUN:	RUN2559
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.35

BEN-BAS-5c03e89e-2_1



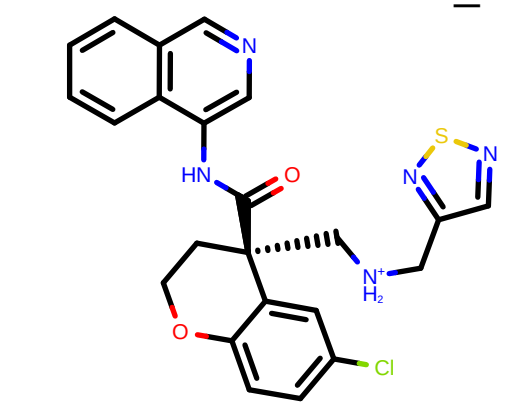
CID:	BEN-BAS-5c03e89e-2_1
SMILES:	CC(C)([C@@H]1C=Nc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN1144
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.33

PET-UNK-acd70dee-3_1



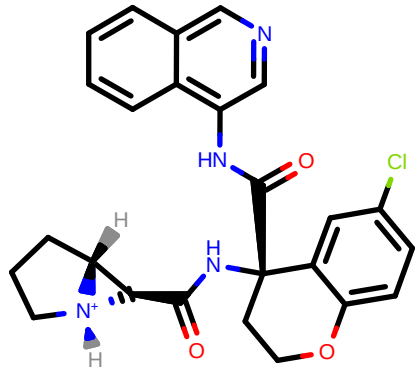
CID:	PET-UNK-acd70dee-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5nccs5
RUN:	RUN4190
DDG (kcal/mol):	-1.35
dDDG (kcal/mol):	0.17

JOH-UNI-ee5ed7c8-9_1



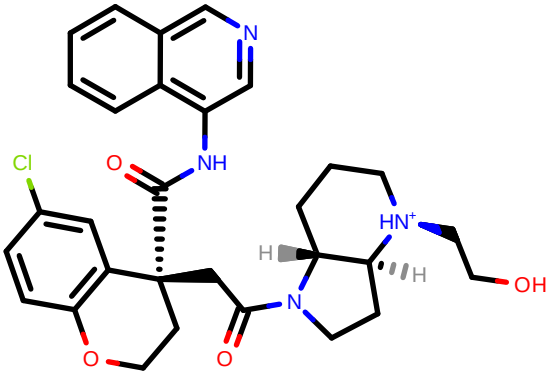
CID:	JOH-UNI-ee5ed7c8-9_1
SMILES:	CN(c1c2ccccc2cnc1C#N)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1907
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.50

LON-WEI-9739a092-10_1



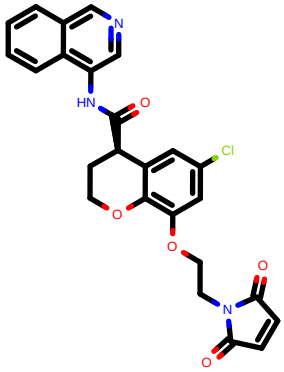
CID:	LON-WEI-9739a092-10_1
SMILES:	COc1c(cc(cn1)Br)Nc2cc(cc(c2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN3276
DDG (kcal/mol):	-1.34
dDDG (kcal/mol):	0.16

DAR-DIA-5ff57136-9_1



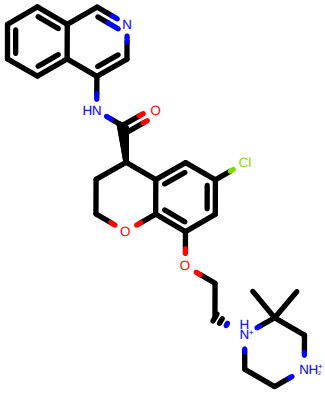
CID:	DAR-DIA-5ff57136-9_1
SMILES:	COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1378
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.53

ALF-EVA-07677224-1_2



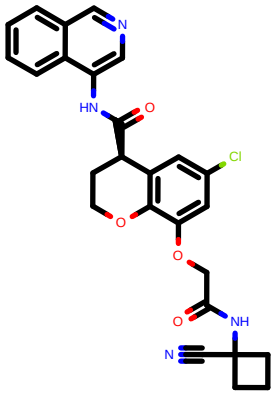
CID:	ALF-EVA-07677224-1_2
SMILES:	Cc1nc(ns1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4895
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.19

MAT-POS-de59a476-2_2



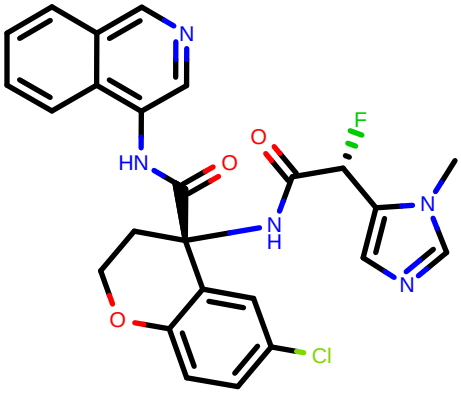
CID:	MAT-POS-de59a476-2_2
SMILES:	CO[C@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2218
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.55

EDG-MED-ba1ac7b9-3_1



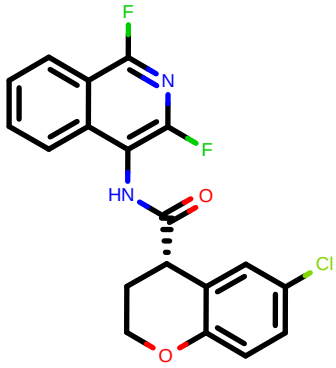
CID:	EDG-MED-ba1ac7b9-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CCO)C5CC5
RUN:	RUN2624
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.51

EDJ-MED-00143744-1_1



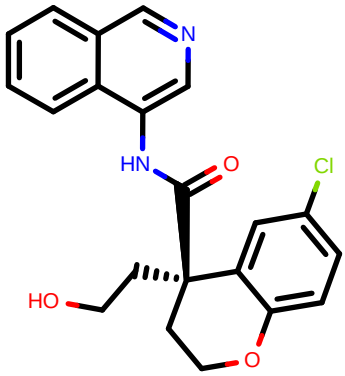
CID:	EDJ-MED-00143744-1_1
SMILES:	Cn1c(nnn1)COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3166
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.16

LON-WEI-4d77710c-1_1



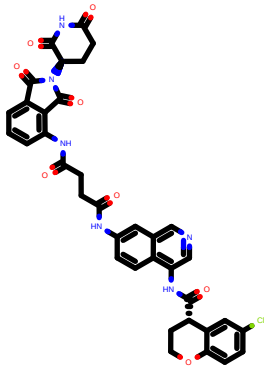
CID:	LON-WEI-4d77710c-1_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCc3cc(ccc3OC)OC
RUN:	RUN193
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.11

ALP-UNI-8e43a71e-4_3



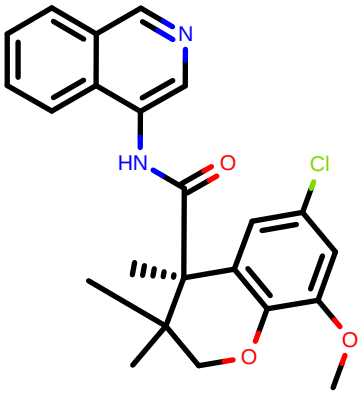
CID:	ALP-UNI-8e43a71e-4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCN(C5=O)c6ccn[nH]6
RUN:	RUN2944
DDG (kcal/mol):	-1.33
dDDG (kcal/mol):	0.06

ALP-UNI-8e43a71e-5_3



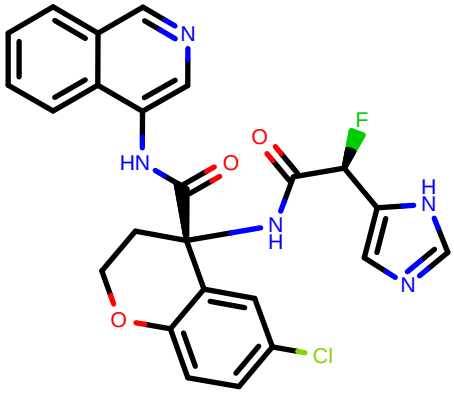
CID:	ALP-UNI-8e43a71e-5_3
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2946
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.42

LON-WEI-4d77710c-35_4



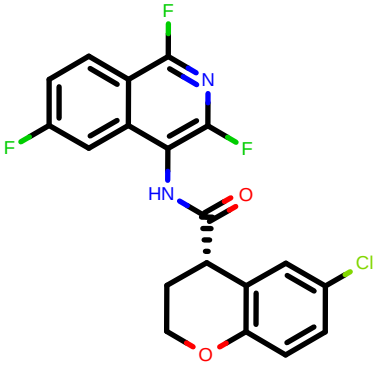
CID:	LON-WEI-4d77710c-35_4
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN225
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.25

DAR-DIA-5d6f1b43-12_1



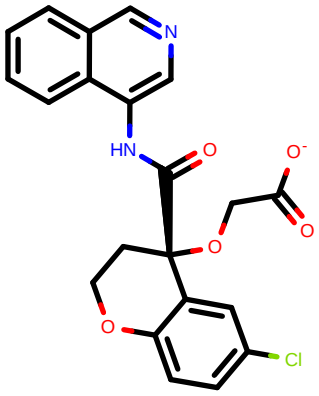
CID:	DAR-DIA-5d6f1b43-12_1
SMILES:	c1ccc2c(c1)cncc2N3CC4(CCCCC4)CN(C3=O)c5cccc(c5)Cl
RUN:	RUN489
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.28

VLA-UCB-1dbca3b4-15_2



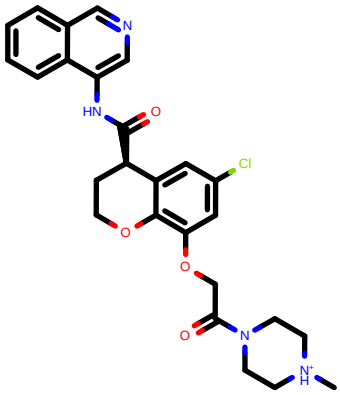
CID:	VLA-UCB-1dbca3b4-15_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN172
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.11

ALP-UNI-44c99a80-1_1



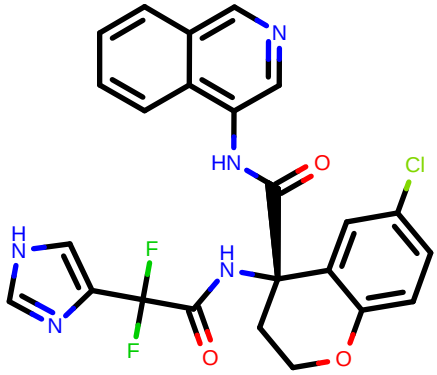
CID:	ALP-UNI-44c99a80-1_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnc[nH]3)C(=O)Cc4cccc(c4)Cl
RUN:	RUN458
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.27

EDJ-MED-d203f206-24_1



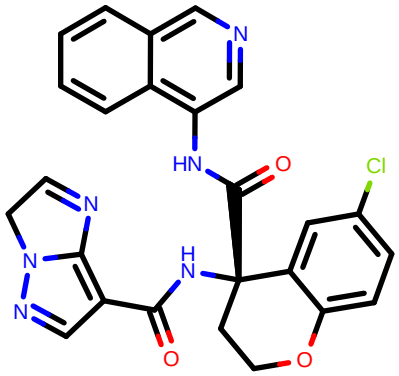
CID:	EDJ-MED-d203f206-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCO[C@@H](C5)Cn6ccnn6
RUN:	RUN2588
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.40

DAR-DIA-0f2f46c9-7_4



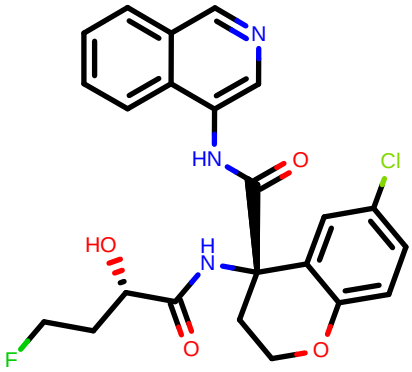
CID:	DAR-DIA-0f2f46c9-7_4
SMILES:	CNS(=O)(=O)[N@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3237
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.16

KAD-UNI-877d7bed-12_2



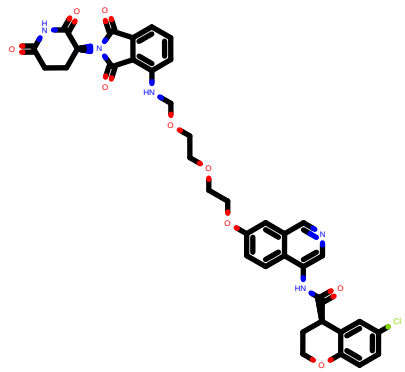
CID:	KAD-UNI-877d7bed-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCC[C@@H]5C(=O)NC(=O)N5)Cl
RUN:	RUN3752
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.12

MAK-UNK-8be7dca9-9_2



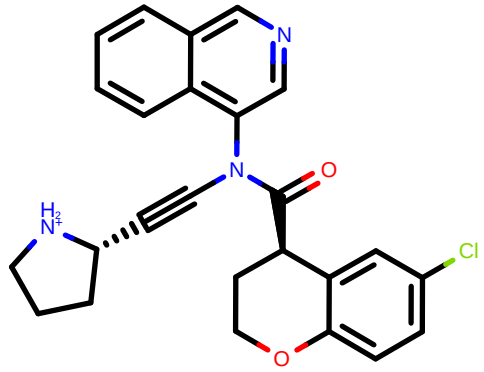
CID:	MAK-UNK-8be7dca9-9_2
SMILES:	c1cc2c(cc1C(=O)[O-])cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN510
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.28

MIC-UNK-9582b2c5-1_4



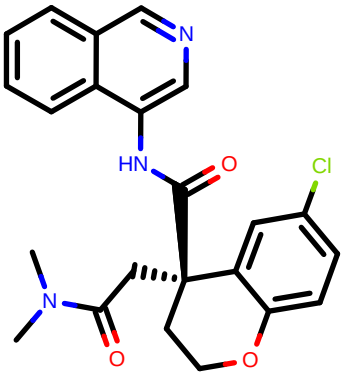
CID:	MIC-UNK-9582b2c5-1_4
SMILES:	CC(=O)N1CC[C@H]2[C@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN255
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.65

ALP-UNI-8e43a71e-2_5



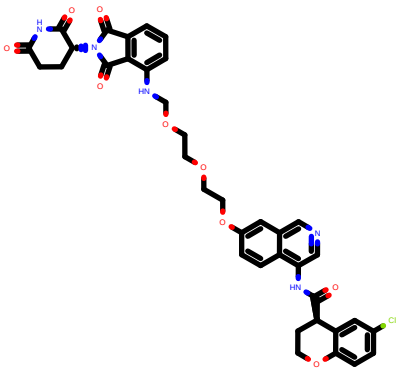
CID:	ALP-UNI-8e43a71e-2_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6[C@H]5CCC[N@@H+]6CCO
RUN:	RUN2928
DDG (kcal/mol):	-1.32
dDDG (kcal/mol):	0.18

MAK-UNK-ffc90da7-6_2



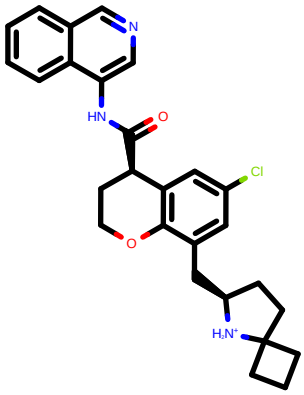
CID:	MAK-UNK-ffc90da7-6_2
SMILES:	C[C@H](C[NH2+]CCCO)c1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN706
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.25

JAG-UCB-f37eaa14-1_1



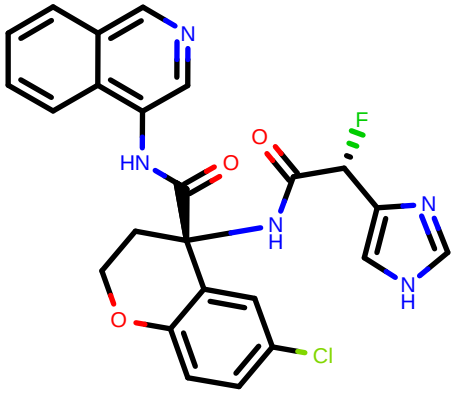
CID:	JAG-UCB-f37eaa14-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)COc5c4cc(c(c5)F)Cl
RUN:	RUN3055
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.30

MIC-UNK-66895286-5_1



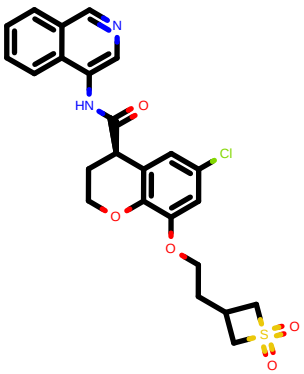
CID:	MIC-UNK-66895286-5_1
SMILES:	c1ccc2c(c1)c(c[nH]c2=O)CC(=O)Nc3cccc(c3)Cl
RUN:	RUN31
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.43

EDJ-MED-37aac4bd-6_1



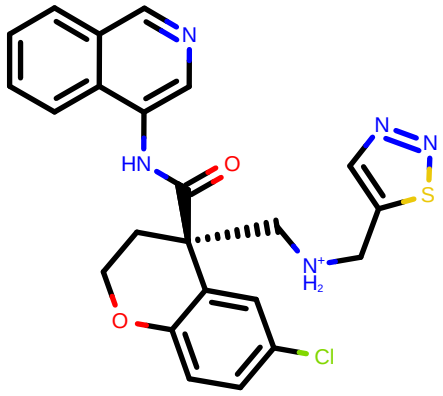
CID:	EDJ-MED-37aac4bd-6_1
SMILES:	COC[C@@]1(CCOc2c1cc(cn2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3149
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.16

ALP-UNI-0676e700-1_1



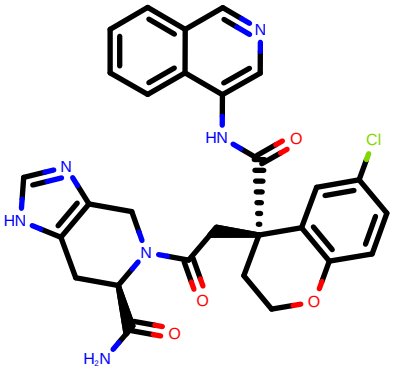
CID:	ALP-UNI-0676e700-1_1
SMILES:	Cc1[nH]n2c(=O)c(cnc2n1)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2442
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.42

MIC-UNK-a28eba03-4_1



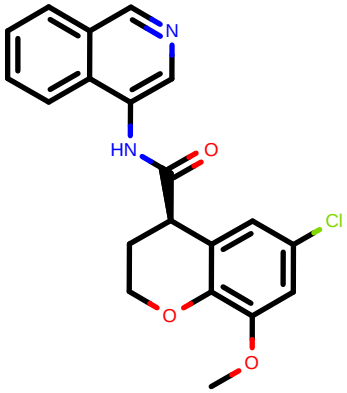
CID:	MIC-UNK-a28eba03-4_1
SMILES:	CC1(CCN(CC1)C(=O)Cc2cncc3c2cccc3)C
RUN:	RUN1877
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.36

JOH-UNI-6fede743-1_1



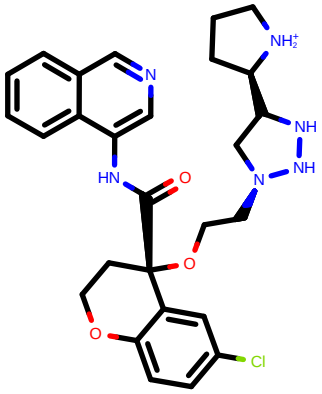
CID:	JOH-UNI-6fede743-1_1
SMILES:	c1ccc2c(c1)c(cnc2C(F)F)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN1166
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.26

ERI-UCB-ce40166b-10_2



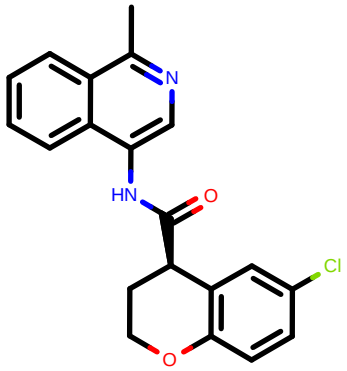
CID:	ERI-UCB-ce40166b-10_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)O[C@H]4CCC(=O)N4)C#N
RUN:	RUN49
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.24

MAK-UNK-8be7dca9-1_2



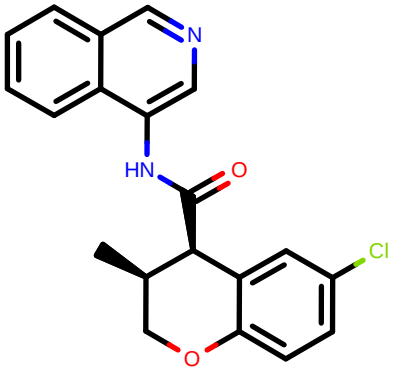
CID:	MAK-UNK-8be7dca9-1_2
SMILES:	c1cc2c(cc1CN3CC[NH2+]CC3)cncc2NC(=O)[C@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN493
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.43

LON-WEI-4d77710c-48_1



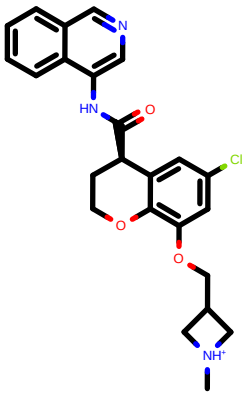
CID:	LON-WEI-4d77710c-48_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3cc(ccc3OC)OC
RUN:	RUN240
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.22

PET-UNK-c9c1e0d8-3_2



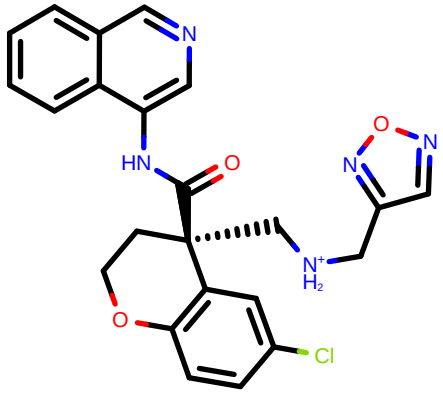
CID:	PET-UNK-c9c1e0d8-3_2
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN121
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.20

ALF-EVA-5b152d2f-4_1



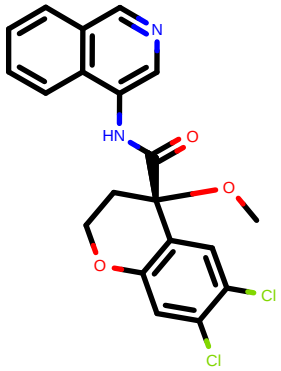
CID:	ALF-EVA-5b152d2f-4_1
SMILES:	c1ccc2c(c1)cncc2NNC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2354
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.37

PET-UNK-03fd2068-4_2



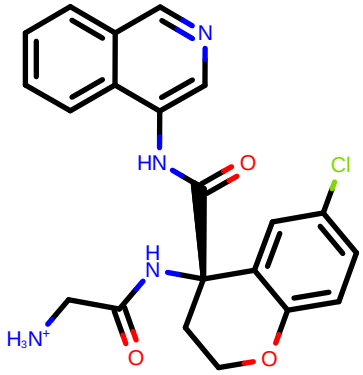
CID:	PET-UNK-03fd2068-4_2
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3ccc(c4)F)Cl
RUN:	RUN4409
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.21

DAR-DIA-0d514e7d-31_14



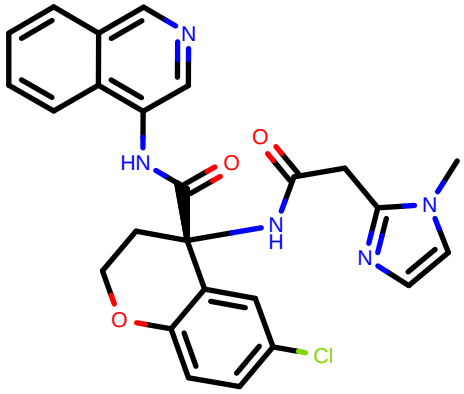
CID:	DAR-DIA-0d514e7d-31_14
SMILES:	C[C@H]1CCO[C@@H]2C=CC(=C[C@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN847
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.25

IVS-FNM-f9a14d04-1_1



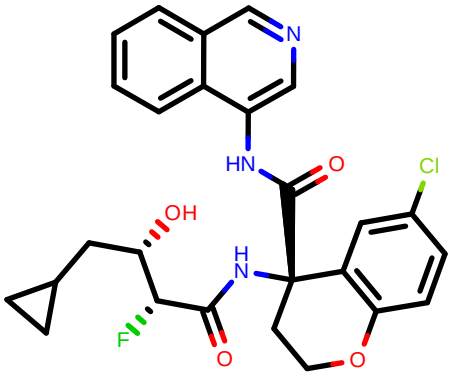
CID:	IVS-FNM-f9a14d04-1_1
SMILES:	COc1c(cccc1Cl)CCCC(=O)Nc2cncc3c2cccc3
RUN:	RUN490
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.27

EDJ-MED-f893e2a1-6_1



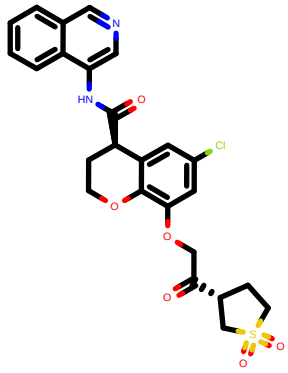
CID:	EDJ-MED-f893e2a1-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@@H]5CC(=O)NC5
RUN:	RUN3203
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.14

MIC-UNK-50cce87d-7_1



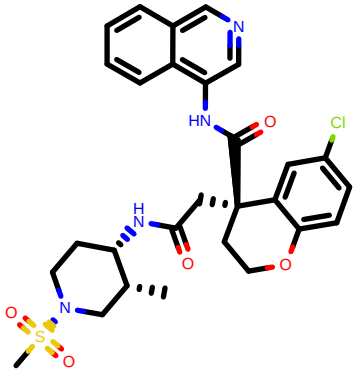
CID:	MIC-UNK-50cce87d-7_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN668
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.28

EDJ-MED-40433386-1_2



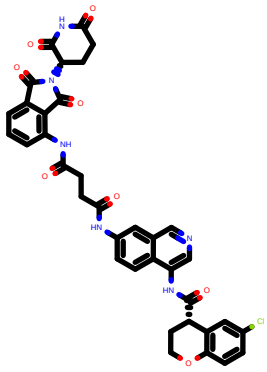
CID:	EDJ-MED-40433386-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@H]5COCC[N@]5CC(F)(F)F
RUN:	RUN2555
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.40

KAD-UNI-877d7bed-9_1



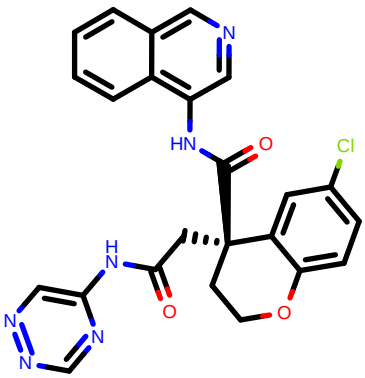
CID:	KAD-UNI-877d7bed-9_1
SMILES:	Cn1cc(cn1)C[N@@H+]2C[C@@H]2COc3cc(cc4c3OCC[C@@H]4C(=O)Nc5cncc6c5cccc6)Cl
RUN:	RUN3736
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.24

NAU-LAT-b7d8c353-8_2



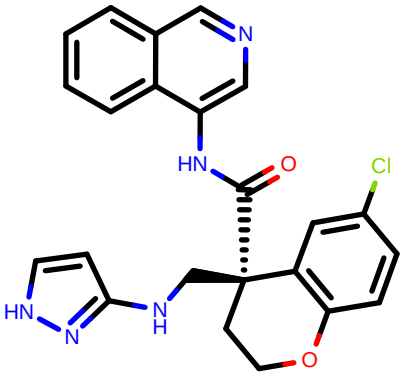
CID:	NAU-LAT-b7d8c353-8_2
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)C[NH3+]
RUN:	RUN457
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.29

KAD-UNI-cb0f2bbc-15_1



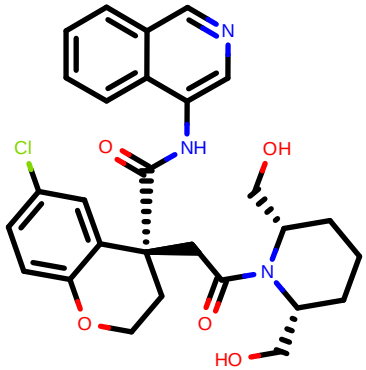
CID:	KAD-UNI-cb0f2bbc-15_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5ccc(cc5S(=O)(=O)[O-])S(=O)(=O)[O-]
RUN:	RUN3700
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.16

EDG-MED-971238d3-3_1



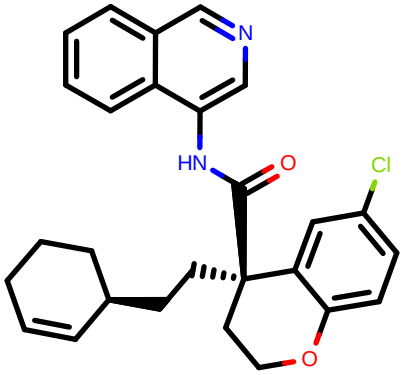
CID:	EDG-MED-971238d3-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCO
RUN:	RUN1468
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.14

MAK-UNK-c749d764-33_6



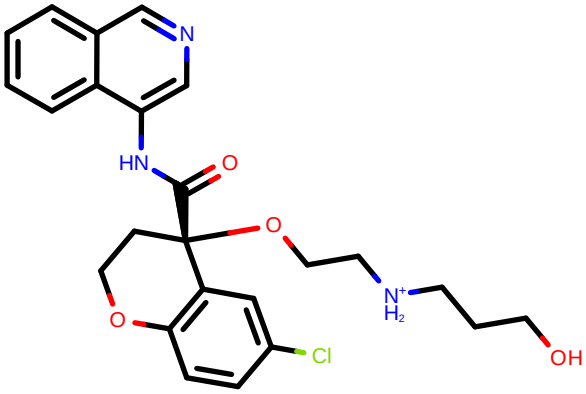
CID:	MAK-UNK-c749d764-33_6
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1083
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.44

DAR-DIA-0cde14eb-57_2



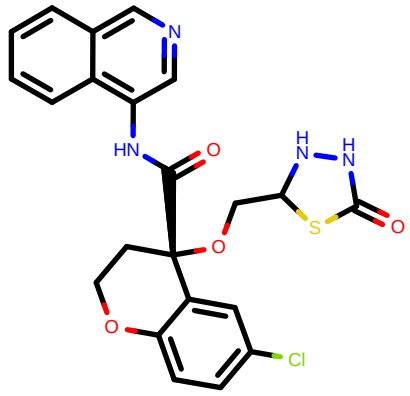
CID:	DAR-DIA-0cde14eb-57_2
SMILES:	C[C@H](c1cccc(c1)C2(CC2)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN26
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.27

DAR-DIA-23e5a6a0-9_1



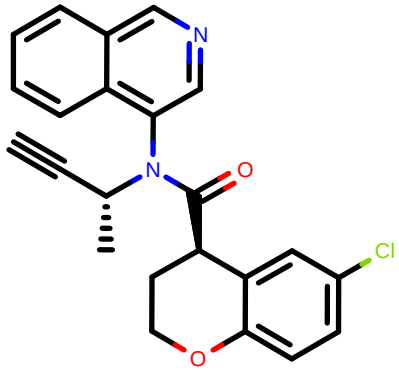
CID:	DAR-DIA-23e5a6a0-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6(CC6)C[NH2+]5)Cl
RUN:	RUN418
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.40

NIR-THE-af15c15d-1_2



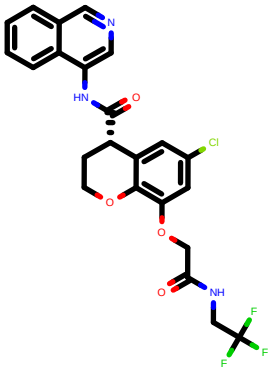
CID:	NIR-THE-af15c15d-1_2
SMILES:	CC#CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN3320
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.13

ALP-UNI-8e43a71e-15_22



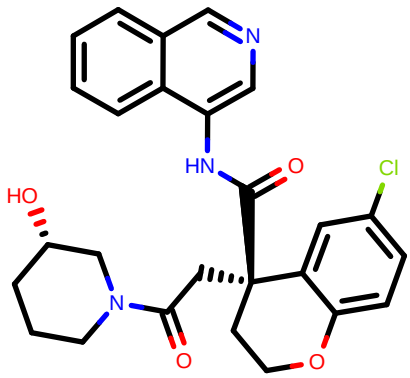
CID:	ALP-UNI-8e43a71e-15_22
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN3003
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.12

JOH-UNI-ea72002d-5_1



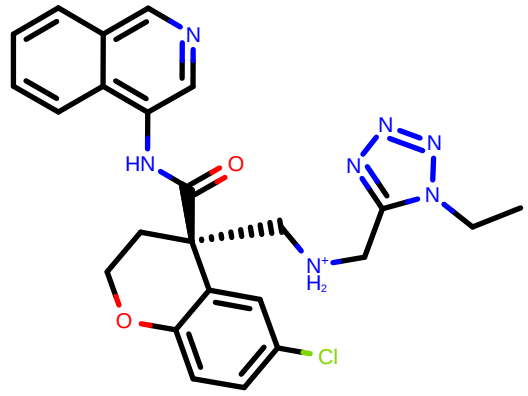
CID:	JOH-UNI-ea72002d-5_1
SMILES:	C=CS(=O)(=O)NN(c1cncc2c1cccc2)C(=O)[C@@]3(CCOc4c3cc(cc4)Cl)F
RUN:	RUN2494
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.31

BEN-BAS-5c03e89e-1_1



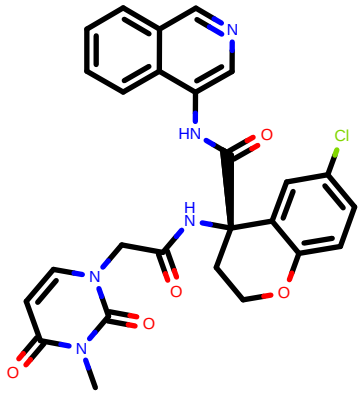
CID:	BEN-BAS-5c03e89e-1_1
SMILES:	CC(C)([C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN1143
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.27

MIC-UNK-ea4eb352-6_1



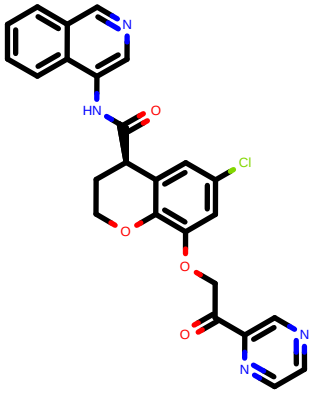
CID:	MIC-UNK-ea4eb352-6_1
SMILES:	CO[C@@]1(C[N@@](Cc2c1cc(c(c2)Cl)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4646
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.29

RAL-THA-c11c1343-1_2



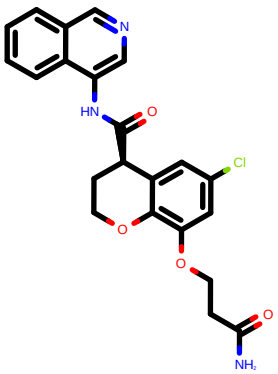
CID:	RAL-THA-c11c1343-1_2
SMILES:	CC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1228
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.27

ALP-UNI-3496895b-15_3



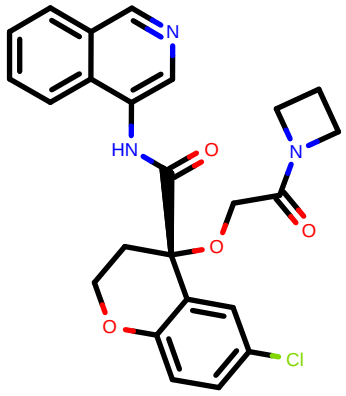
CID:	ALP-UNI-3496895b-15_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N[C@@H]5C[C@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN2533
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.31

MAT-POS-e69ad64a-1_1



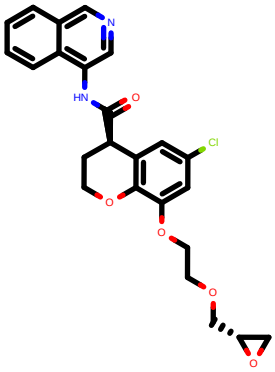
CID:	MAT-POS-e69ad64a-1_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN2328
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.30

VLA-UCB-34f3ed0c-21_2



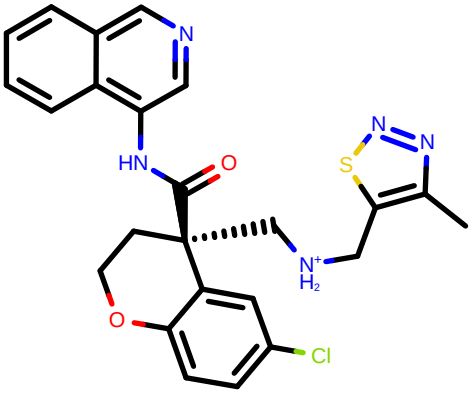
CID:	VLA-UCB-34f3ed0c-21_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@H]5CC(=O)NC5
RUN:	RUN649
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.22

MAT-POS-f9802937-5_1



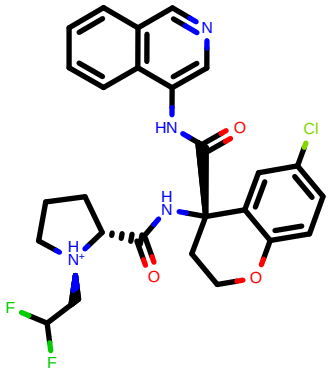
CID:	MAT-POS-f9802937-5_1
SMILES:	CNC(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2396
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.37

MAT-POS-5f1400cf-1_6



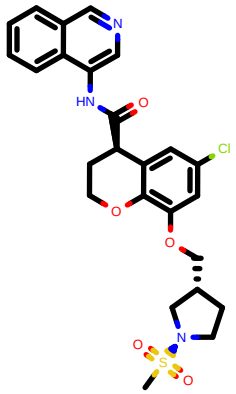
CID:	MAT-POS-5f1400cf-1_6
SMILES:	Cn1cc(cn1)N2CC[C@@H](C2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN4511
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.25

MAT-POS-3b97339c-1_3



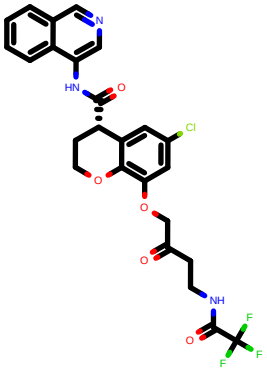
CID:	MAT-POS-3b97339c-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCSC5)O
RUN:	RUN3299
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.17

LEE-CAM-7ab9b158-1_5



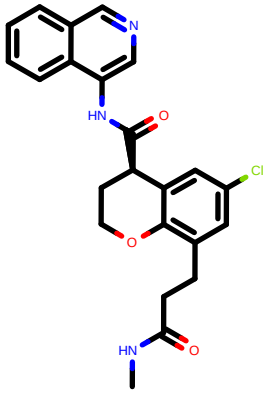
CID:	LEE-CAM-7ab9b158-1_5
SMILES:	C[NH+](C)[C@@H]1COC[C@@H]1OC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2203
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.42

MAT-POS-e9e99895-8_4



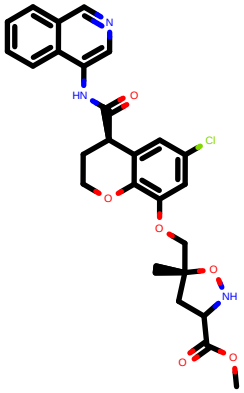
CID:	MAT-POS-e9e99895-8_4
SMILES:	Cc1nc2n(n1)C[C@H](CC2)C(=O)N[C@](C)(c3ccc(c(c3)Cl)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2257
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.26

DAR-DIA-6a508060-5_2



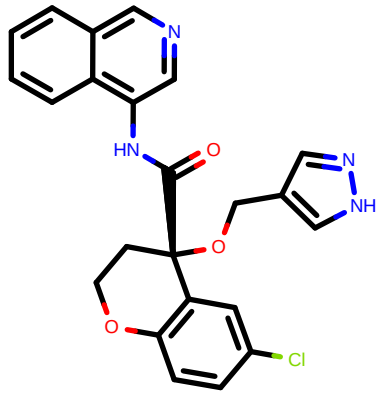
CID:	DAR-DIA-6a508060-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4C[C@@H]5CC(=O)N5)Cl
RUN:	RUN341
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.30

EDJ-MED-d203f206-33_1



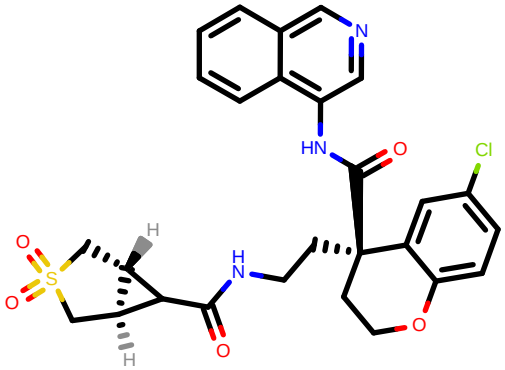
CID:	EDJ-MED-d203f206-33_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5C[C@@H](C[C@@H]5C(=O)N)O
RUN:	RUN2595
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.30

MAT-POS-3b92565d-7_1



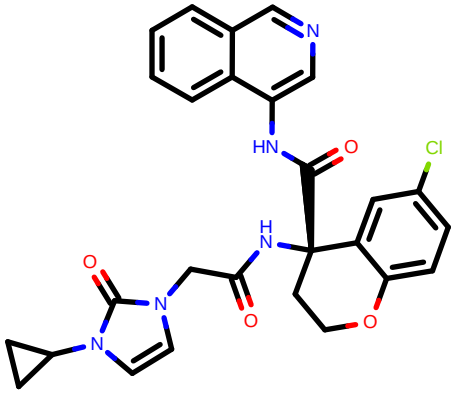
CID:	MAT-POS-3b92565d-7_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Cc3cc(ccc3OC)Cl
RUN:	RUN113
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.30

DAR-DIA-f6ee7aeb-5_1



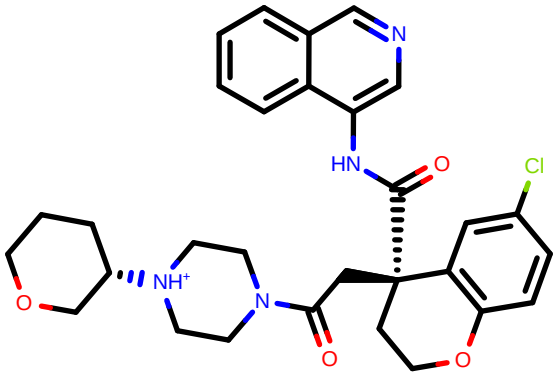
CID:	DAR-DIA-f6ee7aeb-5_1
SMILES:	CCCOc1cc(cc(c1)Cl)[C@@H]2CC(=O)N(C[C@@H]2c3c[nH]c(=O)[nH]c3=O)c4cncc5c4cccc5
RUN:	RUN3414
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.17

MAK-UNK-c749d764-16_4



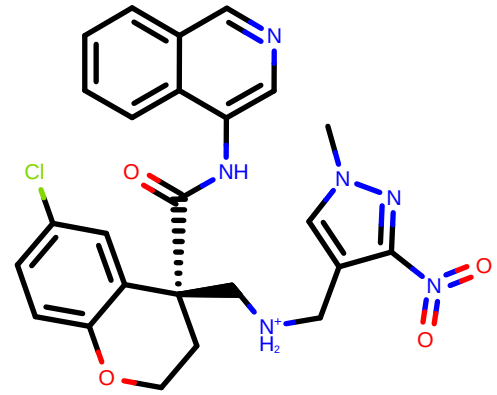
CID:	MAK-UNK-c749d764-16_4
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F)O
RUN:	RUN977
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.34

BEN-DND-c852c98b-4_1



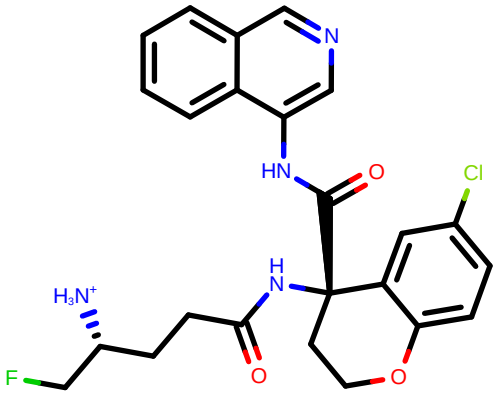
CID:	BEN-DND-c852c98b-4_1
SMILES:	c1cc2cncc(c2cc1O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1207
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.31

EDG-MED-90036822-36_2



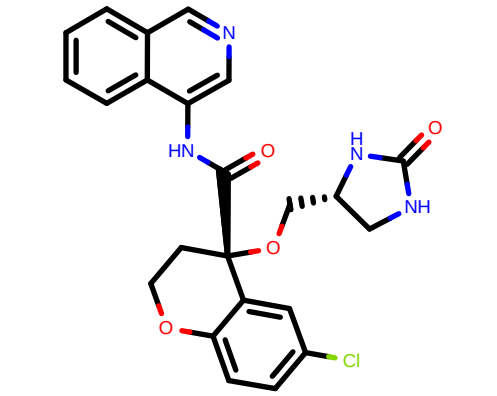
CID:	EDG-MED-90036822-36_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)NC(=O)[C@H](n5ccnc5)F
RUN:	RUN1711
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.46

MIC-UNK-cdc2493e-8_5



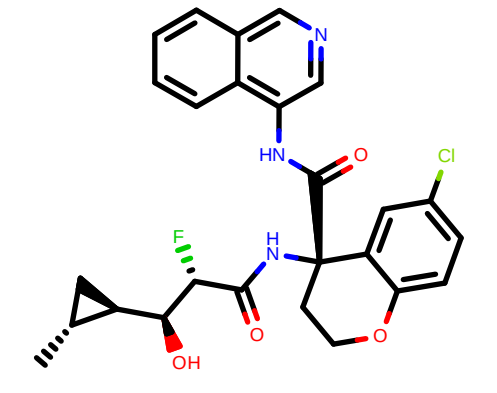
CID:	MIC-UNK-cdc2493e-8_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@@H]5CCCC[C@H]5C4
RUN:	RUN540
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.35

VLA-UCB-50c39ae8-8_2



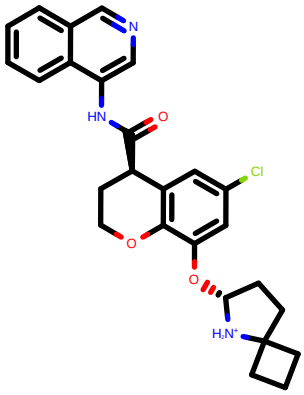
CID:	VLA-UCB-50c39ae8-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@H]5CC(=O)N5)Cl
RUN:	RUN389
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.28

LON-WEI-9739a092-4_2



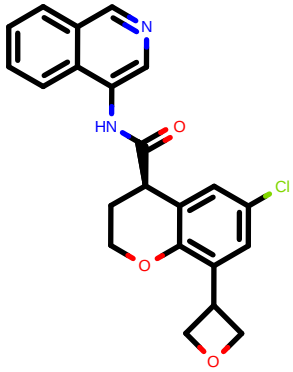
CID:	LON-WEI-9739a092-4_2
SMILES:	CCN(Cc1ccc(cc1)F)c2cc(cc(c2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN3272
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.15

MAT-POS-b5746674-102_1



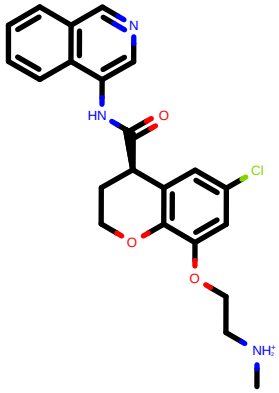
CID:	MAT-POS-b5746674-102_1
SMILES:	CCCCN(CCCNC(=O)Nc1cn(c(=O)c2c1cccc2)CC(C)C)c3ccccc3
RUN:	RUN83
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.41

DAR-DIA-0cde14eb-55_1



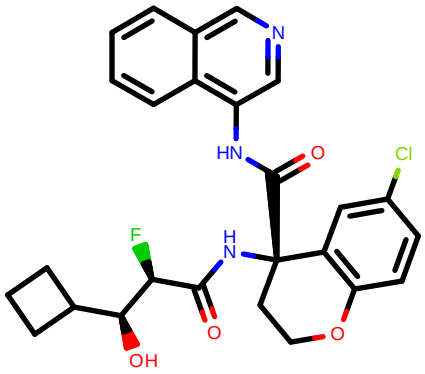
CID:	DAR-DIA-0cde14eb-55_1
SMILES:	C[C@@H](c1cccc(c1)C2(CC2)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN21
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.24

KAD-UNI-8a629cb0-11_1



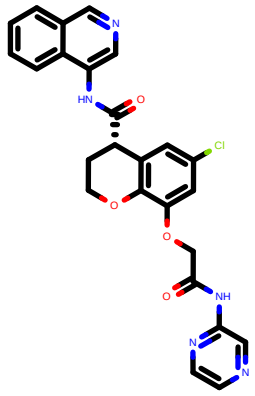
CID:	KAD-UNI-8a629cb0-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)Cc5c(=O)[nH]cnc5[O-]
RUN:	RUN2096
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.55

MAT-POS-dd3ad2b5-1_1



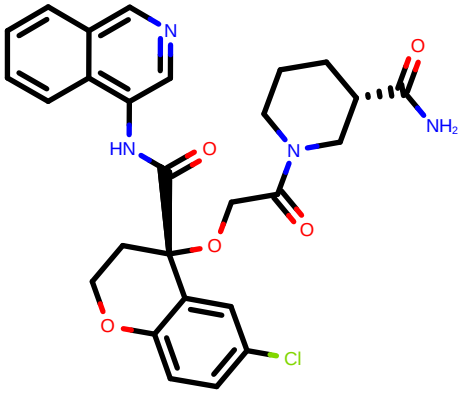
CID:	MAT-POS-dd3ad2b5-1_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3529
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.15

MAT-POS-2905de8c-3_2



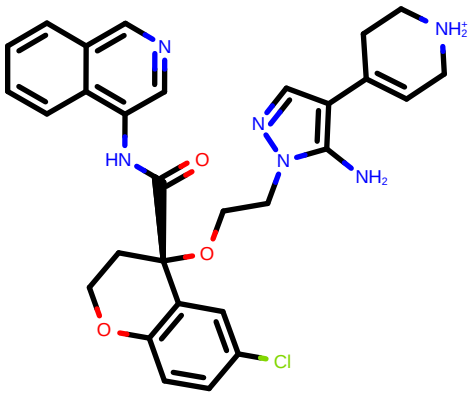
CID:	MAT-POS-2905de8c-3_2
SMILES:	C[NH+](C)[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2232
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.23

MIC-UNK-d854bf4c-4_1



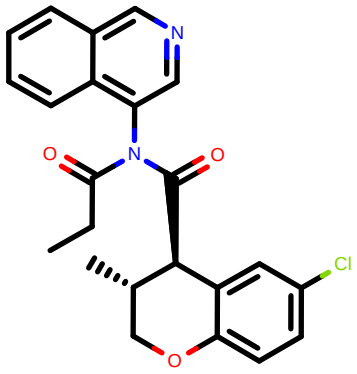
CID:	MIC-UNK-d854bf4c-4_1
SMILES:	CC(=O)N1CCC2(CC1)CCN(C(=O)[C@@H]2c3ccc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN3337
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.21

MIC-UNK-b9827f26-5_1



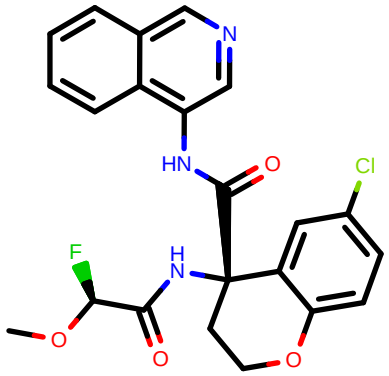
CID:	MIC-UNK-b9827f26-5_1
SMILES:	Cc1ccc(cc1N2CCN(CC2=O)C(=O)c3cncc4c3cccc4)Cl
RUN:	RUN3256
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.19

ALP-UNI-8e43a71e-1_4



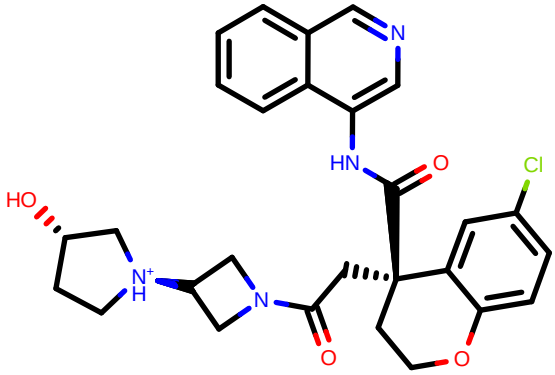
CID:	ALP-UNI-8e43a71e-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CCS(=O)(=O)N@@[C@H]5CCCC6
RUN:	RUN2922
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.13

MAT-POS-fb82b63d-1_1



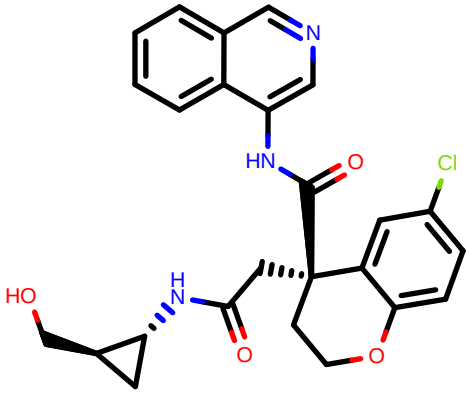
CID:	MAT-POS-fb82b63d-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4CC[NH2+]3)Cl
RUN:	RUN3163
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.10

MIC-UNK-67d4a29a-4_1



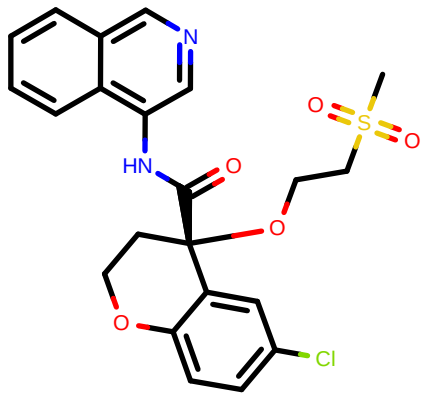
CID:	MIC-UNK-67d4a29a-4_1
SMILES:	CN(c1cncc2c1c(ccc2)OC)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1090
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.44

MAK-UNK-c749d764-33_7



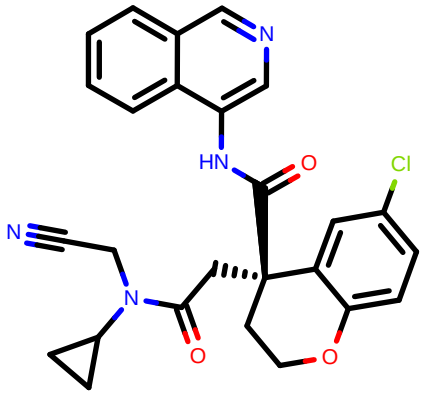
CID:	MAK-UNK-c749d764-33_7
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1085
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.31

MAT-POS-4223bc15-41_2



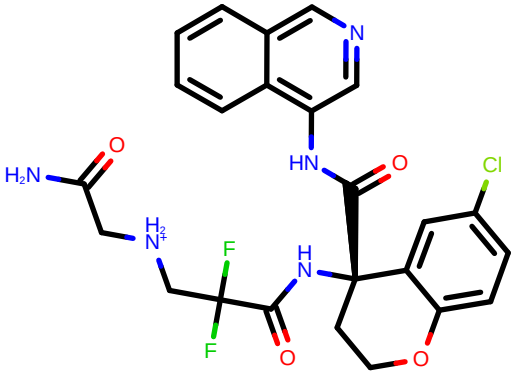
CID:	MAT-POS-4223bc15-41_2
SMILES:	Cn1cncc1C(=O)N2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4164
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.16

JOH-UNI-f51e3bbc-1_2



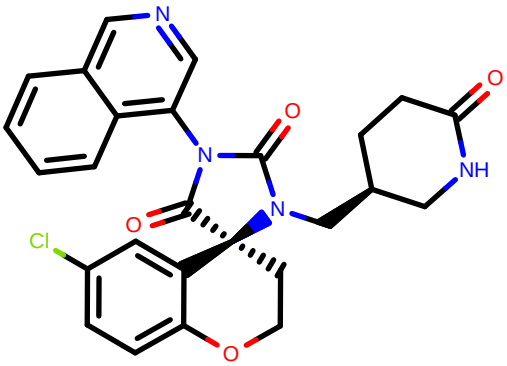
CID:	JOH-UNI-f51e3bbc-1_2
SMILES:	c1ccc2c(c1)c(c[nH]c2=O)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1159
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.25

MIC-UNK-bcd487e9-6_2



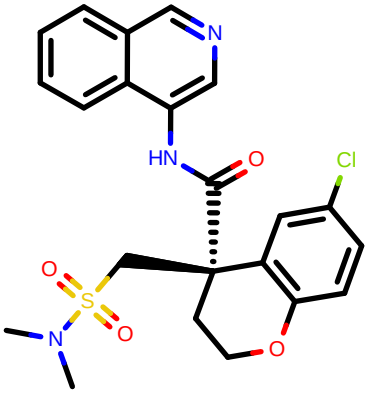
CID:	MIC-UNK-bcd487e9-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(C[C@H]3CCCS3(=O)=O)c4cccc(c4)Cl
RUN:	RUN593
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.42

MIC-UNK-0a05c952-2_6



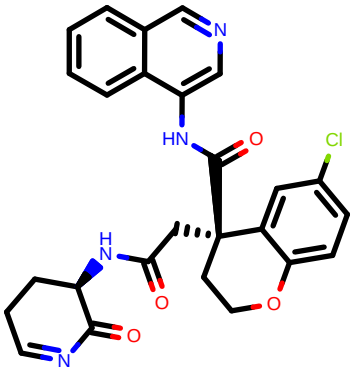
CID:	MIC-UNK-0a05c952-2_6
SMILES:	c1ccc2c(c1)cncc2N3[C@H](CC[C@@H](C3=O)c4cccc(c4)Cl)[C@H]5CO5
RUN:	RUN3510
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.22

LAU-MED-88a3970a-2_1



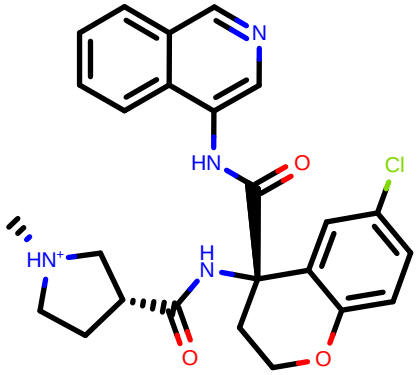
CID:	LAU-MED-88a3970a-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCO)Cl
RUN:	RUN1498
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-25_5



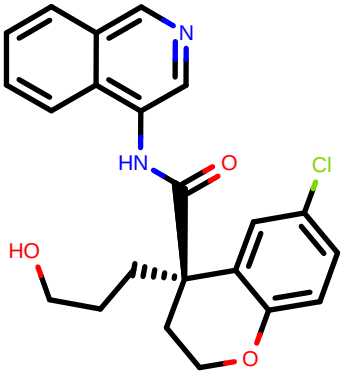
CID:	MAK-UNK-c749d764-25_5
SMILES:	COC(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1042
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.29

RAL-THA-c9f97604-1_1



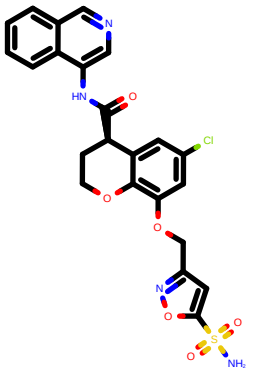
CID:	RAL-THA-c9f97604-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4[C@H]5CC[C@@H]3O5)Cl
RUN:	RUN584
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.36

ALP-UNI-8e43a71e-5_6



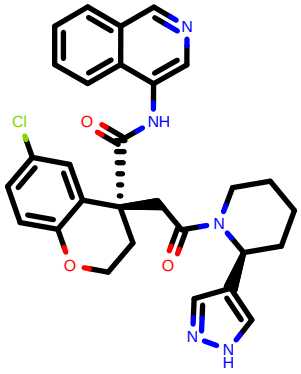
CID:	ALP-UNI-8e43a71e-5_6
SMILES:	C[C@H]1C[N@@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2950
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.10

EDJ-MED-fcba3f31-6_1



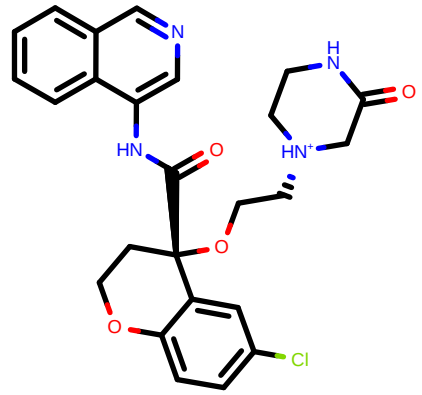
CID:	EDJ-MED-fcba3f31-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CCNC5=O
RUN:	RUN2542
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.38

BEN-DND-c852c98b-3_2



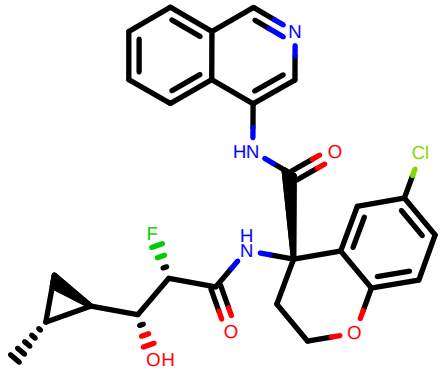
CID:	BEN-DND-c852c98b-3_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)O
RUN:	RUN1209
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.41

DAR-DIA-6a508060-11_2



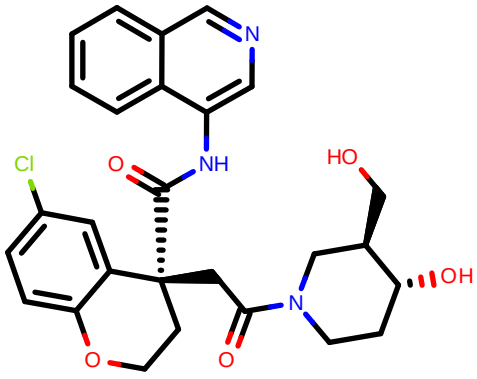
CID:	DAR-DIA-6a508060-11_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@H]4C[C@@H]4Cl
RUN:	RUN347
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.43

ADA-UCB-dc2b944c-6_1



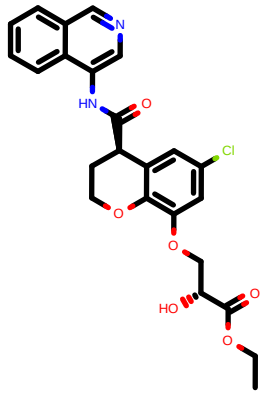
CID:	ADA-UCB-dc2b944c-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC34CCC(O3)CC4)c5cccc(c5)Cl
RUN:	RUN604
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-29_3



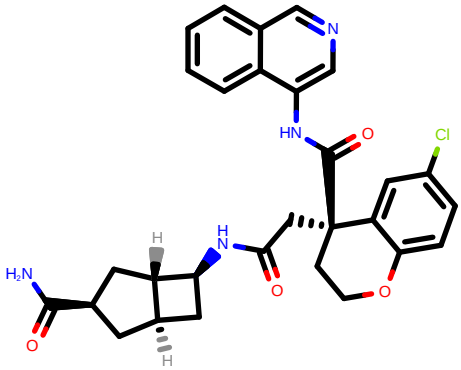
CID:	MAK-UNK-c749d764-29_3
SMILES:	c1ccc2c(c1)cncc2N(C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F)C(=O)ON
RUN:	RUN1064
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.29

CHO-MSK-a31cca77-4_2



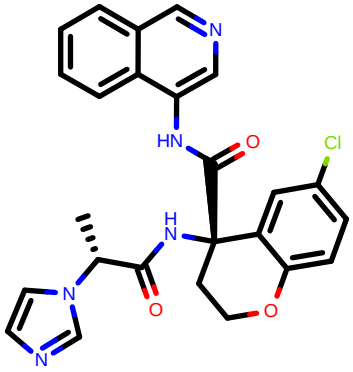
CID:	CHO-MSK-a31cca77-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ncon5
RUN:	RUN2198
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.44

LON-WEI-5e7d1b3e-35_1



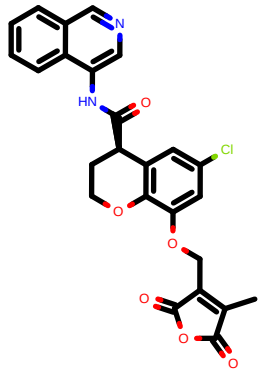
CID:	LON-WEI-5e7d1b3e-35_1
SMILES:	Cc1ccc(cc1)C[N@@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN1342
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.37

MIC-UNK-cdc2493e-7_1



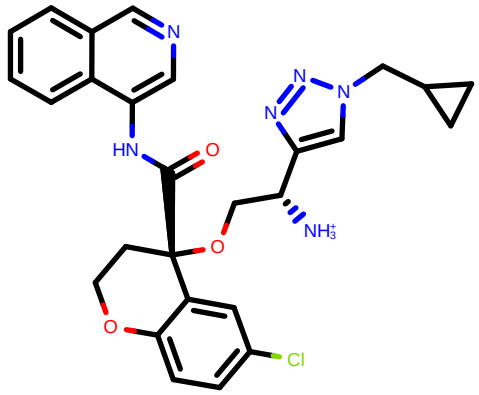
CID:	MIC-UNK-cdc2493e-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CCc5ccccc5C4
RUN:	RUN531
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.27

ALP-UNI-3496895b-5_6



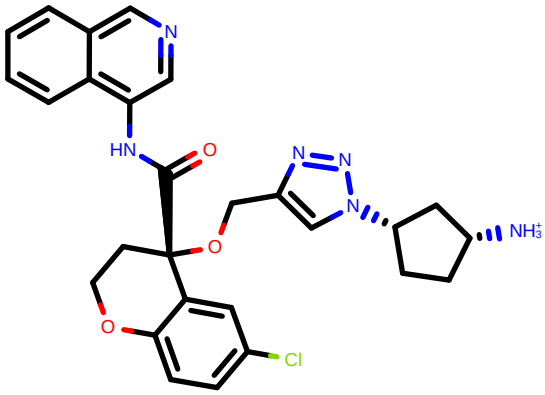
CID:	ALP-UNI-3496895b-5_6
SMILES:	C[C@H]1C[N@@](CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2517
DDG (kcal/mol):	-1.21
dDDG (kcal/mol):	0.36

MAT-POS-8a69d52e-4_1



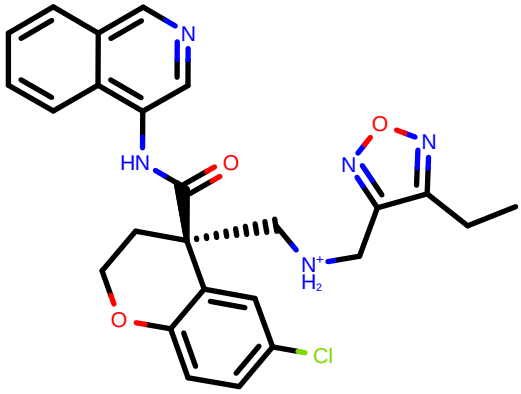
CID:	MAT-POS-8a69d52e-4_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN366
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.46

ALP-POS-fe871b40-2_2



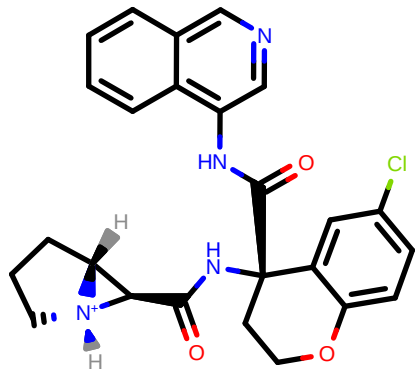
CID:	ALP-POS-fe871b40-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4C#N)Cl
RUN:	RUN3108
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.22

PET-UNK-d61f3ea6-4_1



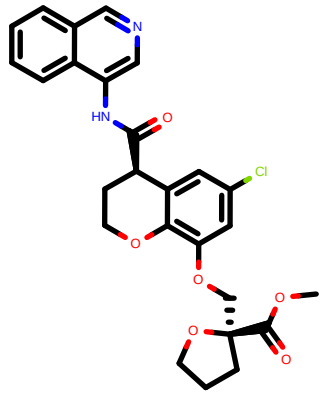
CID:	PET-UNK-d61f3ea6-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)[N@@]5CCC(C5)(F)F
RUN:	RUN4741
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.27

MIC-UNK-d854bf4c-2_1



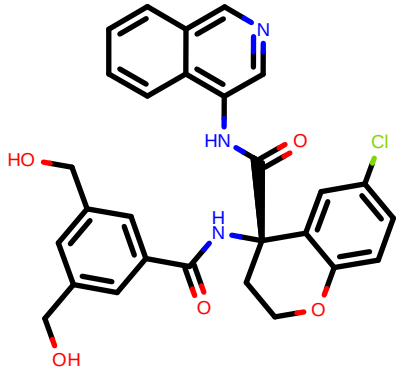
CID:	MIC-UNK-d854bf4c-2_1
SMILES:	CC(=O)N1CCC2(CC1)CN(C(=O)[C@@H]2c3ccc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN3332
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.17

ALP-POS-5bb456a5-7_4



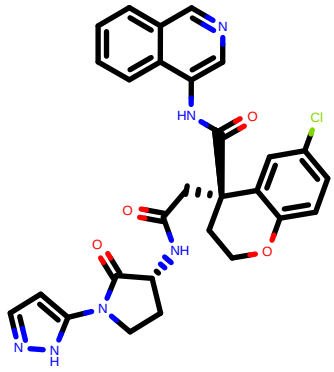
CID:	ALP-POS-5bb456a5-7_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@H]6CCOC6
RUN:	RUN2439
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.36

VLA-UNK-8e76d113-4_1



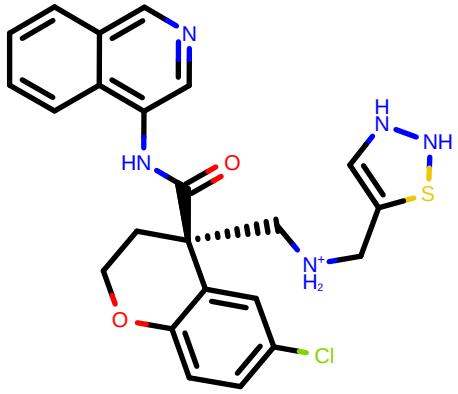
CID:	VLA-UNK-8e76d113-4_1
SMILES:	CO[C@]1(CCNc2c1cc(c(c2C#N)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3856
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.14

LON-WEI-5e7d1b3e-35_4



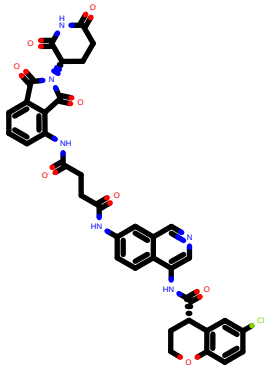
CID:	LON-WEI-5e7d1b3e-35_4
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN1344
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.37

EDJ-MED-cf877e1d-2_3



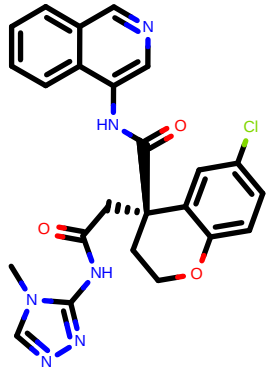
CID:	EDJ-MED-cf877e1d-2_3
SMILES:	CN(C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@](C1)(C(=O)Nc3cncc4c3cccc4)OC)Cl
RUN:	RUN4558
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.22

MIC-UNK-91acba05-3_1



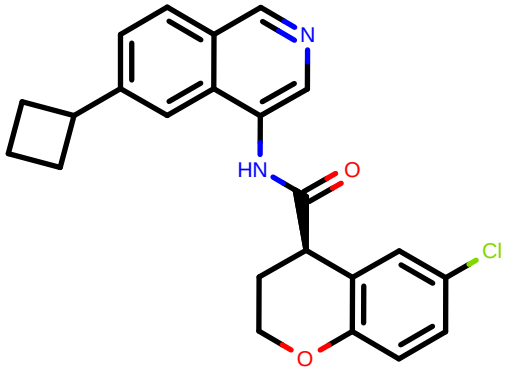
CID:	MIC-UNK-91acba05-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN472
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.32

DAR-DIA-0d514e7d-32_27



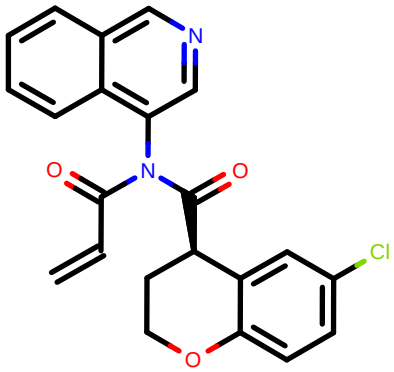
CID:	DAR-DIA-0d514e7d-32_27
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@H]4C[C@@H]4CO[C@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN876
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.35

MAK-UNK-c749d764-20_6



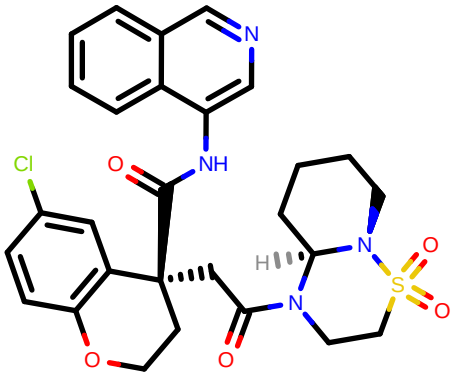
CID:	MAK-UNK-c749d764-20_6
SMILES:	CCCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1011
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.21

EDG-MED-ba1ac7b9-27_3



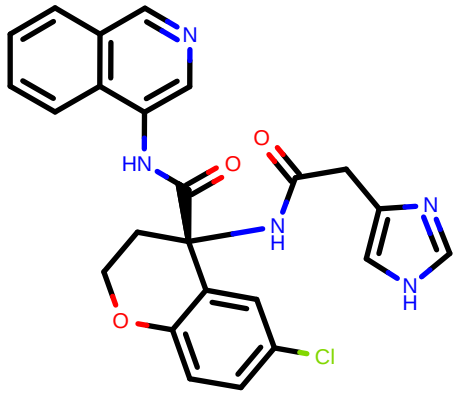
CID:	EDG-MED-ba1ac7b9-27_3
SMILES:	C[C@@H]1C[N@H+](CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)CCO
RUN:	RUN2725
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.16

RAL-THA-8416115c-10_2



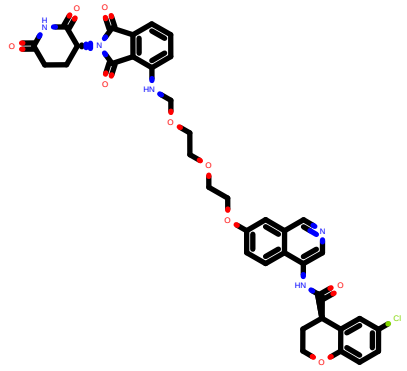
CID:	RAL-THA-8416115c-10_2
SMILES:	CNC(=O)CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1284
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.27

MIC-UNK-cdc2493e-8_1



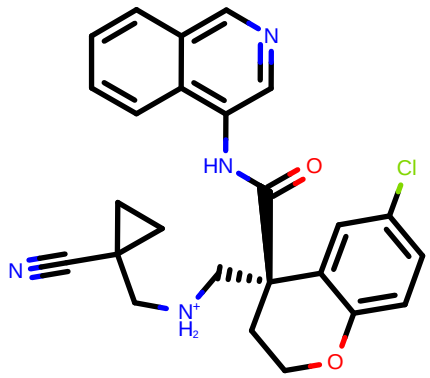
CID:	MIC-UNK-cdc2493e-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@@H]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN536
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.24

ALP-UNI-8e43a71e-15_4



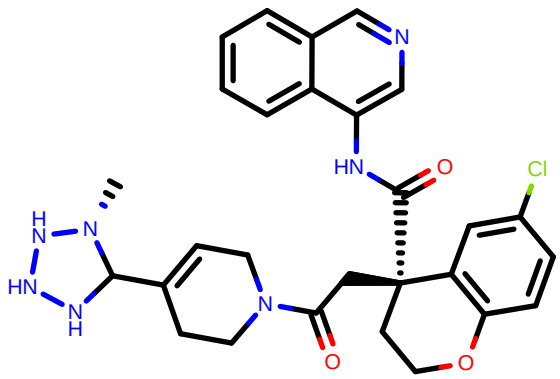
CID:	ALP-UNI-8e43a71e-15_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@@H]6[C@@H]5C[C@@H](C6)C(=O)N
RUN:	RUN2986
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.36

ALP-POS-347519b5-3_59



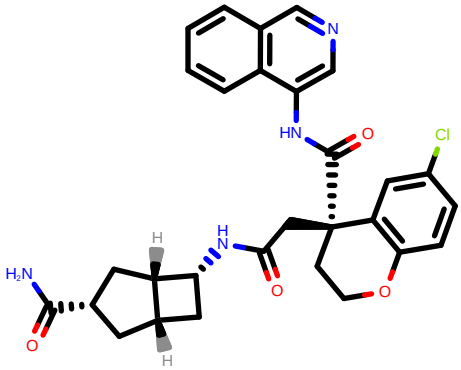
CID:	ALP-POS-347519b5-3_59
SMILES:	CS(=O)(=O)[N@@]1C[C@H]2[C@@H]3CC[C@H]([C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4326
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.17

MAK-UNK-c749d764-3_2



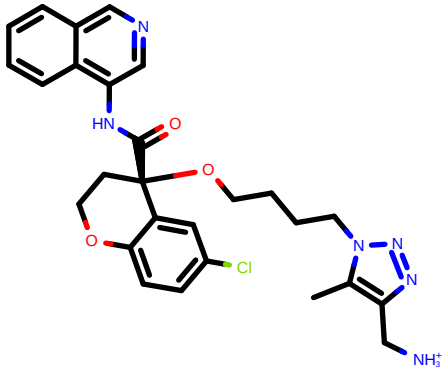
CID:	MAK-UNK-c749d764-3_2
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@H]4CCC[C@@H]([C@@H]4O)C(F)F
RUN:	RUN905
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.24

LON-WEI-5e7d1b3e-49_1



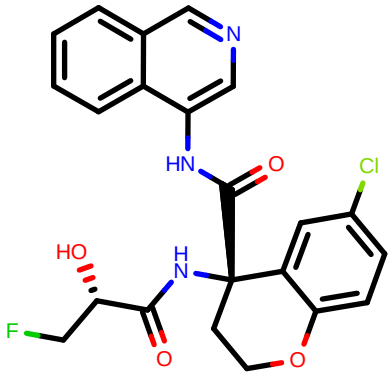
CID:	LON-WEI-5e7d1b3e-49_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCc3ccccn3
RUN:	RUN1357
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.28

EDJ-MED-37aac4bd-3_2



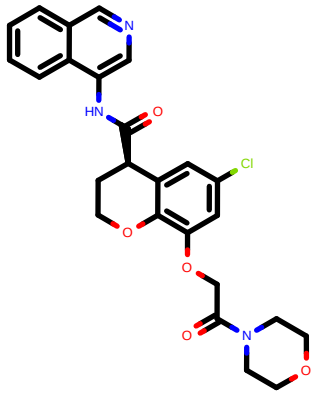
CID:	EDJ-MED-37aac4bd-3_2
SMILES:	COC[C@]1(CCOc2c1cc(cc2F)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3146
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.25

VLA-UCB-34f3ed0c-4_1



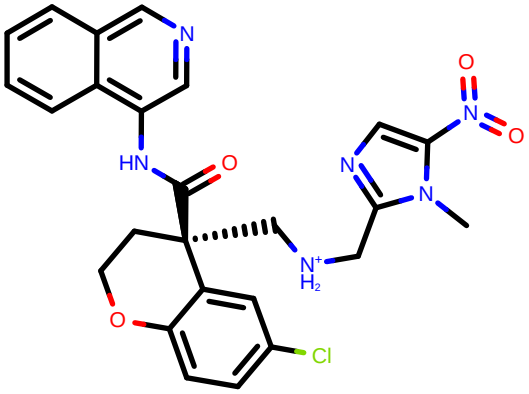
CID:	VLA-UCB-34f3ed0c-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5ccn[nH]5
RUN:	RUN629
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.37

ALP-POS-2da19ca7-2_1



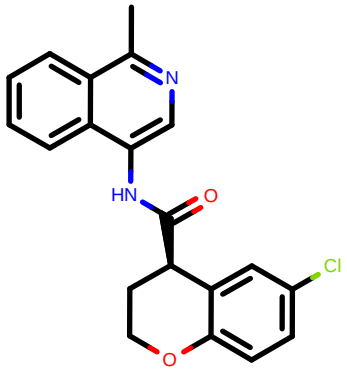
CID:	ALP-POS-2da19ca7-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@@H]6CCOC6
RUN:	RUN2375
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.30

EDJ-MED-c82a5324-1_1



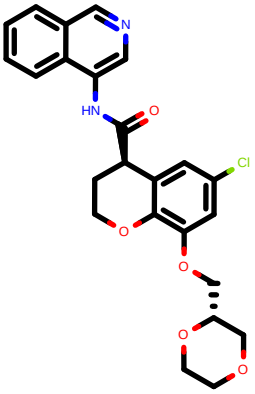
CID:	EDJ-MED-c82a5324-1_1
SMILES:	CNC(=O)[C@@H](CO)[N@@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4719
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.22

MAT-POS-b5746674-98_1



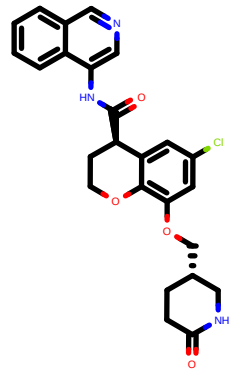
CID:	MAT-POS-b5746674-98_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCC[N@@H+]3CCc4ccccc4C3
RUN:	RUN73
DDG (kcal/mol):	-1.18
dDDG (kcal/mol):	0.20

CHO-MSK-a31cca77-2_2



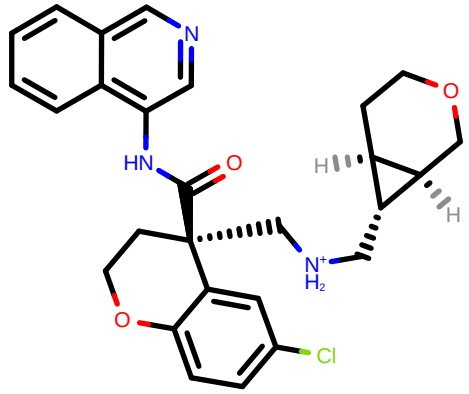
CID:	CHO-MSK-a31cca77-2_2
SMILES:	Cn1cnnc1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2195
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.34

DAR-DIA-e7614d05-1_2



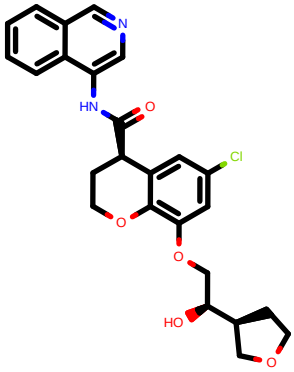
CID:	DAR-DIA-e7614d05-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)OC(F)(F)F
RUN:	RUN2479
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.37

MIC-UNK-ea4eb352-11_1



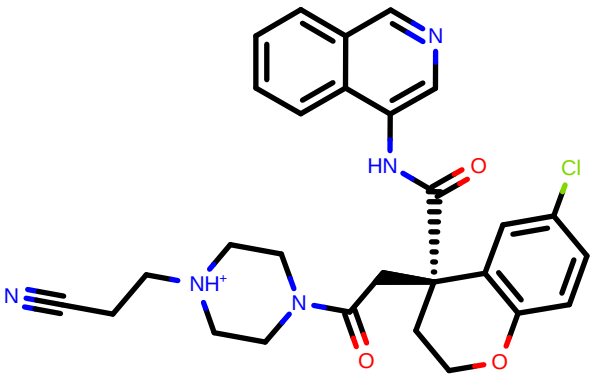
CID:	MIC-UNK-ea4eb352-11_1
SMILES:	CO[C@@]1(CCNc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4657
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.25

ALP-UNI-0676e700-21_1



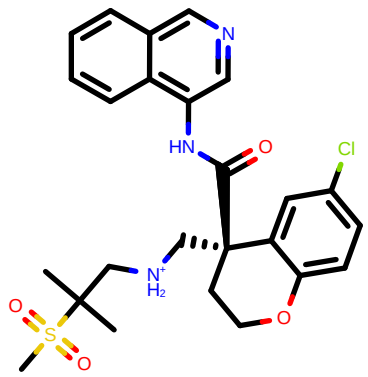
CID:	ALP-UNI-0676e700-21_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5ccc(cc5)OCC(=O)N
RUN:	RUN2472
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.39

LON-WEI-5e7d1b3e-5_1



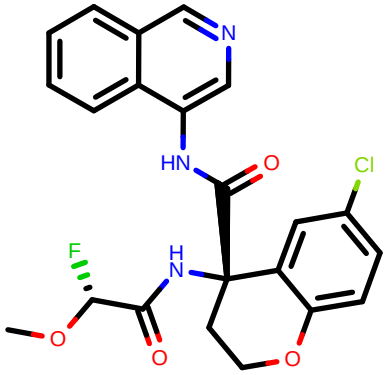
CID:	LON-WEI-5e7d1b3e-5_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccc(c(c3)OC)OC
RUN:	RUN1313
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.27

ALP-POS-347519b5-2_28



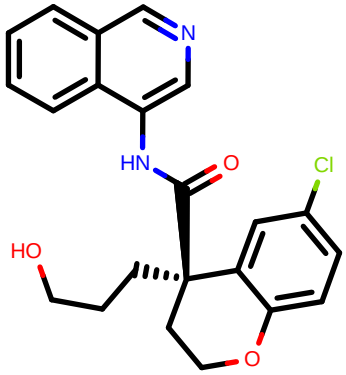
CID:	ALP-POS-347519b5-2_28
SMILES:	CO[C@]1(C[N@][C[C@@H]2[C@H]1[C@H]3CC[C@@H]2C3)S(=O)(=O)C)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4276
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.18

EDG-MED-70ae9412-1_2



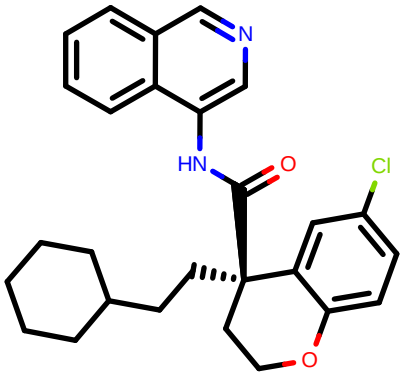
CID:	EDG-MED-70ae9412-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)Cn5ccnc5
RUN:	RUN3164
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.11

EDJ-MED-e4b030d8-2_1



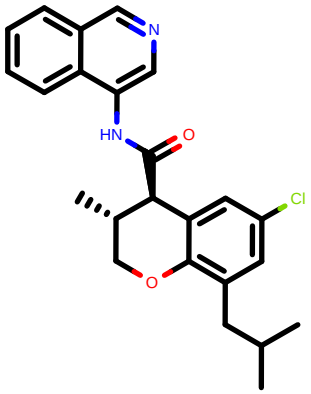
CID:	EDJ-MED-e4b030d8-2_1
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN284
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.25

VLA-UCB-1dbca3b4-14_2



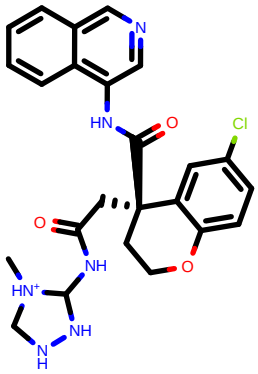
CID:	VLA-UCB-1dbca3b4-14_2
SMILES:	C[C@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN173
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.25

DAR-DIA-53551c05-10_1



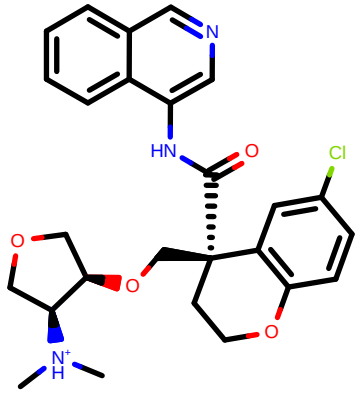
CID:	DAR-DIA-53551c05-10_1
SMILES:	c1ccc2c(c1)cncc2CN3c4cc(ccc4C(=O)C3=O)Br
RUN:	RUN141
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.26

RAL-THA-e002e396-11_2



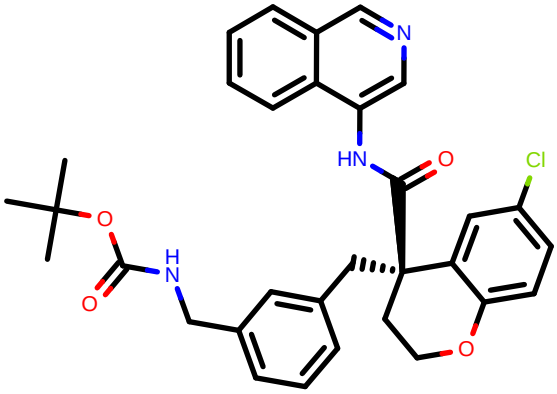
CID:	RAL-THA-e002e396-11_2
SMILES:	COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3470
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.12

MIC-UNK-5a93dd5f-9_5



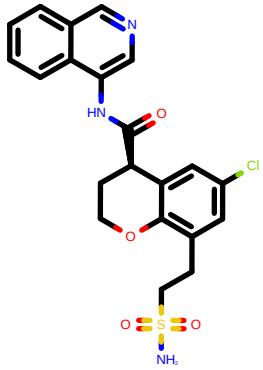
CID:	MIC-UNK-5a93dd5f-9_5
SMILES:	CN(C)[C@@H]1CC[N@@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN782
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.17

EDJ-MED-7320d5d2-1_2



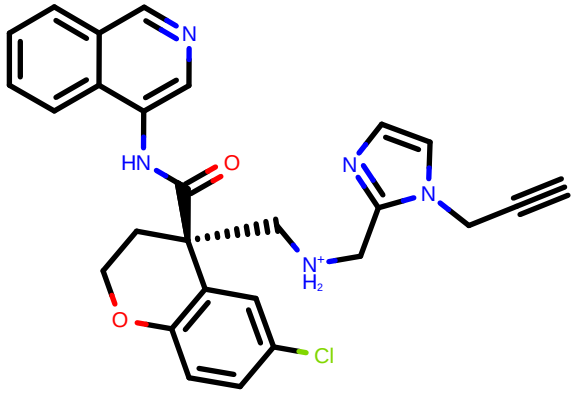
CID:	EDJ-MED-7320d5d2-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN125
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.32

EDJ-MED-50011917-3_2



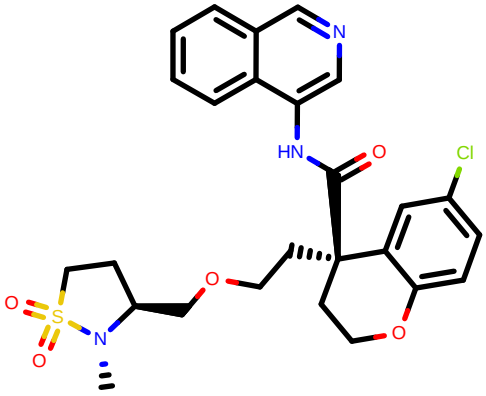
CID:	EDJ-MED-50011917-3_2
SMILES:	COc1c(cc(cc1CC(=O)Nc2cncc3c2cccc3)Cl)C[C@H]4CC(=O)N4
RUN:	RUN380
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.31

RAL-THA-05e671eb-34_1



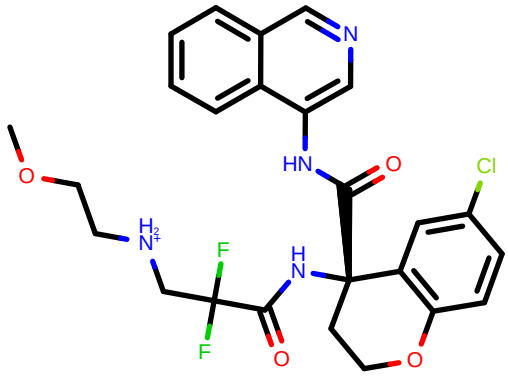
CID:	RAL-THA-05e671eb-34_1
SMILES:	Cc1cccc2c1[C@@H](CCO2)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2072
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.38

MIC-UNK-5a93dd5f-7_5



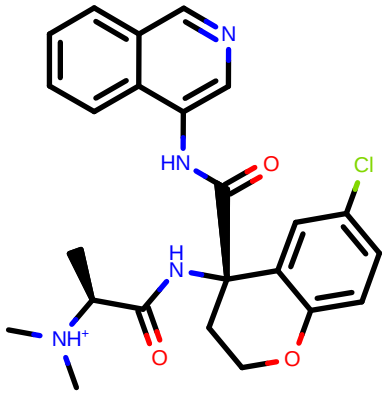
CID:	MIC-UNK-5a93dd5f-7_5
SMILES:	CC(=O)N(C)[C@@H]1CC[N@@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN772
DDG (kcal/mol):	-1.16
dDDG (kcal/mol):	0.26

DAR-DIA-0d514e7d-27_1



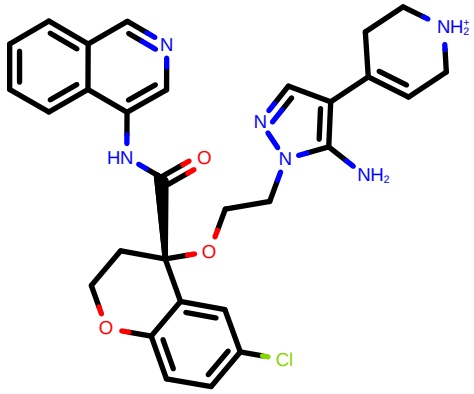
CID:	DAR-DIA-0d514e7d-27_1
SMILES:	C[C@@]1(c2cc(cc(c2OCC1(C)C)OC)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN830
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.34

MAK-UNK-8be7dca9-4_2



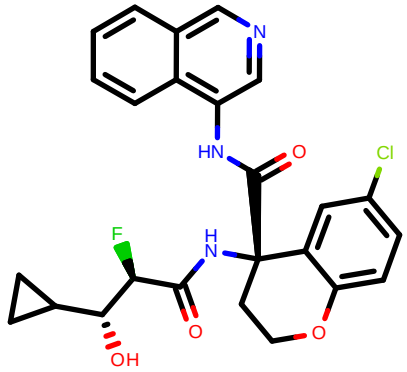
CID:	MAK-UNK-8be7dca9-4_2
SMILES:	c1cc2cncc(c2cc1N3CC[NH2+]CC3)NC(=O)[C@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN505
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.33

MAT-POS-8a69d52e-6_1



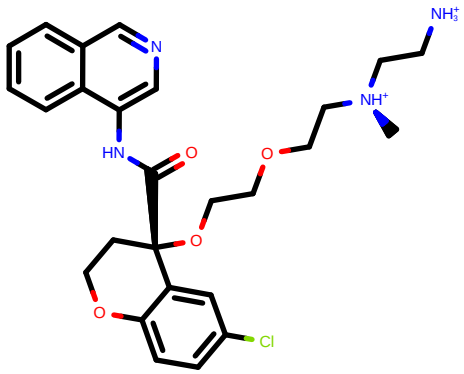
CID:	MAT-POS-8a69d52e-6_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN374
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.38

DAR-DIA-0f2f46c9-9_2



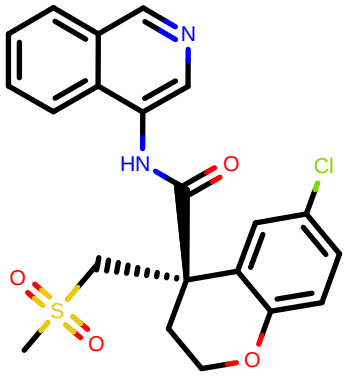
CID:	DAR-DIA-0f2f46c9-9_2
SMILES:	CNS(=O)(=O)[N@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3243
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.15

DAR-DIA-23e5a6a0-7_1



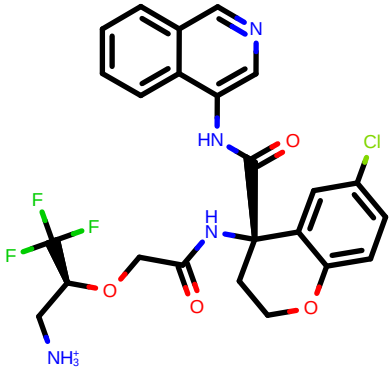
CID:	DAR-DIA-23e5a6a0-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6([NH2+]5)CCC6)Cl
RUN:	RUN413
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.37

PET-UNK-12d8d43f-2_1



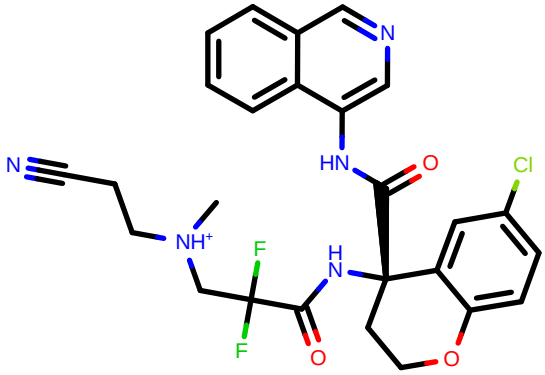
CID:	PET-UNK-12d8d43f-2_1
SMILES:	COC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1496
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.25

MAK-UNK-8be7dca9-6_1



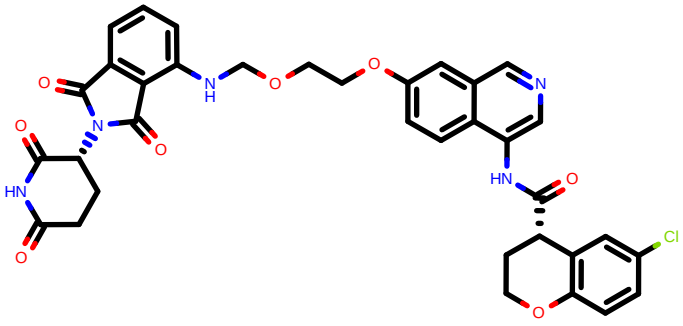
CID:	MAK-UNK-8be7dca9-6_1
SMILES:	c1cc(c2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)C[NH3+]
RUN:	RUN501
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.49

ADA-UCB-dc2b944c-3_1



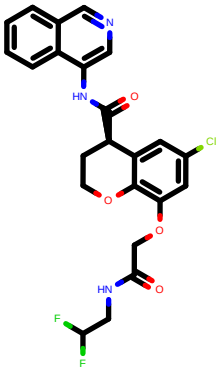
CID:	ADA-UCB-dc2b944c-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cc(ccc4O)Cl
RUN:	RUN602
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.43

DAR-DIA-5d6f1b43-10_1



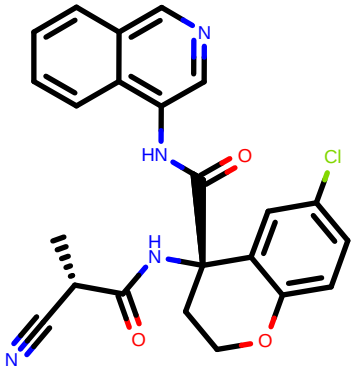
CID:	DAR-DIA-5d6f1b43-10_1
SMILES:	c1ccc2c(c1)cncc2N3CCC4(CCCCC4)N(C3=O)c5cccc(c5)Cl
RUN:	RUN487
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.32

ALP-UNI-3496895b-5_3



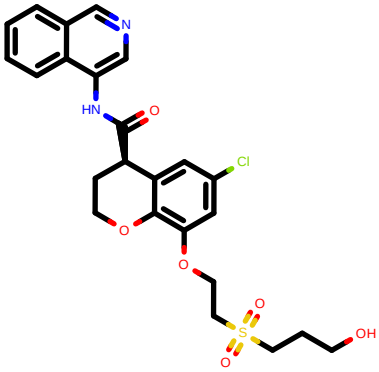
CID:	ALP-UNI-3496895b-5_3
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2514
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.39

DAR-DIA-0f2f46c9-8_1



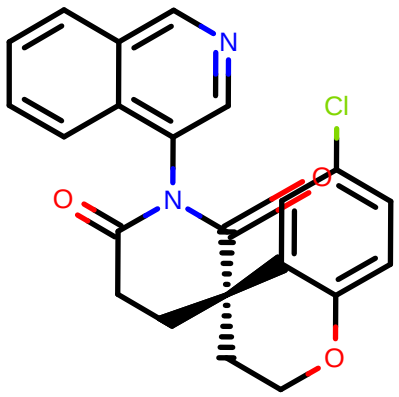
CID:	DAR-DIA-0f2f46c9-8_1
SMILES:	CNS(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3239
DDG (kcal/mol):	-1.15
dDDG (kcal/mol):	0.11

JOH-UNI-ea72002d-3_4



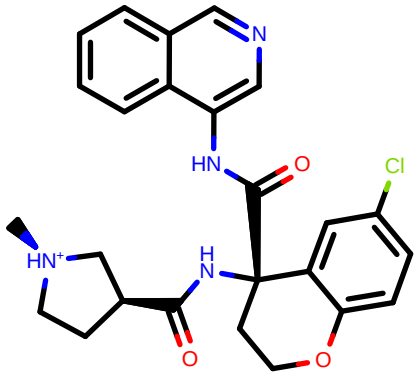
CID:	JOH-UNI-ea72002d-3_4
SMILES:	c1ccc2c(c1)cncc2[C@H](C(=O)[C@H]3CCOc4c3cc(cc4)Cl)N5C(=O)C=CC5=O
RUN:	RUN2487
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.57

EDG-MED-ba1ac7b9-15_5



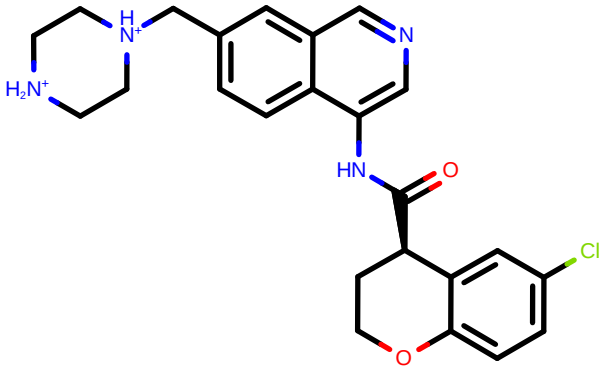
CID:	EDG-MED-ba1ac7b9-15_5
SMILES:	C[C@@H]1C[N@@H+](CCN1C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2679
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.16

MIC-UNK-cdc2493e-19_1



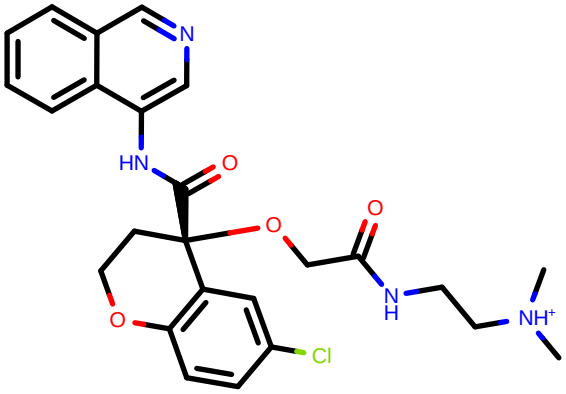
CID:	MIC-UNK-cdc2493e-19_1
SMILES:	CC(C)CCCN(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN567
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.40

MIC-UNK-9582b2c5-3_1



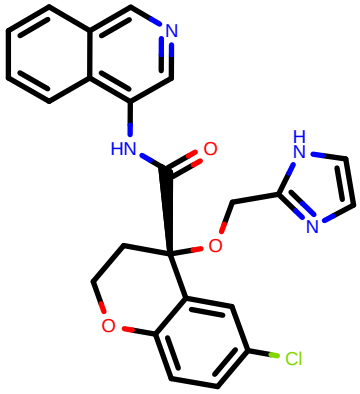
CID:	MIC-UNK-9582b2c5-3_1
SMILES:	CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN270
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.21

FRA-DIA-c7e803f4-1_2



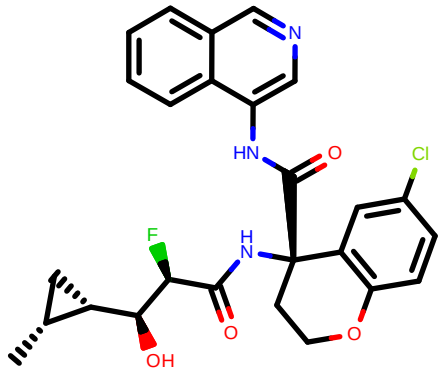
CID:	FRA-DIA-c7e803f4-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cccc4Cl
RUN:	RUN453
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.30

PET-UNK-689df078-4_2



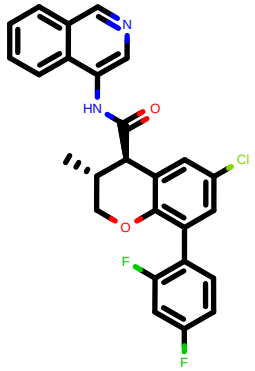
CID:	PET-UNK-689df078-4_2
SMILES:	C[N@H+]1CC(=O)N(C(=O)[C@@H]1c2cccc(c2)Cl)c3cncc4c3cccc4
RUN:	RUN3106
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.12

ADA-UCB-dc2b944c-7_1



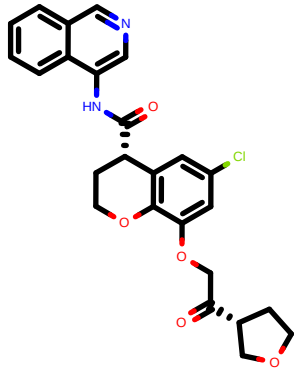
CID:	ADA-UCB-dc2b944c-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)F
RUN:	RUN603
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.24

MIC-UNK-c66144cb-3_2



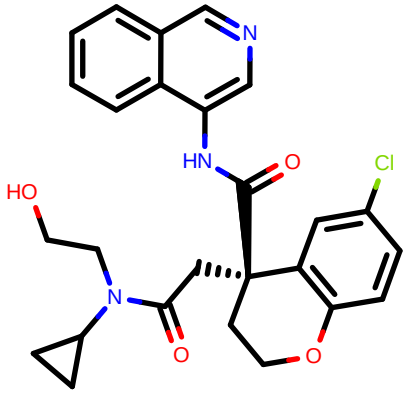
CID:	MIC-UNK-c66144cb-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN134
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.28

EDJ-MED-6864a934-7_1



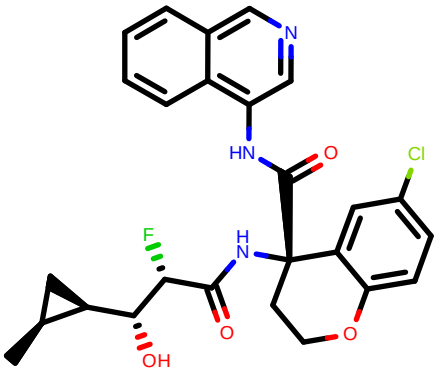
CID:	EDJ-MED-6864a934-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cc6c(nc5)n[nH]n6
RUN:	RUN2612
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.37

JOH-UNI-f51e3bbc-4_2



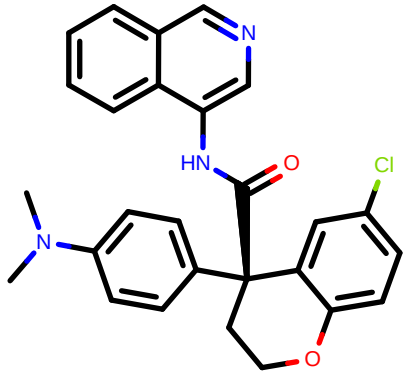
CID:	JOH-UNI-f51e3bbc-4_2
SMILES:	COc1c(c2ccccc2cn1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1165
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.34

VLA-UNK-ba665ac8-1_1



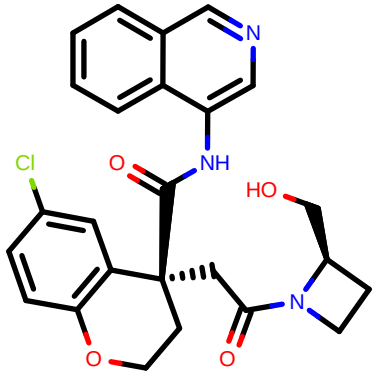
CID:	VLA-UNK-ba665ac8-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[NH2+][C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN3295
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.16

EDJ-MED-50011917-2_2



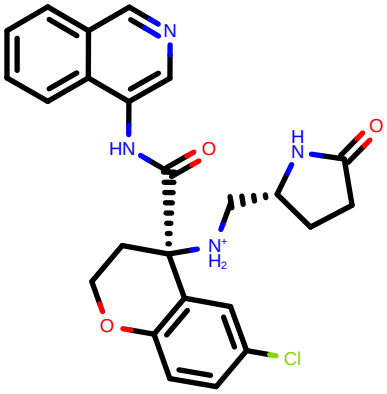
CID:	EDJ-MED-50011917-2_2
SMILES:	Cc1c(cc(cc1O[C@H]2CC(=O)N2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN376
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.21

ALP-POS-d3acb8cc-2_1



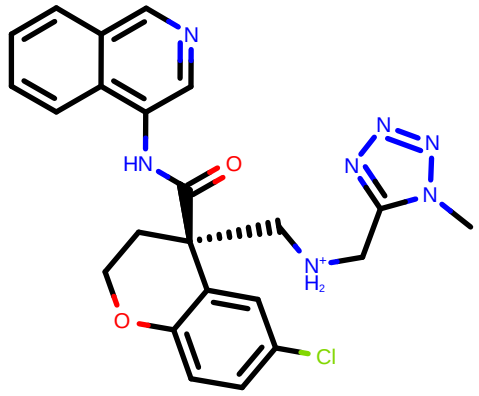
CID:	ALP-POS-d3acb8cc-2_1
SMILES:	C[C@@H]1C[C@@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1093
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.20

EDG-MED-90036822-29_1



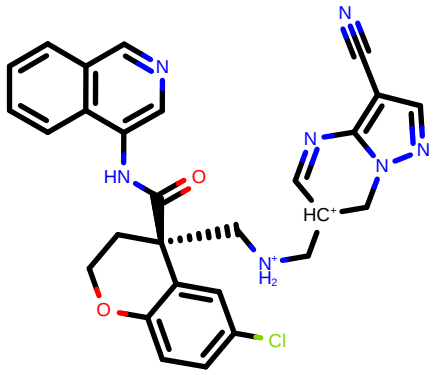
CID:	EDG-MED-90036822-29_1
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1698
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.28

EDJ-MED-1981ceba-2_3



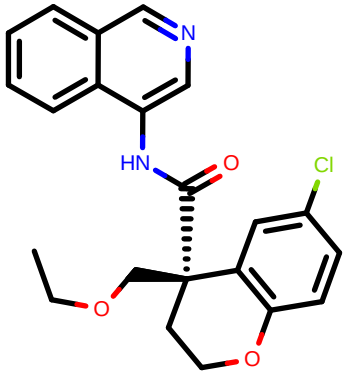
CID:	EDJ-MED-1981ceba-2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)N5CCC5
RUN:	RUN4687
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.26

MIC-UNK-89b52b17-4_1



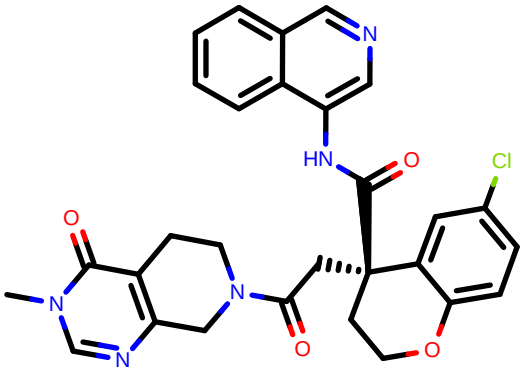
CID:	MIC-UNK-89b52b17-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4C[N@]5[C@@H]3CCCS5(=O)=O)Cl
RUN:	RUN4666
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.26

LAU-MED-88a3970a-4_1



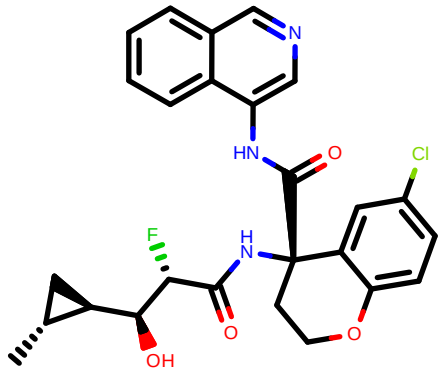
CID:	LAU-MED-88a3970a-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCCO)Cl
RUN:	RUN1503
DDG (kcal/mol):	-1.12
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-20_4



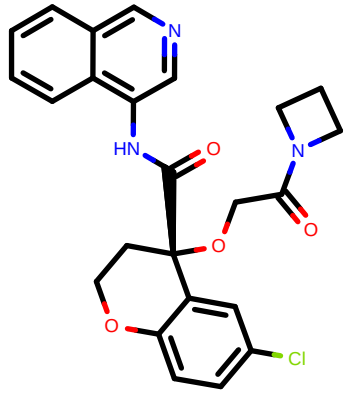
CID:	MAK-UNK-c749d764-20_4
SMILES:	CCCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1009
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.29

MIC-UNK-bcd487e9-8_1



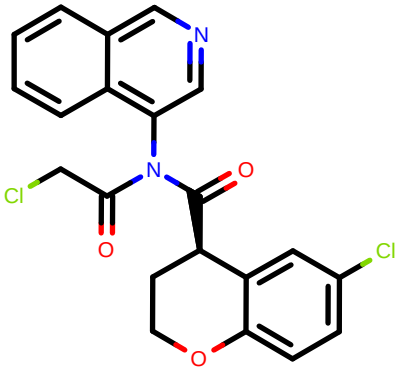
CID:	MIC-UNK-bcd487e9-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(Cc3[nH]ncn3)c4cccc(c4)Cl
RUN:	RUN596
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.24

EDJ-MED-6d9ff7d0-10_1



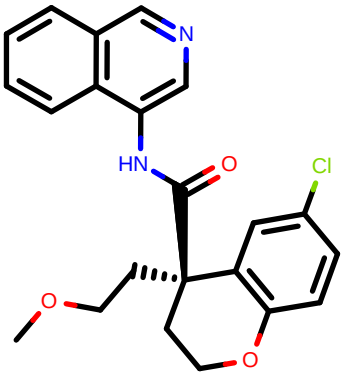
CID:	EDJ-MED-6d9ff7d0-10_1
SMILES:	CS(=O)(=O)CCC[NH2+][C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3438
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.14

EDG-MED-ba1ac7b9-23_3



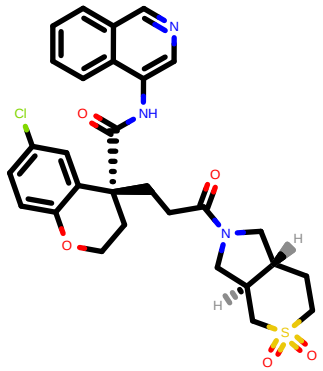
CID:	EDG-MED-ba1ac7b9-23_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5C[C@@H]6C[C@H]5C[N@]6CC(F)F
RUN:	RUN2709
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.15

VLA-UCB-1dbca3b4-6_2



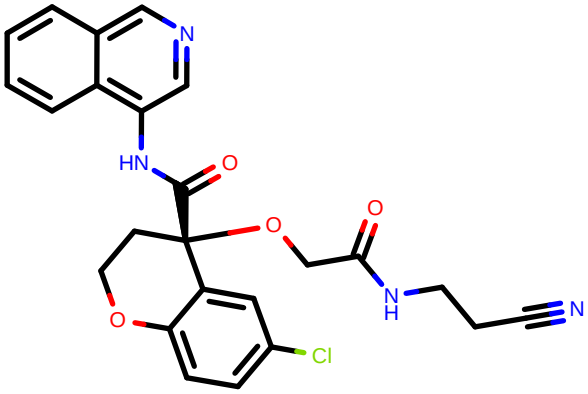
CID:	VLA-UCB-1dbca3b4-6_2
SMILES:	c1ccc2c(c1)cncc2n3c(cc(c3O)c4cccc(c4)Cl)O
RUN:	RUN157
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.22

ALP-POS-6d96567b-2_2



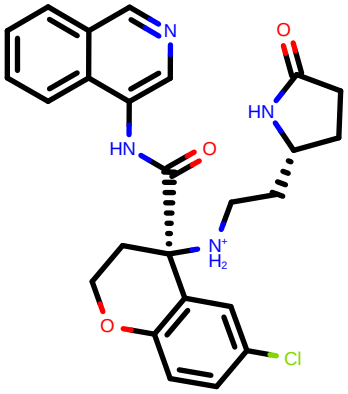
CID:	ALP-POS-6d96567b-2_2
SMILES:	c1ccc2c(c1)cncc2N(Cc3c[nH]c(=O)[nH]c3=O)C(=O)[C@H]4CCOc5c4ccc(c5)Cl
RUN:	RUN3586
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.16

PET-UNK-bb7ffe78-2_1



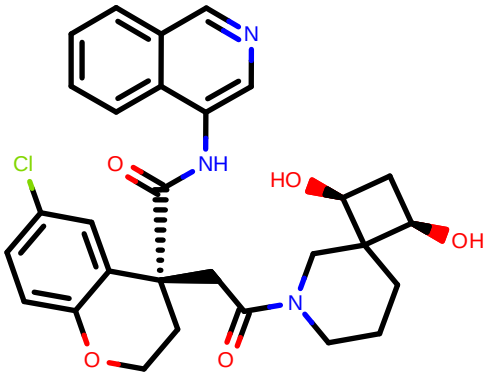
CID:	PET-UNK-bb7ffe78-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OC(F)(F)F
RUN:	RUN3331
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.16

BEN-DND-a7517465-2_1



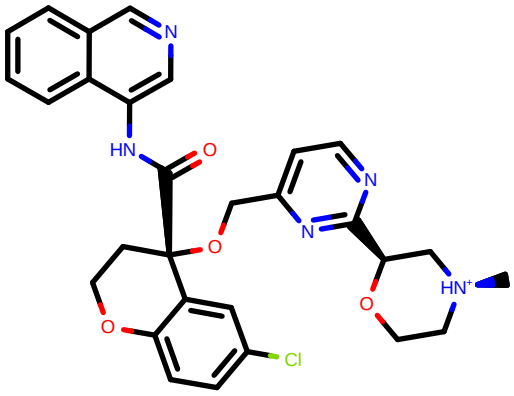
CID:	BEN-DND-a7517465-2_1
SMILES:	c1cc2cncc(c2c(c1)O)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1479
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.25

NAU-LAT-2fed8305-1_1



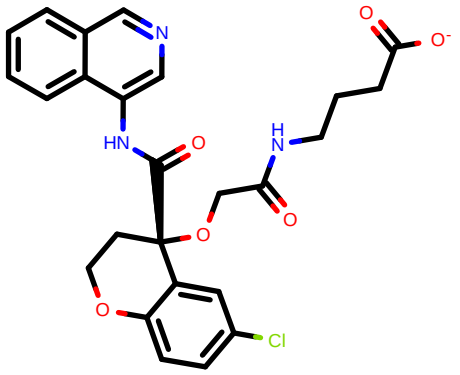
CID:	NAU-LAT-2fed8305-1_1
SMILES:	CC(C)(c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN1104
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.46

PET-UNK-dd44aeb6-1_1



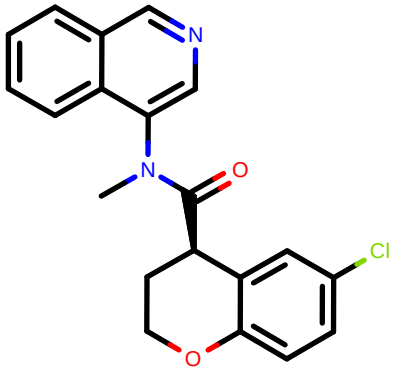
CID:	PET-UNK-dd44aeb6-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(ccc3F)Cl
RUN:	RUN426
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.36

MIC-UNK-cdc2493e-4_2



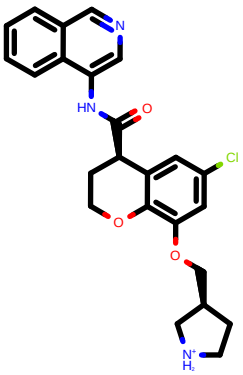
CID:	MIC-UNK-cdc2493e-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@H]5CCC[C@@H]5C4
RUN:	RUN528
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.34

ALF-EVA-ced740bd-1_2



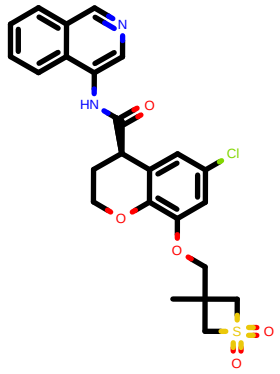
CID:	ALF-EVA-ced740bd-1_2
SMILES:	COc1c(ccc2c1c(cnc2)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl)Cl
RUN:	RUN2789
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.09

KAD-UNI-8a629cb0-17_1



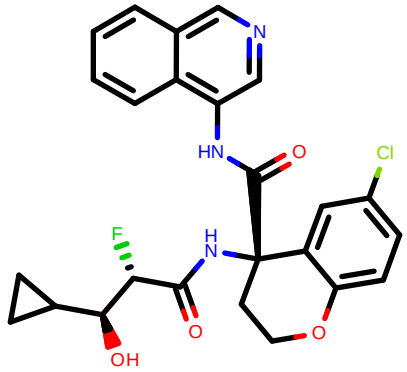
CID:	KAD-UNI-8a629cb0-17_1
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2099
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.36

ALP-POS-5bb456a5-9_1



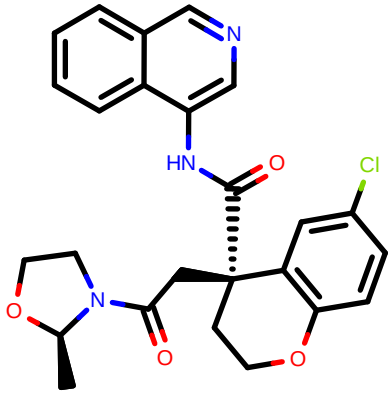
CID:	ALP-POS-5bb456a5-9_1
SMILES:	CCNC(=O)C[NH+]1CCN(CC1)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2443
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.44

DAR-DIA-0f2f46c9-13_3



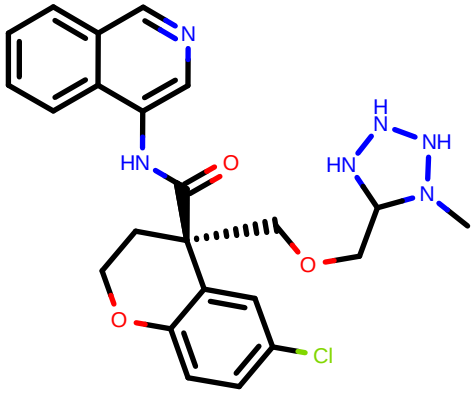
CID:	DAR-DIA-0f2f46c9-13_3
SMILES:	CN(C)S(=O)(=O)[N@@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3249
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.14

BEN-DND-f2e727cd-2_1



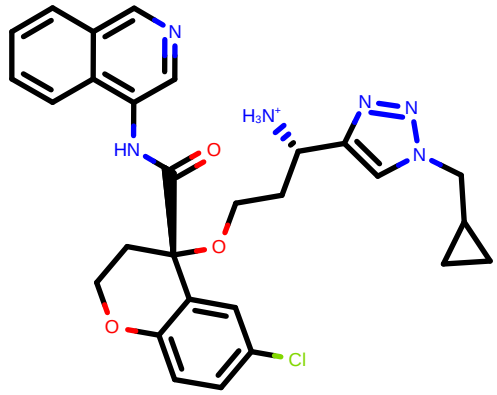
CID:	BEN-DND-f2e727cd-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N3CCNc4c3cc(cc4)Cl
RUN:	RUN1191
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.19

MAT-POS-4223bc15-16_1



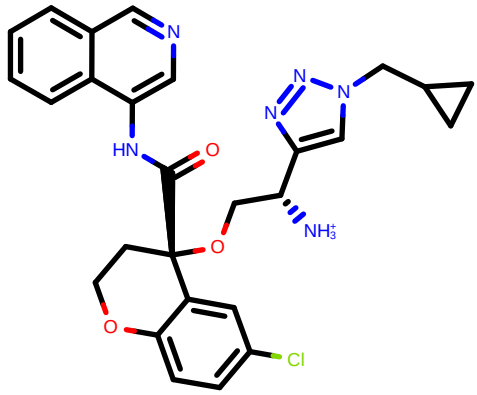
CID:	MAT-POS-4223bc15-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)N[C@@H]5CCC[C@@H]5CO
RUN:	RUN4073
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.11

ERI-UCB-b3e6b0c2-7_1



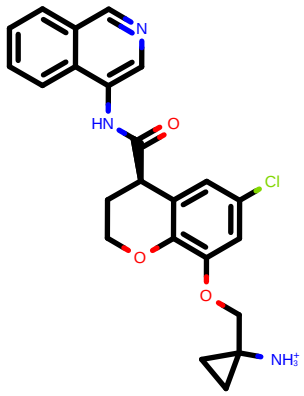
CID:	ERI-UCB-b3e6b0c2-7_1
SMILES:	COCCOc1ccc2cncc(c2c1)NC(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN3040
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.26

DAR-DIA-6a508060-5_3



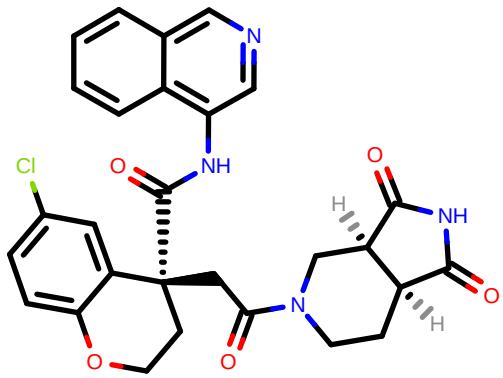
CID:	DAR-DIA-6a508060-5_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC(=O)N5)Cl
RUN:	RUN342
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.55

ALP-POS-5bb456a5-1_1



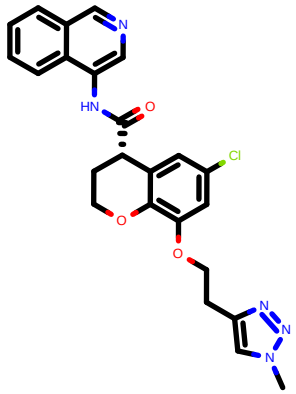
CID:	ALP-POS-5bb456a5-1_1
SMILES:	C[C@@H]1C[N@@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2406
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.44

VLA-UNK-5b0345c3-1_1



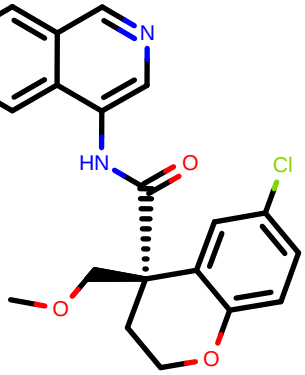
CID:	VLA-UNK-5b0345c3-1_1
SMILES:	COc1cccc2c1cc([nH]2)C(=O)N3Cc4ccc(cc4[C@@H](C3)C(=O)Nc5cncc6c5cccc6)Cl
RUN:	RUN3883
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.16

MAT-POS-e9e99895-9_1



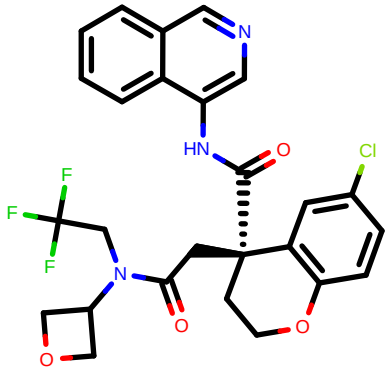
CID:	MAT-POS-e9e99895-9_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)COc4ccc(cc4)C(=O)N
RUN:	RUN2261
DDG (kcal/mol):	-1.09
dDDG (kcal/mol):	0.25

EDG-MED-90036822-9_1



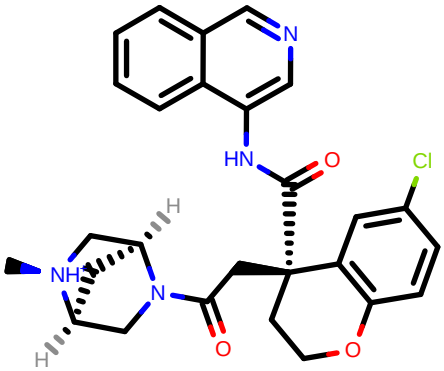
CID:	EDG-MED-90036822-9_1
SMILES:	C[NH2+]CC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1665
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.18

RAL-THA-8416115c-5_3



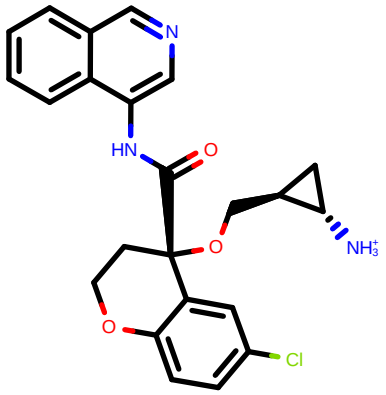
CID:	RAL-THA-8416115c-5_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5[nH]ccn5
RUN:	RUN1265
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.21

JOH-SUS-a69c159d-1_1



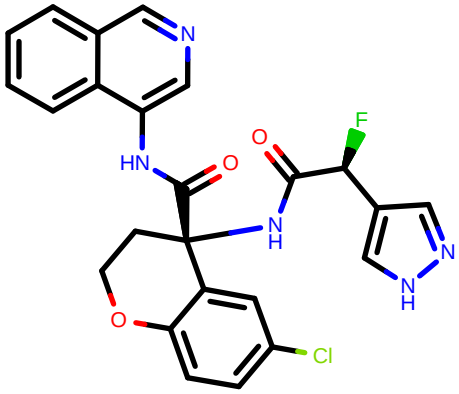
CID:	JOH-SUS-a69c159d-1_1
SMILES:	Cc1c2ccccc2c(cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1116
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.23

ADA-UCB-dc2b944c-2_1



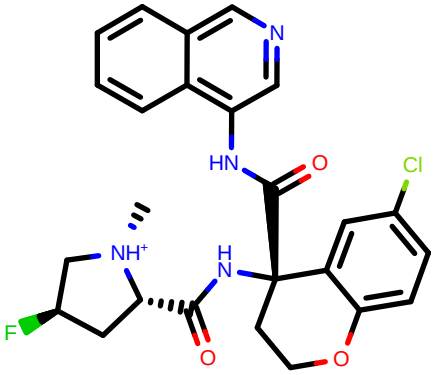
CID:	ADA-UCB-dc2b944c-2_1
SMILES:	COc1ccc(cc1N(CCC2CCCCC2)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN605
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.21

ALP-POS-64a710fa-1_1



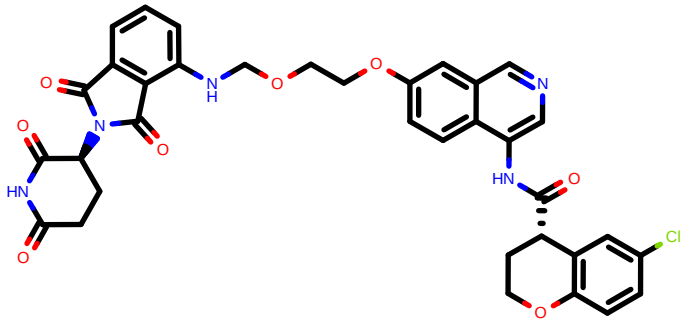
CID:	ALP-POS-64a710fa-1_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)N(CCC3CCCCC3)Cc4cccs4
RUN:	RUN464
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.29

DAR-DIA-0f2f46c9-7_1



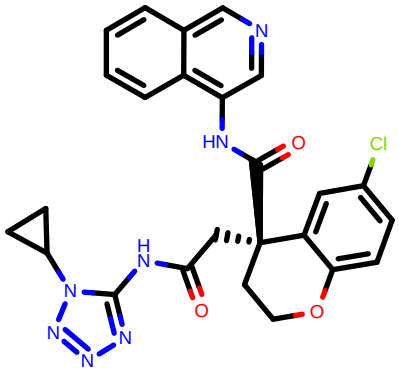
CID:	DAR-DIA-0f2f46c9-7_1
SMILES:	CNS(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3234
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.23

EDJ-MED-e4b030d8-4_1



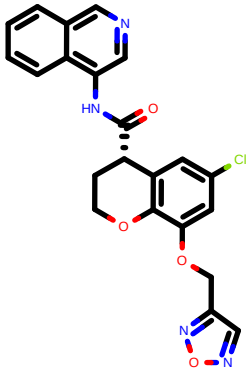
CID:	EDJ-MED-e4b030d8-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OC5COC5)Cl
RUN:	RUN287
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.39

KAD-UNI-cb0f2bbc-21_1



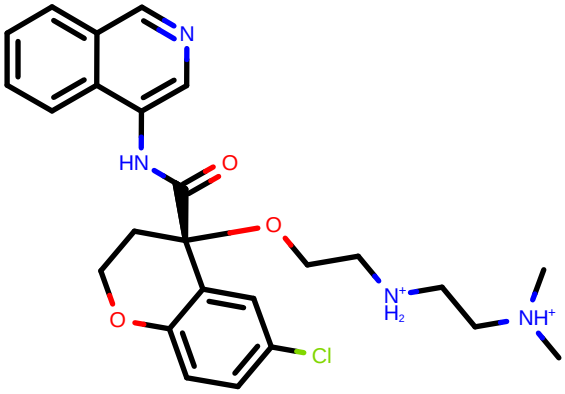
CID:	KAD-UNI-cb0f2bbc-21_1
SMILES:	Cn1cc(n2c1c(cn2)C#N)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3707
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.17

MAT-POS-8293a91a-6_2



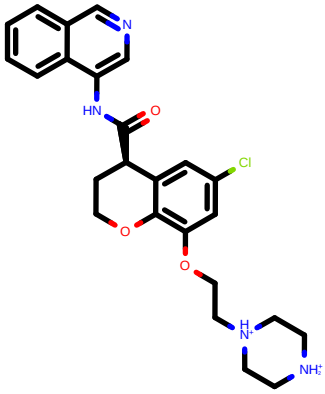
CID:	MAT-POS-8293a91a-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN5097
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.32

MAT-POS-8a69d52e-4_2



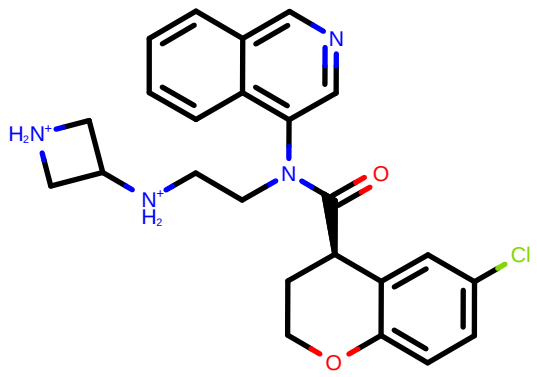
CID:	MAT-POS-8a69d52e-4_2
SMILES:	C[C@H]1COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN367
DDG (kcal/mol):	-1.08
dDDG (kcal/mol):	0.46

MAT-POS-e9e99895-13_4



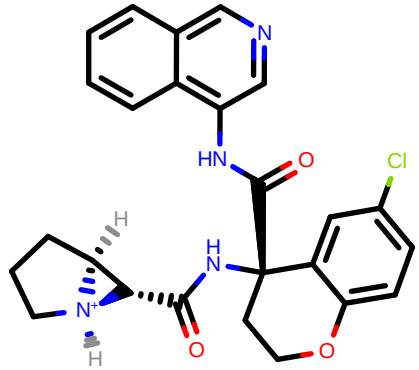
CID:	MAT-POS-e9e99895-13_4
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@H]4CC[N@@H+](C4)C
RUN:	RUN2270
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.43

EDJ-MED-ee07cf00-17_2



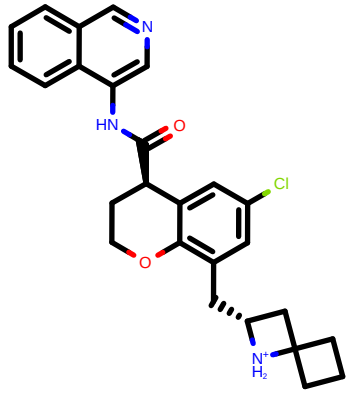
CID:	EDJ-MED-ee07cf00-17_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)Cn4c(=O)c5ccnn5cn4
RUN:	RUN2844
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.30

MAT-POS-78e1d523-1_2



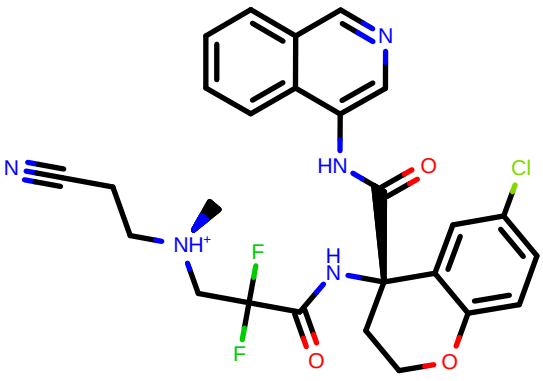
CID:	MAT-POS-78e1d523-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCSc4c3cc(cc4)Cl
RUN:	RUN3279
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.16

DAR-DIA-53551c05-11_2



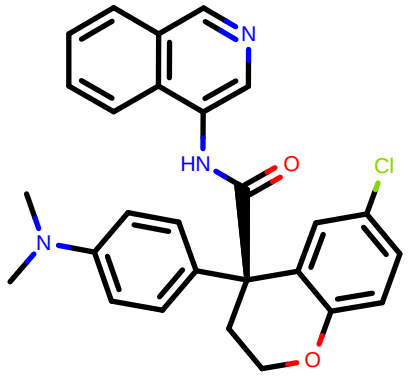
CID:	DAR-DIA-53551c05-11_2
SMILES:	c1ccc2c(c1)cncc2CN3c4cc(ccc4C(=O)C3=O)c5cc(cc(c5)Cl)O[C@H]6CC(=O)N6
RUN:	RUN145
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.34

MIC-UNK-5a93dd5f-2_5



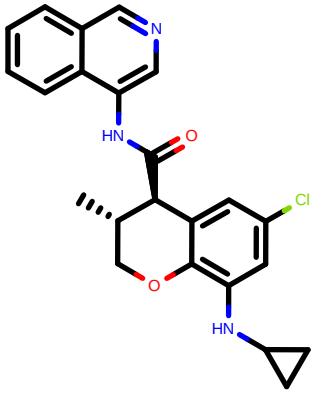
CID:	MIC-UNK-5a93dd5f-2_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@@H]5CCCC[C@H]5C4
RUN:	RUN738
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.33

LON-WEI-4d77710c-39_1



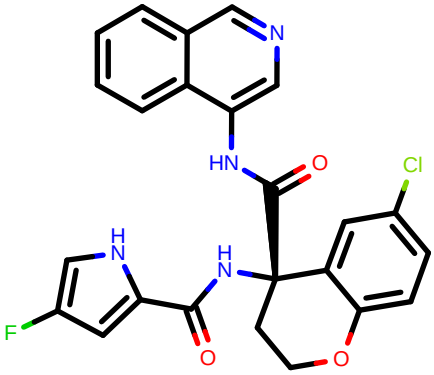
CID:	LON-WEI-4d77710c-39_1
SMILES:	C[C@@H](CCc1ccco1)NC(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN226
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.24

PET-UNK-c9c1e0d8-4_1



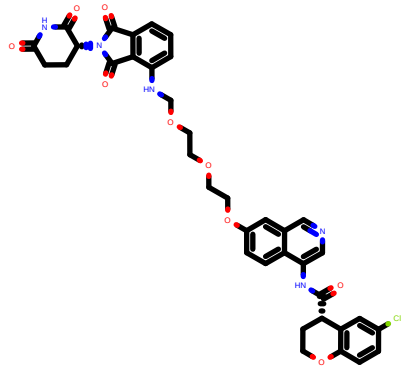
CID:	PET-UNK-c9c1e0d8-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN122
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.27

VLA-UNK-70dd90ef-1_1



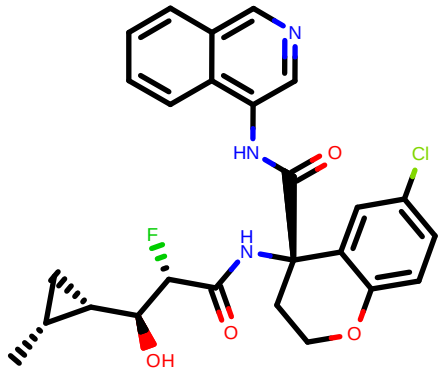
CID:	VLA-UNK-70dd90ef-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CNc5c4cc(cc5)Cl)NC3=O
RUN:	RUN3302
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.11

FRA-DIA-0fa076fe-1_1



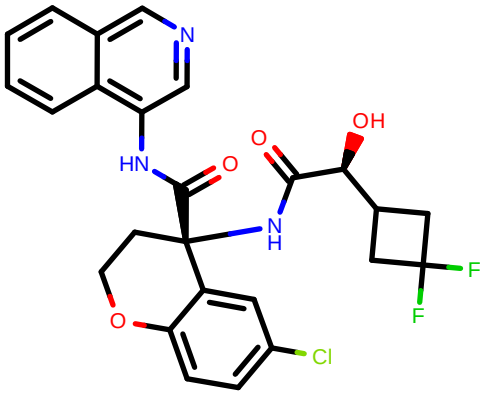
CID:	FRA-DIA-0fa076fe-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cccc4Cl
RUN:	RUN417
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.48

MAT-POS-78e1d523-4_1



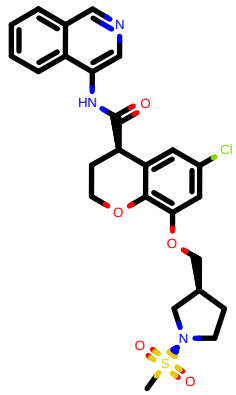
CID:	MAT-POS-78e1d523-4_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3286
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.15

VLA-UNK-70dd90ef-2_1



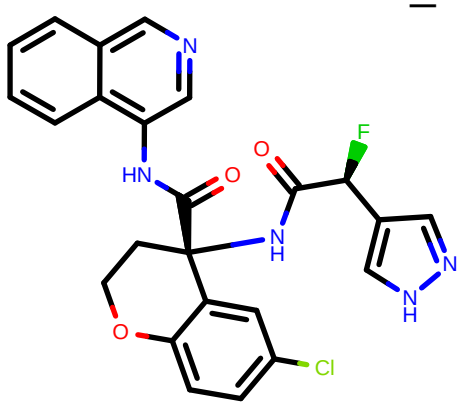
CID:	VLA-UNK-70dd90ef-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(c5cc(ccc5NC4=O)Cl)NC3=O
RUN:	RUN3303
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.16

KAD-UNI-80f122c8-3_1



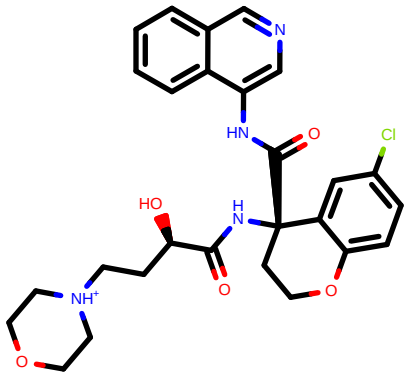
CID:	KAD-UNI-80f122c8-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)Cl)CC(=O)N5CC[C@@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN2288
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.46

ALP-POS-fe871b40-11_1



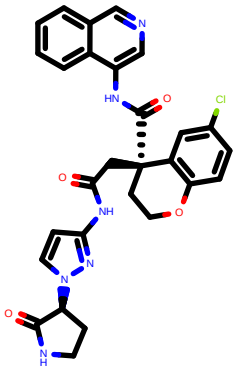
CID:	ALP-POS-fe871b40-11_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3129
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.15

NAU-LAT-a5c7d7cb-4_1



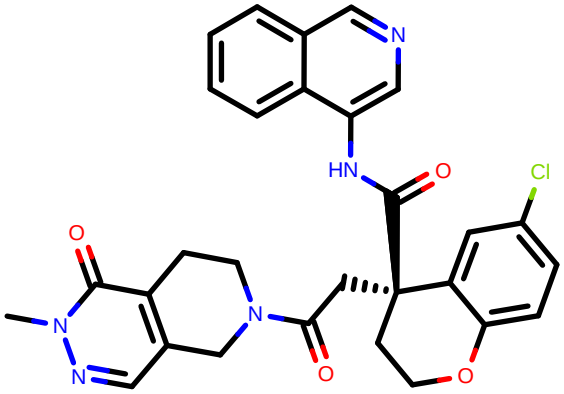
CID:	NAU-LAT-a5c7d7cb-4_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)N(Cc3ccsc3)c4cccc(c4)Cl
RUN:	RUN576
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.31

LON-WEI-5e7d1b3e-17_1



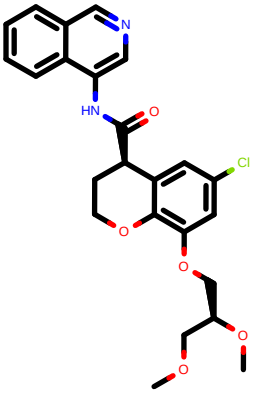
CID:	LON-WEI-5e7d1b3e-17_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccc(cc3)Cl
RUN:	RUN1324
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.23

MAK-UNK-ffc90da7-7_4



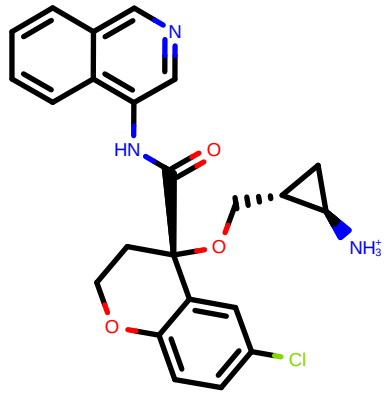
CID:	MAK-UNK-ffc90da7-7_4
SMILES:	CC(C)OC[C@H]([C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)[NH2+]C
RUN:	RUN713
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.26

ALF-EVA-5b152d2f-8_1



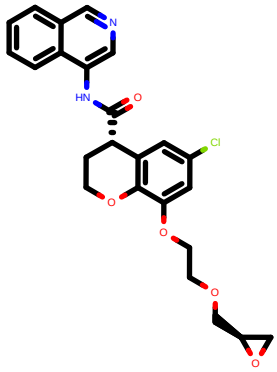
CID:	ALF-EVA-5b152d2f-8_1
SMILES:	c1cc2c(cc1CC3CC3)cncc2NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN2362
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.48

VLA-UNK-f49ebb87-1_2



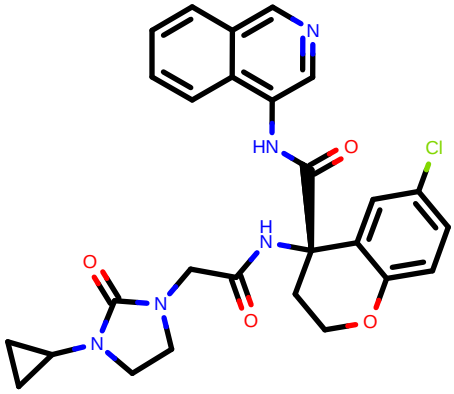
CID:	VLA-UNK-f49ebb87-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4NC(=O)O3)Cl
RUN:	RUN3102
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.16

EDG-MED-ba1ac7b9-4_2



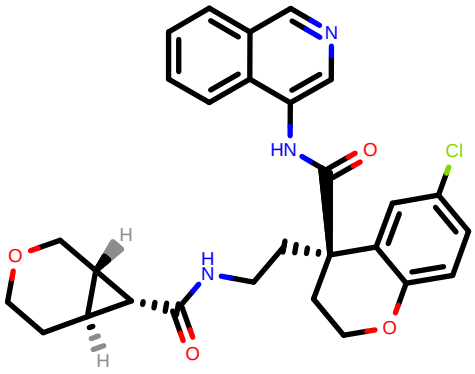
CID:	EDG-MED-ba1ac7b9-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[N@@H+]6CC[C@@H](C6)O
RUN:	RUN2625
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.25

RAL-THA-8416115c-6_2



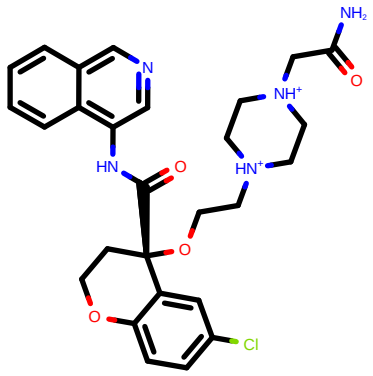
CID:	RAL-THA-8416115c-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5ccn[nH]5
RUN:	RUN1268
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.34

DAR-DIA-f6ee7aeb-4_4



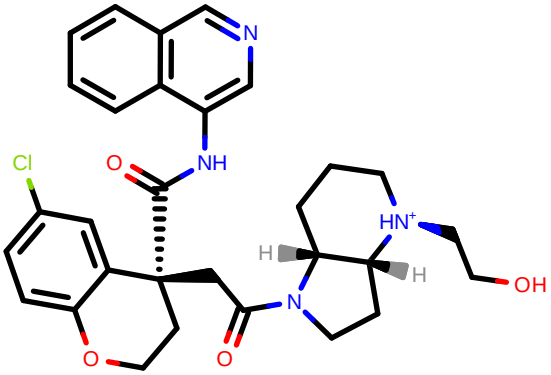
CID:	DAR-DIA-f6ee7aeb-4_4
SMILES:	c1ccc2c(c1)cncc2N3C[C@H]([C@H](CC3=O)c4cc(cc(c4)Cl)OCCC(F)(F)F)c5c[nH]c(=O)[nH]c5=O
RUN:	RUN3417
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.17

MAR-UCB-6ab2ec87-4_1



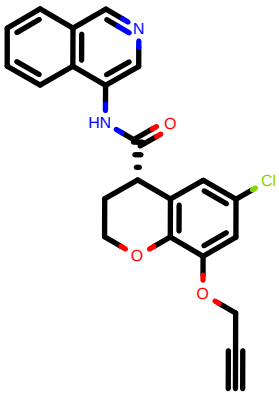
CID:	MAR-UCB-6ab2ec87-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3COc4c3cc(cc4O)Cl
RUN:	RUN3027
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.32

MAT-POS-4223bc15-24_2



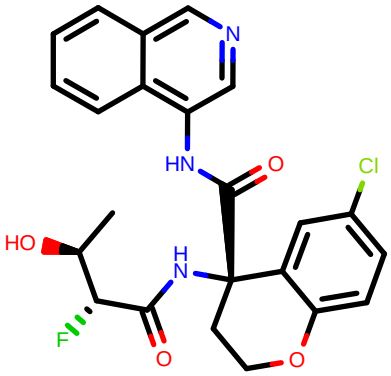
CID:	MAT-POS-4223bc15-24_2
SMILES:	CN(C)C(=O)C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4110
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.27

MAT-POS-e9e99895-2_5



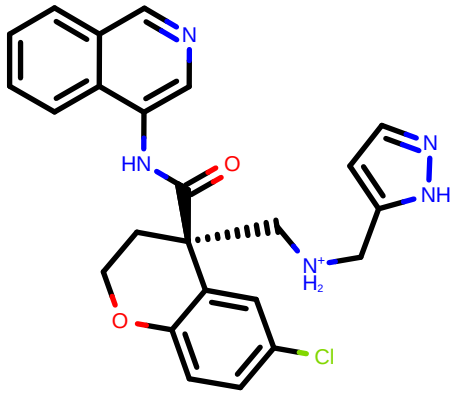
CID:	MAT-POS-e9e99895-2_5
SMILES:	CC(C)[N@@H+]1CCO[C@@H](C1)C(=O)N[C@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2239
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.21

NIR-THE-3fc2bec4-1_1



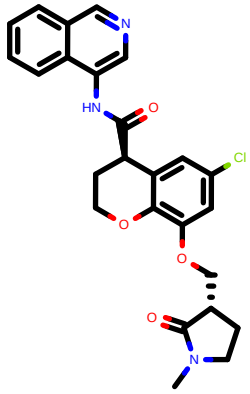
CID:	NIR-THE-3fc2bec4-1_1
SMILES:	CO[C@]1(CCNc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3275
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.11

EDG-MED-90036822-91_1



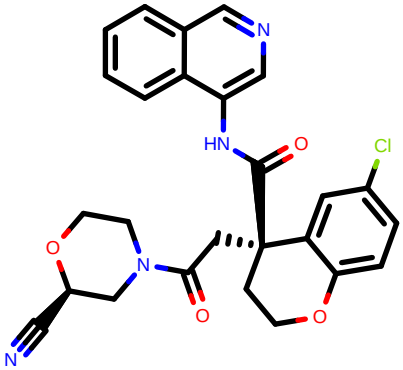
CID:	EDG-MED-90036822-91_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5cccc(c5)F)[NH3+]
RUN:	RUN1799
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.41

MAT-POS-fce787c2-4_2



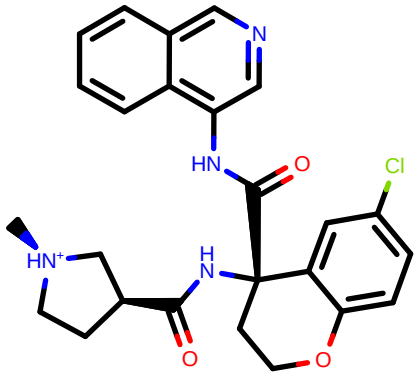
CID:	MAT-POS-fce787c2-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)O
RUN:	RUN2148
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.42

MIC-UNK-67d4a29a-2_1



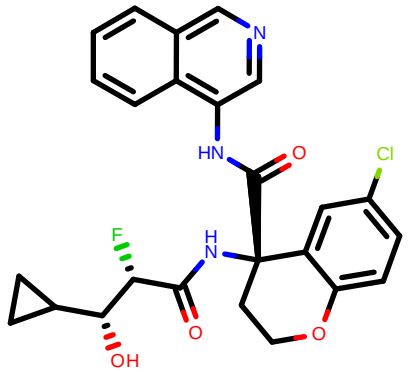
CID:	MIC-UNK-67d4a29a-2_1
SMILES:	CN(c1cncc2c1c(ccc2)F)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1088
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.28

DAR-DIA-0587064e-10_1



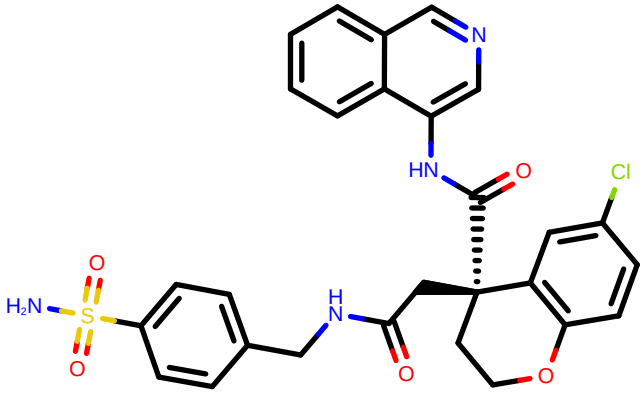
CID:	DAR-DIA-0587064e-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCCC(F)(F)F)Cl
RUN:	RUN3355
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.17

DAR-DIA-0f2f46c9-10_3



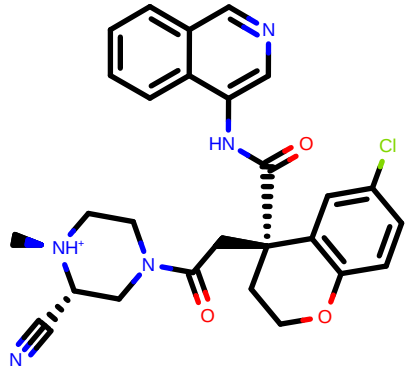
CID:	DAR-DIA-0f2f46c9-10_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC[N@](c4c3cc(cc4)Cl)S(=O)(=O)[O-]
RUN:	RUN3244
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.17

NAU-LAT-4ce8bf23-1_1



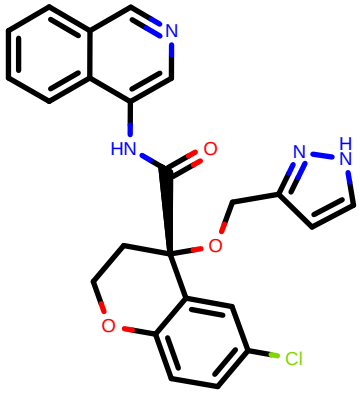
CID:	NAU-LAT-4ce8bf23-1_1
SMILES:	CC(=O)NC[C@@H](c1cncc2c1cccc2)C(=O)Nc3cccc(c3)Cl
RUN:	RUN1389
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.25

JOH-SUS-a69c159d-3_2



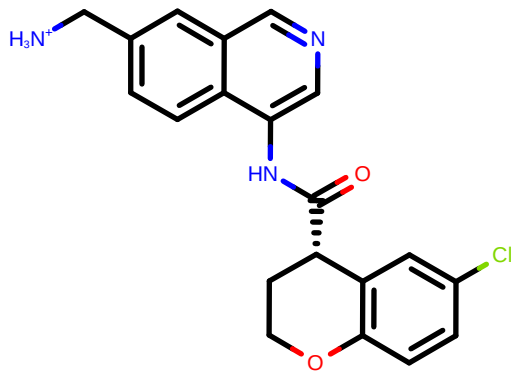
CID:	JOH-SUS-a69c159d-3_2
SMILES:	c1ccc2c(c1)c(cnc2C(F)F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1121
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.22

MAT-POS-3b97339c-2_1



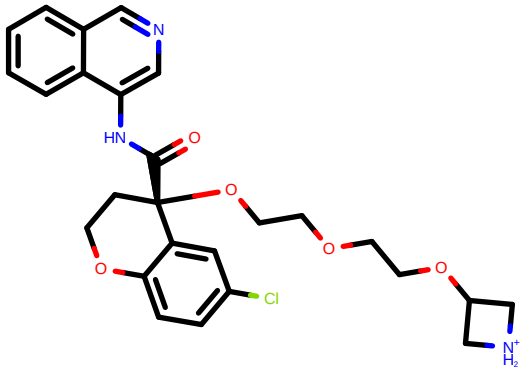
CID:	MAT-POS-3b97339c-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)[NH3+]
RUN:	RUN3296
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.11

ERI-UCB-ce40166b-12_1



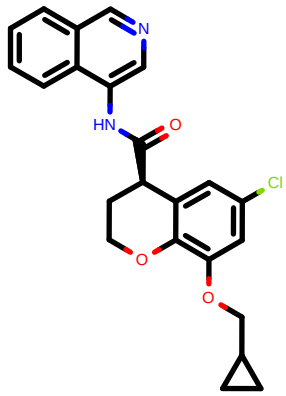
CID:	ERI-UCB-ce40166b-12_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Oc4cccnc4)C#N
RUN:	RUN51
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.16

MIC-UNK-cdc2493e-1_1



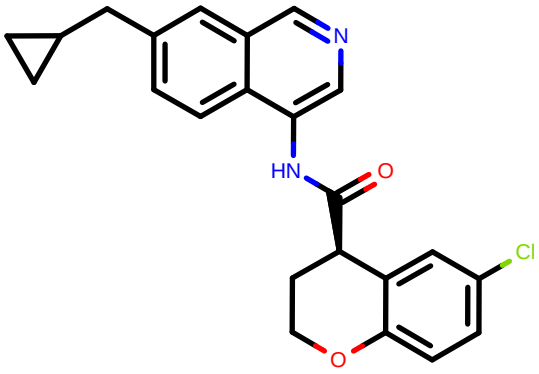
CID:	MIC-UNK-cdc2493e-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCC3)c4cccc(c4)Cl
RUN:	RUN521
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.37

DAR-DIA-9e4459de-15_10



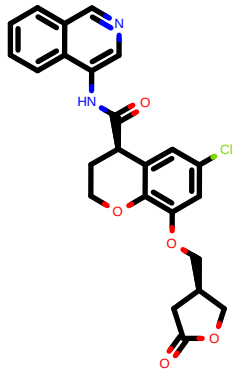
CID:	DAR-DIA-9e4459de-15_10
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1450
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.32

DAR-DIA-0d514e7d-32_9



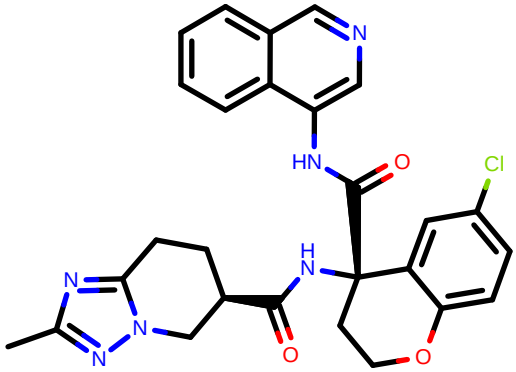
CID:	DAR-DIA-0d514e7d-32_9
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H]4C[C@@H]4CO[C@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN858
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.23

ALP-POS-2da19ca7-7_4



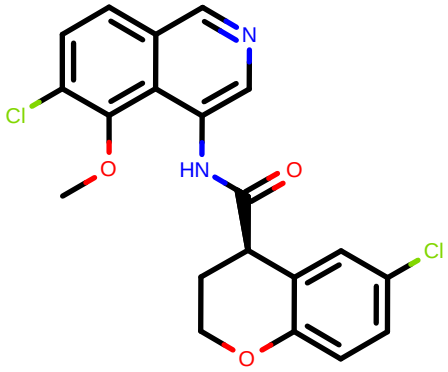
CID:	ALP-POS-2da19ca7-7_4
SMILES:	C[C@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2383
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.40

BEN-DND-c852c98b-5_1



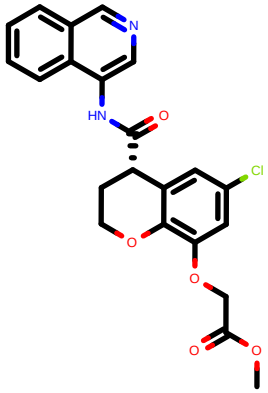
CID:	BEN-DND-c852c98b-5_1
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1210
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.27

LON-WEI-5e7d1b3e-34_1



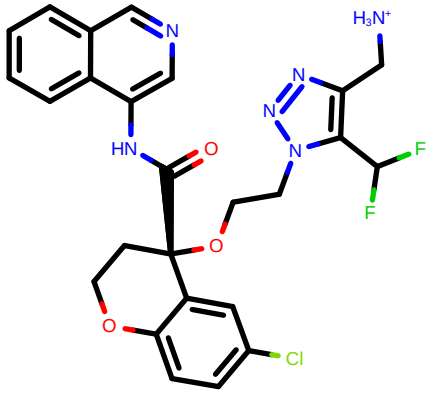
CID:	LON-WEI-5e7d1b3e-34_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CC[C@@H](C3)c4ccccc4
RUN:	RUN1335
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.20

MAT-POS-e9e99895-13_7



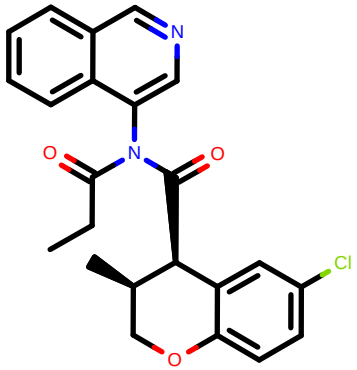
CID:	MAT-POS-e9e99895-13_7
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@H]4CC[N@H+](C4)C
RUN:	RUN2273
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.23

DAR-DIA-6a508060-8_2



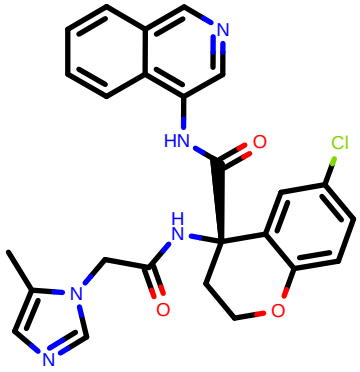
CID:	DAR-DIA-6a508060-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)C5CC5
RUN:	RUN345
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.37

LON-WEI-4d77710c-27_1



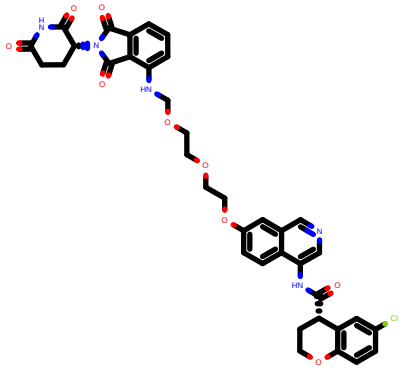
CID:	LON-WEI-4d77710c-27_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NC3CCCCCC3
RUN:	RUN211
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.22

VLA-UNK-3a43cd95-4_1



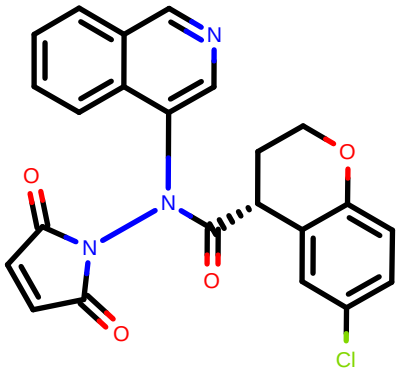
CID:	VLA-UNK-3a43cd95-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)COc5c4cc(c(c5)F)Cl
RUN:	RUN3191
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.14

DAR-DIA-6a508060-5_1



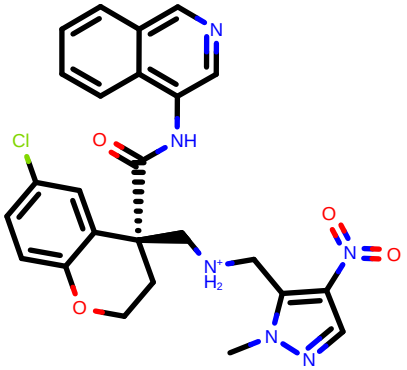
CID:	DAR-DIA-6a508060-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC(=O)N5)Cl
RUN:	RUN340
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.45

MAK-UNK-c749d764-10_3



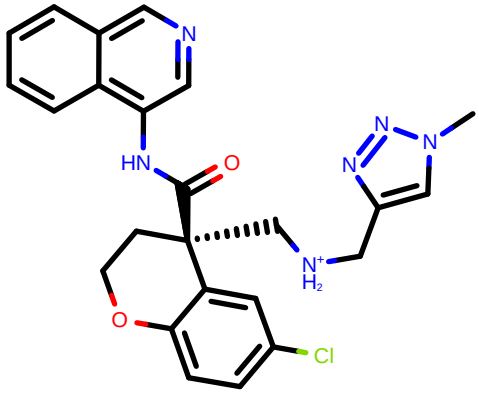
CID:	MAK-UNK-c749d764-10_3
SMILES:	CSN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN943
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.30

MIC-UNK-ea4eb352-4_1



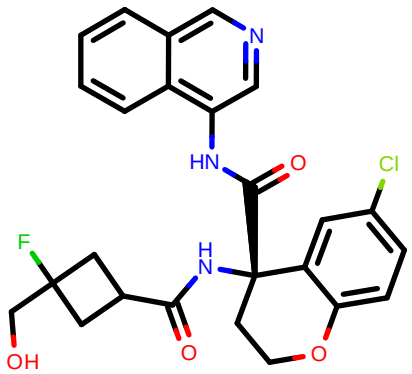
CID:	MIC-UNK-ea4eb352-4_1
SMILES:	CO[C@@]1(CCSc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4640
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.24

EDJ-MED-1981ceba-4_2



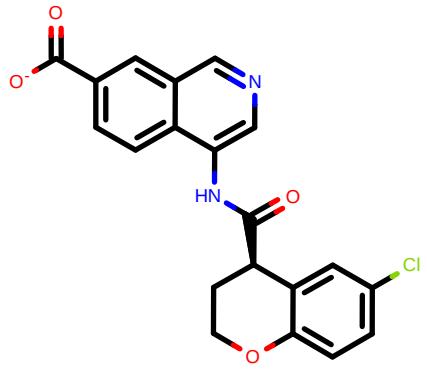
CID:	EDJ-MED-1981ceba-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)N5CC(C5)C#N
RUN:	RUN4694
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.20

LON-WEI-9739a092-3_1



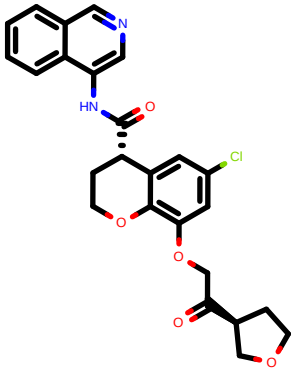
CID:	LON-WEI-9739a092-3_1
SMILES:	COc1cc(ccc1Nc2cc(cc(c2)Cl)CC(=O)Nc3cncc4c3cccc4)Br
RUN:	RUN3267
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.14

MAT-POS-2492181e-10_4



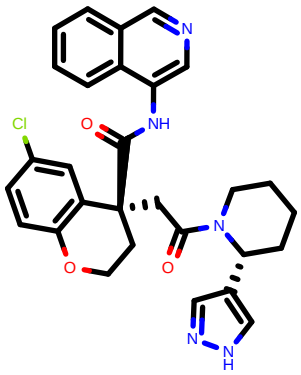
CID:	MAT-POS-2492181e-10_4
SMILES:	C[C@H]1CCCC[N@H+]1CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN110
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.18

ALP-UNI-0676e700-18_2



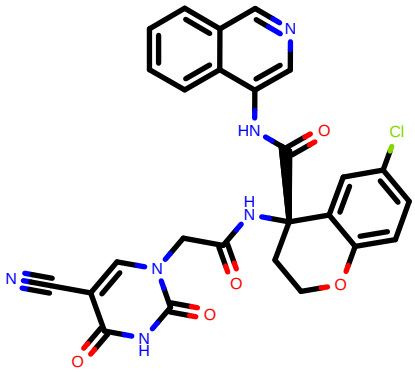
CID:	ALP-UNI-0676e700-18_2
SMILES:	Cc1nnc2n1C[C@@H]([N@H+](C2)C)C(=O)NC[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2464
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.34

RAL-THA-8416115c-2_3



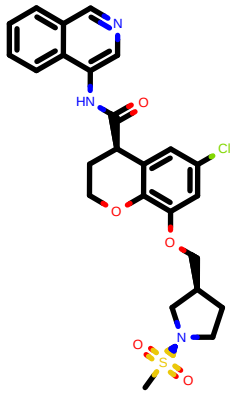
CID:	RAL-THA-8416115c-2_3
SMILES:	CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1253
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.25

MIC-UNK-08fa0751-1_1



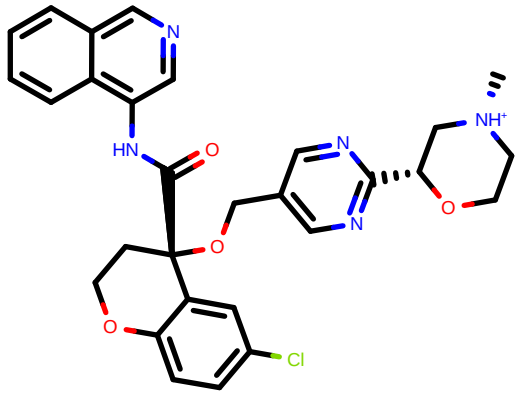
CID:	MIC-UNK-08fa0751-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C(CO)(F)F)Cl
RUN:	RUN1519
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.30

LEE-CAM-7ab9b158-1_3



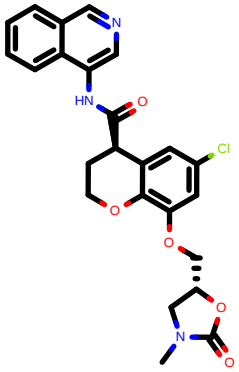
CID:	LEE-CAM-7ab9b158-1_3
SMILES:	C[NH+](C)[C@@H]1COC[C@H]1OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2202
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.44

JAG-UCB-f37eaa14-9_2



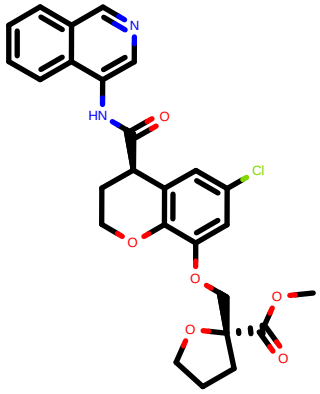
CID:	JAG-UCB-f37eaa14-9_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](c5c4cc(cc5)Cl)C6CC(=O)C6
RUN:	RUN3071
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.21

ALP-UNI-0676e700-5_1



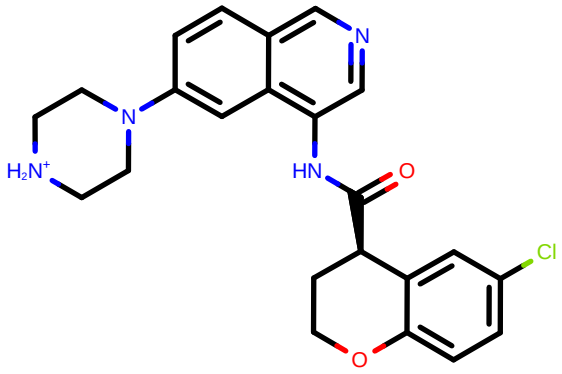
CID:	ALP-UNI-0676e700-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cccc(c5)OCC(=O)N
RUN:	RUN2449
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.37

MAT-POS-2905de8c-2_2



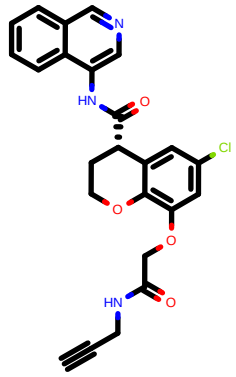
CID:	MAT-POS-2905de8c-2_2
SMILES:	C[NH2+][C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2230
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.48

EDG-MED-ba1ac7b9-30_2



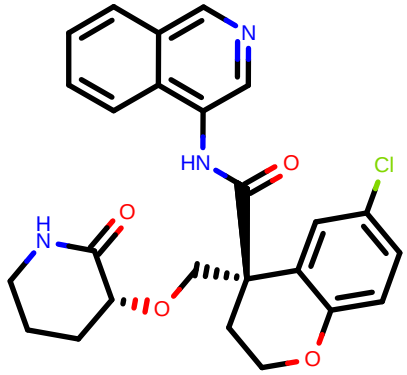
CID:	EDG-MED-ba1ac7b9-30_2
SMILES:	C[NH+]1CCC(CC1)N(CCO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2741
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.10

JOH-UNI-ea72002d-4_2



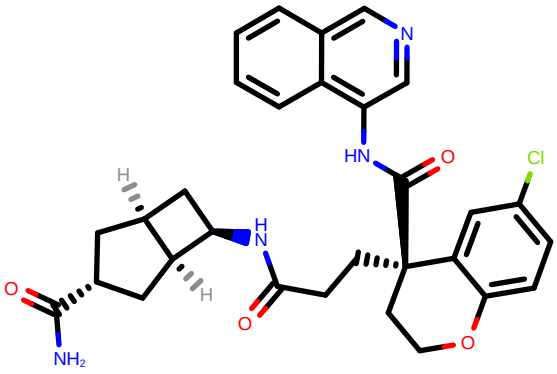
CID:	JOH-UNI-ea72002d-4_2
SMILES:	c1ccc2c(c1)cncc2[C@](C(=O)[C@@H]3CCOc4c3cc(cc4)Cl)(N5C(=O)C=CC5=O)F
RUN:	RUN2490
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.29

BEN-DND-a02b439d-15_2



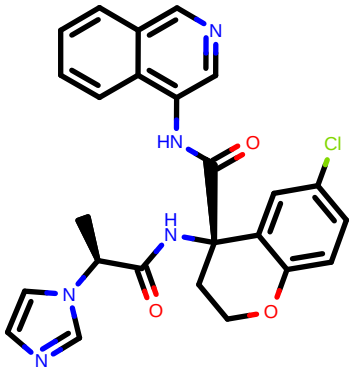
CID:	BEN-DND-a02b439d-15_2
SMILES:	C[N@H+]1Cc2cc(c(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl)Cl
RUN:	RUN3673
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.11

MIC-UNK-0a05c952-3_6



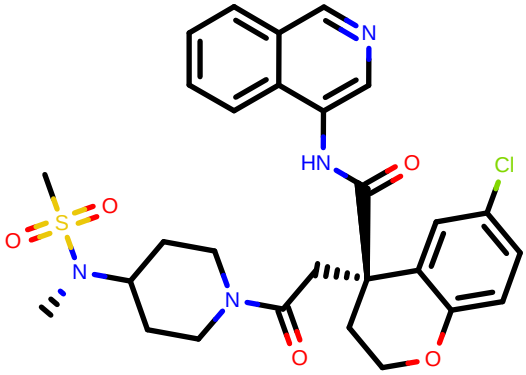
CID:	MIC-UNK-0a05c952-3_6
SMILES:	c1ccc2c(c1)cncc2N3[C@H](C[C@@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@H]5CO5
RUN:	RUN3517
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.24

EDJ-MED-f893e2a1-7_2



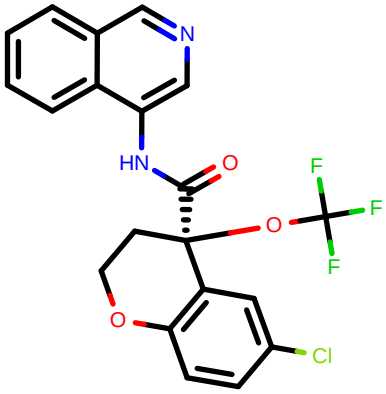
CID:	EDJ-MED-f893e2a1-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5c[nH]c(=O)o5
RUN:	RUN3207
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.16

ALP-UNI-4b8a177c-1_1



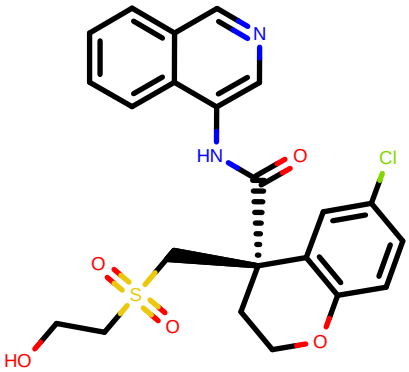
CID:	ALP-UNI-4b8a177c-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3c(ccc4O)Cl
RUN:	RUN1173
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-15_1



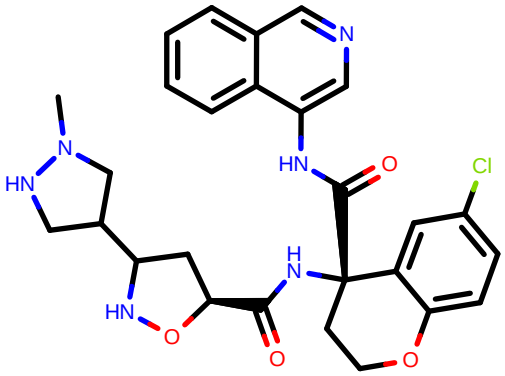
CID:	MAK-UNK-c749d764-15_1
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN959
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.08

ED_-GRI-5b13fbe2-12_1



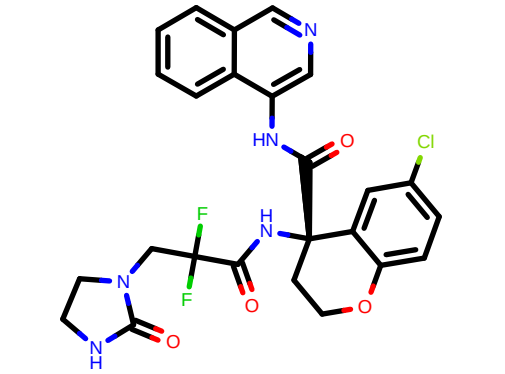
CID:	ED_-GRI-5b13fbe2-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@@H+](CCO)CCOCCO
RUN:	RUN1540
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.32

EDJ-MED-009f762b-4_2



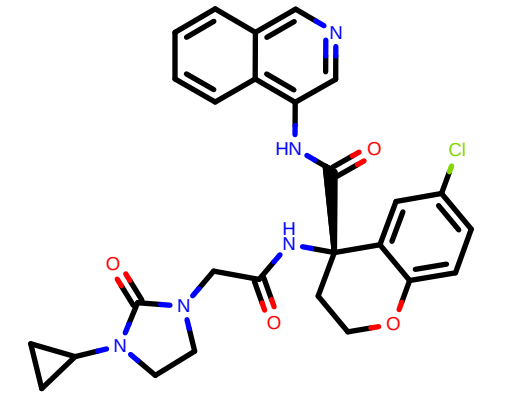
CID:	EDJ-MED-009f762b-4_2
SMILES:	Cc1[nH]c(c[nH+]1)C[N@H+]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cc(cc5)F)Cl
RUN:	RUN3913
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.14

MIC-UNK-cdc2493e-14_2



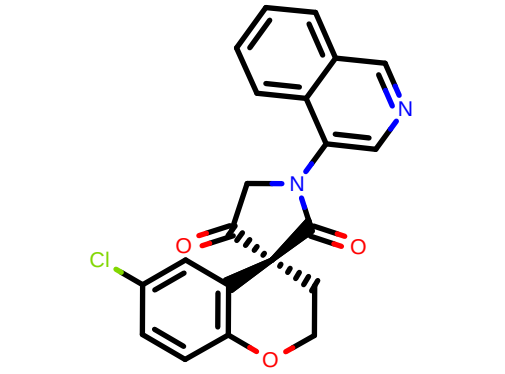
CID:	MIC-UNK-cdc2493e-14_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@H]4CC[C@@H](C4)[NH+]5CCCCC5
RUN:	RUN556
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.33

ALP-POS-a0a4abd7-1_2



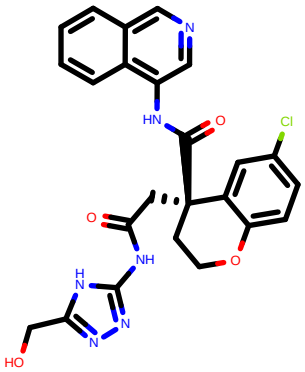
CID:	ALP-POS-a0a4abd7-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3ccc(c4)Cl)CNc5c[nH]c(=O)[nH]c5=O
RUN:	RUN3562
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.18

LON-WEI-5e7d1b3e-51_1



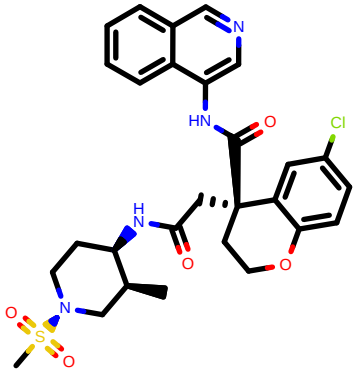
CID:	LON-WEI-5e7d1b3e-51_1
SMILES:	Cc1c(c(on1)C)CCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN1360
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.17

KAD-UNI-cb0f2bbc-14_1



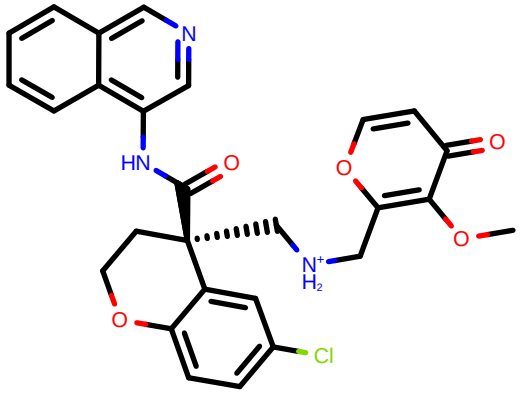
CID:	KAD-UNI-cb0f2bbc-14_1
SMILES:	COC(=O)c1cnc(cn1)Cn2ccc(n2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3705
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.17

DAR-DIA-0d514e7d-33_1



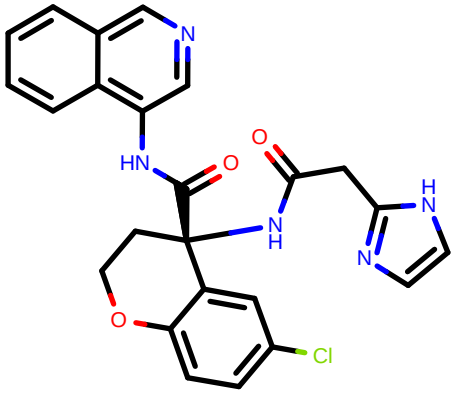
CID:	DAR-DIA-0d514e7d-33_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4O[C@@H]5[C@@H]3C5)Cl
RUN:	RUN880
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.34

ALP-POS-a577c8a2-3_1



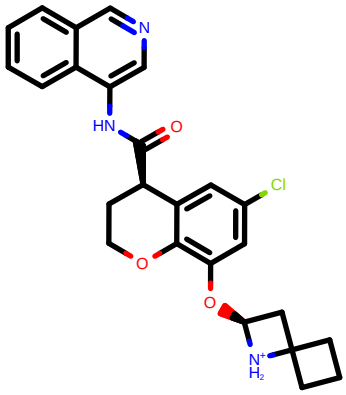
CID:	ALP-POS-a577c8a2-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@]([S(=O)(=O)c4c3cc(cc4)Cl)Cc5[nH]ccn5
RUN:	RUN4628
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.27

LON-WEI-9739a092-9_1



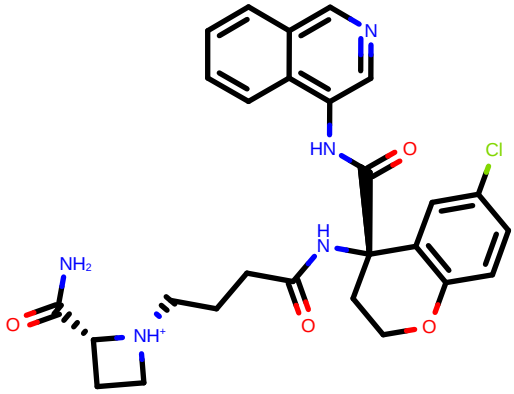
CID:	LON-WEI-9739a092-9_1
SMILES:	CCS(=O)(=O)N1CCN(CC1)c2cc(cc(c2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN3278
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.13

MAT-POS-2492181e-5_1



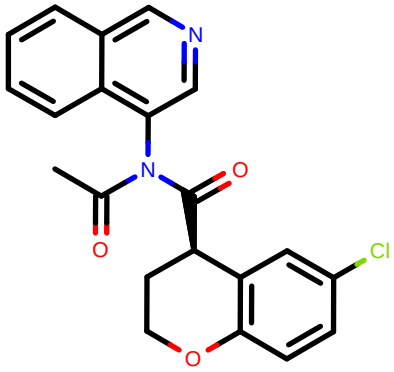
CID:	MAT-POS-2492181e-5_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccsc3
RUN:	RUN96
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.43

ADA-UCB-dc2b944c-16_1



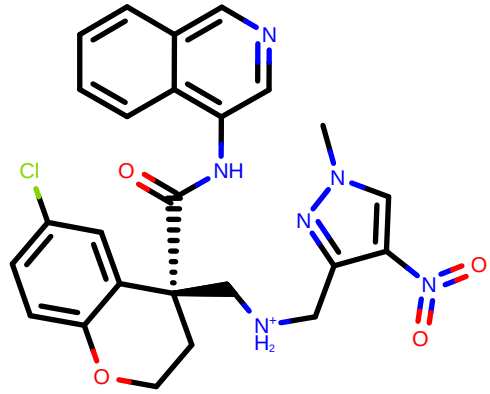
CID:	ADA-UCB-dc2b944c-16_1
SMILES:	CC1(C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4)C
RUN:	RUN614
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.33

EDG-MED-ba1ac7b9-25_5



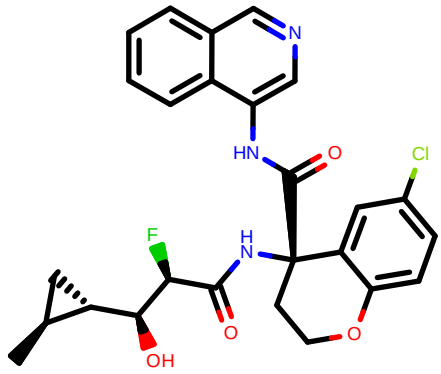
CID:	EDG-MED-ba1ac7b9-25_5
SMILES:	C[C@@H]1CN(CC[N@@H+]1CCO)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2716
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.12

MIC-UNK-ddc6ad53-2_2



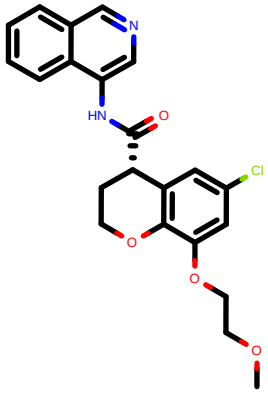
CID:	MIC-UNK-ddc6ad53-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)OCCOC(F)(F)F
RUN:	RUN4761
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.26

EDJ-MED-28ec730d-1_1



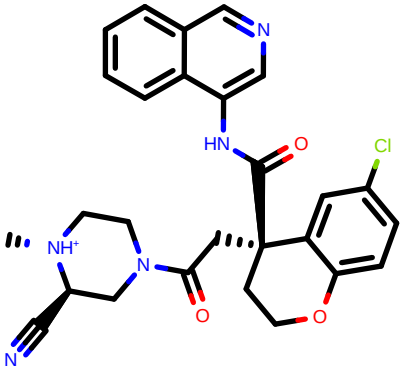
CID:	EDJ-MED-28ec730d-1_1
SMILES:	COCCC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN651
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.29

EDG-MED-90036822-24_1



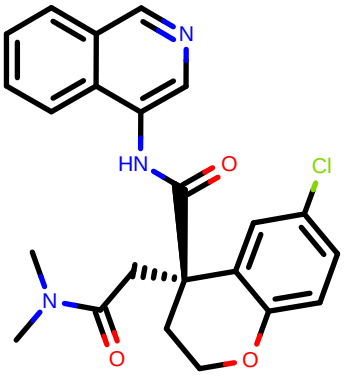
CID:	EDG-MED-90036822-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C5(COC5)F
RUN:	RUN1688
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.22

JOH-UNI-ea1df7a8-1_1



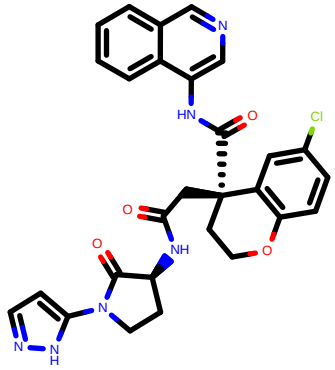
CID:	JOH-UNI-ea1df7a8-1_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)N3CCOc4c3cc(cc4)Cl
RUN:	RUN1212
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.34

MAK-UNK-c749d764-18_6



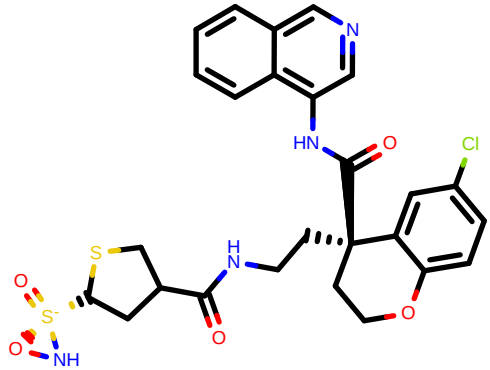
CID:	MAK-UNK-c749d764-18_6
SMILES:	CC(C)SCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN995
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.31

ALP-POS-fab80cf2-1_2



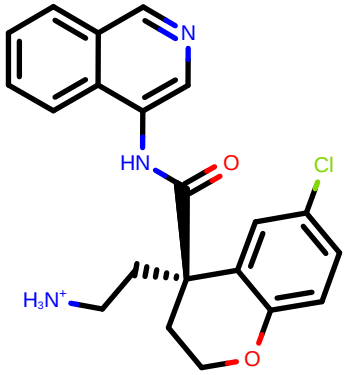
CID:	ALP-POS-fab80cf2-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C([C@H]4CC(=O)N4)(F)F
RUN:	RUN1515
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.24

DAR-DIA-0587064e-27_2



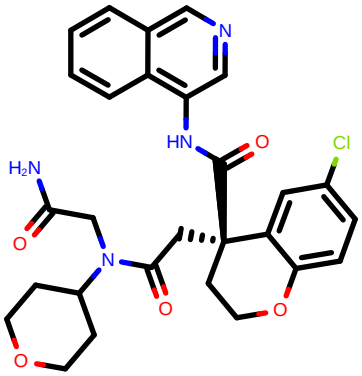
CID:	DAR-DIA-0587064e-27_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(c(c4OCc5ccc(cc5Cl)F)F)Cl
RUN:	RUN3388
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.21

EDJ-MED-e4b030d8-13_1



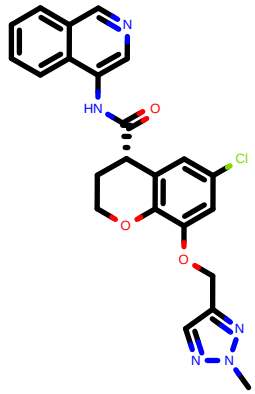
CID:	EDJ-MED-e4b030d8-13_1
SMILES:	C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN297
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.29

KAD-UNI-877d7bed-11_4



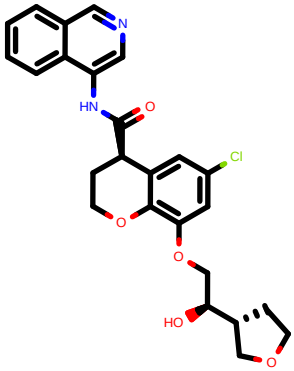
CID:	KAD-UNI-877d7bed-11_4
SMILES:	CC(C)([C@H]1CCN(C1)C(=O)COc2cc(cc3c2OCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl)O
RUN:	RUN3750
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.16

EDG-MED-ba1ac7b9-4_8



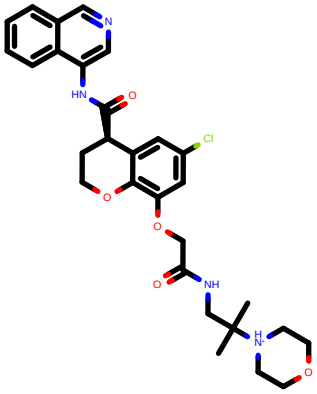
CID:	EDG-MED-ba1ac7b9-4_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[N@H+]6CC[C@H](C6)O
RUN:	RUN2633
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.27

EDJ-MED-d203f206-35_1



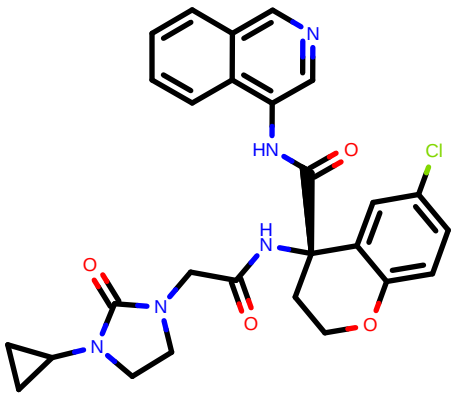
CID:	EDJ-MED-d203f206-35_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@@H](C5)C(=O)NC6=O
RUN:	RUN2596
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.40

ALP-POS-5bb456a5-9_2



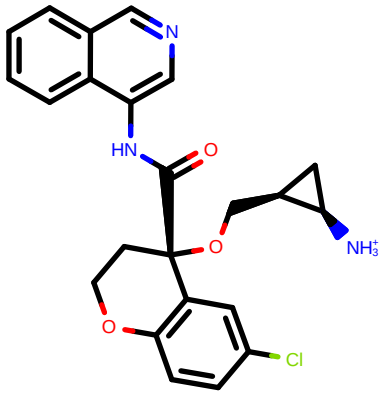
CID:	ALP-POS-5bb456a5-9_2
SMILES:	CCNC(=O)C[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2445
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.40

MAT-POS-4223bc15-9_10



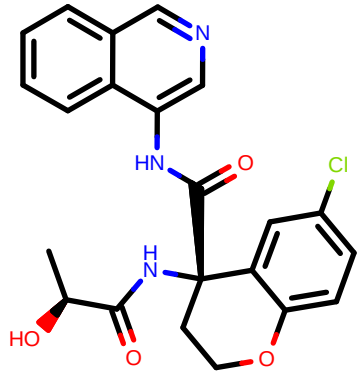
CID:	MAT-POS-4223bc15-9_10
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)[C@@H]5CCC[C@H]5O
RUN:	RUN4018
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.17

DAR-DIA-23e5a6a0-7_2



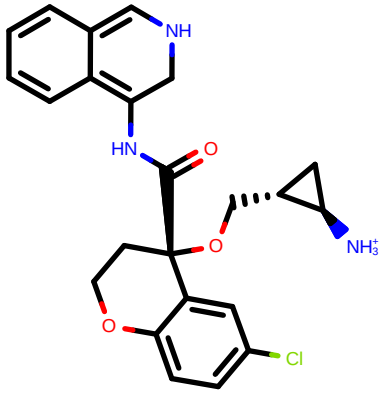
CID:	DAR-DIA-23e5a6a0-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC6([NH2+]5)CCC6)Cl
RUN:	RUN415
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.29

MIC-UNK-91acba05-4_1



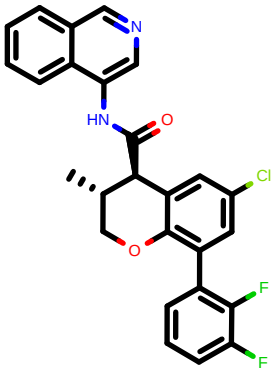
CID:	MIC-UNK-91acba05-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCCc4c3cc(cc4)Cl
RUN:	RUN474
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.29

VLA-UNK-9a7dc93f-4_1



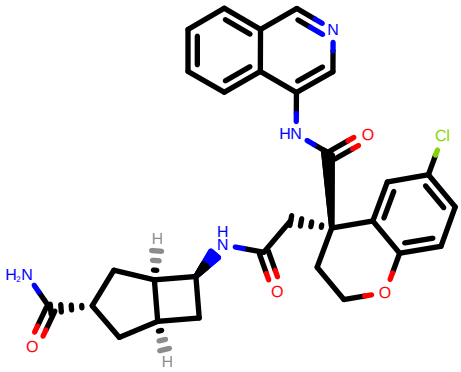
CID:	VLA-UNK-9a7dc93f-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(c(c4F)F)C#N
RUN:	RUN3086
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.16

DAR-DIA-53551c05-11_1



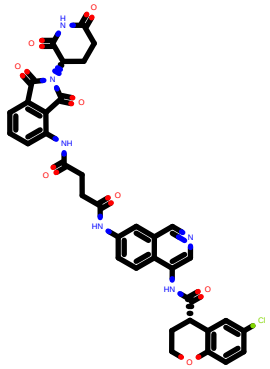
CID:	DAR-DIA-53551c05-11_1
SMILES:	c1ccc2c(c1)cncc2CN3c4cc(ccc4C(=O)C3=O)c5cc(cc(c5)Cl)O[C@@H]6CC(=O)N6
RUN:	RUN144
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.29

NAU-LAT-2fed8305-3_2



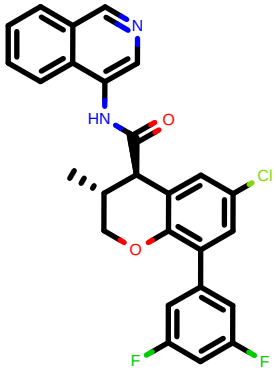
CID:	NAU-LAT-2fed8305-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[N@H+]3CCC=C(C3)Cl
RUN:	RUN1109
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.38

VLA-UCB-05e51b3f-14_1



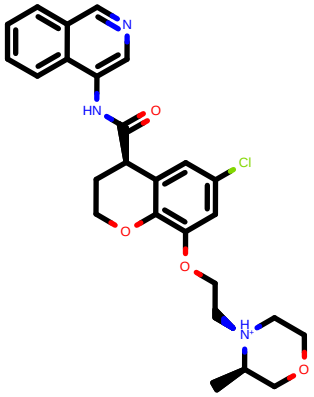
CID:	VLA-UCB-05e51b3f-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN324
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.33

MIC-UNK-c66144cb-1_2



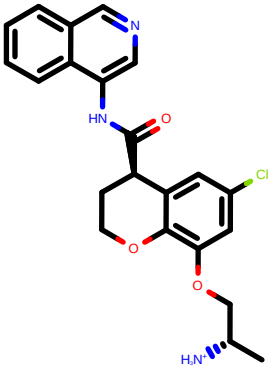
CID:	MIC-UNK-c66144cb-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](CCc3cccc(c3)F)c4cccc(c4)Cl
RUN:	RUN129
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.29

EDJ-MED-fcba3f31-8_1



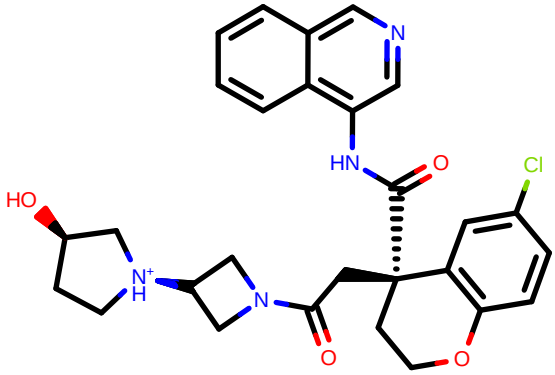
CID:	EDJ-MED-fcba3f31-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCOC5=O
RUN:	RUN2545
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.50

MAT-POS-e9e99895-6_2



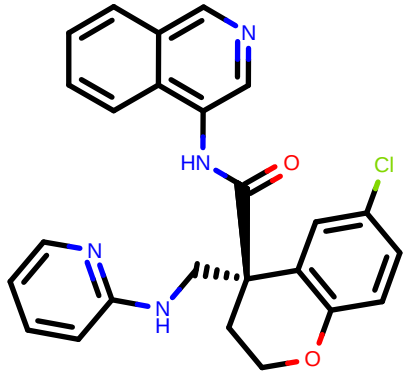
CID:	MAT-POS-e9e99895-6_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)CN4CCN(C4=O)C5CC5
RUN:	RUN2258
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.36

ERI-UCB-d6de1f3c-7_2



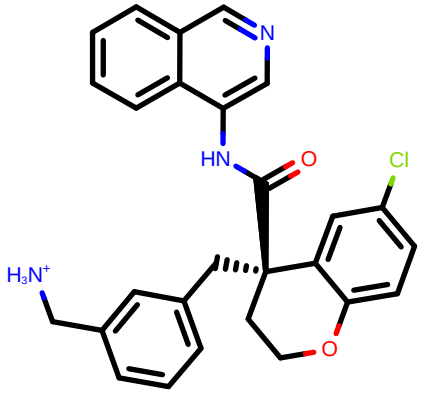
CID:	ERI-UCB-d6de1f3c-7_2
SMILES:	C[C@H]1CN(CC(=O)N1c2cccc(c2)Cl)C(=O)c3cncc4c3cccc4
RUN:	RUN1100
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.25

EDG-MED-971238d3-7_1



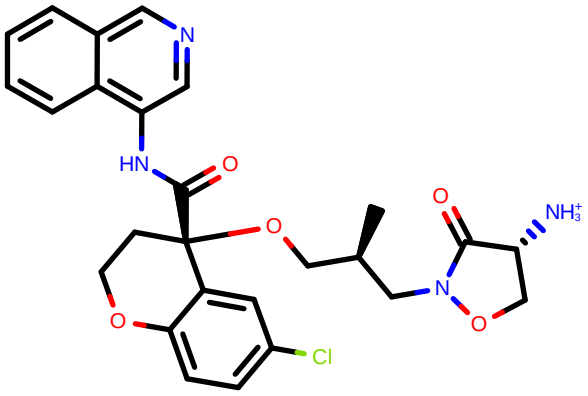
CID:	EDG-MED-971238d3-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC[NH3+]
RUN:	RUN1472
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.29

MAT-POS-b5746674-108_1



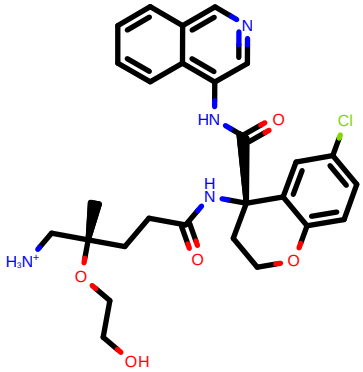
CID:	MAT-POS-b5746674-108_1
SMILES:	Cc1ccc(cc1)C[N@@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN88
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.33

ALP-POS-fe871b40-4_1



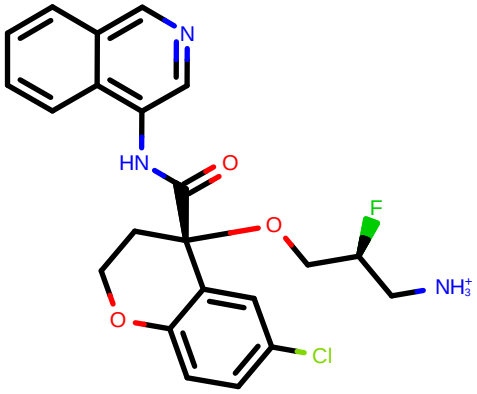
CID:	ALP-POS-fe871b40-4_1
SMILES:	CO[C@@]1(CCNc2c1cc(cc2C#N)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3111
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.27

MAT-POS-fb82b63d-4_1



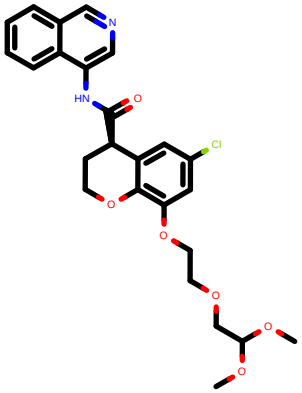
CID:	MAT-POS-fb82b63d-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3c4cc(ccc4CC[N@@H+]3CC5CC5)Cl
RUN:	RUN3177
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.28

ERI-UCB-b3e6b0c2-13_2



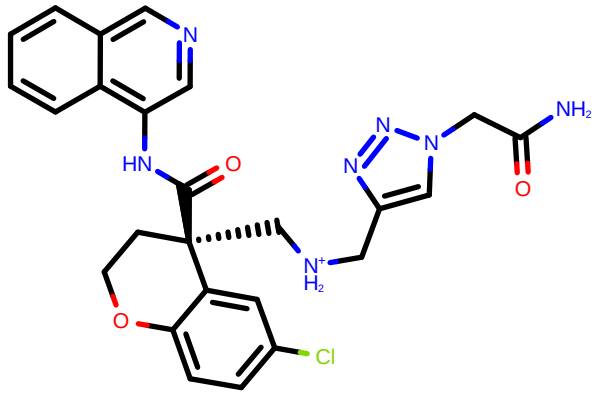
CID:	ERI-UCB-b3e6b0c2-13_2
SMILES:	C[N@]1C[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3ccc(c4)CN5CC[NH2+]CC5
RUN:	RUN3049
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.25

ALP-UNI-3496895b-2_7



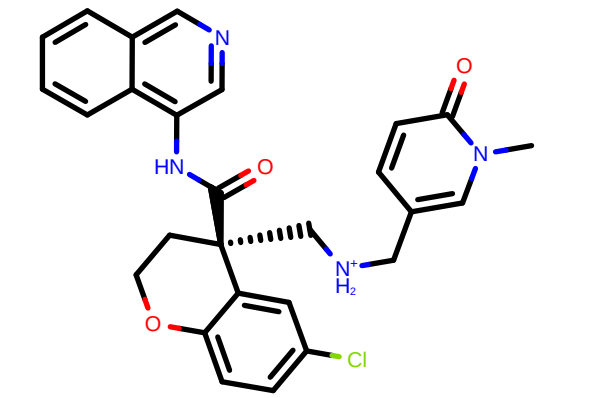
CID:	ALP-UNI-3496895b-2_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CC(=O)N5CC[C@@H]6[C@H]5CCC[N@H+]6CCO
RUN:	RUN2508
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.38

MAT-POS-61f37a1a-15_1



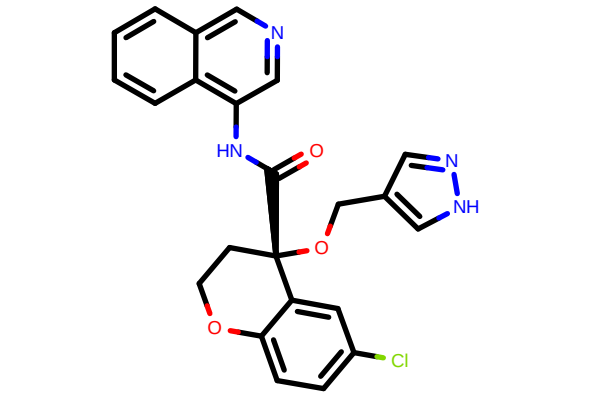
CID:	MAT-POS-61f37a1a-15_1
SMILES:	Cn1c(nc2c1c(=O)[nH]c(=O)n2C)C[NH2+]C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN4624
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.32

MAT-POS-61f37a1a-13_2



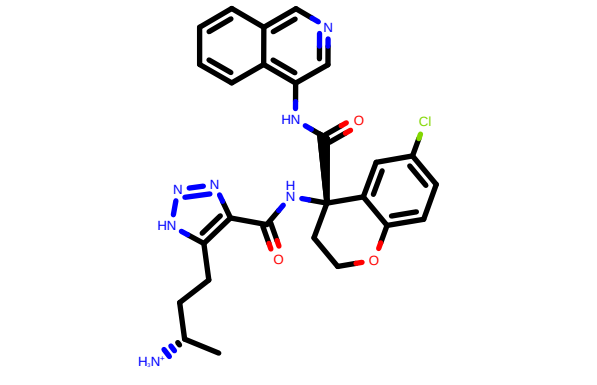
CID:	MAT-POS-61f37a1a-13_2
SMILES:	Cc1[nH]c(c[nH+]1)C[N@H+]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cc(cc5)F)Cl
RUN:	RUN4615
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.21

JAG-UCB-f37eaa14-2_1



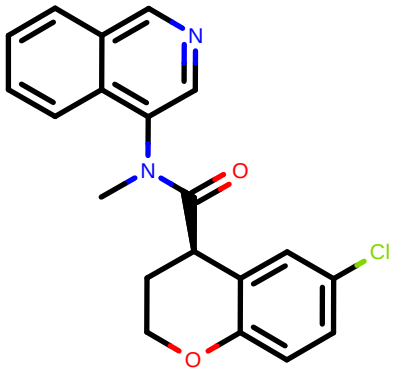
CID:	JAG-UCB-f37eaa14-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNc5c4cc(cc5)Cl
RUN:	RUN3058
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.17

MAT-POS-fb82b63d-4_4



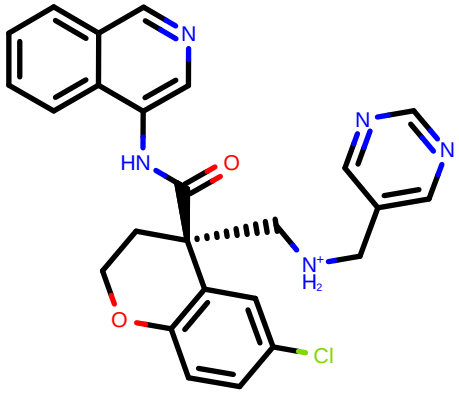
CID:	MAT-POS-fb82b63d-4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4CC[N@H+]3CC5CC5)Cl
RUN:	RUN3183
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.20

MAT-POS-4223bc15-11_9



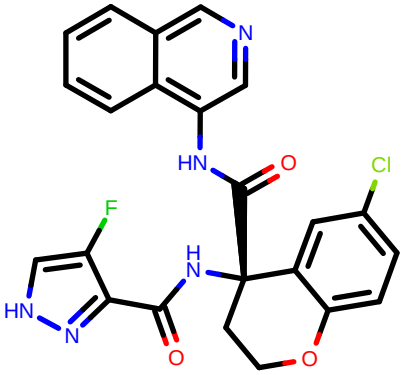
CID:	MAT-POS-4223bc15-11_9
SMILES:	C[C@@H]1CC[N@@](C1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4037
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.09

ED_-GRI-5b13fbe2-51_1



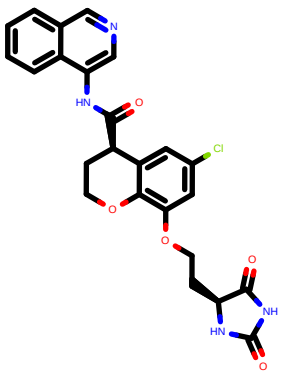
CID:	ED_-GRI-5b13fbe2-51_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5(COC5)COC6C[NH2+]C6
RUN:	RUN1598
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.37

EDJ-MED-00143744-2_1



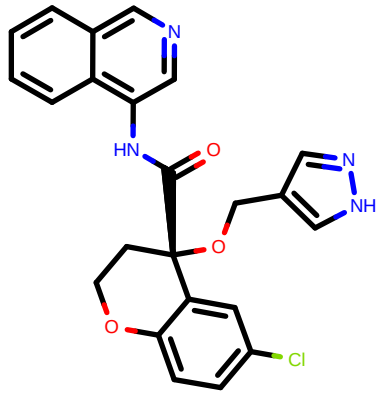
CID:	EDJ-MED-00143744-2_1
SMILES:	CNS(=O)(=O)CCOC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3178
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.11

MAT-POS-e9e99895-2_2



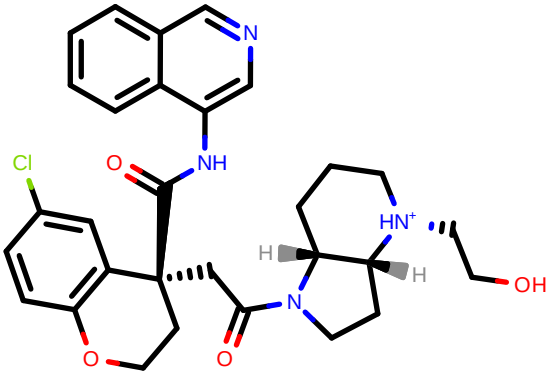
CID:	MAT-POS-e9e99895-2_2
SMILES:	CC(C)[N@H+]1CCO[C@@H](C1)C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2238
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.40

ALP-UNI-8e43a71e-4_1



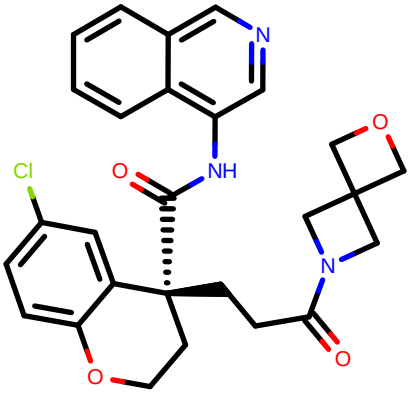
CID:	ALP-UNI-8e43a71e-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5CCN(C5=O)c6ccn[nH]6
RUN:	RUN2941
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.16

RAL-THA-8416115c-11_4



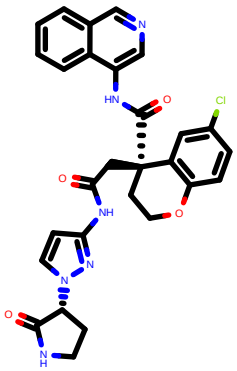
CID:	RAL-THA-8416115c-11_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1289
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.53

RAL-THA-e002e396-2_1



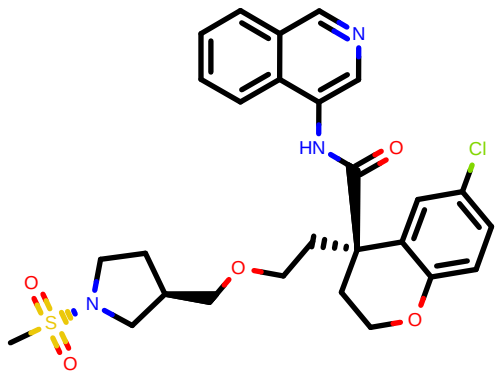
CID:	RAL-THA-e002e396-2_1
SMILES:	CCS(=O)(=O)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3453
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.15

DAR-DIA-9e4459de-11_7



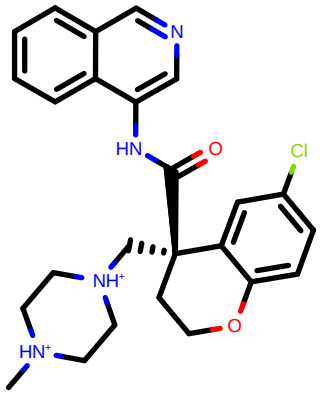
CID:	DAR-DIA-9e4459de-11_7
SMILES:	c1cc2c(c(c1)NCOCCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1415
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-2_2



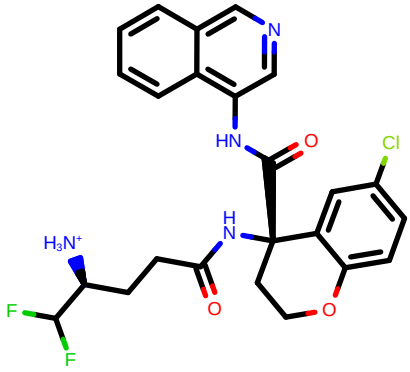
CID:	MIC-UNK-5a93dd5f-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCCC[C@H]5C4
RUN:	RUN735
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.41

RAL-THA-4aa06b95-7_4



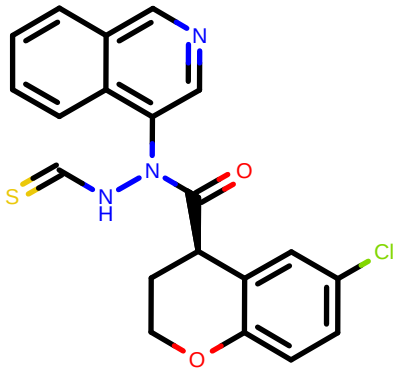
CID:	RAL-THA-4aa06b95-7_4
SMILES:	COCCN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1246
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.29

PET-UNK-824b5c6a-3_1



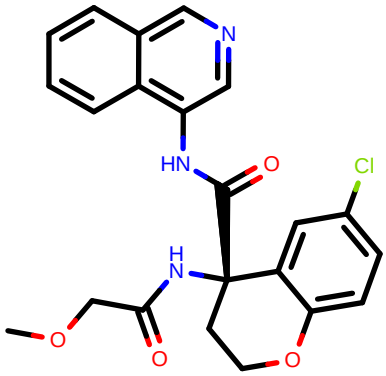
CID:	PET-UNK-824b5c6a-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC5CC5
RUN:	RUN3291
DDG (kcal/mol):	-0.91
dDDG (kcal/mol):	0.23

DAR-DIA-ecdbc7dd-19_1



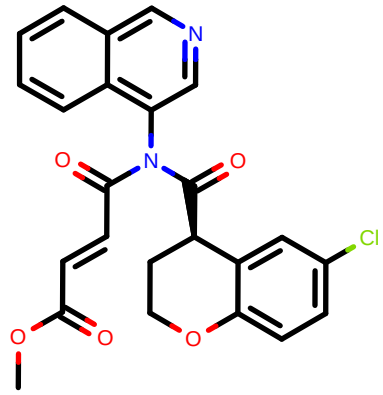
CID:	DAR-DIA-ecdbc7dd-19_1
SMILES:	CC(=O)N1CC[NH+](CC1)C[C@@]2(CCNc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2909
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.12

EDJ-MED-4f704dc9-1_2



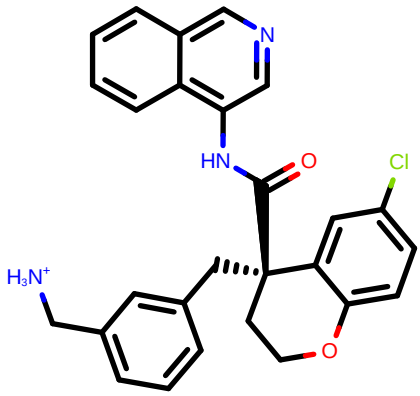
CID:	EDJ-MED-4f704dc9-1_2
SMILES:	CO[C@]1(CCNc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3160
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.10

MIC-UNK-9582b2c5-2_4



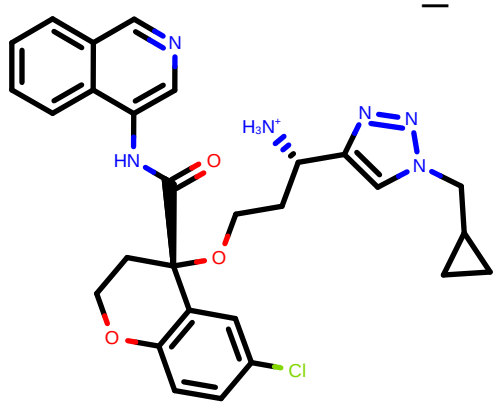
CID:	MIC-UNK-9582b2c5-2_4
SMILES:	CC(=O)N1CC[C@H]2[C@H](C1)C[C@@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN265
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.36

ALF-EVA-650655fc-4_4



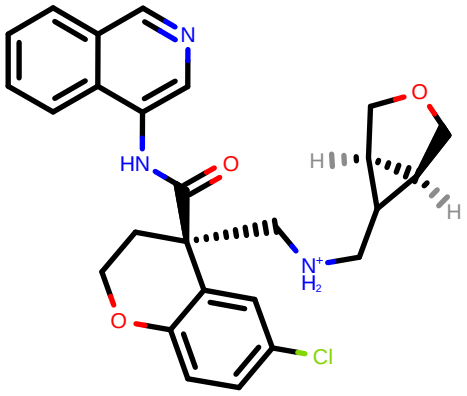
CID:	ALF-EVA-650655fc-4_4
SMILES:	C[N@H+]1CC[C@H](C1)CCN(c2cc(cc(c2)Cl)O[C@@H]3CC(=O)N3)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2860
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.14

DAR-DIA-23e5a6a0-8_2



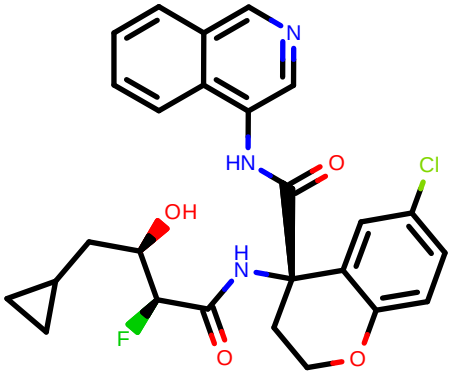
CID:	DAR-DIA-23e5a6a0-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC6([NH2+]5)COC6)Cl
RUN:	RUN416
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.36

EDG-MED-90036822-108_1



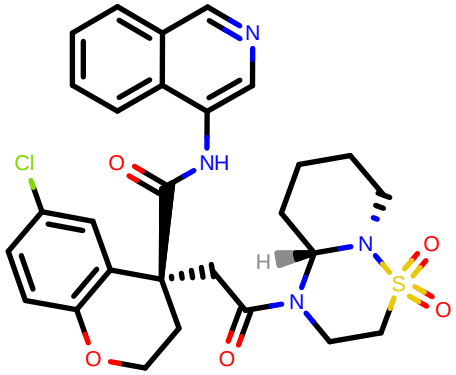
CID:	EDG-MED-90036822-108_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H]([C@@H](CC5CC5)O)F
RUN:	RUN1846
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.34

DAR-DIA-f6ee7aeb-2_2



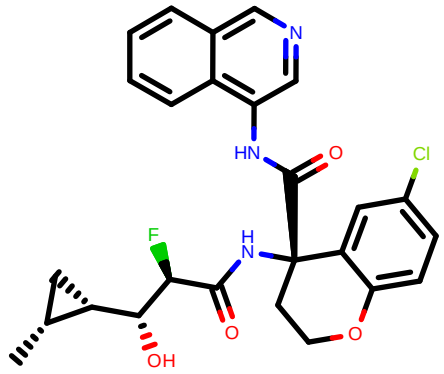
CID:	DAR-DIA-f6ee7aeb-2_2
SMILES:	c1ccc2c(c1)cncc2N3C[C@H]([C@@H](CC3=O)c4cc(cc(c4)Cl)OCCC(F)(F)F)c5ccccc5C#N
RUN:	RUN3405
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.18

BEN-DND-a7517465-1_1



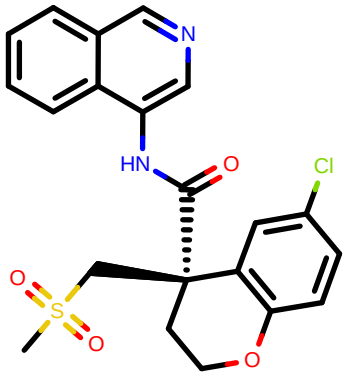
CID:	BEN-DND-a7517465-1_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1477
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.26

MAT-POS-78e1d523-3_1



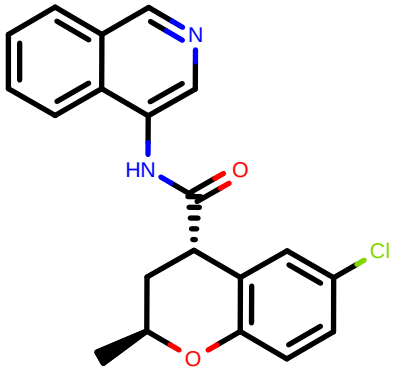
CID:	MAT-POS-78e1d523-3_1
SMILES:	CO[C@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3284
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.16

ED_-GRI-5b13fbe2-19_1



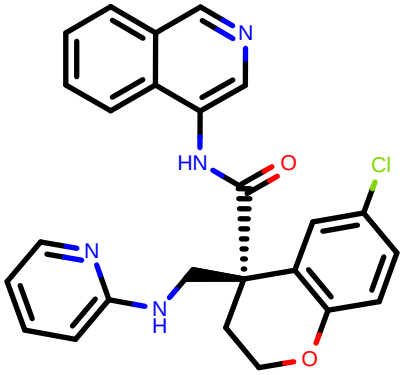
CID:	ED_-GRI-5b13fbe2-19_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCC[NH2+]CCOCCO
RUN:	RUN1553
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.14

DAR-DIA-0cde14eb-56_2



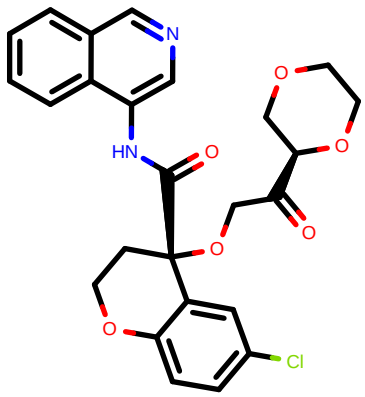
CID:	DAR-DIA-0cde14eb-56_2
SMILES:	C[C@H](c1cccc(c1)C2(CC2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN24
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.10

EDG-MED-90036822-50_1



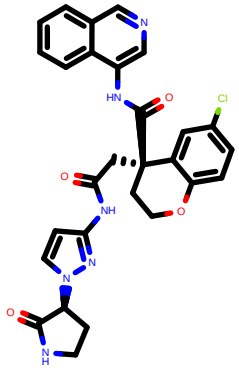
CID:	EDG-MED-90036822-50_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnc[nH]5
RUN:	RUN1728
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.26

MAK-UNK-ffc90da7-9_4



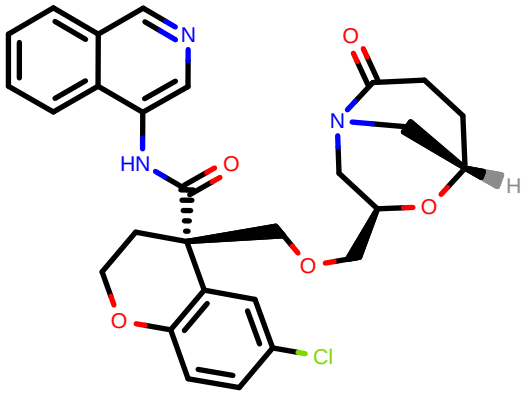
CID:	MAK-UNK-ffc90da7-9_4
SMILES:	C[C@H]1[C@H](CCO1)SC[C@@H](C)c2ccc3c(c2)cncc3NC(=O)Cc4cccc(c4)Cl
RUN:	RUN715
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-22_4



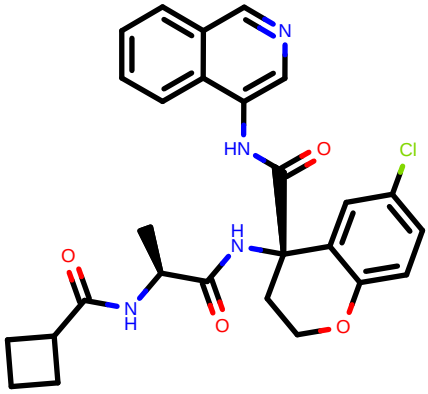
CID:	MAK-UNK-c749d764-22_4
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1025
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.45

DAR-DIA-0d514e7d-2_1



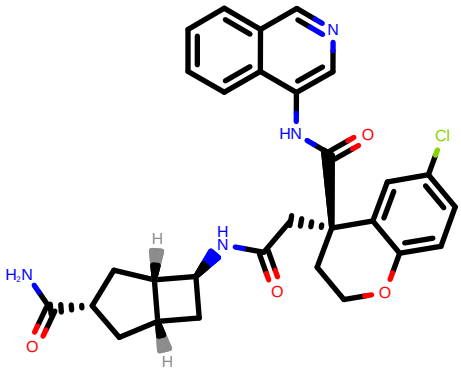
CID:	DAR-DIA-0d514e7d-2_1
SMILES:	C[C@@H]1COc2c(cc(cc2OC)Cl)[C@@H]1C(=O)Nc3cncc4c3cccc4
RUN:	RUN806
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.28

RAL-THA-4aa06b95-3_2



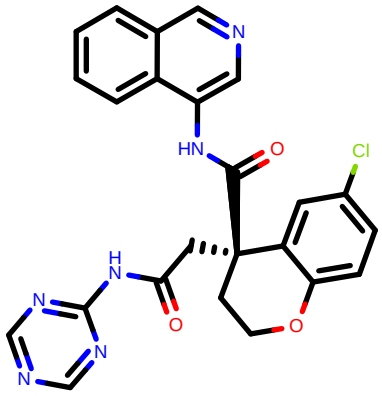
CID:	RAL-THA-4aa06b95-3_2
SMILES:	CNC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1234
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.28

MAK-UNK-c749d764-33_3



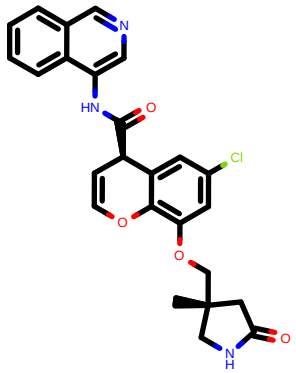
CID:	MAK-UNK-c749d764-33_3
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1081
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.43

KAD-UNI-cb0f2bbc-24_1



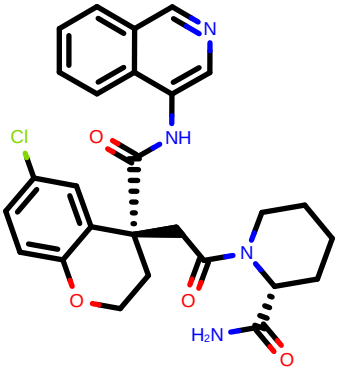
CID:	KAD-UNI-cb0f2bbc-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cn(nn5)C[C@@H]6CCOC6
RUN:	RUN3716
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.12

MAT-POS-2905de8c-2_1



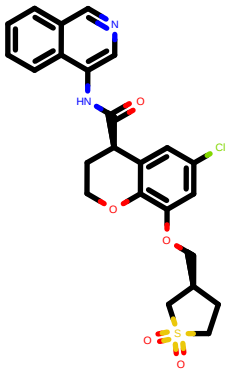
CID:	MAT-POS-2905de8c-2_1
SMILES:	C[NH2+][C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2229
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.38

MAK-UNK-c749d764-33_1



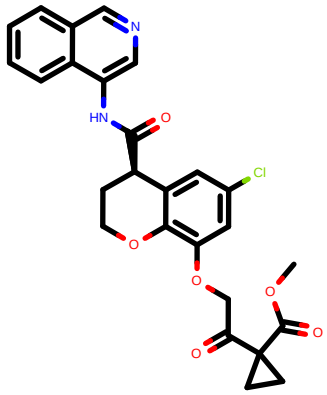
CID:	MAK-UNK-c749d764-33_1
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1079
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.29

ALP-POS-5bb456a5-7_1



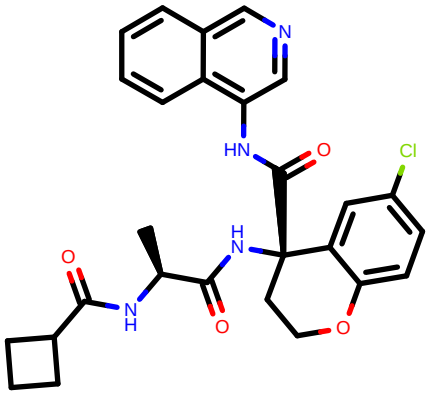
CID:	ALP-POS-5bb456a5-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@@H]6CCOC6
RUN:	RUN2435
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.36

EDJ-MED-d203f206-8_1



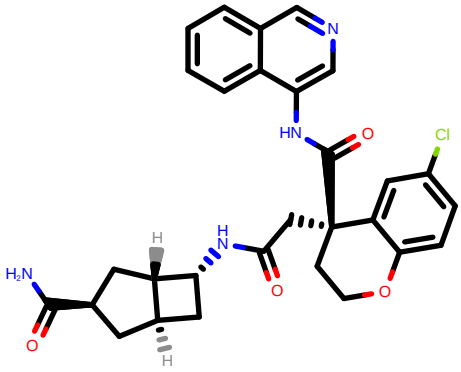
CID:	EDJ-MED-d203f206-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5CC(=O)N
RUN:	RUN2571
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.42

EDJ-MED-009f762b-2_2



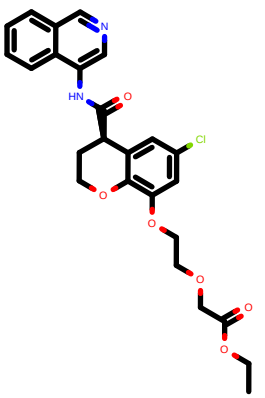
CID:	EDJ-MED-009f762b-2_2
SMILES:	Cc1nc(cs1)C[N@H+]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cc(cc5)F)Cl
RUN:	RUN3911
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.15

DAR-DIA-9e4459de-13_16



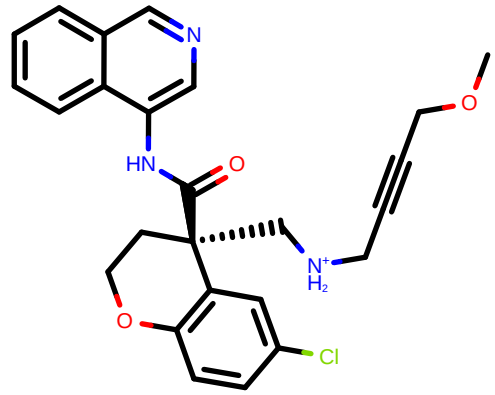
CID:	DAR-DIA-9e4459de-13_16
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1440
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.36

EDG-MED-ba1ac7b9-7_3



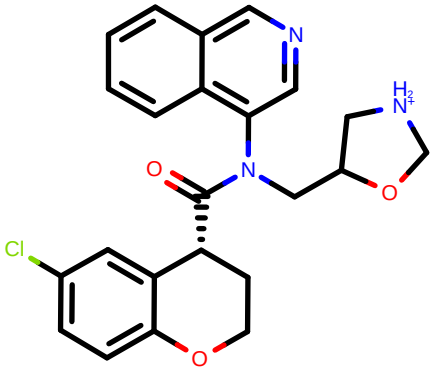
CID:	EDG-MED-ba1ac7b9-7_3
SMILES:	C[C@@H]1N(CCO1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2642
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.45

PET-UNK-b87f07d0-2_1



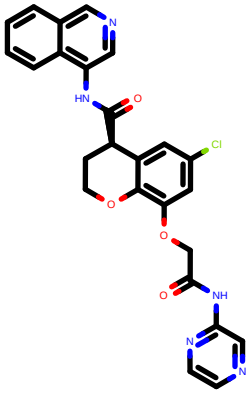
CID:	PET-UNK-b87f07d0-2_1
SMILES:	C[C@H](CCc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3)NC(=O)C
RUN:	RUN1899
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.44

ALF-EVA-ced740bd-3_2



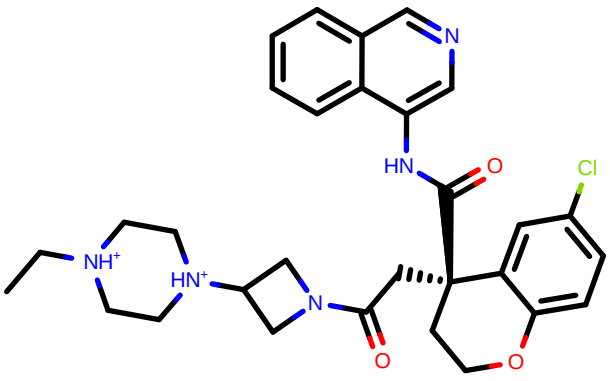
CID:	ALF-EVA-ced740bd-3_2
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@H]3COc4c3cc(cc4)F
RUN:	RUN2793
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.14

PET-UNK-1320d94d-8_1



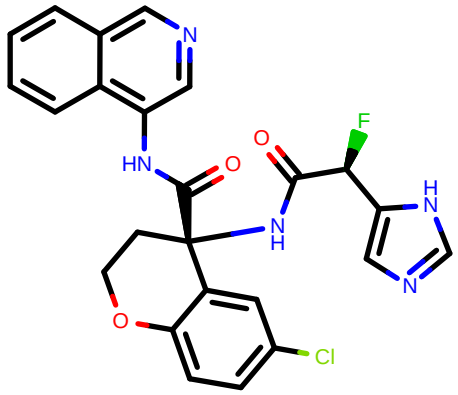
CID:	PET-UNK-1320d94d-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4C[C@@H](O4)C(=O)N5CCCC5
RUN:	RUN4979
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.20

LON-WEI-5e7d1b3e-18_1



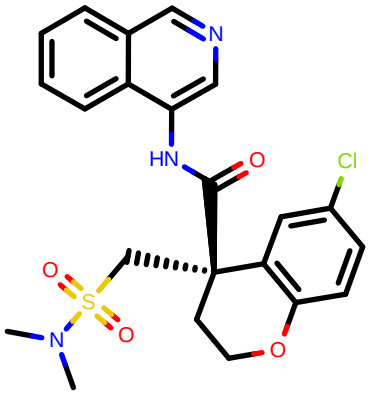
CID:	LON-WEI-5e7d1b3e-18_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccc(cc3OC)OC
RUN:	RUN1322
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.33

VLA-UNK-ba665ac8-2_1



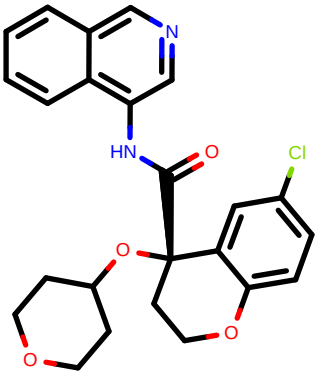
CID:	VLA-UNK-ba665ac8-2_1
SMILES:	C[N@@H+]1CC(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN3301
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.17

ED_-GRI-5b13fbe2-4_1



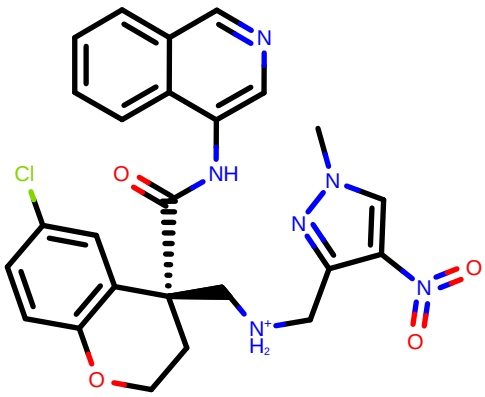
CID:	ED_-GRI-5b13fbe2-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5n[n-]nn5)[NH3+]
RUN:	RUN1525
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.27

VLA-UNK-5c5a631c-1_3



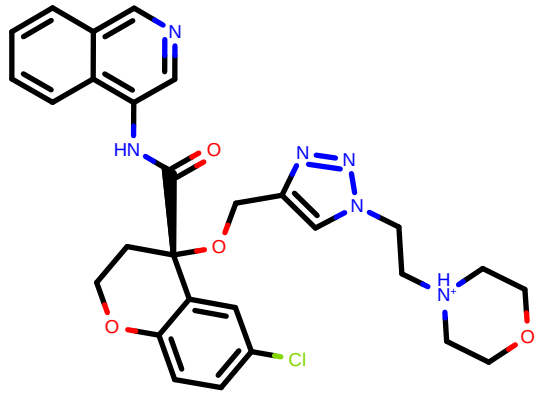
CID:	VLA-UNK-5c5a631c-1_3
SMILES:	c1ccc2c(c1)cncc2N(CC[C@@H](O)S(=O)(=O)[O-])C(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN2917
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.12

KAD-UNI-8a629cb0-30_1



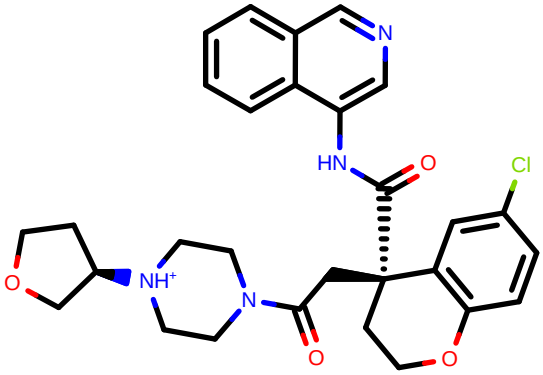
CID:	KAD-UNI-8a629cb0-30_1
SMILES:	C[C@H](C(=O)N1CCC[C@@H](C1)C(=O)N)O[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2114
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.36

MAT-POS-78e1d523-2_1



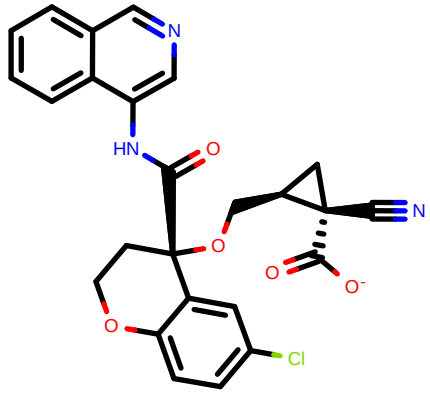
CID:	MAT-POS-78e1d523-2_1
SMILES:	CNC(=O)[C@@]1(CCOc2c1cc(cc2)Cl)CC(=O)Nc3cncc4c3cccc4
RUN:	RUN3280
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.22

RAL-THA-8416115c-12_4



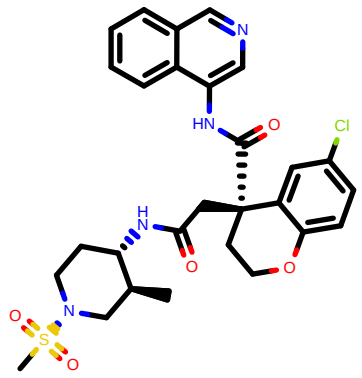
CID:	RAL-THA-8416115c-12_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5n[n-]nn5
RUN:	RUN1294
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.28

JAG-UCB-f37eaa14-5_2



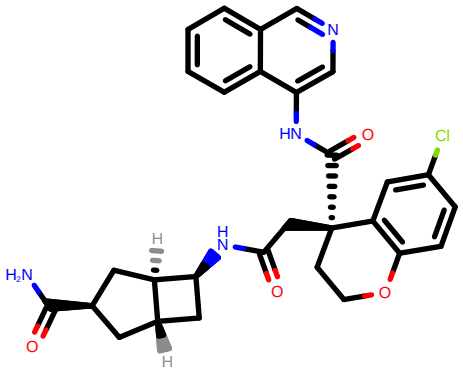
CID:	JAG-UCB-f37eaa14-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](c5c4cc(cc5)Cl)CCN6CCNC6=O
RUN:	RUN3065
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.19

MAK-UNK-c749d764-21_3



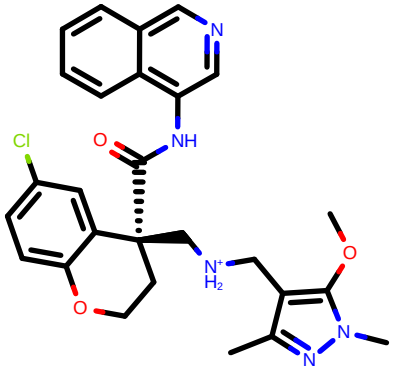
CID:	MAK-UNK-c749d764-21_3
SMILES:	CCCCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1016
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.23

LON-WEI-5e7d1b3e-40_1



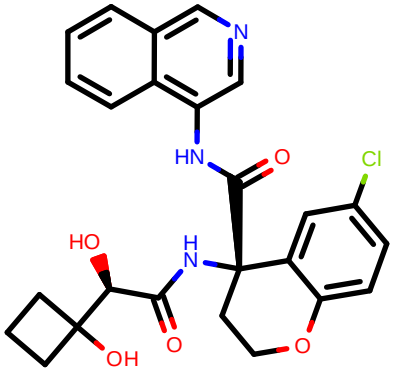
CID:	LON-WEI-5e7d1b3e-40_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCC3=CCCCC3
RUN:	RUN1352
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.22

ALP-POS-347519b5-2_46



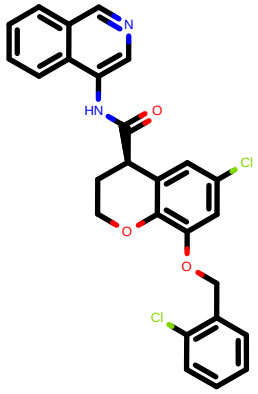
CID:	ALP-POS-347519b5-2_46
SMILES:	CO[C@]1(C[N@@]([C[C@H]2[C@H]1[C@@H]3CC[C@H]2C3)S(=O)(=O)C)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4293
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.25

KAD-UNI-877d7bed-14_1



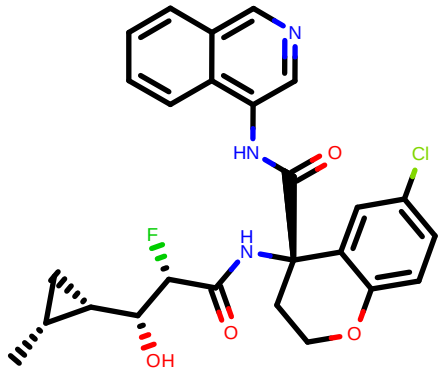
CID:	KAD-UNI-877d7bed-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCC(=O)CCNC(=O)C(F)(F)F)Cl
RUN:	RUN3760
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.16

DAR-DIA-9e4459de-15_15



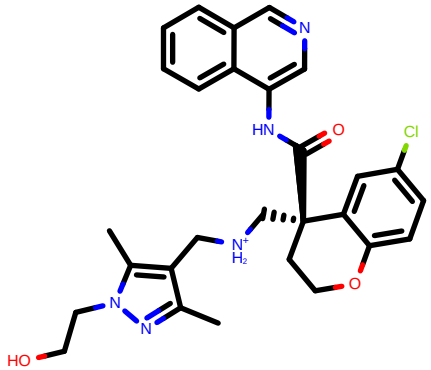
CID:	DAR-DIA-9e4459de-15_15
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1453
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.46

PET-UNK-7a31b064-2_1



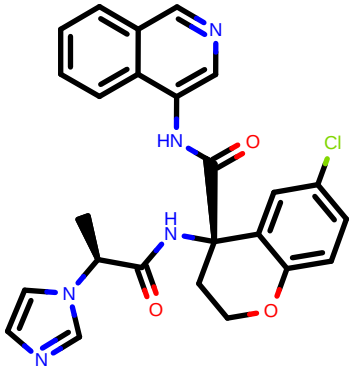
CID:	PET-UNK-7a31b064-2_1
SMILES:	CCN1C[C@H](C(=O)N(C1=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN3290
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.17

ALP-POS-869ac754-2_2



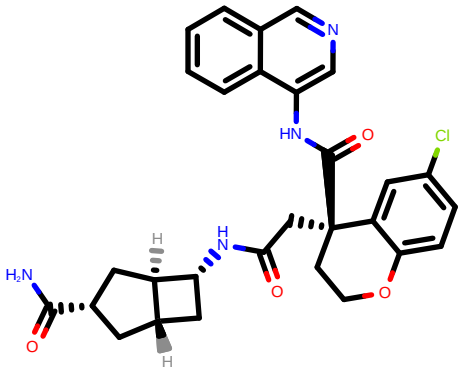
CID:	ALP-POS-869ac754-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3ccc(c4Cl)Cl
RUN:	RUN1953
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.59

ADA-UCB-dc2b944c-9_1



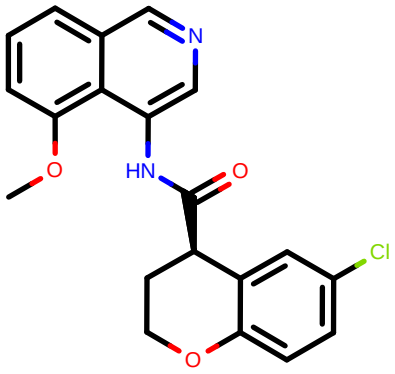
CID:	ADA-UCB-dc2b944c-9_1
SMILES:	c1ccc2c(c1)cnc(c2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl)Br
RUN:	RUN607
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.28

NAU-LAT-4ce8bf23-1_2



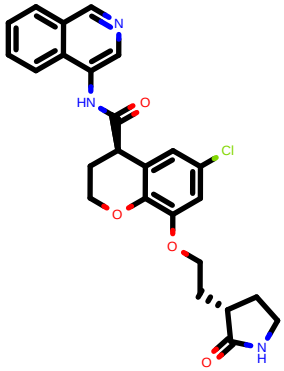
CID:	NAU-LAT-4ce8bf23-1_2
SMILES:	CC(=O)NC[C@H](c1cncc2c1cccc2)C(=O)Nc3cccc(c3)Cl
RUN:	RUN1394
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.41

MAT-POS-8a69d52e-1_3



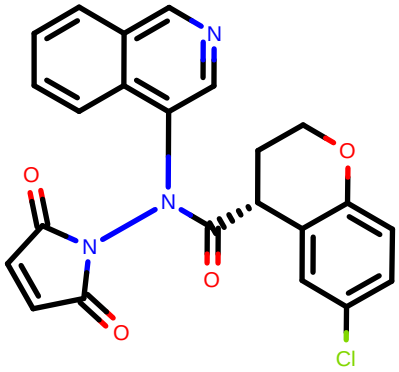
CID:	MAT-POS-8a69d52e-1_3
SMILES:	C[C@@H]1C[C@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN362
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.24

MAT-POS-e9e99895-1_2



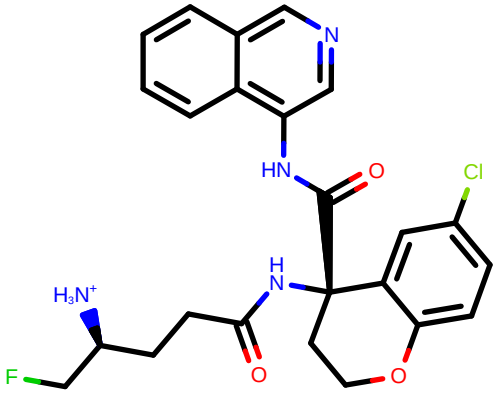
CID:	MAT-POS-e9e99895-1_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)[NH3+]
RUN:	RUN2234
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.44

BEN-DND-34fc7f90-8_1



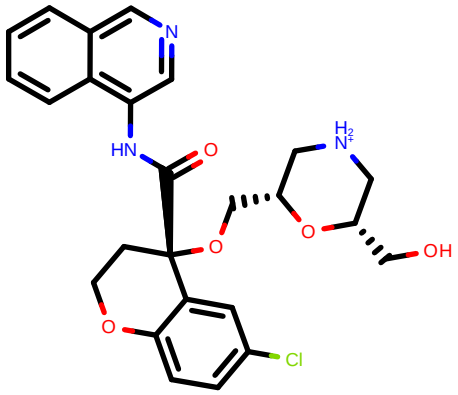
CID:	BEN-DND-34fc7f90-8_1
SMILES:	C[N@@H+]1Cc2cc(c(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl)Cl
RUN:	RUN3674
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.12

MIC-UNK-cdc2493e-10_3



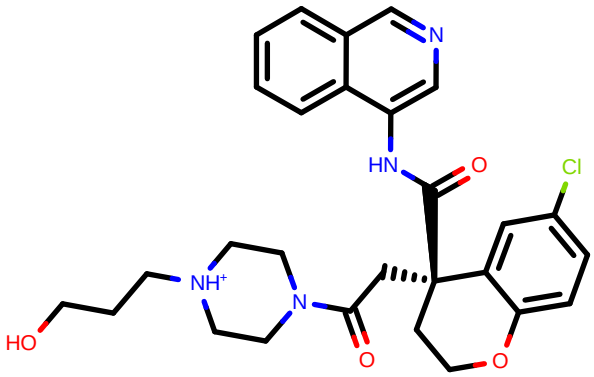
CID:	MIC-UNK-cdc2493e-10_3
SMILES:	CC(=O)N[C@@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN547
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.31

DAR-DIA-0f2f46c9-1_2



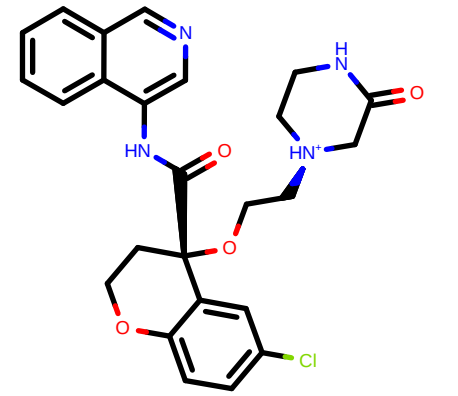
CID:	DAR-DIA-0f2f46c9-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC[N@@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3219
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.23

BEN-DND-c852c98b-6_2



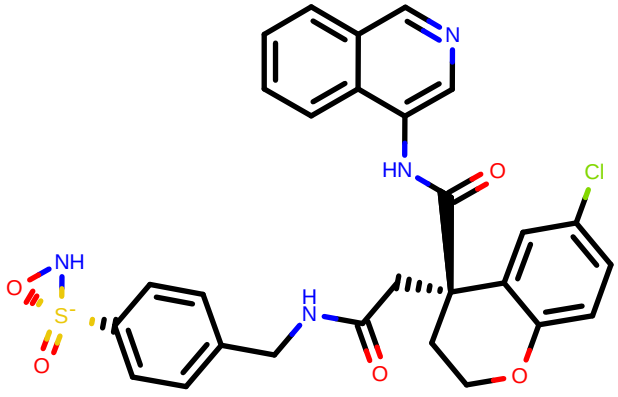
CID:	BEN-DND-c852c98b-6_2
SMILES:	c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1216
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.34

DAR-DIA-6a508060-10_1



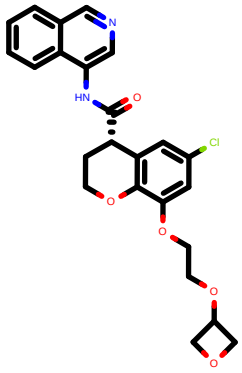
CID:	DAR-DIA-6a508060-10_1
SMILES:	C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN349
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.36

MAK-UNK-b7886382-1_1



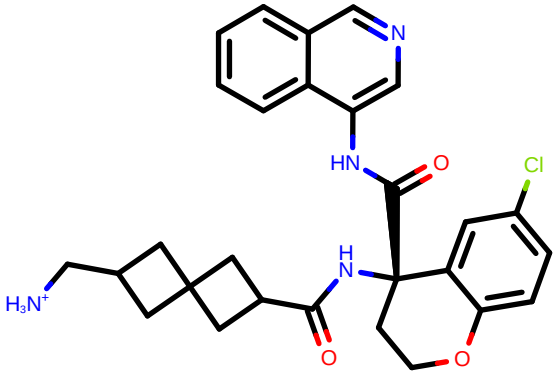
CID:	MAK-UNK-b7886382-1_1
SMILES:	C[C@@H](C[NH2+]CCCO)N(Cc1ccsc1)C(=O)Cc2cncc3c2cccc3
RUN:	RUN1155
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.33

MAT-POS-f9802937-4_1



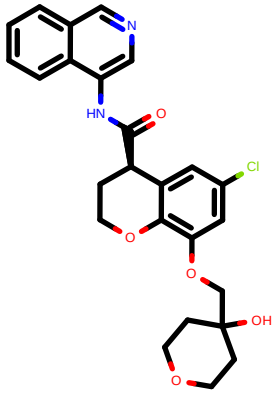
CID:	MAT-POS-f9802937-4_1
SMILES:	CN(C)C(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2397
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.29

EDJ-MED-28ec730d-5_1



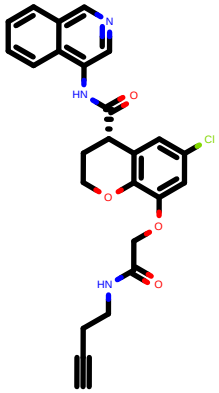
CID:	EDJ-MED-28ec730d-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5c[nH]nc5
RUN:	RUN655
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.39

MAT-POS-fce787c2-10_2



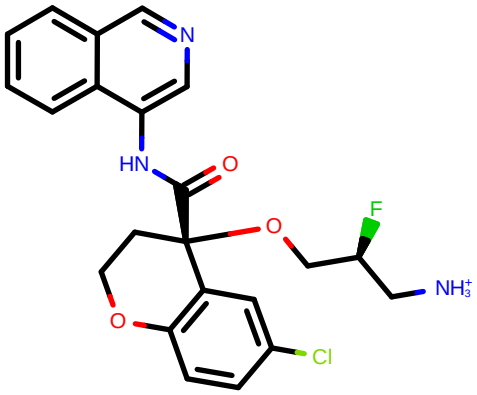
CID:	MAT-POS-fce787c2-10_2
SMILES:	CN(C)CC[NH2+][C@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2161
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.31

ALP-POS-5bb456a5-1_8



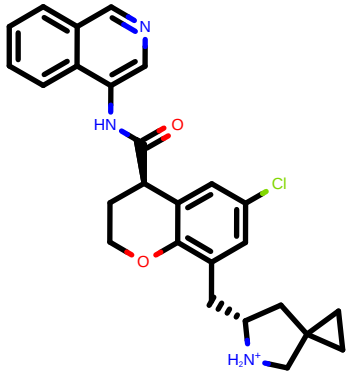
CID:	ALP-POS-5bb456a5-1_8
SMILES:	C[C@H]1C[N@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2413
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.30

MAK-UNK-8be7dca9-10_1



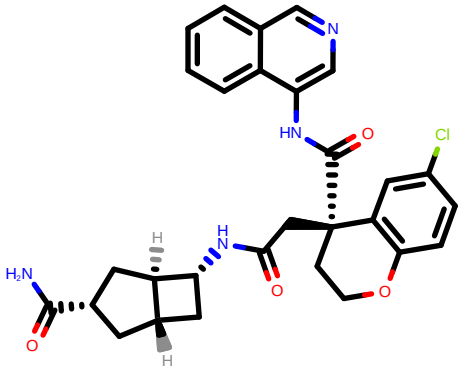
CID:	MAK-UNK-8be7dca9-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[C@@H](Oc4c3cc(cc4)Cl)C(=O)[O-]
RUN:	RUN511
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.32

ALP-POS-3b848b35-4_1



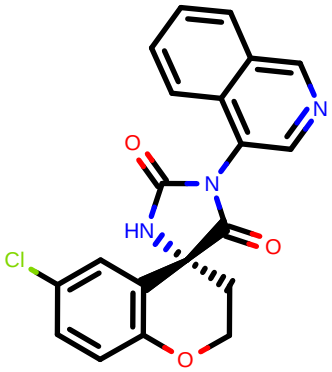
CID:	ALP-POS-3b848b35-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](CCC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN61
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.34

DAR-DIA-9e4459de-15_3



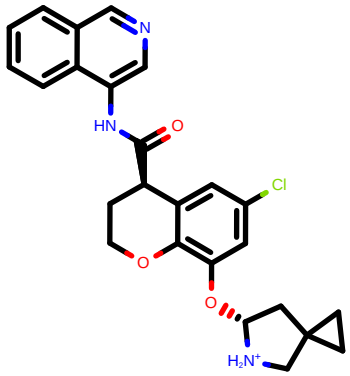
CID:	DAR-DIA-9e4459de-15_3
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1442
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.24

MIC-UNK-0a05c952-4_1



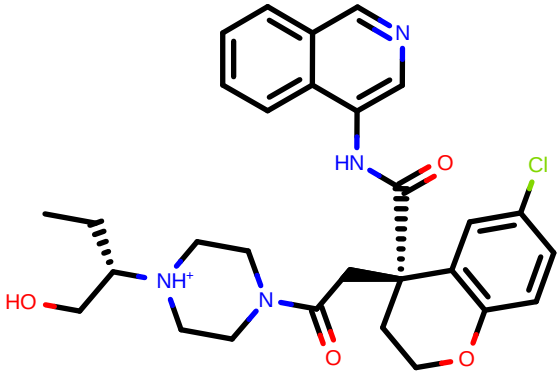
CID:	MIC-UNK-0a05c952-4_1
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](CC[C@@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@@H]5CO5
RUN:	RUN3521
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.20

MIC-UNK-6ab519a7-1_1



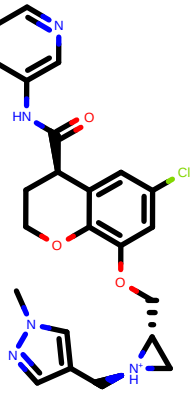
CID:	MIC-UNK-6ab519a7-1_1
SMILES:	CC(=O)N1CC[NH+](CC1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN191
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.44

VLA-UNK-5b0345c3-3_2



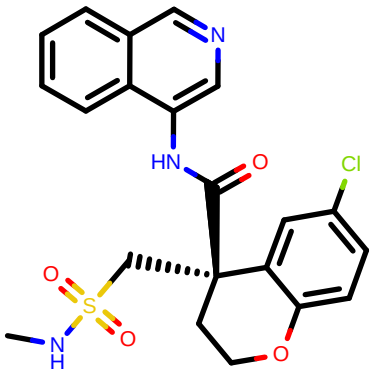
CID:	VLA-UNK-5b0345c3-3_2
SMILES:	c1ccc(cc1)COS(=O)(=O)[N@]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3887
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.51

EDG-MED-ba1ac7b9-9_4



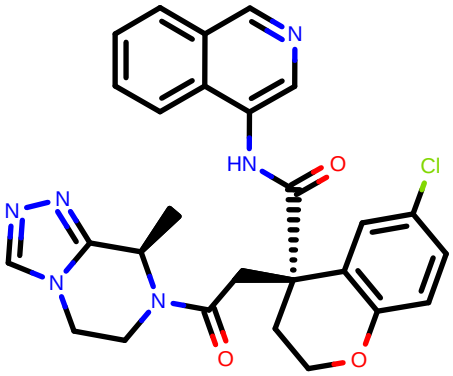
CID:	EDG-MED-ba1ac7b9-9_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC[C@H]5c6[nH]ncn6
RUN:	RUN2649
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.48

ED_-GRI-5b13fbe2-12_2



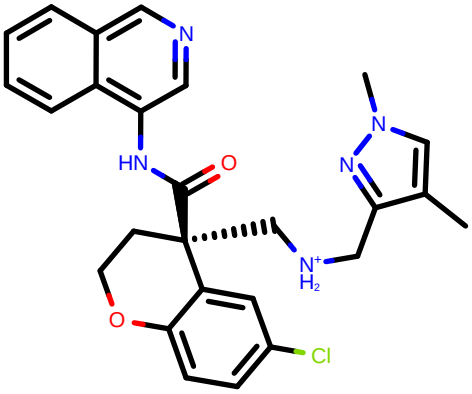
CID:	ED_-GRI-5b13fbe2-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@H+](CCO)CCOCCO
RUN:	RUN1539
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.24

BEN-DND-f2e727cd-5_1



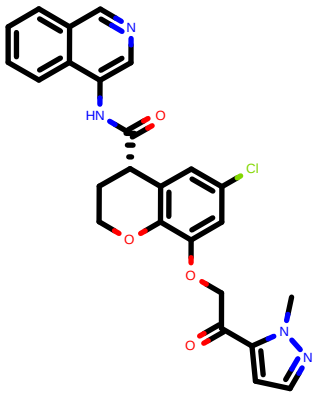
CID:	BEN-DND-f2e727cd-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[NH2+]Cc4c3cc(cc4)Cl
RUN:	RUN1196
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.22

EDJ-MED-fa7708b3-2_3



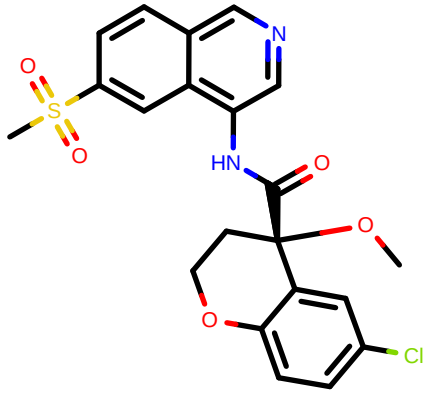
CID:	EDJ-MED-fa7708b3-2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@H+](Cc4c3cc(cc4)Cl)Cc5[nH]ncn5
RUN:	RUN4675
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.23

ALP-UNI-3496895b-2_5



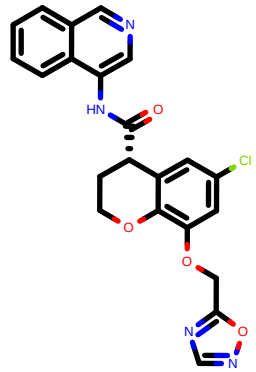
CID:	ALP-UNI-3496895b-2_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@H]6[C@@H]5CCC[N@H+]6CCO
RUN:	RUN2506
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.25

PET-UNK-acd70dee-5_1



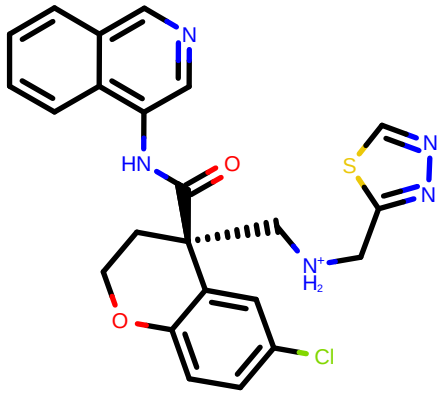
CID:	PET-UNK-acd70dee-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5=NCCO5
RUN:	RUN4191
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.08

EDG-MED-5d232de5-5_2



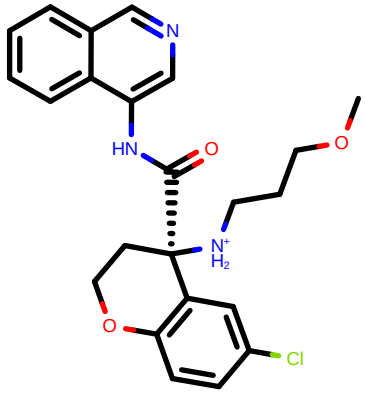
CID:	EDG-MED-5d232de5-5_2
SMILES:	CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2368
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.24

EDJ-MED-1981ceba-3_4



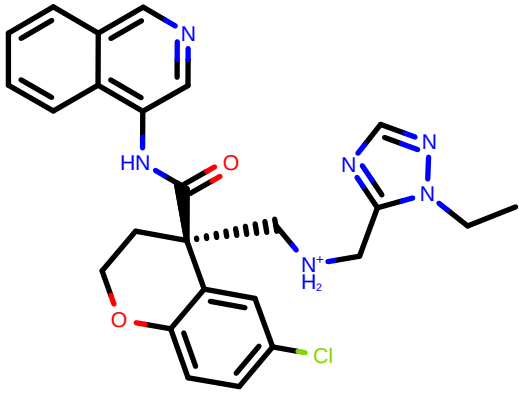
CID:	EDJ-MED-1981ceba-3_4
SMILES:	COC1CN(C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4692
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.24

ED_-GRI-5b13fbe2-3_1



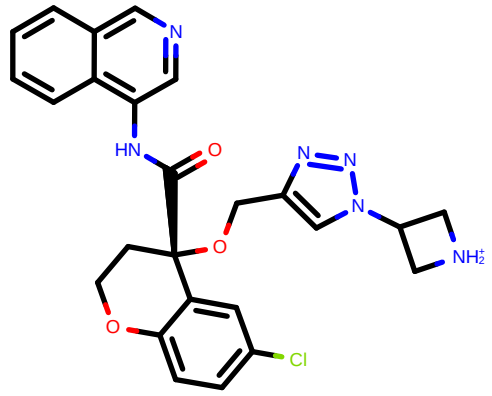
CID:	ED_-GRI-5b13fbe2-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](c5n[n-]nn5)[NH3+]
RUN:	RUN1523
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.24

MAT-POS-61f37a1a-4_2



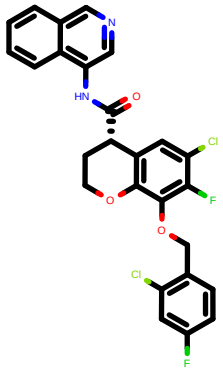
CID:	MAT-POS-61f37a1a-4_2
SMILES:	CC(C)(C)OC(=O)NCc1c(nn1)C)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4594
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.28

MAT-POS-fb82b63d-2_1



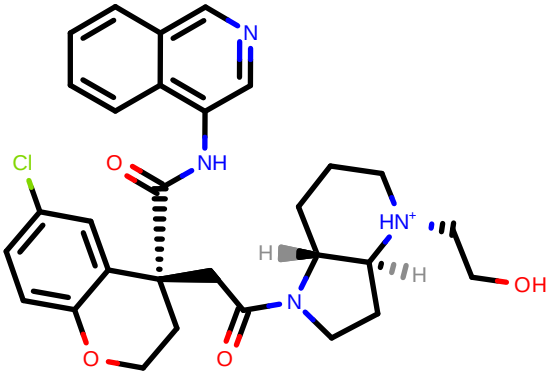
CID:	MAT-POS-fb82b63d-2_1
SMILES:	C[C@@]1(c2cc(ccc2CC[NH2+]1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3171
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.19

EDG-MED-90036822-39_2



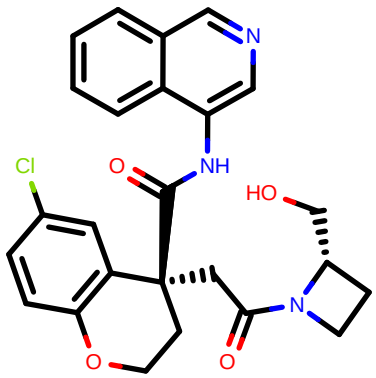
CID:	EDG-MED-90036822-39_2
SMILES:	C[C@H](CO)NCC(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F
RUN:	RUN1722
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.28

ALF-EVA-b701bd13-5_1



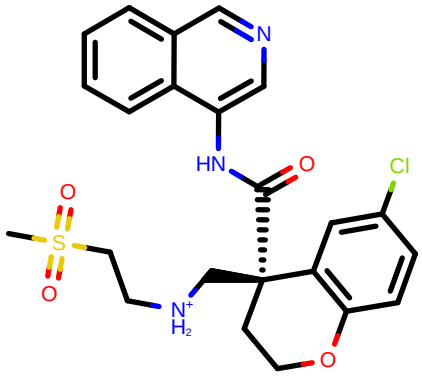
CID:	ALF-EVA-b701bd13-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN3638
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.37

RAL-THA-8416115c-10_3



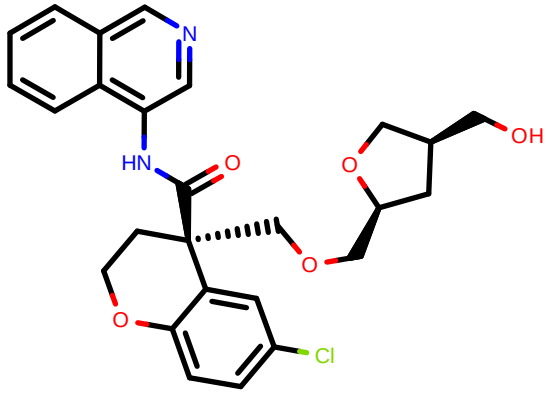
CID:	RAL-THA-8416115c-10_3
SMILES:	CNC(=O)CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1285
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.21

ED_-GRI-5b13fbe2-30_1



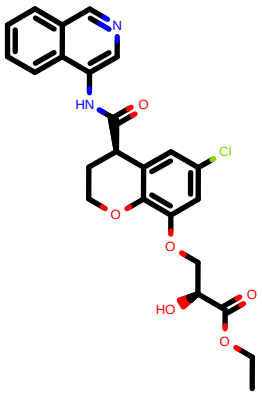
CID:	ED_-GRI-5b13fbe2-30_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+]CCO
RUN:	RUN1558
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.42

KAD-UNI-cb0f2bbc-10_2



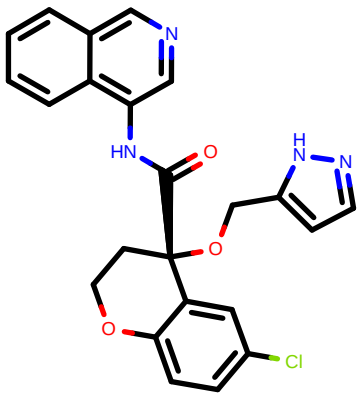
CID:	KAD-UNI-cb0f2bbc-10_2
SMILES:	CC(C)(C)OC(=O)N[C@H](CCO)C[NH2+]C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3699
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.12

KAD-UNI-8a629cb0-38_2



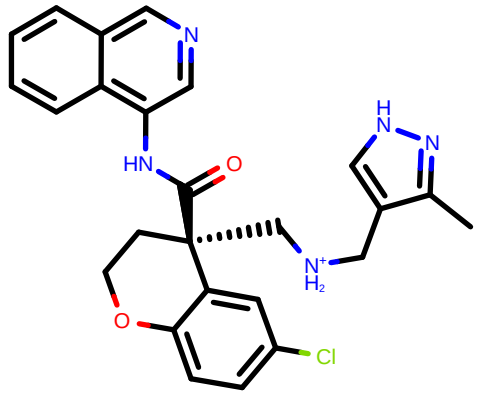
CID:	KAD-UNI-8a629cb0-38_2
SMILES:	C[N@]1[C@@H](CCS1(=O)=O)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2124
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.41

ALP-UNI-ba800595-1_2



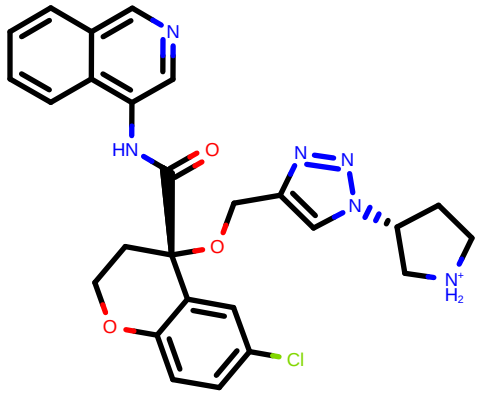
CID:	ALP-UNI-ba800595-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4Cl)Cl
RUN:	RUN3073
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.11

ALP-UNI-dbb9503d-1_1



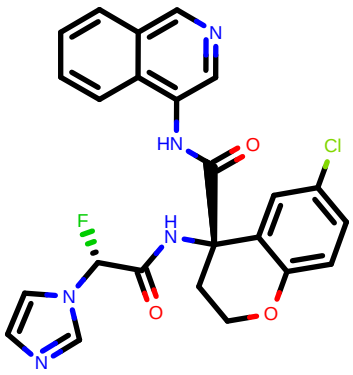
CID:	ALP-UNI-dbb9503d-1_1
SMILES:	CO[C@@]1(CCN(C1=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN4328
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.25

JAG-UCB-f37eaa14-8_1



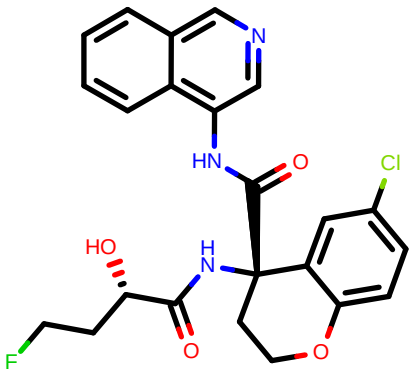
CID:	JAG-UCB-f37eaa14-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](c5c4cc(cc5)Cl)CCn6ccnc6
RUN:	RUN3068
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.20

MAT-POS-fb82b63d-3_1



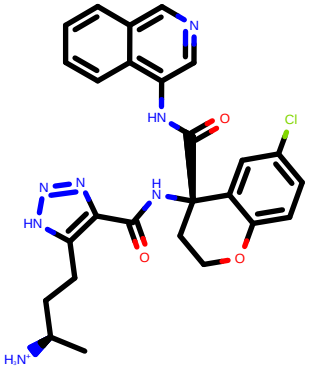
CID:	MAT-POS-fb82b63d-3_1
SMILES:	C[N@@H+]1CCc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3173
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.14

MIC-UNK-b9827f26-4_1



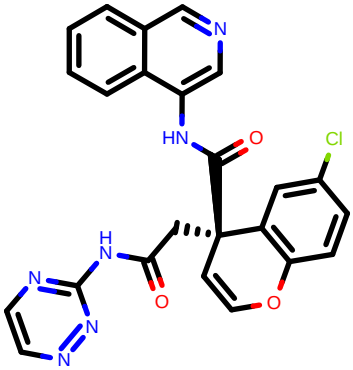
CID:	MIC-UNK-b9827f26-4_1
SMILES:	COc1ccc(cc1N2CCN(CC2=O)C(=O)c3cncc4c3cccc4)Cl
RUN:	RUN3255
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.15

EDJ-MED-4f704dc9-1_1



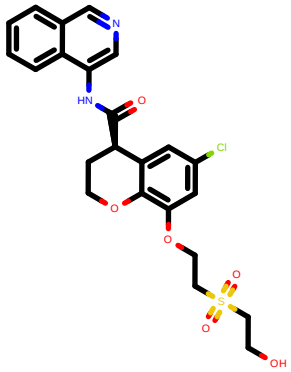
CID:	EDJ-MED-4f704dc9-1_1
SMILES:	CO[C@@]1(CCNc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3159
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.23

MIC-UNK-5a93dd5f-11_2



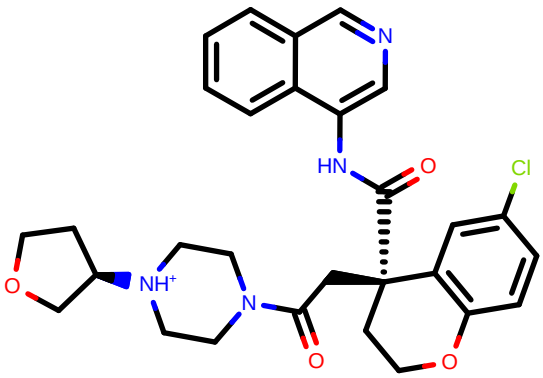
CID:	MIC-UNK-5a93dd5f-11_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3Cl)[NH+]4CCC(CC4)[NH+]5CCCCC5
RUN:	RUN789
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.31

MAT-POS-e9e99895-12_1



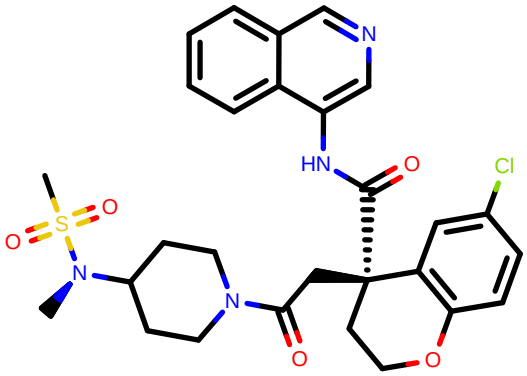
CID:	MAT-POS-e9e99895-12_1
SMILES:	C[C@@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)CC[NH+](C)C
RUN:	RUN2265
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.56

MAK-UNK-c749d764-15_15



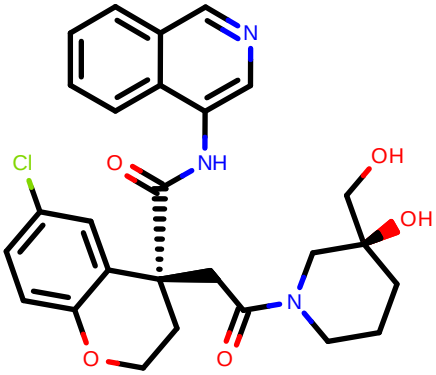
CID:	MAK-UNK-c749d764-15_15
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN972
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.26

JOH-UNI-a38a7bdd-5_4



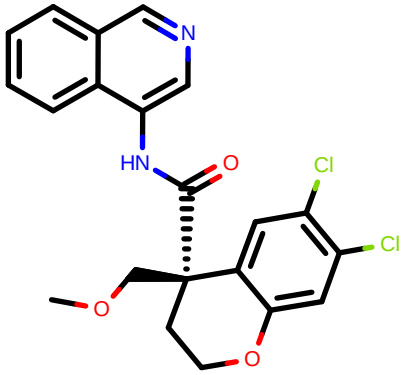
CID:	JOH-UNI-a38a7bdd-5_4
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@H]4C[C@H]4F
RUN:	RUN1486
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.46

MAK-UNK-c749d764-26_8



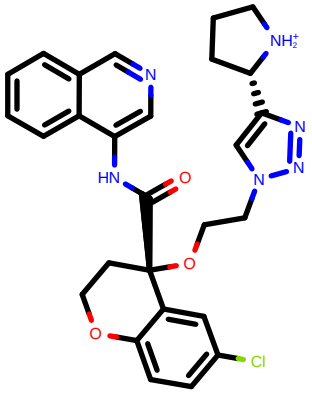
CID:	MAK-UNK-c749d764-26_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCCC[C@H]([C@H]3O)Cl
RUN:	RUN1053
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.45

DAR-DIA-56cf811e-5_1



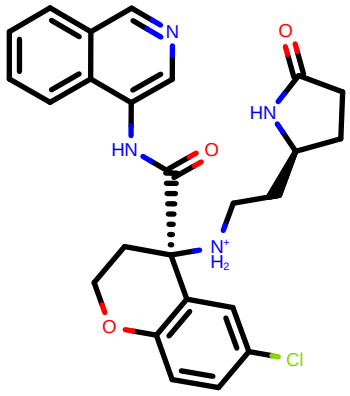
CID:	DAR-DIA-56cf811e-5_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)/C=C/C(F)(F)F
RUN:	RUN1522
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.19

MIC-UNK-bcd487e9-6_1



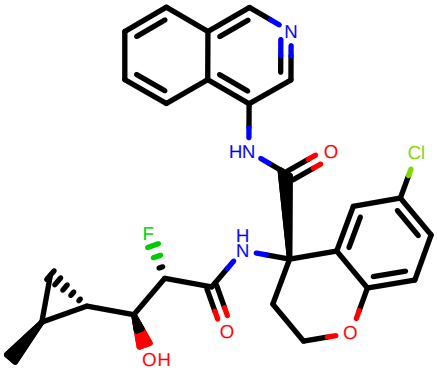
CID:	MIC-UNK-bcd487e9-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(C[C@@H]3CCCS3(=O)=O)c4cccc(c4)Cl
RUN:	RUN592
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.40

ED_-GRI-5b13fbe2-23_2



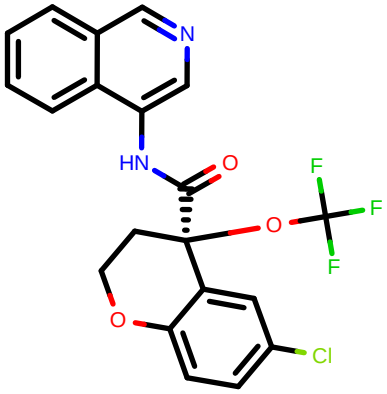
CID:	ED_-GRI-5b13fbe2-23_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[N@H+]5CCn6c(c(cn6)C[NH3+])C5
RUN:	RUN1554
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.29

MIC-UNK-0a05c952-4_2



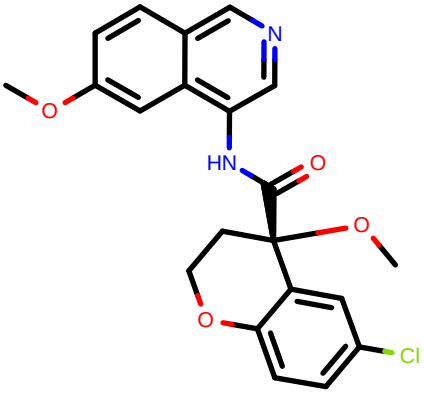
CID:	MIC-UNK-0a05c952-4_2
SMILES:	c1ccc2c(c1)cncc2N3[C@H](CC[C@@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@@H]5CO5
RUN:	RUN3522
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.17

MAK-UNK-c749d764-10_4



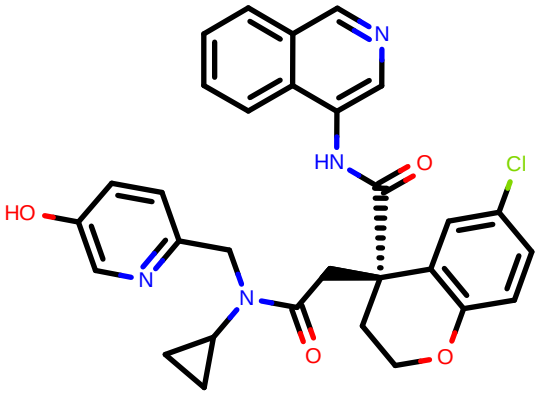
CID:	MAK-UNK-c749d764-10_4
SMILES:	CSN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN944
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.08

ROB-UNI-7b37d95b-1_1



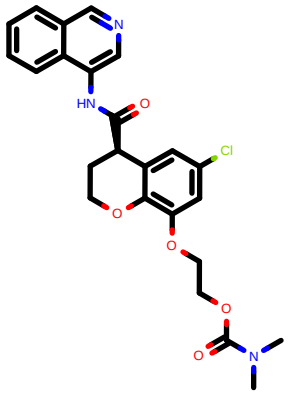
CID:	ROB-UNI-7b37d95b-1_1
SMILES:	C[C@H]1CNc2cc(c(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)F)F
RUN:	RUN4380
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.06

BEN-DND-c852c98b-6_1



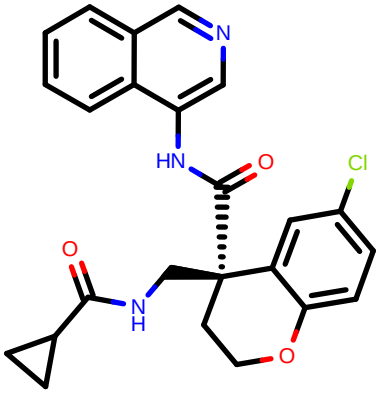
CID:	BEN-DND-c852c98b-6_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1213
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.28

ALP-POS-5bb456a5-1_5



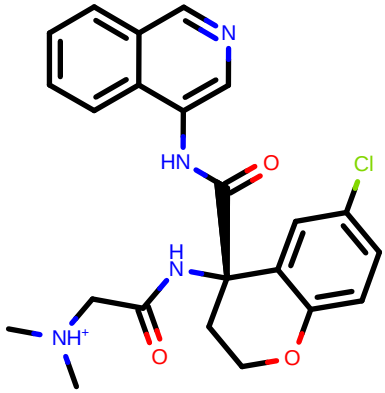
CID:	ALP-POS-5bb456a5-1_5
SMILES:	C[C@@H]1C[N@@]([CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2410
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.42

RAL-THA-8416115c-5_2



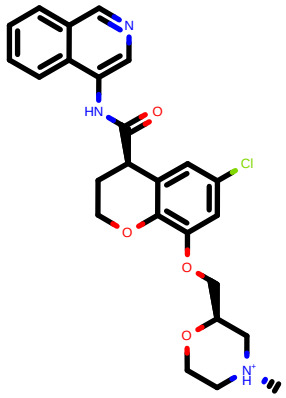
CID:	RAL-THA-8416115c-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5[nH]ccn5
RUN:	RUN1264
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.23

ALP-UNI-44c99a80-2_1



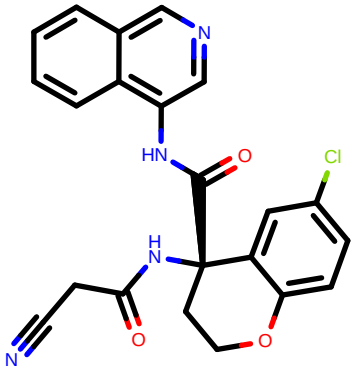
CID:	ALP-UNI-44c99a80-2_1
SMILES:	c1ccc2c(c1)cncc2N(Cc3cnc[nH]3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN463
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.34

MAT-POS-1f3f1a6f-4_1



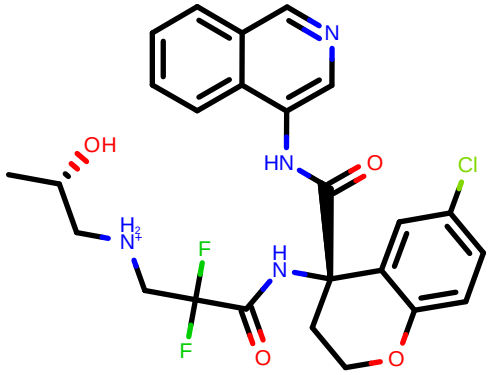
CID:	MAT-POS-1f3f1a6f-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3ccc(c(c3)Cl)Cl)[NH2+]CC4CC4
RUN:	RUN2283
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.40

EDJ-MED-f893e2a1-2_2



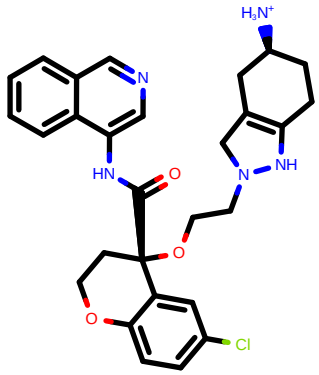
CID:	EDJ-MED-f893e2a1-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC[C@]5(CCOC5)C#N
RUN:	RUN3194
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.10

MAK-UNK-8be7dca9-10_2



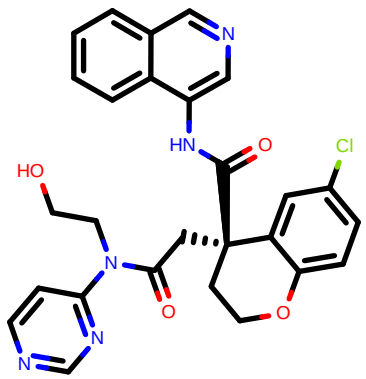
CID:	MAK-UNK-8be7dca9-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[C@@H](Oc4c3cc(cc4)Cl)C(=O)[O-]
RUN:	RUN512
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.38

FRA-DIA-b66f7109-2_2



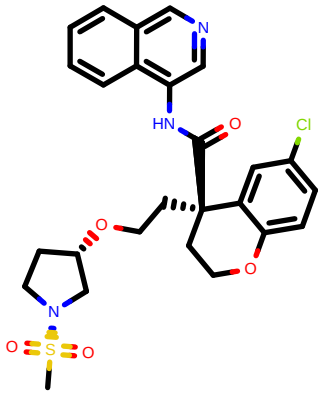
CID:	FRA-DIA-b66f7109-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cc(cc4Cl)O[C@H]5CC(=O)N5
RUN:	RUN394
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.37

MAK-UNK-c749d764-24_8



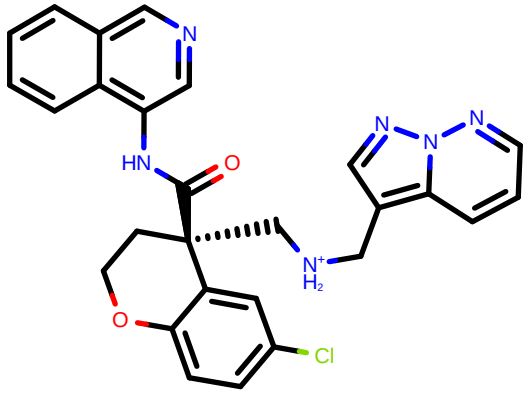
CID:	MAK-UNK-c749d764-24_8
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1036
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.35

EDJ-MED-15e90dfc-1_2



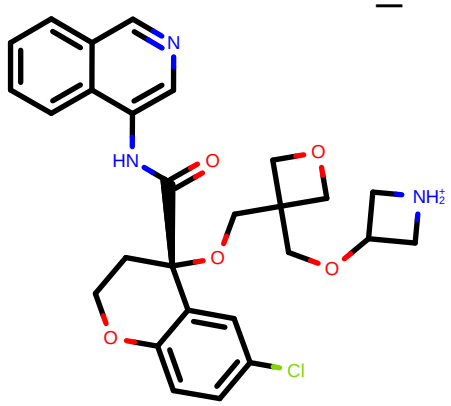
CID:	EDJ-MED-15e90dfc-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5ccn[nH]5
RUN:	RUN3437
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.19

EDG-MED-4c68219f-14_1



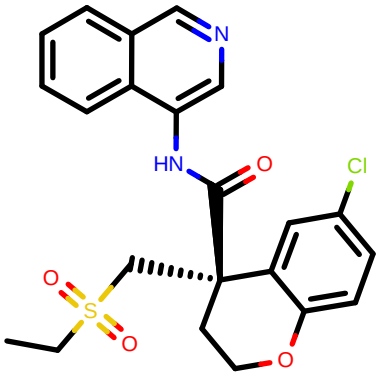
CID:	EDG-MED-4c68219f-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)O[C@H]5C[C@H]([NH2+]C5)CO
RUN:	RUN1649
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.40

FRA-DIA-b66f7109-1_1



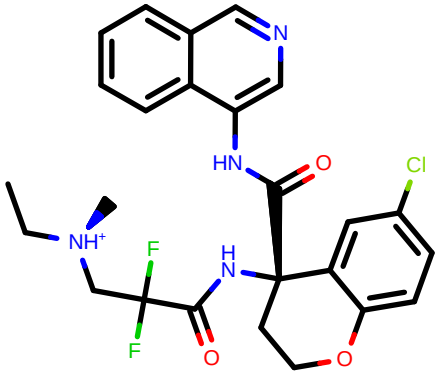
CID:	FRA-DIA-b66f7109-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CNc4c3cc(cc4Cl)O[C@@H]5CC(=O)N5
RUN:	RUN391
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.33

JOH-UNI-a38a7bdd-6_1



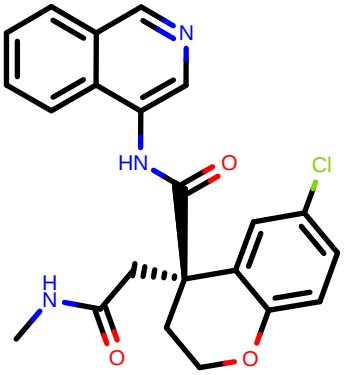
CID:	JOH-UNI-a38a7bdd-6_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@@H]4C[C@@H]4C(F)(F)F
RUN:	RUN1489
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.28

ROB-UNI-611831f5-2_2



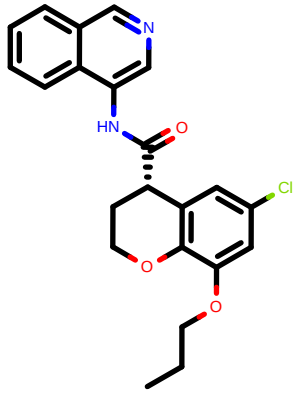
CID:	ROB-UNI-611831f5-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cn4)Cl
RUN:	RUN3324
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.18

MAK-UNK-ffc90da7-4_8



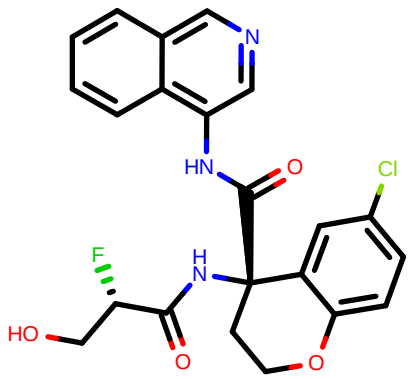
CID:	MAK-UNK-ffc90da7-4_8
SMILES:	C[C@H](C[NH2+]C[C@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN705
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.25

ED_-GRI-5b13fbe2-6_1



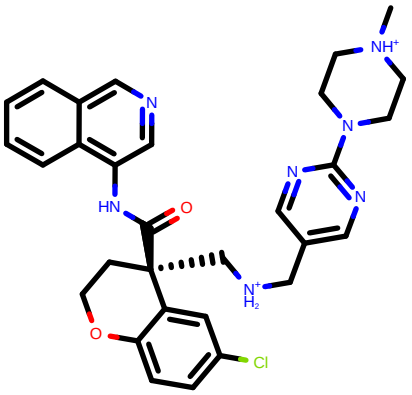
CID:	ED_-GRI-5b13fbe2-6_1
SMILES:	C[NH+](C)CC(=O)NC[C@H](CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1536
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.21

PET-UNK-7a31b064-1_1



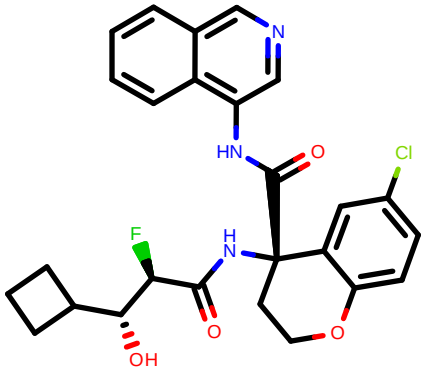
CID:	PET-UNK-7a31b064-1_1
SMILES:	CN1C[C@H](C(=O)N(C1=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN3289
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.15

ALP-POS-347519b5-3_58



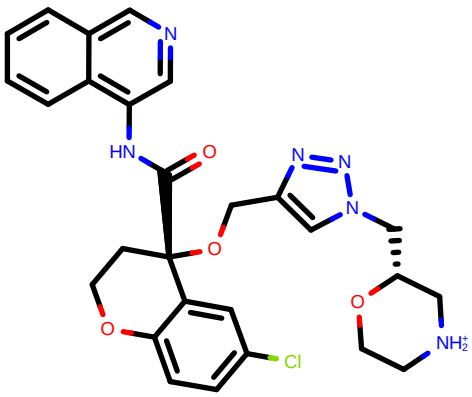
CID:	ALP-POS-347519b5-3_58
SMILES:	CS(=O)(=O)[N@]1C[C@@H]2[C@@H]3CC[C@H]([C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4325
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.32

DAR-DIA-0587064e-1_1



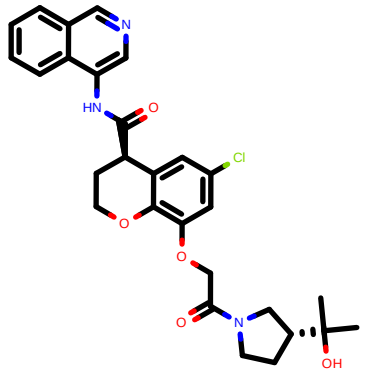
CID:	DAR-DIA-0587064e-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)OCCC(F)(F)F
RUN:	RUN3348
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.15

ALP-UNI-8e43a71e-15_13



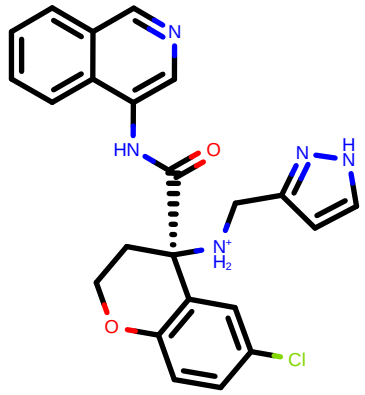
CID:	ALP-UNI-8e43a71e-15_13
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@H]6[C@H]5C[C@@H](C6)C(=O)N
RUN:	RUN2996
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.23

MAT-POS-e9e99895-2_1



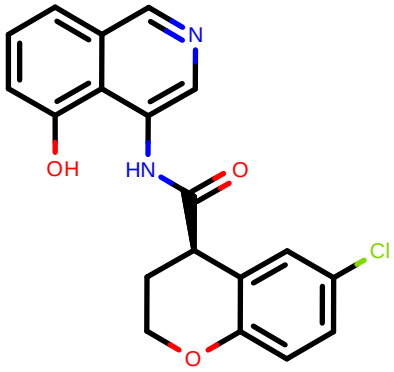
CID:	MAT-POS-e9e99895-2_1
SMILES:	CC(C)[N@@H+]1CCO[C@@H](C1)C(=O)N[C@@](C)(c2ccc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2235
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.35

EDG-MED-90036822-61_1



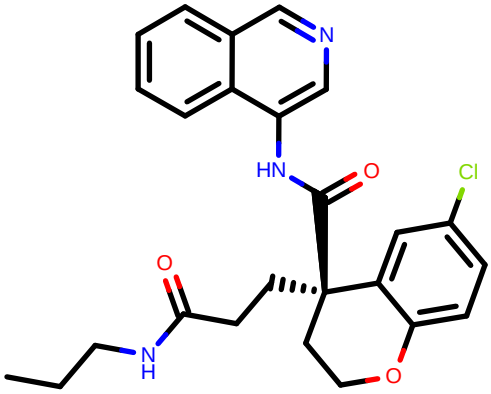
CID:	EDG-MED-90036822-61_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C[NH+]5CCC5
RUN:	RUN1745
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.26

DAR-DIA-6a508060-11_4



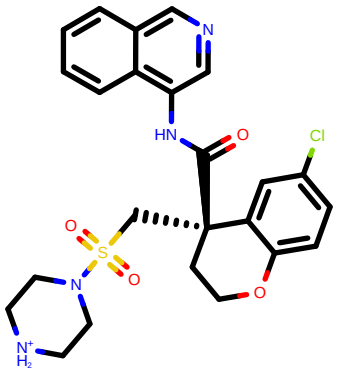
CID:	DAR-DIA-6a508060-11_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@H]4C[C@H]4Cl
RUN:	RUN353
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.19

MAT-POS-2492181e-11_1



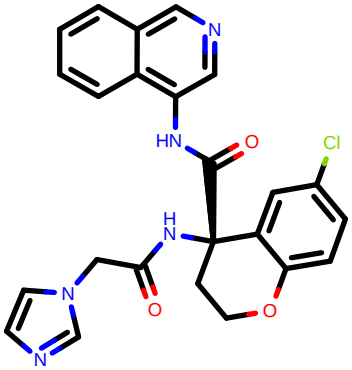
CID:	MAT-POS-2492181e-11_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCC[NH+]3CCOCC3
RUN:	RUN108
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.24

ALP-POS-347519b5-1_35



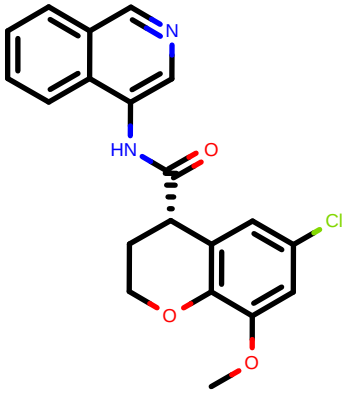
CID:	ALP-POS-347519b5-1_35
SMILES:	CS(=O)(=O)[N@@]1C[C@H]2[C@@H]3CC[C@@H](C3)[C@@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4250
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.24

EDJ-MED-37aac4bd-4_1



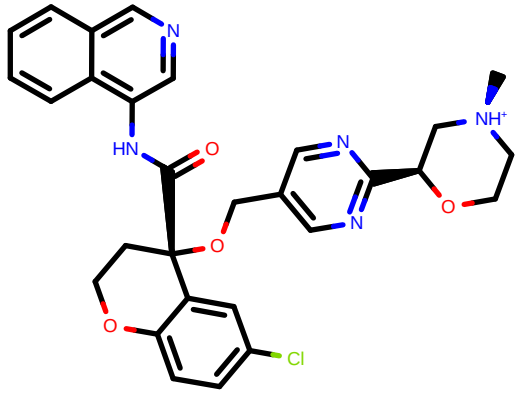
CID:	EDJ-MED-37aac4bd-4_1
SMILES:	CO[C@@]1(CCOc2c1cc(cc2F)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3145
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-2_3



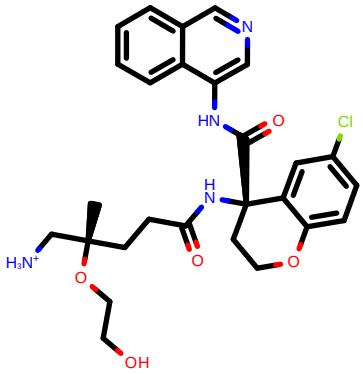
CID:	MIC-UNK-5a93dd5f-2_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCCC[C@@H]5C4
RUN:	RUN736
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.14

EDJ-MED-f893e2a1-2_1



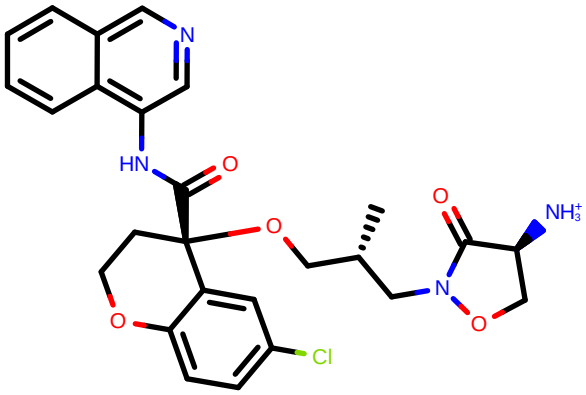
CID:	EDJ-MED-f893e2a1-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC[C@]5(CCOC5)C#N
RUN:	RUN3195
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.27

PET-UNK-5ecb6237-1_1



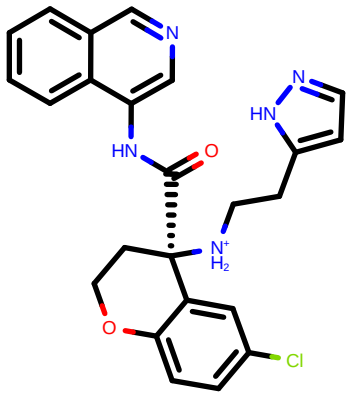
CID:	PET-UNK-5ecb6237-1_1
SMILES:	c1ccc2c(c1)cncc2N(C#N)C(=O)Cc3cccc(c3)Cl
RUN:	RUN519
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.64

ALP-POS-fe871b40-3_1



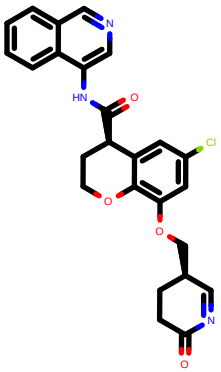
CID:	ALP-POS-fe871b40-3_1
SMILES:	CO[C@@]1(CCOc2c1cc(cc2C#N)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3113
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.22

ALP-POS-ce760d3f-7_2



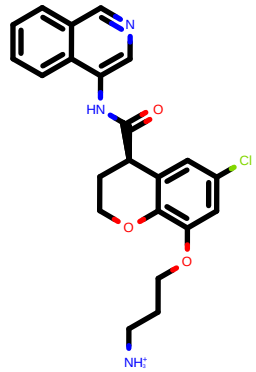
CID:	ALP-POS-ce760d3f-7_2
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1464
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.29

JOH-UNI-ea72002d-3_3



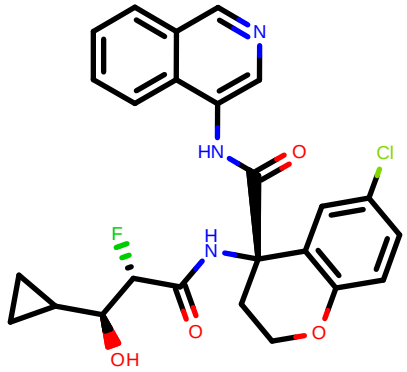
CID:	JOH-UNI-ea72002d-3_3
SMILES:	c1ccc2c(c1)cncc2[C@@H](C(=O)[C@H]3CCOc4c3cc(cc4)Cl)N5C(=O)C=CC5=O
RUN:	RUN2486
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.52

RAL-THA-05e671eb-24_1



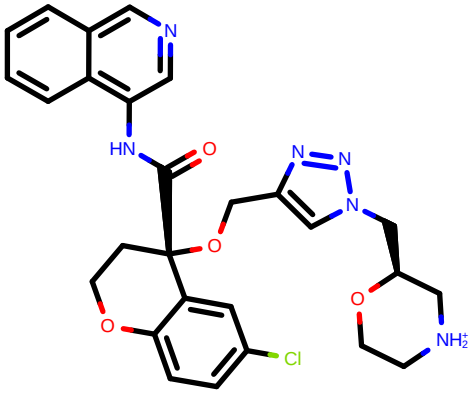
CID:	RAL-THA-05e671eb-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cccc4C#N
RUN:	RUN2052
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.32

PET-UNK-a692de38-1_1



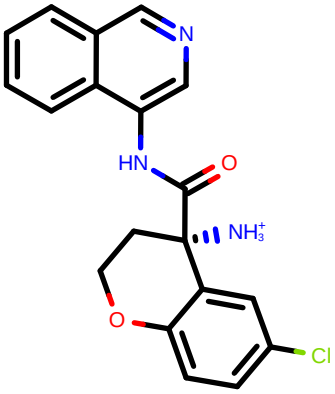
CID:	PET-UNK-a692de38-1_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)NC#N
RUN:	RUN583
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.26

WIL-UCB-7ba4ac3a-2_1



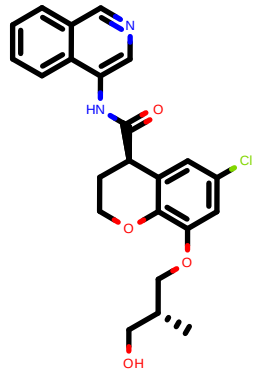
CID:	WIL-UCB-7ba4ac3a-2_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN3024
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.23

DAR-DIA-0d514e7d-31_4



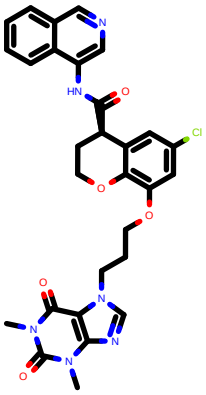
CID:	DAR-DIA-0d514e7d-31_4
SMILES:	C[C@H]1CCO[C@H]2C=CC(=C[C@@H]2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN836
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.23

EDJ-MED-9e38fd34-1_2



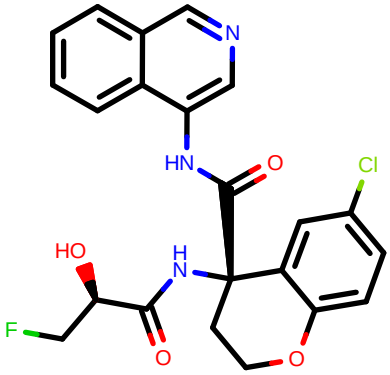
CID:	EDJ-MED-9e38fd34-1_2
SMILES:	C[C@]1(c2cc(ccc2NC1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2344
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.35

EDJ-MED-2f867453-1_2



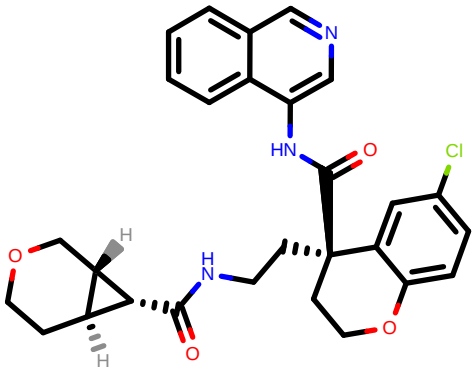
CID:	EDJ-MED-2f867453-1_2
SMILES:	C[C@]1(CNc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2336
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.45

VLA-UCB-34f3ed0c-21_1



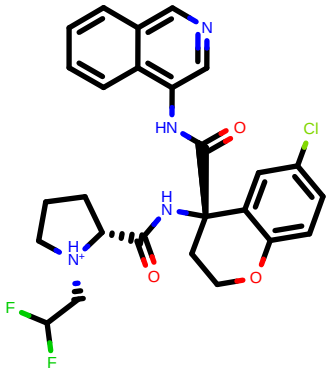
CID:	VLA-UCB-34f3ed0c-21_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)CC[C@@H]5CC(=O)NC5
RUN:	RUN648
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.29

MIC-UNK-5a93dd5f-3_4



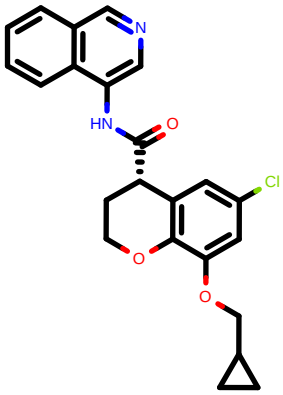
CID:	MIC-UNK-5a93dd5f-3_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3Cl)[N@H+]4CC[C@@H]5CCCC[C@@H]5C4
RUN:	RUN743
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.23

MAT-POS-dd3ad2b5-5_2



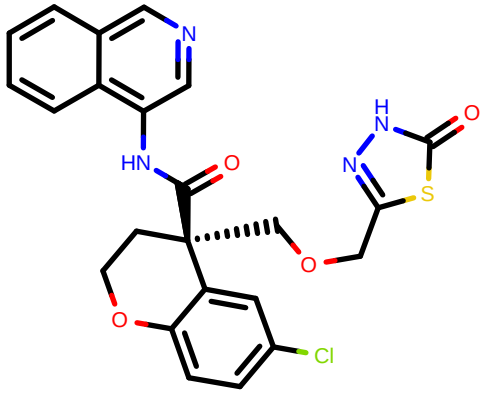
CID:	MAT-POS-dd3ad2b5-5_2
SMILES:	CNC(=O)N1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3544
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.16

ED_-GRI-5b13fbe2-25_1



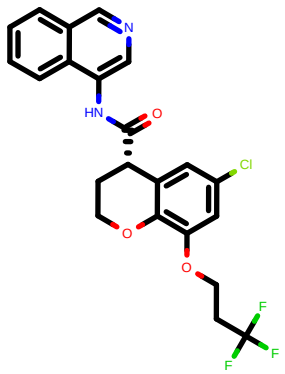
CID:	ED_-GRI-5b13fbe2-25_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+]CCOCCO
RUN:	RUN1560
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.28

KAD-UNI-cb0f2bbc-7_1



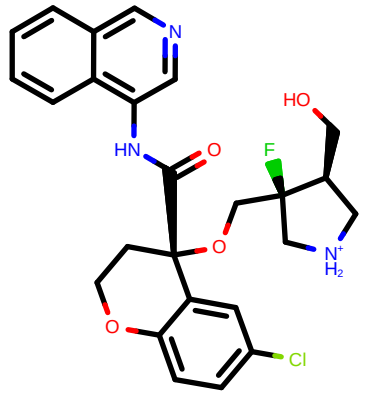
CID:	KAD-UNI-cb0f2bbc-7_1
SMILES:	C[C@@]1(CCS(=O)(=O)C1)n2cc(cn2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3686
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.11

JOH-UNI-a38a7bdd-6_4



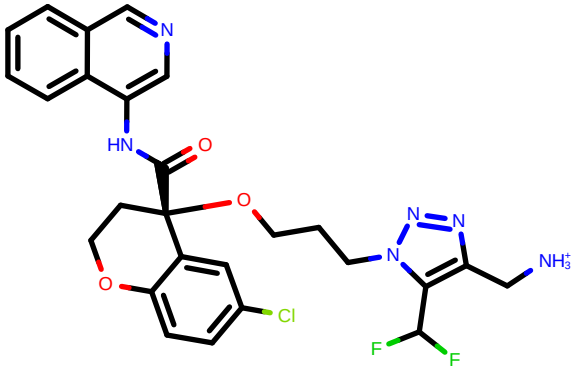
CID:	JOH-UNI-a38a7bdd-6_4
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@H]4C[C@H]4C(F)(F)F
RUN:	RUN1494
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.31

VLA-UCB-50c39ae8-7_1



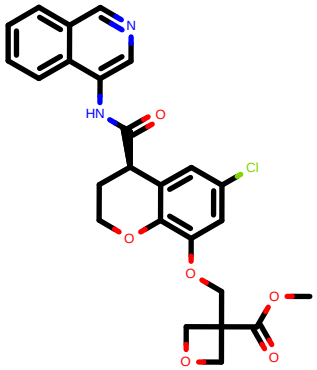
CID:	VLA-UCB-50c39ae8-7_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN386
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.30

DAR-DIA-0587064e-21_2



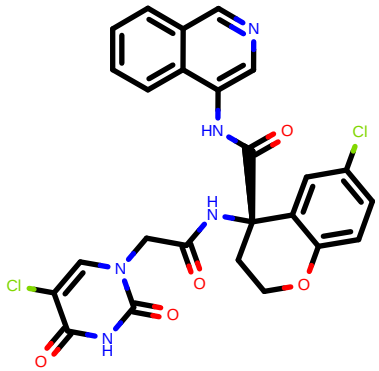
CID:	DAR-DIA-0587064e-21_2
SMILES:	c1ccc(cc1)CCOc2cc(cc3c2NCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3376
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.22

ALP-UNI-3496895b-5_2



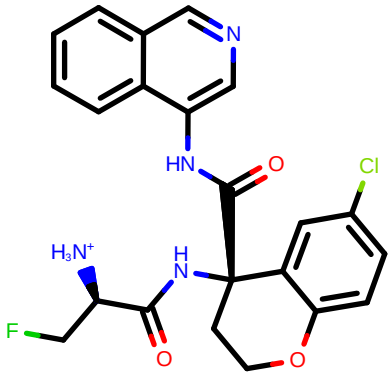
CID:	ALP-UNI-3496895b-5_2
SMILES:	C[C@H]1C[N@@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2513
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.42

MIC-UNK-5a93dd5f-3_8



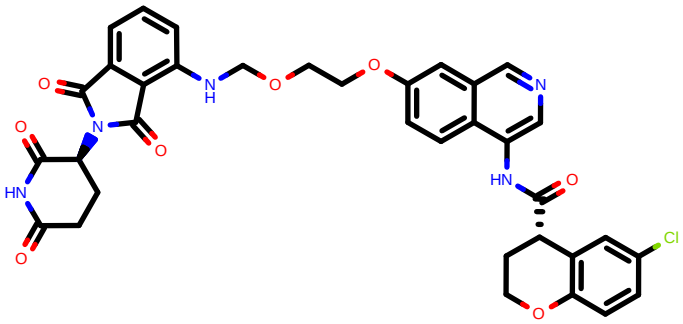
CID:	MIC-UNK-5a93dd5f-3_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@H+]4CC[C@H]5CCCC[C@@H]5C4
RUN:	RUN746
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.33

NIR-WEI-acbd6416-2_1



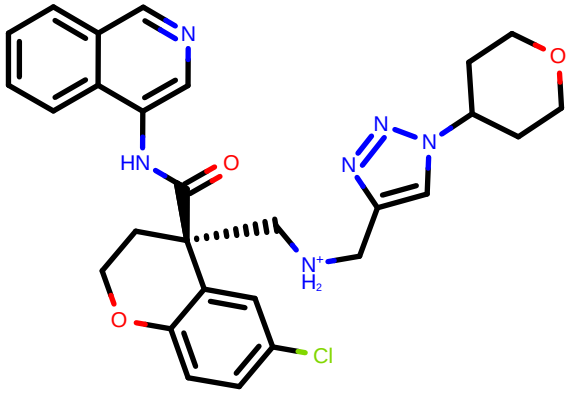
CID:	NIR-WEI-acbd6416-2_1
SMILES:	C=C(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN454
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.26

EDJ-MED-e4b030d8-5_1



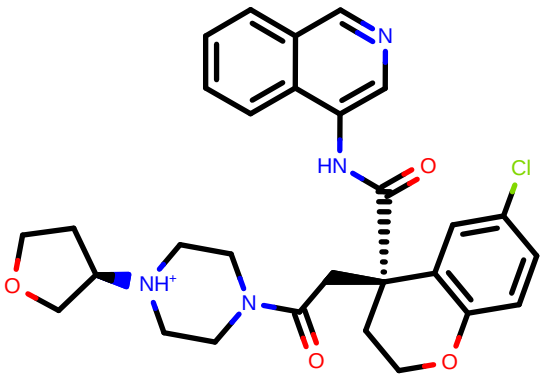
CID:	EDJ-MED-e4b030d8-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C5COC5)Cl
RUN:	RUN286
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.37

CHO-MSK-5891c1ff-6_1



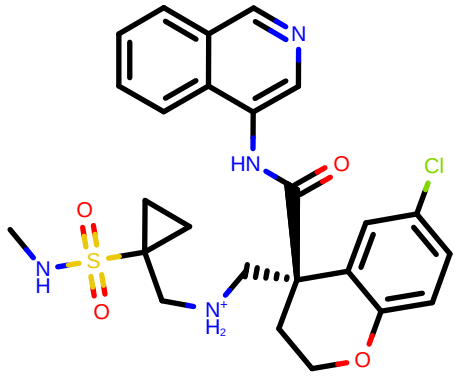
CID:	CHO-MSK-5891c1ff-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCN5CCOCC5=O
RUN:	RUN1860
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.39

MAK-UNK-c749d764-3_7



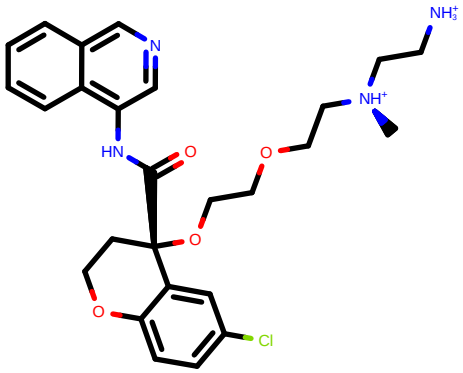
CID:	MAK-UNK-c749d764-3_7
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@@H]4CCC[C@H]([C@H]4O)C(F)F
RUN:	RUN911
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.27

ALF-EVA-07677224-9_3



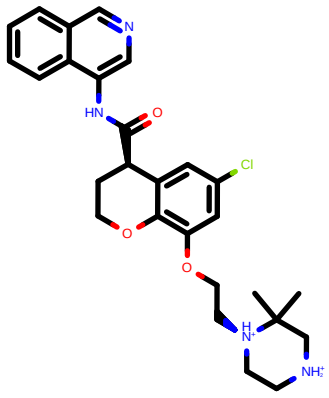
CID:	ALF-EVA-07677224-9_3
SMILES:	CC1(C[NH2+]C1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4942
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.28

DAR-DIA-0f7b7cd9-5_1



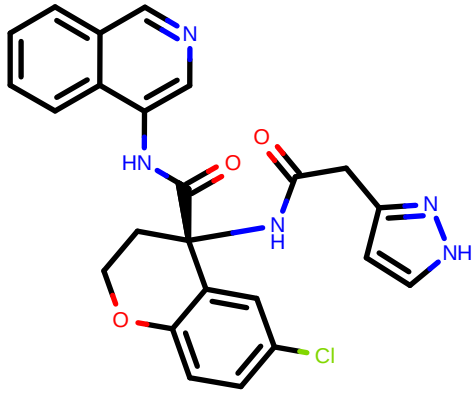
CID:	DAR-DIA-0f7b7cd9-5_1
SMILES:	c1ccc2c(c1)cncc2n3cc(n(c3=O)Cc4cccc(c4)Cl)[O-]
RUN:	RUN3011
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.25

MAT-POS-de59a476-4_1



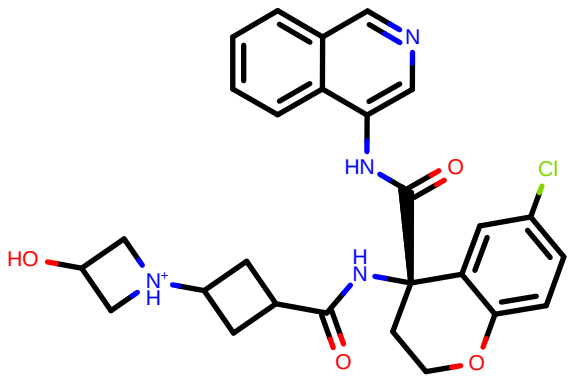
CID:	MAT-POS-de59a476-4_1
SMILES:	COCCO[C@@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2222
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.48

EDJ-MED-ee07cf00-11_6



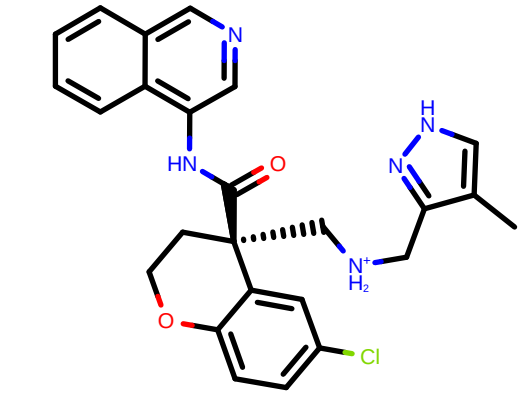
CID:	EDJ-MED-ee07cf00-11_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN2830
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.13

PAU-WEI-df8f33bc-1_1



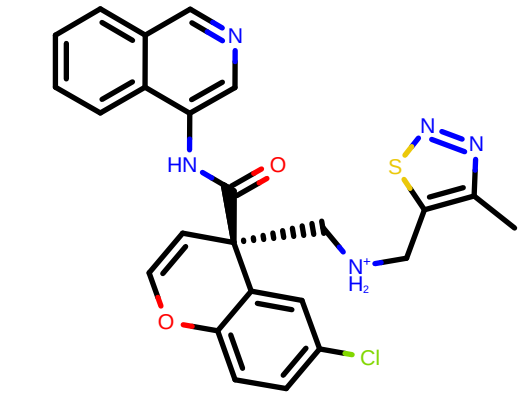
CID:	PAU-WEI-df8f33bc-1_1
SMILES:	CC(C)(C)c1ccc(cc1)N([C@@H](c2cncc3c2cccc3)C(=O)NCCc4cccc(c4)F)C(=O)c5ccco5
RUN:	RUN516
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.33

ALP-POS-347519b5-3_27



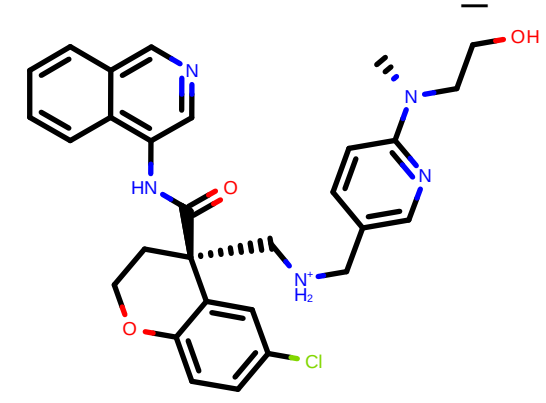
CID:	ALP-POS-347519b5-3_27
SMILES:	CS(=O)(=O)[N@@]1C[C@H]2[C@@H]3CC[C@H]([C@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4310
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.22

EDG-MED-90036822-17_1



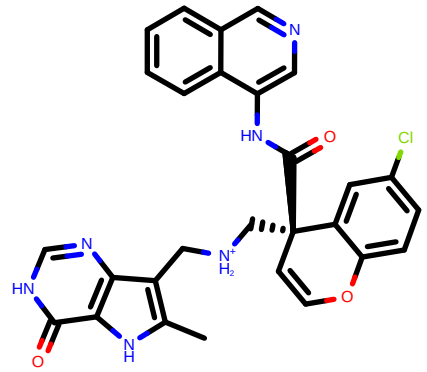
CID:	EDG-MED-90036822-17_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CF)O
RUN:	RUN1680
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.42

EDJ-MED-b7309adf-2_1



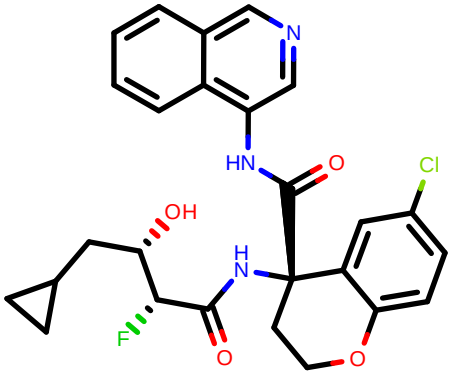
CID:	EDJ-MED-b7309adf-2_1
SMILES:	c1cc2c(cc1Cl)cncc2NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN4526
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.45

EDG-MED-90036822-94_7



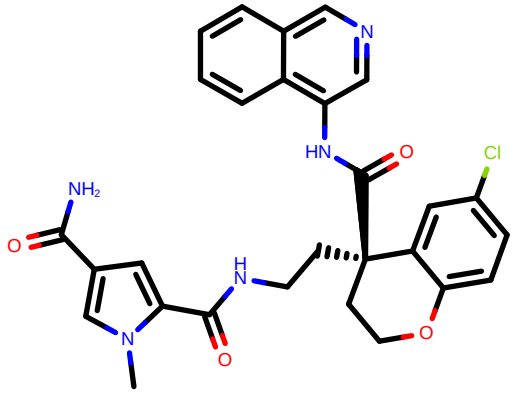
CID:	EDG-MED-90036822-94_7
SMILES:	C[C@@H]1C[C@H]1[C@H]([C@@H](C(=O)N[C@]2(CCOc3c2ccc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)F)O
RUN:	RUN1810
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.46

DAR-DIA-b4e9dd8d-5_2



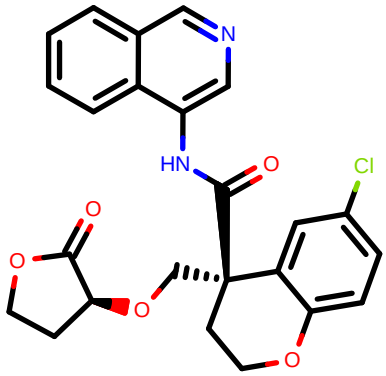
CID:	DAR-DIA-b4e9dd8d-5_2
SMILES:	COC(=O)/C=C/C(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3CNc4c3cc(cc4)Cl
RUN:	RUN3400
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.15

DAR-DIA-0587064e-27_1



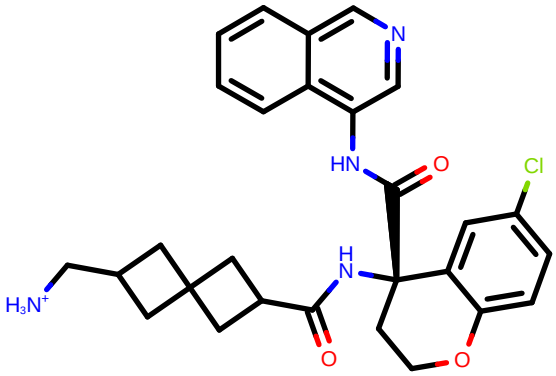
CID:	DAR-DIA-0587064e-27_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNc4c3cc(c(c4OCc5ccc(cc5Cl)F)F)Cl
RUN:	RUN3387
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.16

MIC-UNK-d58dbb53-2_2



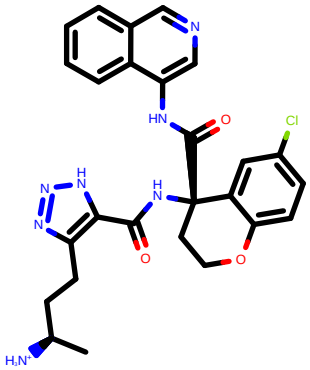
CID:	MIC-UNK-d58dbb53-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)O[C@H]5CCS(=O)(=O)C5
RUN:	RUN3678
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.10

MIC-UNK-8758c41d-1_1



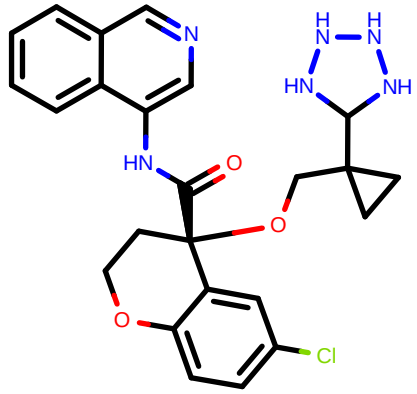
CID:	MIC-UNK-8758c41d-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(c(c4)Cl)Cl
RUN:	RUN3312
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.18

PET-UNK-55f647aa-2_1



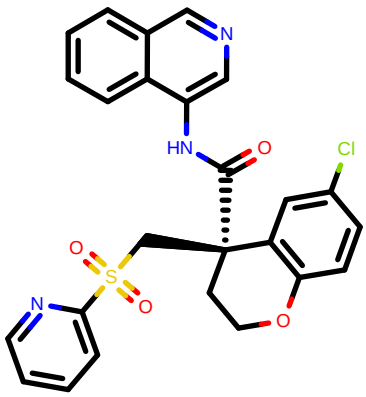
CID:	PET-UNK-55f647aa-2_1
SMILES:	CN(C)c1ccc(cn1)N(Cc2ccsc2)C(=O)Cc3cncc4c3cccc4
RUN:	RUN570
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.33

DAR-DIA-23e5a6a0-8_1



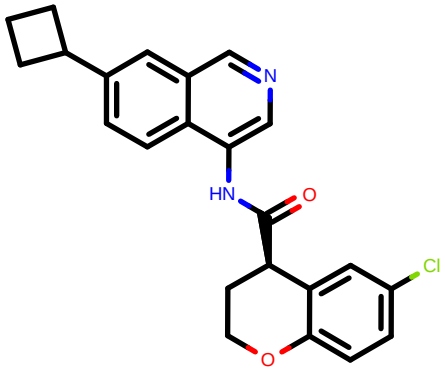
CID:	DAR-DIA-23e5a6a0-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CC6([NH2+]5)COC6)Cl
RUN:	RUN414
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.37

MIC-UNK-08fa0751-1_2



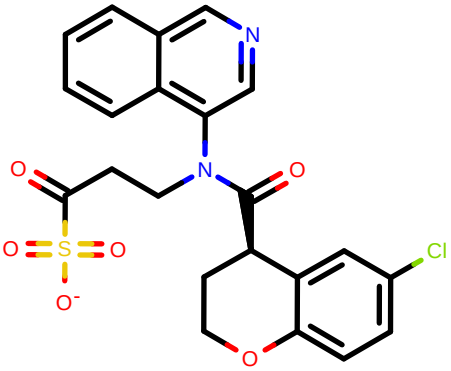
CID:	MIC-UNK-08fa0751-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4C(CO)(F)F)Cl
RUN:	RUN1520
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.19

DAR-DIA-0d514e7d-31_12



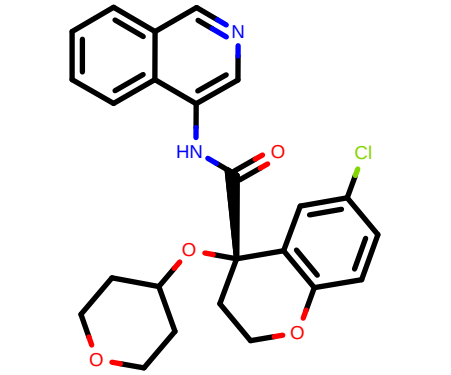
CID:	DAR-DIA-0d514e7d-31_12
SMILES:	C[C@H]1CCO[C@H]2C=CC(=C[C@@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN845
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.21

MAT-POS-e6dd326d-5_1



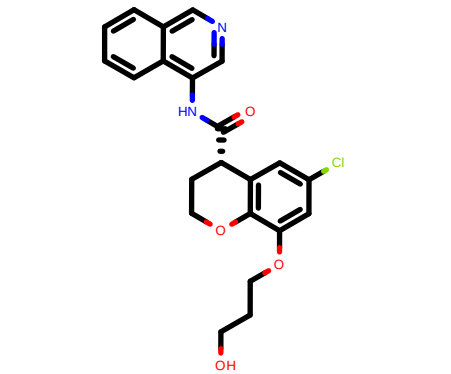
CID:	MAT-POS-e6dd326d-5_1
SMILES:	CN(C)S(=O)(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3946
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.24

MIC-UNK-9582b2c5-1_5



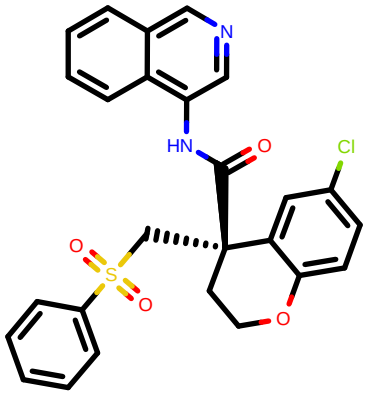
CID:	MIC-UNK-9582b2c5-1_5
SMILES:	CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)[C@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN257
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.27

VLA-UNK-f702bf1c-2_1



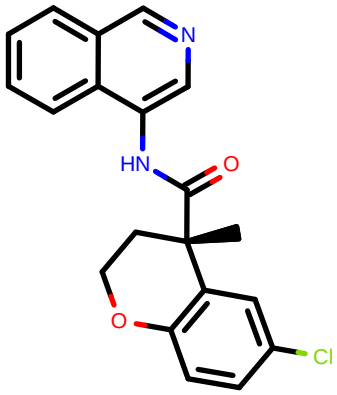
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6ccn[nH]6
RUN:	RUN2306
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.31

PET-UNK-1b92fa34-1_1



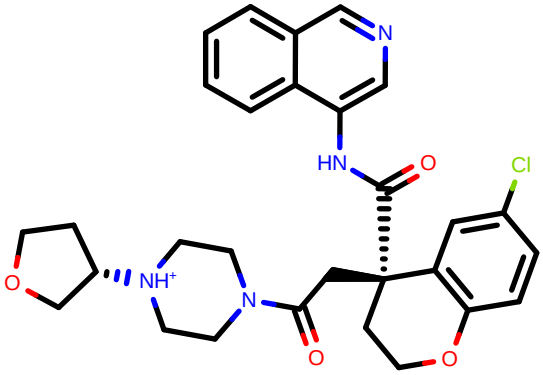
CID:	PET-UNK-1b92fa34-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CS(=O)(=O)Cc4c3cc(cc4)Cl
RUN:	RUN4169
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.17

NAU-LAT-356bd3c2-7_1



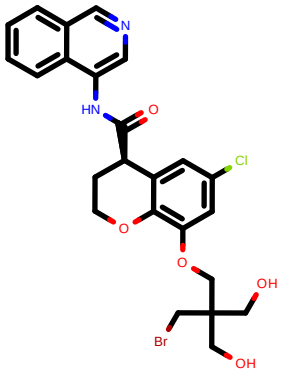
CID:	NAU-LAT-356bd3c2-7_1
SMILES:	c1ccc2c(c1)cncc2OC(=O)c3cccc4c3cc[nH]4
RUN:	RUN58
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.13

BEN-DND-c852c98b-2_1



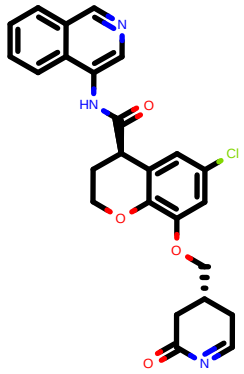
CID:	BEN-DND-c852c98b-2_1
SMILES:	c1cc2cncc(c2cc1OC(F)(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1204
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.28

ALP-POS-5bb456a5-1_11



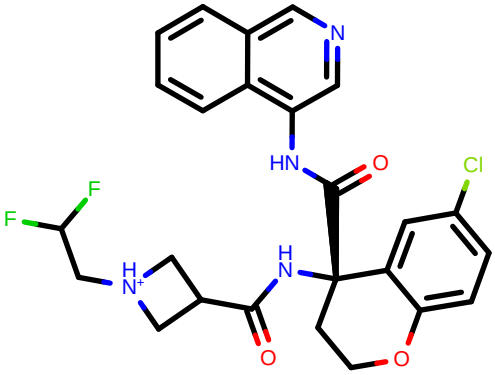
CID:	ALP-POS-5bb456a5-1_11
SMILES:	C[C@@H]1C[N@](CC[C@@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2418
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.40

EDJ-MED-fcba3f31-1_1



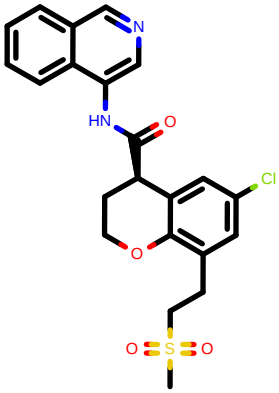
CID:	EDJ-MED-fcba3f31-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@@H]5CCCNC5=O
RUN:	RUN2538
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.33

DAR-DIA-0f2f46c9-1_1



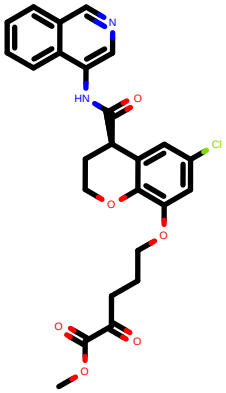
CID:	DAR-DIA-0f2f46c9-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC[N@@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3218
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.15

MAT-POS-afd4d4fd-1_1



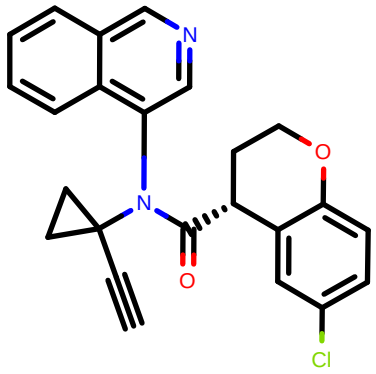
CID:	MAT-POS-afd4d4fd-1_1
SMILES:	Cc1c(cccc1Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN303
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.33

EDG-MED-ba1ac7b9-14_2



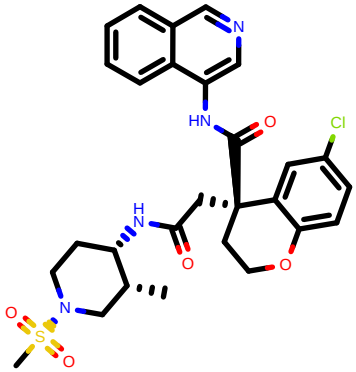
CID:	EDG-MED-ba1ac7b9-14_2
SMILES:	C[N@]1CCN(C[C@@H]1C#N)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2667
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.40

ALP-UNI-8e43a71e-2_12



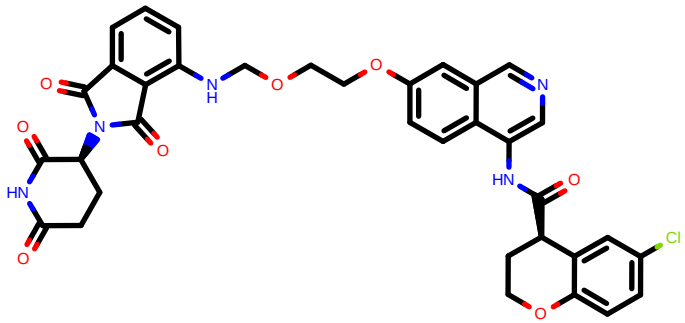
CID:	ALP-UNI-8e43a71e-2_12
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@@H]5CCC[N@H+]6CCO
RUN:	RUN2933
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.12

MAK-UNK-c749d764-16_13



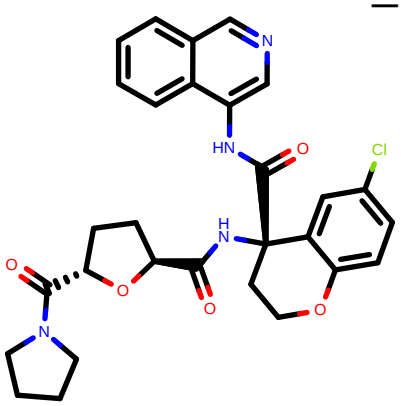
CID:	MAK-UNK-c749d764-16_13
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F)O
RUN:	RUN986
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.44

ROB-UNI-322e8f70-2_2



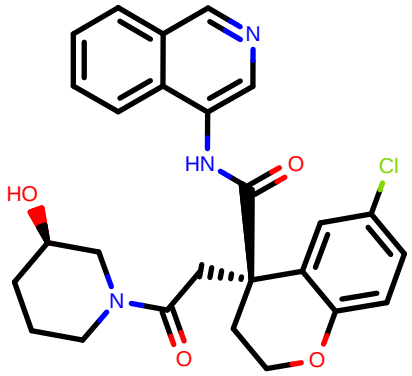
CID:	ROB-UNI-322e8f70-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CS(=O)(=O)Nc4c3cc(cc4)Cl
RUN:	RUN3156
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.28

MAT-POS-91829f0d-1_1



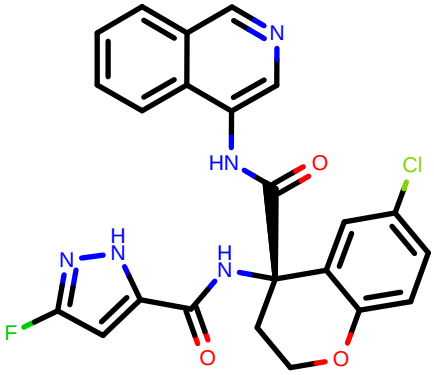
CID:	MAT-POS-91829f0d-1_1
SMILES:	COc1ccccc1OCCNC(=O)c2cncc3c2cccc3
RUN:	RUN1224
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.38

RAL-THA-8416115c-6_3



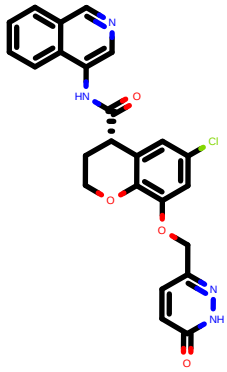
CID:	RAL-THA-8416115c-6_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5ccn[nH]5
RUN:	RUN1269
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.33

EDJ-MED-f893e2a1-10_1



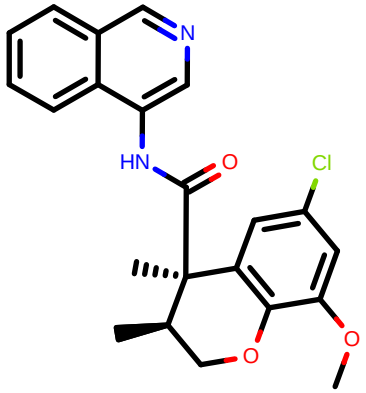
CID:	EDJ-MED-f893e2a1-10_1
SMILES:	CC(C)(CNC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)C#N
RUN:	RUN3214
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.11

EDJ-MED-40433386-4_1



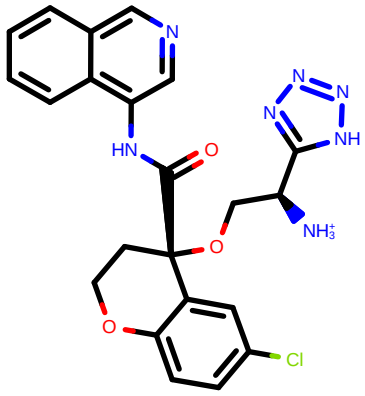
CID:	EDJ-MED-40433386-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)C5(CCC5)CO
RUN:	RUN2556
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.24

LON-WEI-4d77710c-7_2



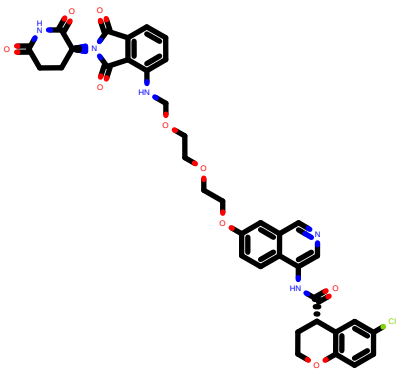
CID:	LON-WEI-4d77710c-7_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCC[N@H+]3CCc4ccccc4C3
RUN:	RUN198
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.22

ALP-UNI-8e43a71e-15_8



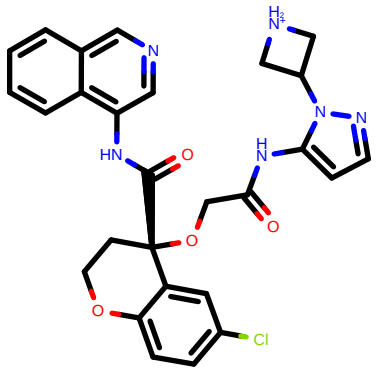
CID:	ALP-UNI-8e43a71e-15_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]6[C@@H]5C[C@@H](C6)C(=O)N
RUN:	RUN2989
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.22

MAT-POS-8a69d52e-3_1



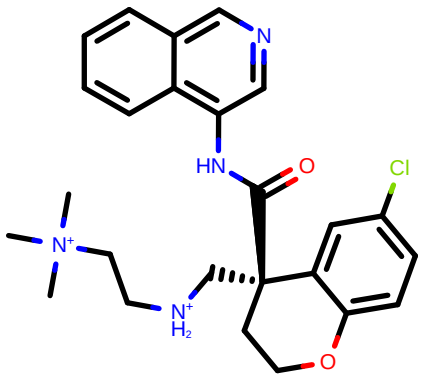
CID:	MAT-POS-8a69d52e-3_1
SMILES:	C[C@H]1C[C@@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN365
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.40

VLA-UNK-c65c1026-1_1



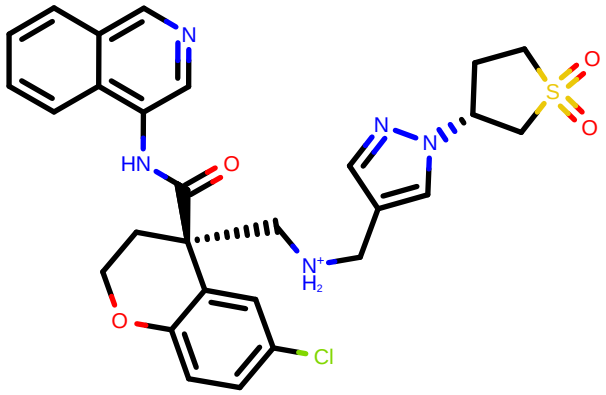
CID:	VLA-UNK-c65c1026-1_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@@]4(C3=O)COc5c4cc(cc5)Cl
RUN:	RUN3179
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.25

BEN-DND-d1eb1f41-16_2



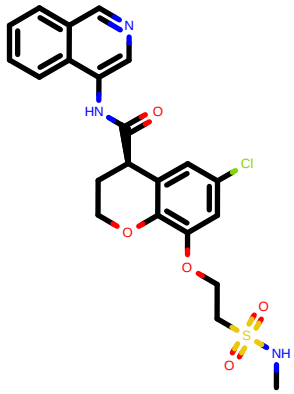
CID:	BEN-DND-d1eb1f41-16_2
SMILES:	c1ccc2c(c1)cncc2N[C@H](Cc3ccc(c(c3)Cl)Cl)C(F)(F)F
RUN:	RUN4366
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.19

ALP-POS-347519b5-2_23



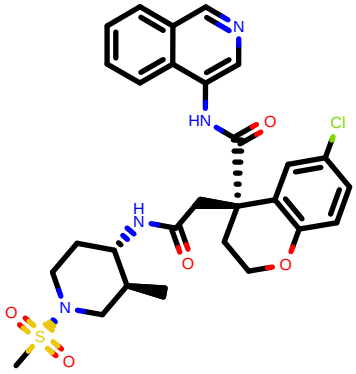
CID:	ALP-POS-347519b5-2_23
SMILES:	CO[C@@]1(C[N@](C[C@H]2[C@@H]1[C@H]3CC[C@@H]2C3)S(=O)(=O)C)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4270
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.28

KAD-UNI-8a629cb0-13_1



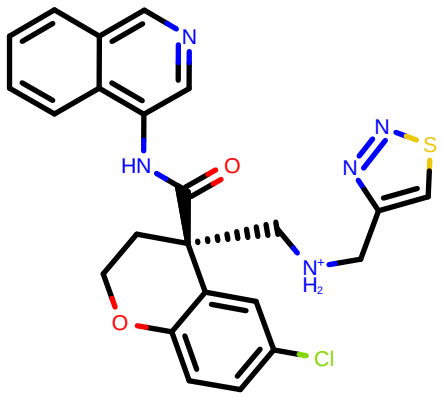
CID:	KAD-UNI-8a629cb0-13_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CN5CCN(C5=O)C6CC6
RUN:	RUN2095
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.34

ED_-GRI-5b13fbe2-15_2



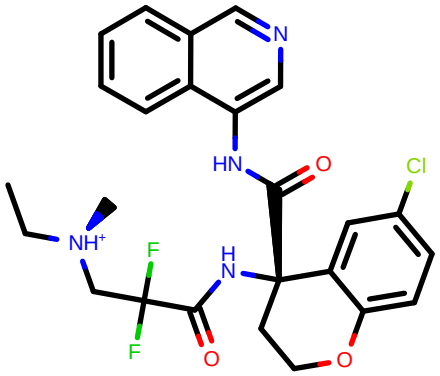
CID:	ED_-GRI-5b13fbe2-15_2
SMILES:	C[N@](CC[NH3+])CCOCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1544
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.26

ALP-POS-347519b5-1_3



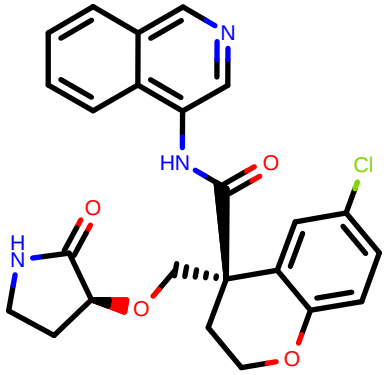
CID:	ALP-POS-347519b5-1_3
SMILES:	CS(=O)(=O)N@@]1C[C@H]2[C@@H]3CC[C@@H](C3)[C@@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4233
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.20

DAR-DIA-0d514e7d-33_3



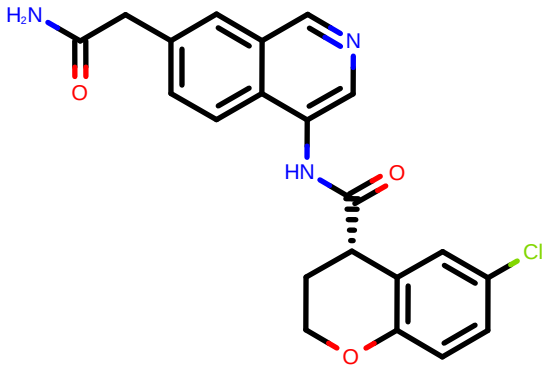
CID:	DAR-DIA-0d514e7d-33_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4O[C@@H]5[C@H]3C5)Cl
RUN:	RUN884
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.34

BEN-DND-a02b439d-14_1



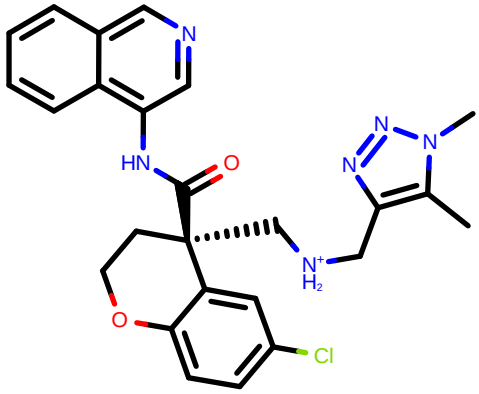
CID:	BEN-DND-a02b439d-14_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[NH2+]Cc4c3cc(c(c4)Cl)Cl
RUN:	RUN3671
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.10

MAT-POS-b5746674-37_2



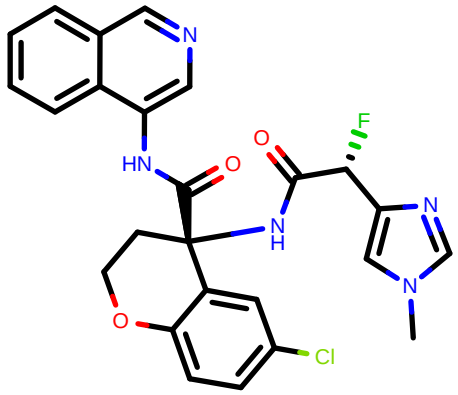
CID:	MAT-POS-b5746674-37_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N(Cc3ccco3)C[C@H]4CCCO4
RUN:	RUN67
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.13

PET-UNK-0cc03aae-4_2



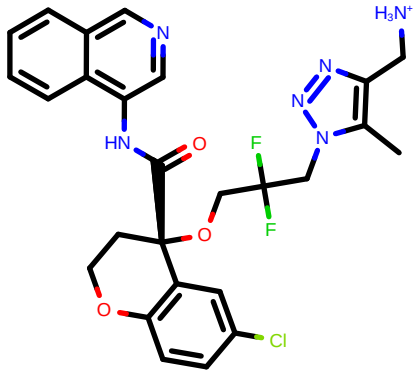
CID:	PET-UNK-0cc03aae-4_2
SMILES:	C[N@@](CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)S(=O)(=O)C
RUN:	RUN4482
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.25

EDJ-MED-4f704dc9-2_2



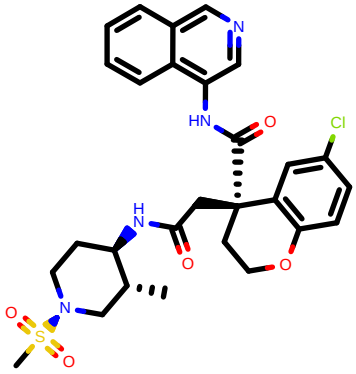
CID:	EDJ-MED-4f704dc9-2_2
SMILES:	COC[C@]1(CC(=O)Nc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3162
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.14

ERI-UCB-b3e6b0c2-12_1



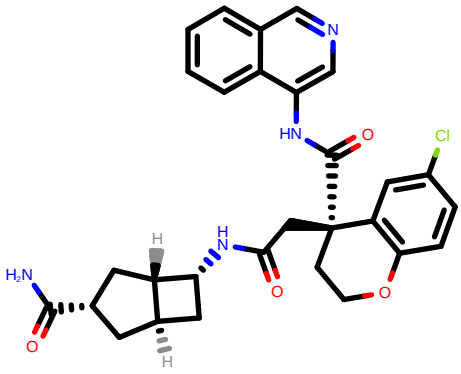
CID:	ERI-UCB-b3e6b0c2-12_1
SMILES:	C[N@@]1C[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3ccc(c4)C[NH3+]
RUN:	RUN3046
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.21

MAT-POS-4223bc15-14_2



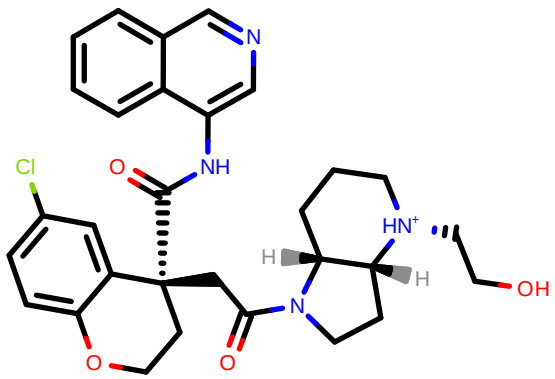
CID:	MAT-POS-4223bc15-14_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5C[NH2+]C5
RUN:	RUN4067
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.34

LON-WEI-5e7d1b3e-52_1



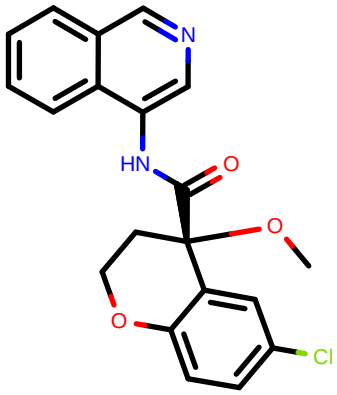
CID:	LON-WEI-5e7d1b3e-52_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3ccc(cc3)Cl
RUN:	RUN1358
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.26

RAL-THA-8416115c-9_3



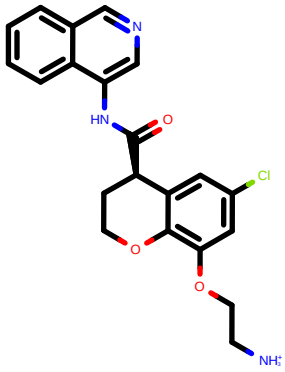
CID:	RAL-THA-8416115c-9_3
SMILES:	CN(C)C(=O)CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1281
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.48

MAT-POS-2492181e-10_2



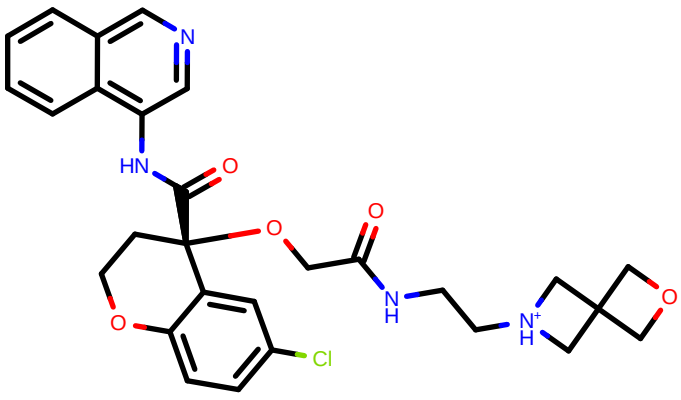
CID:	MAT-POS-2492181e-10_2
SMILES:	C[C@H]1CCCC[N@@H+]1CCCNC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN105
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.23

RAL-THA-05e671eb-21_2



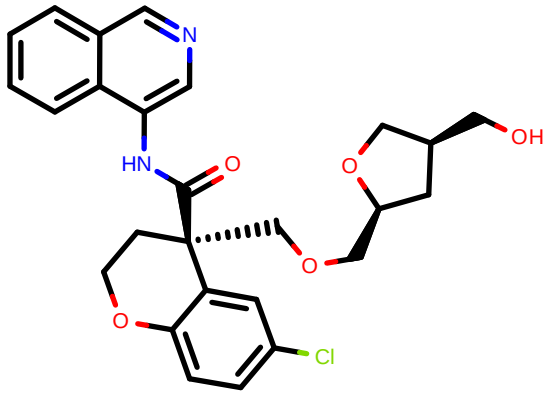
CID:	RAL-THA-05e671eb-21_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cccc4Cl
RUN:	RUN2047
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.40

MIC-UNK-8758c41d-2_1



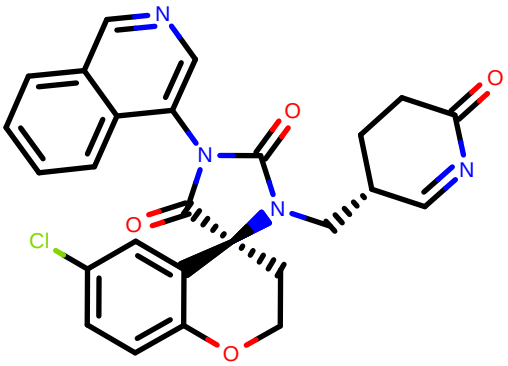
CID:	MIC-UNK-8758c41d-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CNC(=O)c4c3cc(c(c4)Cl)Cl
RUN:	RUN3310
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.24

MAK-UNK-c749d764-24_2



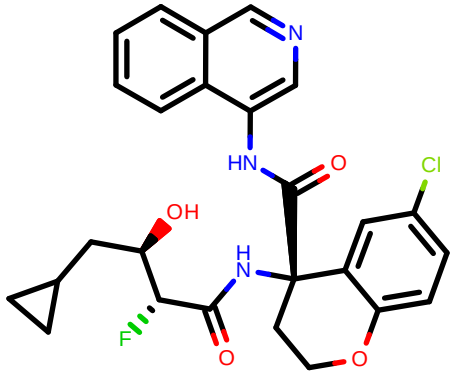
CID:	MAK-UNK-c749d764-24_2
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1031
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.21

MAK-UNK-c749d764-15_13



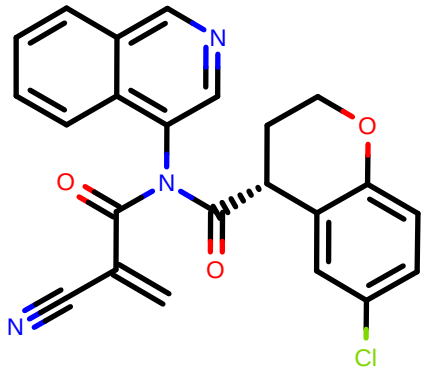
CID:	MAK-UNK-c749d764-15_13
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN969
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.25

MIC-UNK-0a05c952-1_8



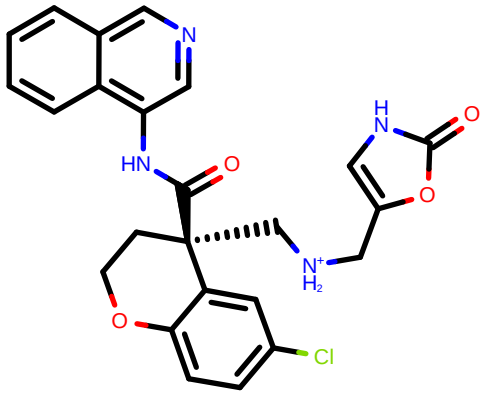
CID:	MIC-UNK-0a05c952-1_8
SMILES:	c1ccc2c(c1)cncc2N3[C@H](C[C@H](C3=O)c4cccc(c4Cl)Cl)[C@H]5CO5
RUN:	RUN3504
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.18

DAR-DIA-ecdbc7dd-9_2



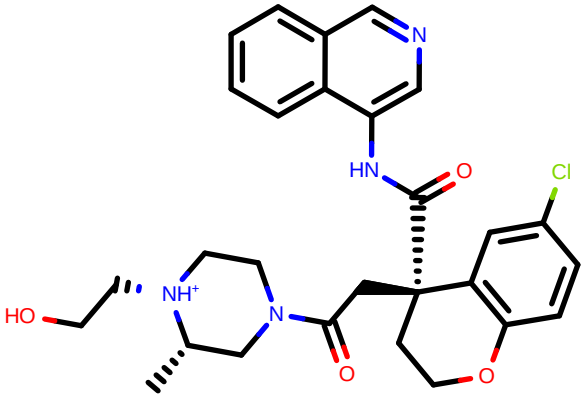
CID:	DAR-DIA-ecdbc7dd-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCNc4c3cc(cc4)Cl)C[NH+]5CCC5
RUN:	RUN2892
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.13

ALP-POS-347519b5-3_24



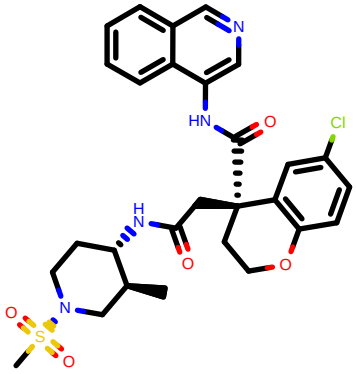
CID:	ALP-POS-347519b5-3_24
SMILES:	CS(=O)(=O)N@]1C[C@H]2[C@H]3CC[C@@H][C@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4307
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.32

RAL-THA-8416115c-7_1



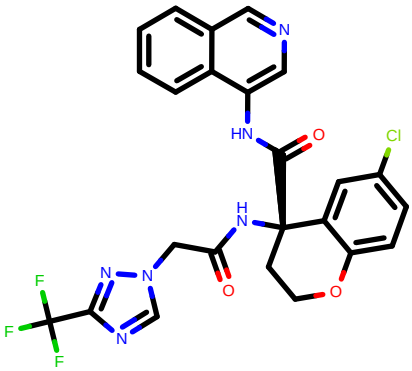
CID:	RAL-THA-8416115c-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)CC(=O)[O-]
RUN:	RUN1270
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.50

EDJ-MED-12f7f543-1_1



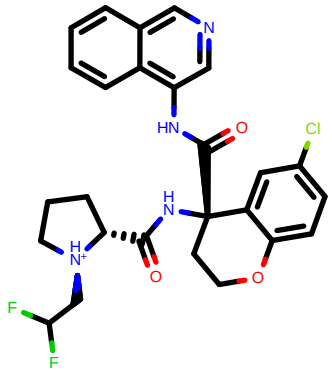
CID:	EDJ-MED-12f7f543-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cn4)Cl
RUN:	RUN1387
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.32

MAT-POS-96f51285-4_2



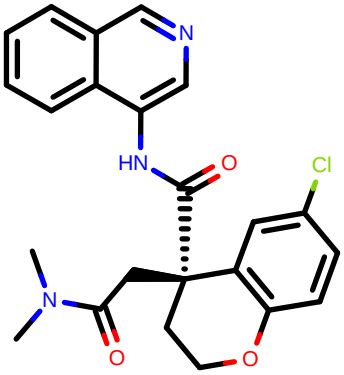
CID:	MAT-POS-96f51285-4_2
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@H]3CCOc4c3cc(c(c4)F)Cl
RUN:	RUN3933
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.14

MIC-UNK-5a93dd5f-9_4



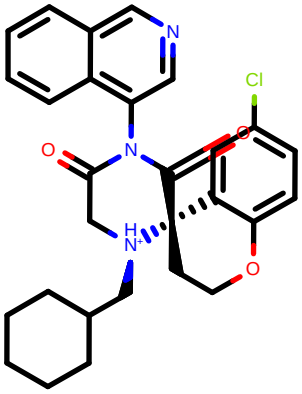
CID:	MIC-UNK-5a93dd5f-9_4
SMILES:	CN(C)[C@H]1CC[N@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN781
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.28

MAK-UNK-ffc90da7-6_1



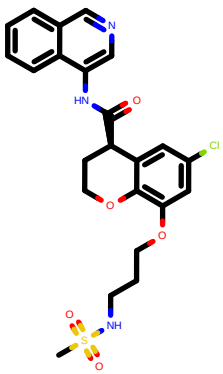
CID:	MAK-UNK-ffc90da7-6_1
SMILES:	C[C@@H](C[NH2+]CCCO)c1ccc2cncc(c2c1)NC(=O)Cc3cccc(c3)Cl
RUN:	RUN703
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.18

EDJ-MED-ee07cf00-11_5



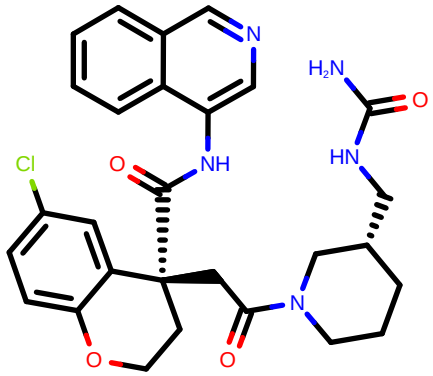
CID:	EDJ-MED-ee07cf00-11_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)[C@@H]4CC[C@H](O4)C(=O)N5CCCC5
RUN:	RUN2829
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.32

ALP-POS-5bb456a5-1_4



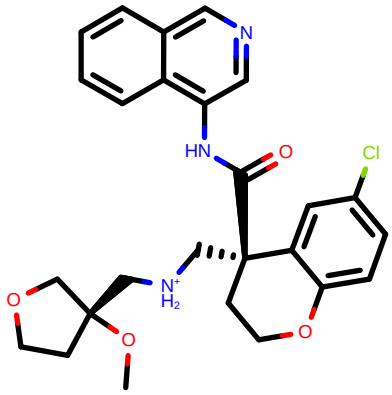
CID:	ALP-POS-5bb456a5-1_4
SMILES:	C[C@H]1C[N@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2408
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.40

NAU-LAT-2fed8305-6_1



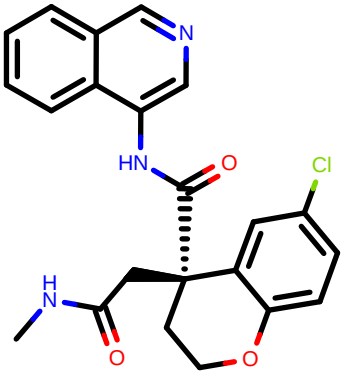
CID:	NAU-LAT-2fed8305-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3ccc(s3)Cl
RUN:	RUN1113
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.41

JOH-UNI-6e27fddc-7_1



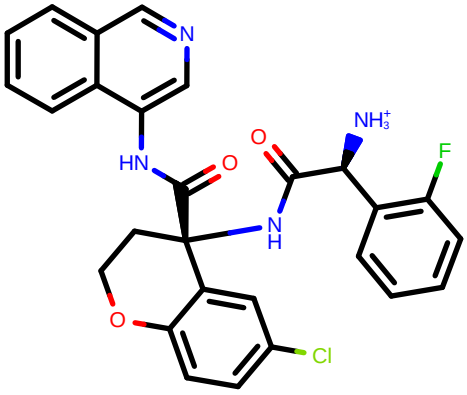
CID:	JOH-UNI-6e27fddc-7_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=S)[C@@]3(CCOc4c3cc(cc4)Cl)OC
RUN:	RUN4379
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.37

DAR-DIA-0d514e7d-32_1



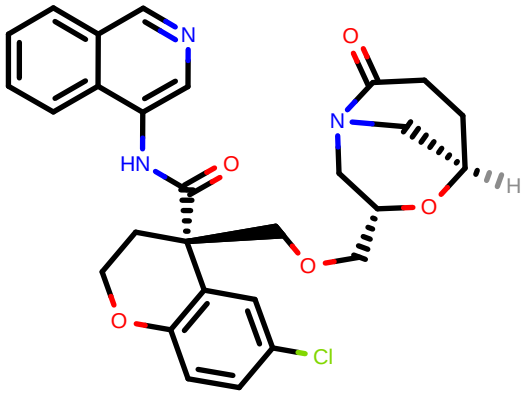
CID:	DAR-DIA-0d514e7d-32_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@@H]4C[C@@H]4CO[C@@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN850
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.16

ADA-UCB-dc2b944c-1_2



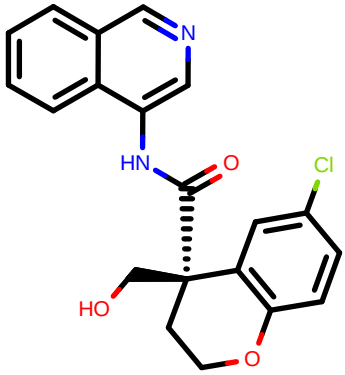
CID:	ADA-UCB-dc2b944c-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[N@H+][C@@]4(C3=O)CCOc5c4cc(cc5)Cl)CC6CCCCC6
RUN:	RUN598
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.31

MAK-UNK-3875bbc8-3_1



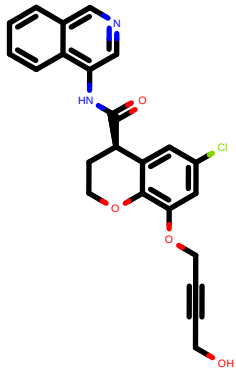
CID:	MAK-UNK-3875bbc8-3_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H]3CCOc4c3cccc4
RUN:	RUN802
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.28

RAL-THA-4aa06b95-5_2



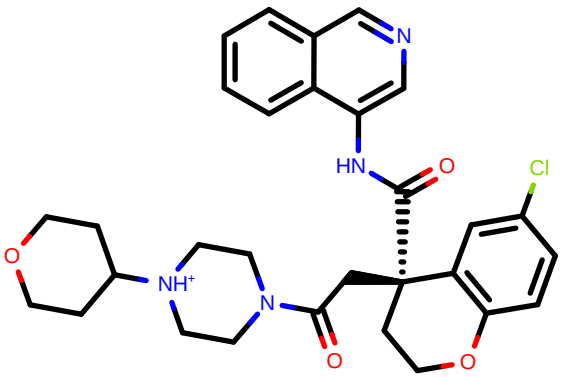
CID:	RAL-THA-4aa06b95-5_2
SMILES:	COCC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1238
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.16

ALF-EVA-a24cc7ce-2_1



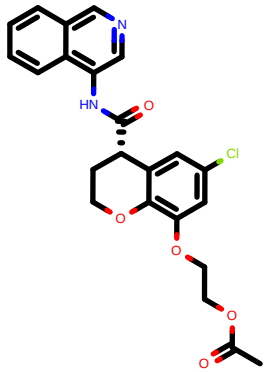
CID:	ALF-EVA-a24cc7ce-2_1
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN4955
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.15

ALP-POS-ce760d3f-1_2



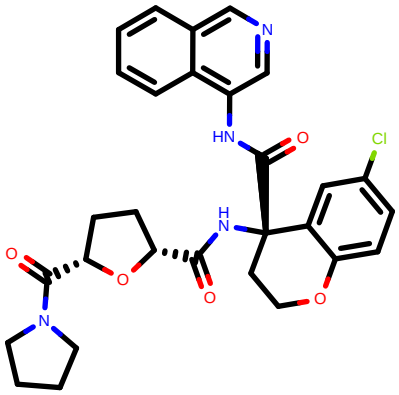
CID:	ALP-POS-ce760d3f-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4O)Cl
RUN:	RUN1462
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.33

EDG-MED-ba1ac7b9-1_4



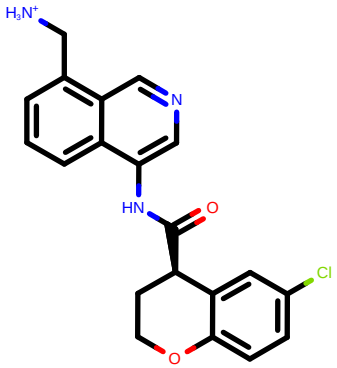
CID:	EDG-MED-ba1ac7b9-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]5C(=O)N
RUN:	RUN2618
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.24

ALP-POS-966f8da6-1_1



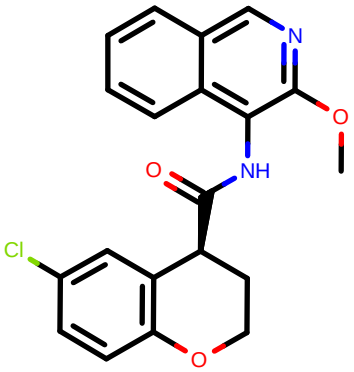
CID:	ALP-POS-966f8da6-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1218
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.33

DAR-DIA-0cde14eb-57_1



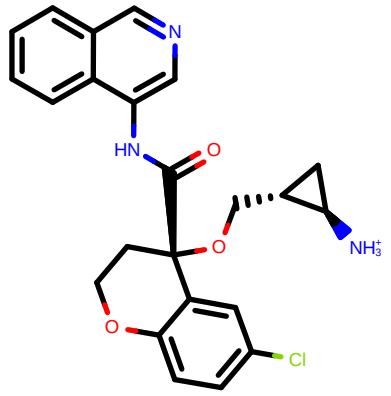
CID:	DAR-DIA-0cde14eb-57_1
SMILES:	C[C@@H](c1cccc(c1)C2(CC2)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN25
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.23

LON-WEI-4d77710c-35_3



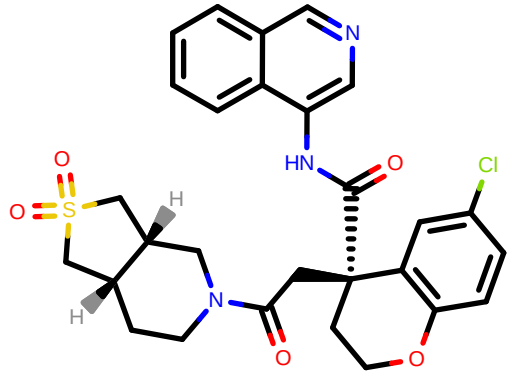
CID:	LON-WEI-4d77710c-35_3
SMILES:	Cc1ccc(cc1)C[N@@H+]2CC[C@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN224
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.15

DAR-DIA-23e5a6a0-6_1



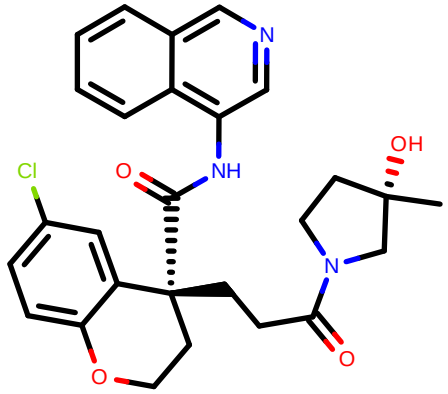
CID:	DAR-DIA-23e5a6a0-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@@H]5CCC6([NH2+]5)CCC6)Cl
RUN:	RUN411
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.23

DAR-DIA-0d514e7d-12_1



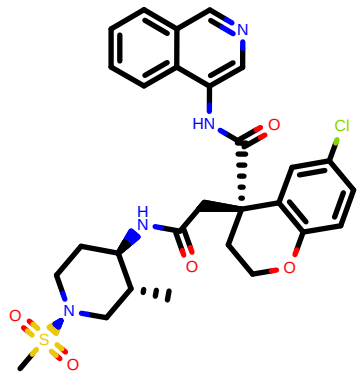
CID:	DAR-DIA-0d514e7d-12_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5ccc(cc5F)F
RUN:	RUN816
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.28

MAT-POS-932d1078-1_1



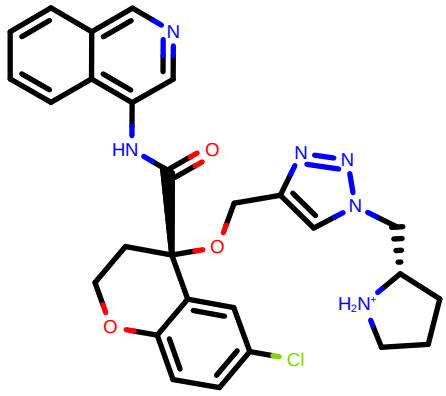
CID:	MAT-POS-932d1078-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4Cl)CNC(=O)[C@@H]5COCC[N@@]5CC(F)(F)F
RUN:	RUN3588
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-3_1



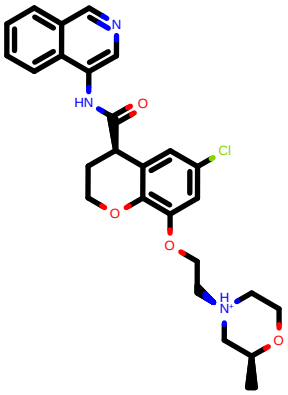
CID:	MAK-UNK-c749d764-3_1
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@@H]4CCC[C@@H]([C@@H]4O)C(F)F
RUN:	RUN906
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.27

ALP-POS-fe871b40-12_2



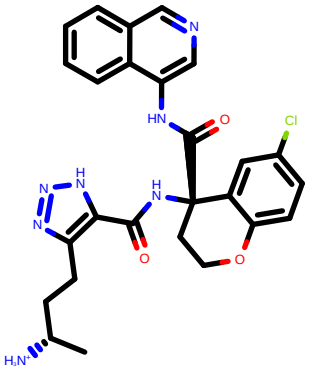
CID:	ALP-POS-fe871b40-12_2
SMILES:	CO[C@]1(CCNc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3128
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.20

ALP-UNI-3496895b-15_8



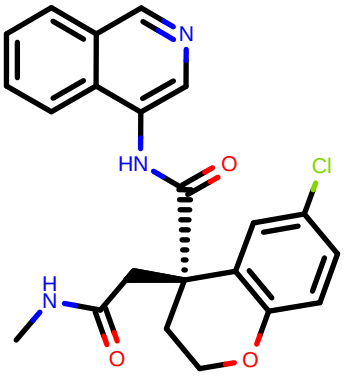
CID:	ALP-UNI-3496895b-15_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5C[C@H]6[C@H]5C[C@H](C6)C(=O)N
RUN:	RUN2539
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.39

MIC-UNK-91acba05-4_2



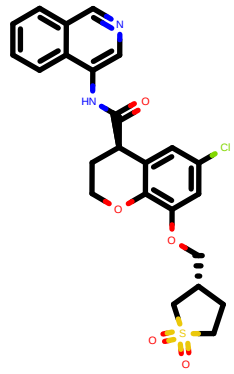
CID:	MIC-UNK-91acba05-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCCc4c3cc(cc4)Cl
RUN:	RUN475
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.39

DAR-DIA-0d514e7d-32_14



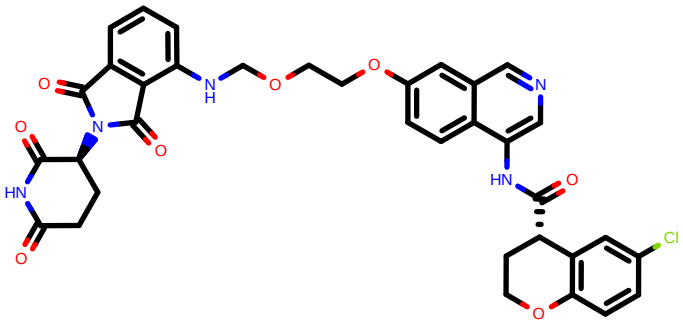
CID:	DAR-DIA-0d514e7d-32_14
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@@H]4C[C@H]4CO[C@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN863
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.16

ALP-UNI-0676e700-4_1



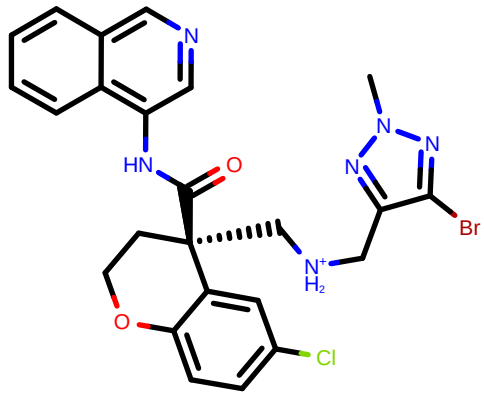
CID:	ALP-UNI-0676e700-4_1
SMILES:	Cc1nc(on1)COCC(=O)NC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2447
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.34

EDJ-MED-e4b030d8-9_1



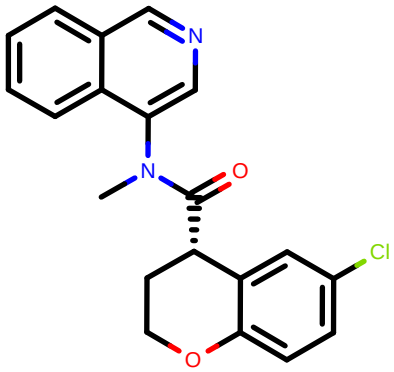
CID:	EDJ-MED-e4b030d8-9_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3nc(cc4)Cl
RUN:	RUN290
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.35

EDJ-MED-1b5395f9-3_2



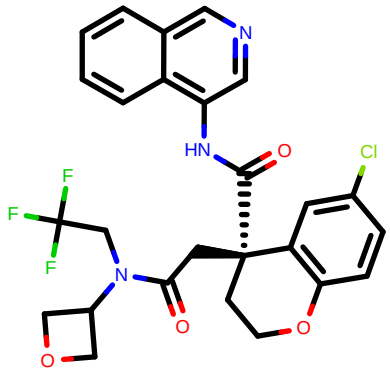
CID:	EDJ-MED-1b5395f9-3_2
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@H]3C[N@](Cc4c3cc(c(c4)Cl)Cl)S(=O)(=O)C
RUN:	RUN4466
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.28

LON-WEI-4d77710c-35_1



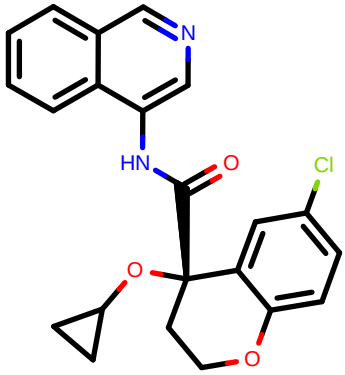
CID:	LON-WEI-4d77710c-35_1
SMILES:	Cc1ccc(cc1)C[N@@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN222
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.22

MAT-POS-e6dd326d-4_1



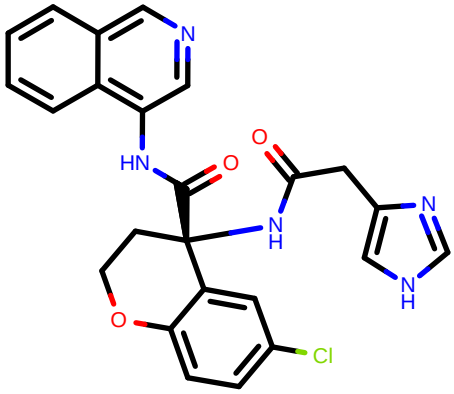
CID:	MAT-POS-e6dd326d-4_1
SMILES:	CS(=O)(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3943
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.29

MAT-POS-4223bc15-31_3



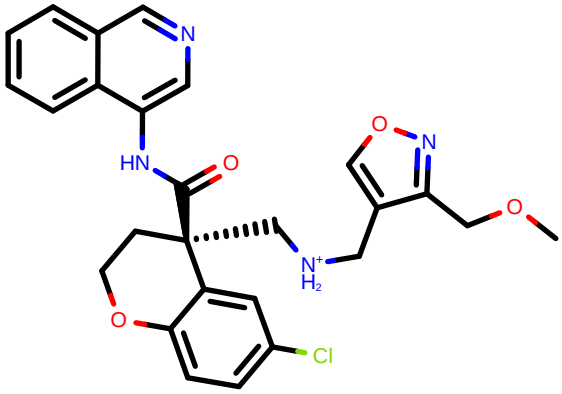
CID:	MAT-POS-4223bc15-31_3
SMILES:	Cn1ncc(n1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4140
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.08

DAR-DIA-0f2f46c9-14_1



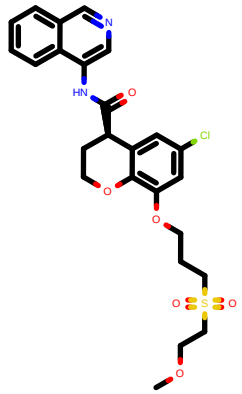
CID:	DAR-DIA-0f2f46c9-14_1
SMILES:	CN(C)S(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3252
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.15

MIC-UNK-460e637d-2_6



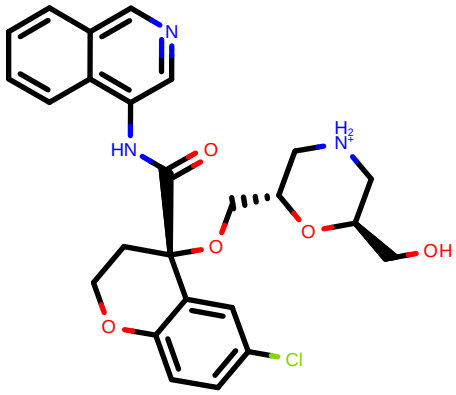
CID:	MIC-UNK-460e637d-2_6
SMILES:	C[N@H+]1CCN(C[C@@H]1CO[C@H]2CC(=O)N2)C(=O)Cc3cncc4c3cccc4
RUN:	RUN1887
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.52

EDG-MED-ba1ac7b9-8_2



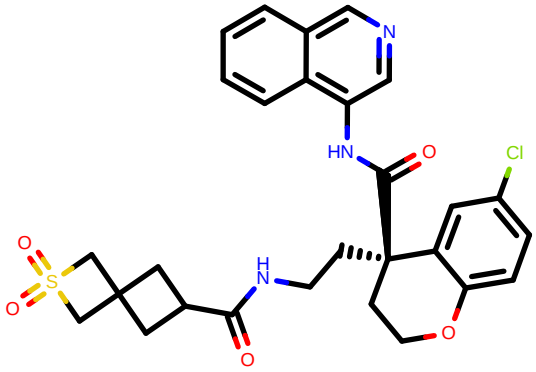
CID:	EDG-MED-ba1ac7b9-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N(CC#N)C5CC5
RUN:	RUN2645
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.51

ALP-UNI-ba800595-2_2



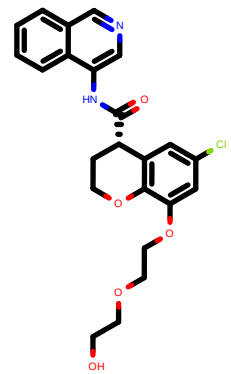
CID:	ALP-UNI-ba800595-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(c(c4)F)Cl
RUN:	RUN3077
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.21

DAR-DIA-f6ee7aeb-3_3



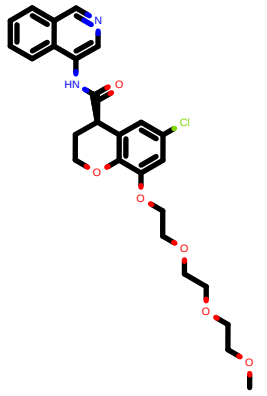
CID:	DAR-DIA-f6ee7aeb-3_3
SMILES:	CCCOc1cc(cc(c1)Cl)[C@@H]2CC(=O)N(C[C@H]2c3ccccc3C#N)c4cncc5c4cccc5
RUN:	RUN3409
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.20

ALP-POS-2da19ca7-8_1



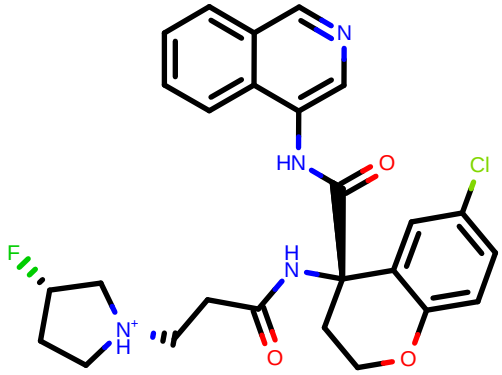
CID:	ALP-POS-2da19ca7-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H](CC(=O)N)C5CCOCC5
RUN:	RUN2394
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.28

ALP-UNI-3496895b-11_1



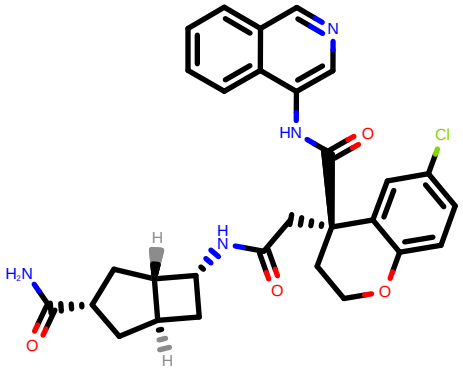
CID:	ALP-UNI-3496895b-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)Cc6n[n-]nn6
RUN:	RUN2526
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.47

MAK-UNK-c749d764-4_4



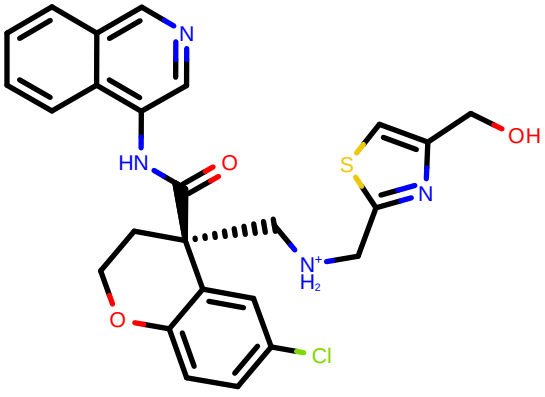
CID:	MAK-UNK-c749d764-4_4
SMILES:	CS[C@H]1CCC[C@H]([C@@H]1O)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN917
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.36

EDG-MED-971238d3-11_1



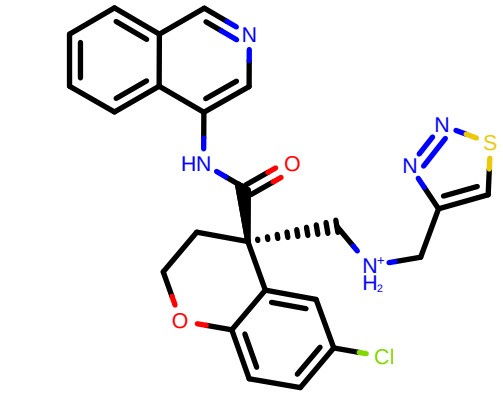
CID:	EDG-MED-971238d3-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)[O-]
RUN:	RUN1476
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.34

EDJ-MED-93390d0c-4_1



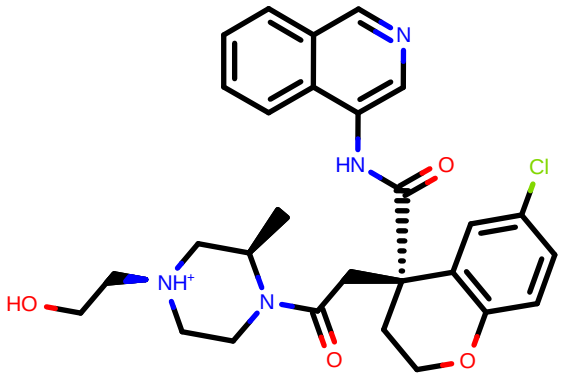
CID:	EDJ-MED-93390d0c-4_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cc(cc4)S(=O)(=O)C
RUN:	RUN4525
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.25

ED_-GRI-5b13fbe2-24_1



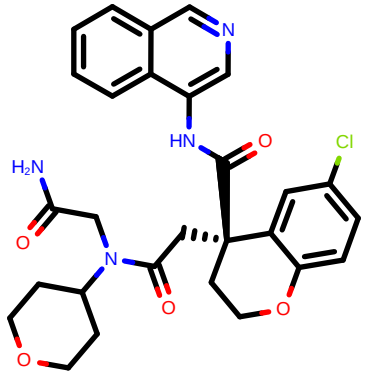
CID:	ED_-GRI-5b13fbe2-24_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(nn5)CC6C[NH2+]C6
RUN:	RUN1555
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.36

ALP-POS-c3a96089-4_1



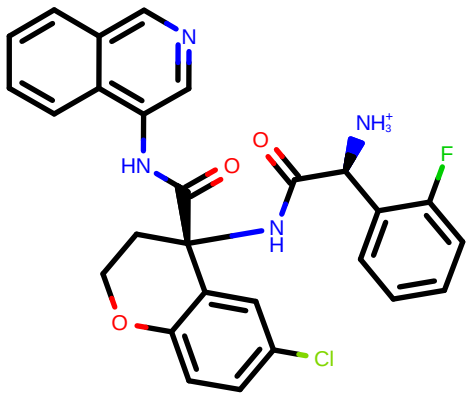
CID:	ALP-POS-c3a96089-4_1
SMILES:	CC(=O)Nc1ccc(cn1)N(Cc2cccc(c2)Cl)C(=O)Cc3cncc4c3cccc4
RUN:	RUN1188
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.32

ERI-UCB-d6de1f3c-6_2



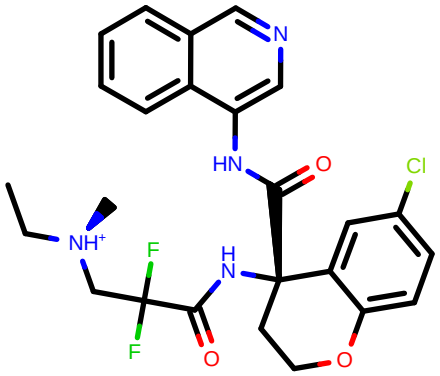
CID:	ERI-UCB-d6de1f3c-6_2
SMILES:	c1ccc2c(c1)cncc2C(=O)N3C[C@H](N(C(=O)C3)c4cccc(c4)Cl)C[NH+]5CCCCC5
RUN:	RUN1102
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.35

MIC-UNK-d854bf4c-8_1



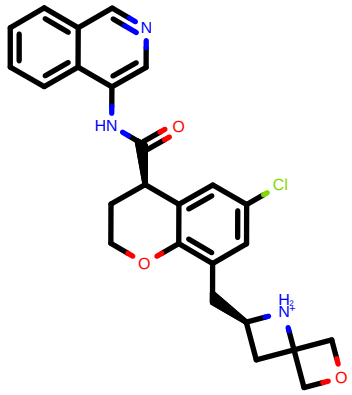
CID:	MIC-UNK-d854bf4c-8_1
SMILES:	CS(=O)(=O)N1CCC2(CC1)CCN(C(=O)[C@@H]2c3ccc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN3344
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.17

MAK-UNK-ffc90da7-4_5



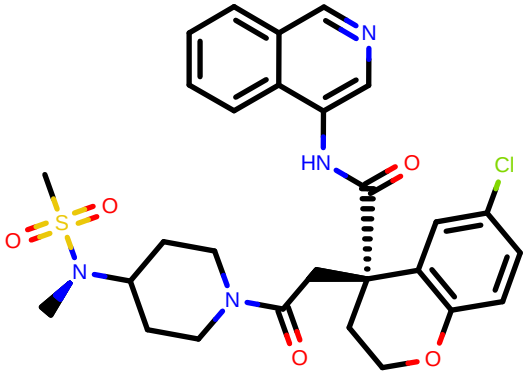
CID:	MAK-UNK-ffc90da7-4_5
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN700
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.29

DAR-DIA-0cde14eb-60_2



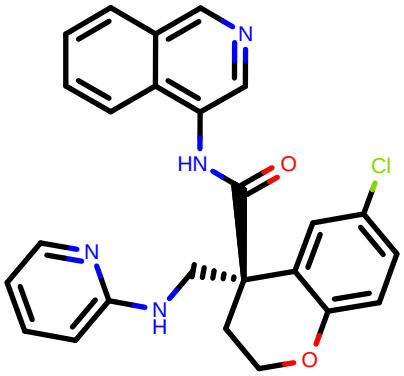
CID:	DAR-DIA-0cde14eb-60_2
SMILES:	C[C@H](c1cccc(c1)C2(CC2)C#N)C(=O)Nc3cncc4c3cccc4
RUN:	RUN32
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.38

LON-WEI-5e7d1b3e-21_1



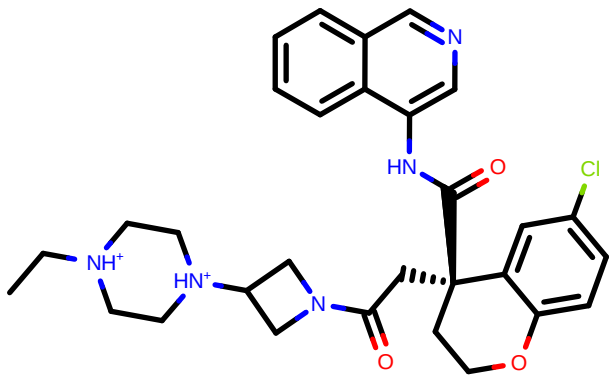
CID:	LON-WEI-5e7d1b3e-21_1
SMILES:	Cc1cccnc1NC(=O)Nc2cn(c(=O)c3c2cccc3)CC(C)C
RUN:	RUN1326
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.67

EDJ-MED-7587a9ee-2_2



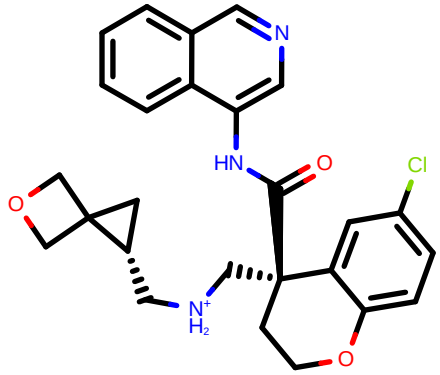
CID:	EDJ-MED-7587a9ee-2_2
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@@]3(C1)CCCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN4335
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.19

DAR-DIA-0d514e7d-31_15



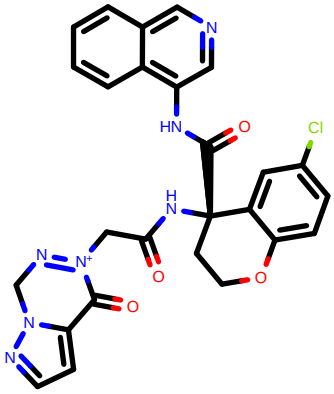
CID:	DAR-DIA-0d514e7d-31_15
SMILES:	C[C@@H]1CCO[C@H]2C=CC(=C[C@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN848
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.32

RAL-THA-05e671eb-20_1



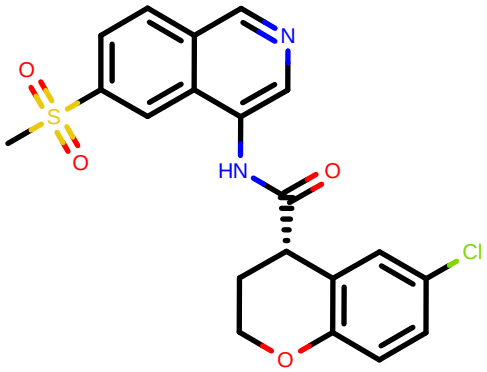
CID:	RAL-THA-05e671eb-20_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C#N)Cl
RUN:	RUN2044
DDG (kcal/mol):	-0.63
dDDG (kcal/mol):	0.33

RAL-THA-6e4c80cf-3_1



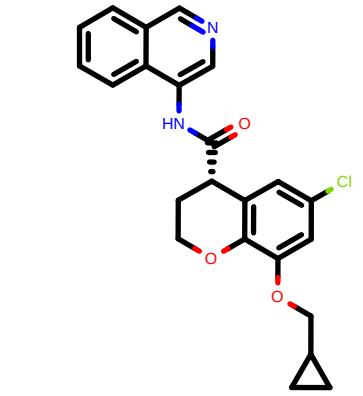
CID:	RAL-THA-6e4c80cf-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CN(Cc4c3cc(cc4)Cl)C(=O)OCc5cncs5
RUN:	RUN3898
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.18

MAT-POS-b3e365b9-2_1



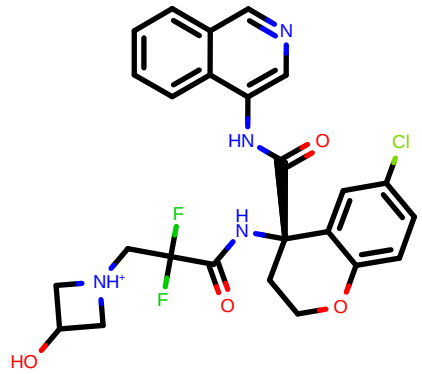
CID:	MAT-POS-b3e365b9-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN277
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.12

DAR-DIA-9e4459de-15_4



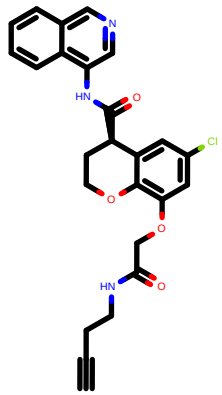
CID:	DAR-DIA-9e4459de-15_4
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1446
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.24

DAR-DIA-2964957d-9_1



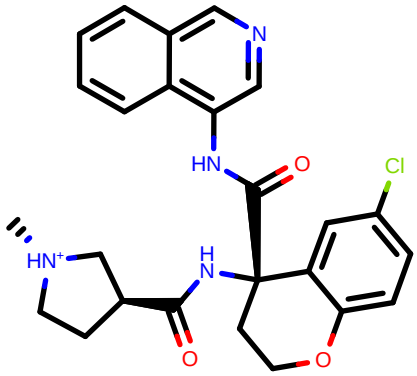
CID:	DAR-DIA-2964957d-9_1
SMILES:	CN(c1cccc(c1)Cl)c2c(c(=O)c2=O)Nc3cncc4c3cccc4
RUN:	RUN518
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.29

MAT-POS-8293a91a-3_2



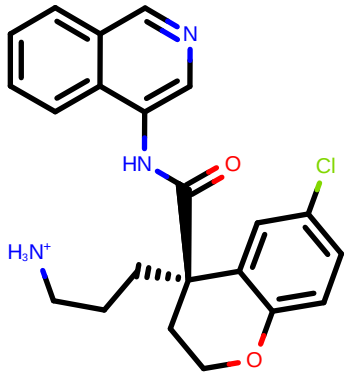
CID:	MAT-POS-8293a91a-3_2
SMILES:	c1cc2cncc(c2cc1C(F)(F)F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN5086
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.21

LON-WEI-9739a092-7_1



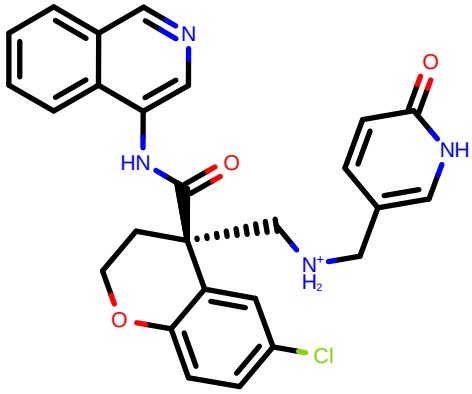
CID:	LON-WEI-9739a092-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)NCc4ccc(cc4)Br
RUN:	RUN3271
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.22

EDJ-MED-e4b030d8-1_1



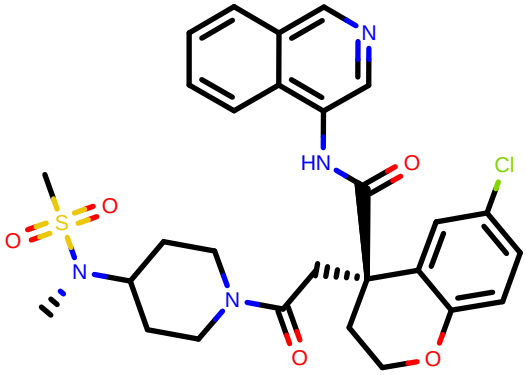
CID:	EDJ-MED-e4b030d8-1_1
SMILES:	C[C@@]1(c2cc(ccc2OCC1=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN283
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.29

EDG-MED-90036822-49_1



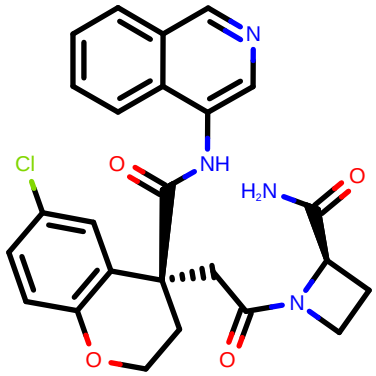
CID:	EDG-MED-90036822-49_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cc5cnc[nH]5
RUN:	RUN1727
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.42

RAL-THA-e002e396-13_1



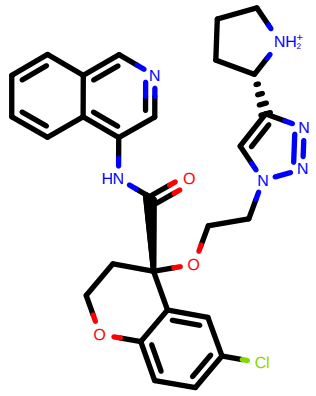
CID:	RAL-THA-e002e396-13_1
SMILES:	c1ccc(cc1)OC[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3479
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.14

MAK-UNK-c749d764-33_2



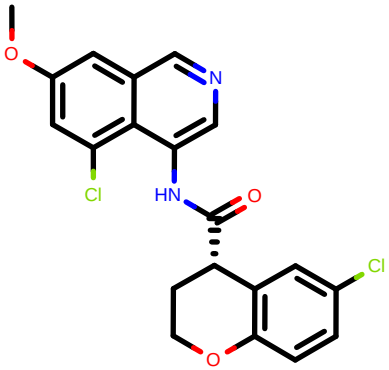
CID:	MAK-UNK-c749d764-33_2
SMILES:	CS(=O)(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1080
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.20

DAR-DIA-0f2f46c9-8_2



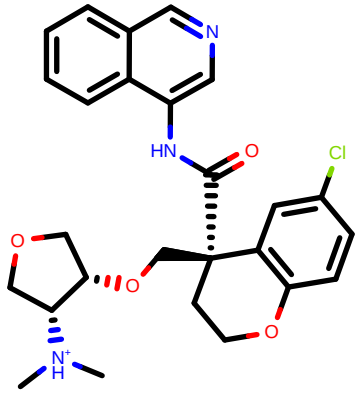
CID:	DAR-DIA-0f2f46c9-8_2
SMILES:	CNS(=O)(=O)[N@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3238
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.23

RAL-THA-4aa06b95-7_3



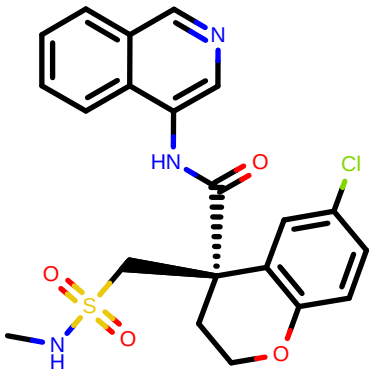
CID:	RAL-THA-4aa06b95-7_3
SMILES:	COCCN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1245
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.13

MIC-UNK-5a93dd5f-7_8



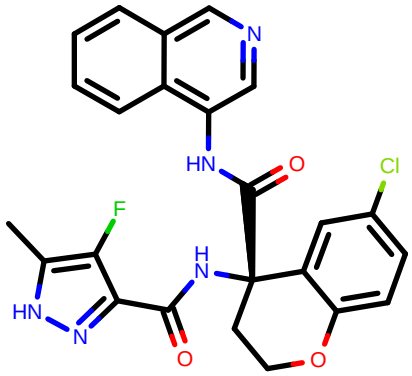
CID:	MIC-UNK-5a93dd5f-7_8
SMILES:	CC(=O)N(C)[C@H]1CC[N@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN777
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.25

LAU-MED-88a3970a-3_1



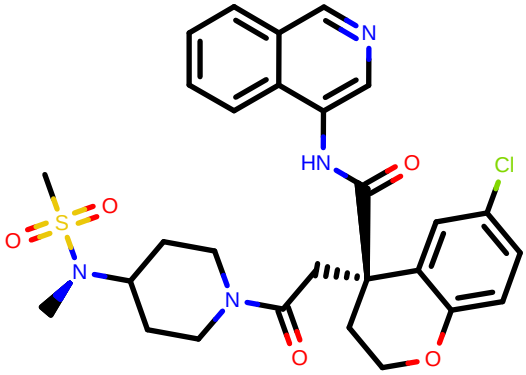
CID:	LAU-MED-88a3970a-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCCCO)Cl
RUN:	RUN1501
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.15

DAR-DIA-0f2f46c9-9_1



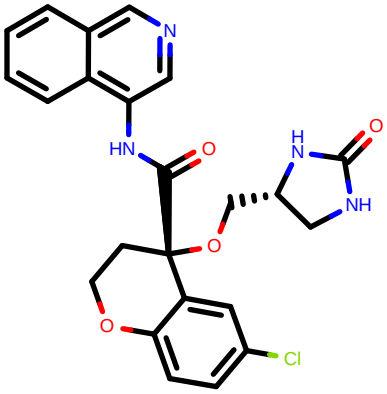
CID:	DAR-DIA-0f2f46c9-9_1
SMILES:	CNS(=O)(=O)[N@@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3240
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-3_14



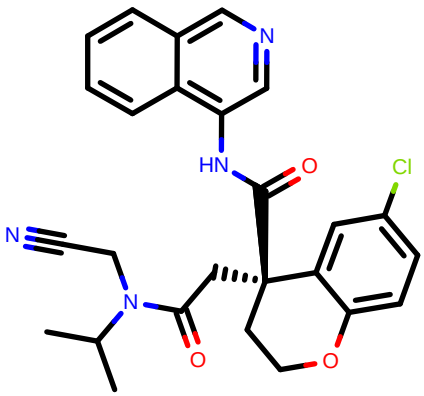
CID:	MIC-UNK-5a93dd5f-3_14
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@@H+]4CC[C@H]5CCCC[C@H]5C4
RUN:	RUN753
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.23

MAR-UCB-6ab2ec87-6_1



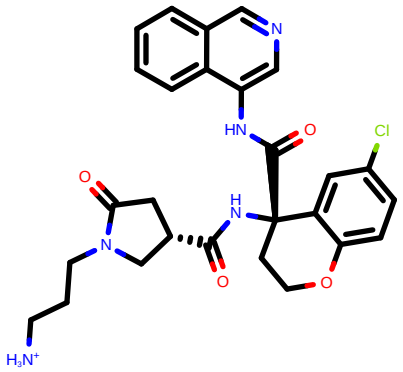
CID:	MAR-UCB-6ab2ec87-6_1
SMILES:	C[N@@]1C[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3029
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.14

ERI-UCB-d6de1f3c-7_1



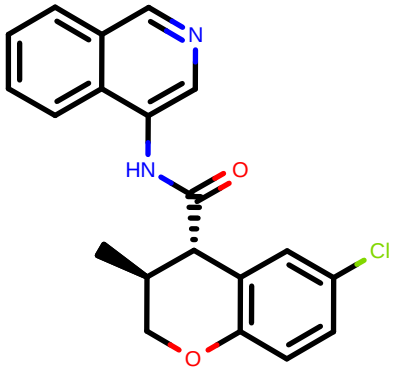
CID:	ERI-UCB-d6de1f3c-7_1
SMILES:	C[C@@H]1CN(CC(=O)N1c2cccc(c2)Cl)C(=O)c3cncc4c3cccc4
RUN:	RUN1099
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.36

ALP-POS-64a710fa-2_1



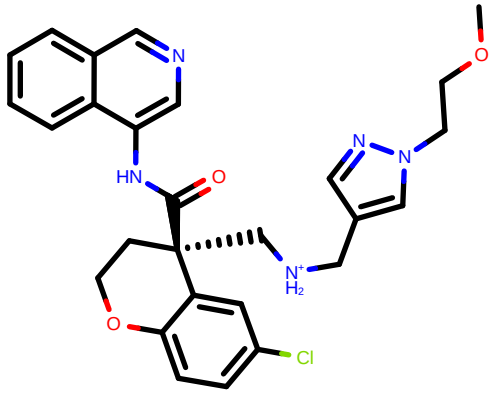
CID:	ALP-POS-64a710fa-2_1
SMILES:	C[NH+](C)CCCN(Cc1cccs1)C(=O)Cc2cncc3c2cccc3
RUN:	RUN465
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.35

MAT-POS-b5746674-34_1



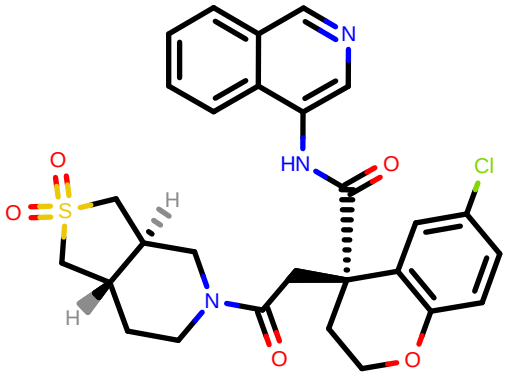
CID:	MAT-POS-b5746674-34_1
SMILES:	CCCC[N@@H+](CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C)Cc3ccco3
RUN:	RUN66
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.12

EDG-MED-90036822-23_2



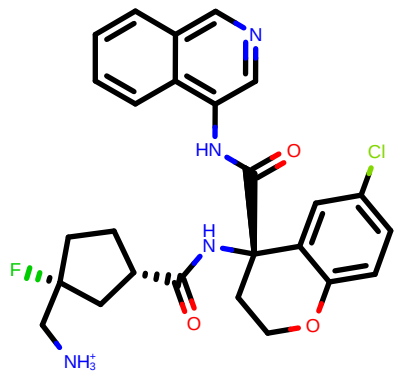
CID:	EDG-MED-90036822-23_2
SMILES:	C[C@H](CCc1c(n[nH]n1)C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)[NH3+]
RUN:	RUN1694
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.50

DAR-DIA-0d514e7d-32_23



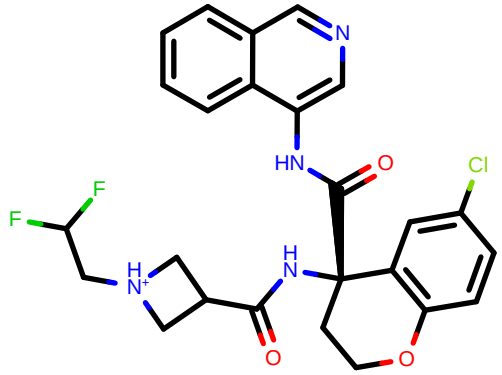
CID:	DAR-DIA-0d514e7d-32_23
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3[C@H]4C[C@H]4CO[C@@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN872
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.24

DAR-DIA-0f2f46c9-2_1



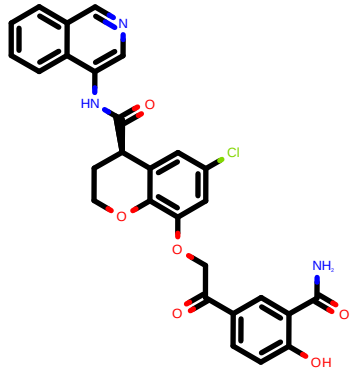
CID:	DAR-DIA-0f2f46c9-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC[N@@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3222
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.19

VLA-UCB-34f3ed0c-15_1



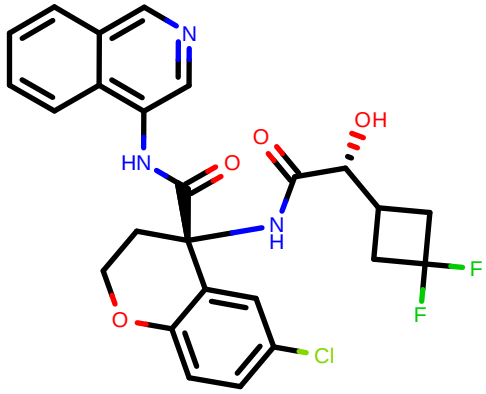
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+]CC6
RUN:	RUN639
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.27

EDG-MED-ba1ac7b9-12_2



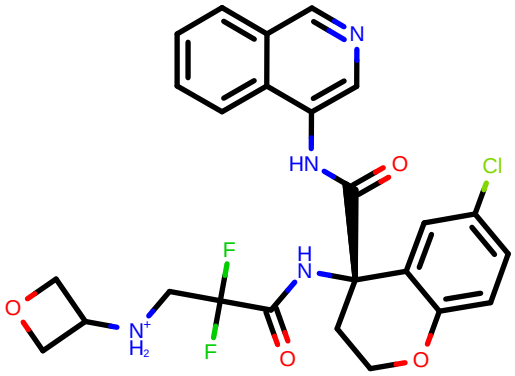
CID:	EDG-MED-ba1ac7b9-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@@H]5c6n[n-]nn6
RUN:	RUN2659
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.43

EDJ-MED-6d9ff7d0-8_1



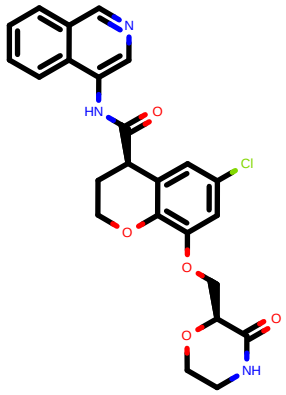
CID:	EDJ-MED-6d9ff7d0-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)[NH2+]C[C@@H]5CCC(=O)N5
RUN:	RUN3433
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.15

PET-UNK-55f647aa-1_1



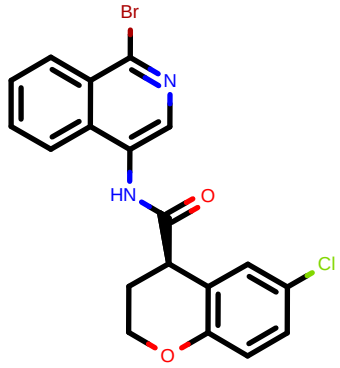
CID:	PET-UNK-55f647aa-1_1
SMILES:	CN(C)c1ccc(nc1)N(Cc2ccsc2)C(=O)Cc3cncc4c3cccc4
RUN:	RUN569
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.42

ALP-POS-5bb456a5-2_8



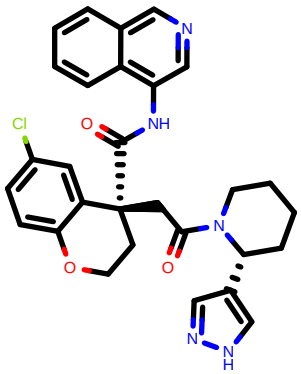
CID:	ALP-POS-5bb456a5-2_8
SMILES:	C[C@H]1C[N@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2429
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.42

MAT-POS-b5746674-109_1



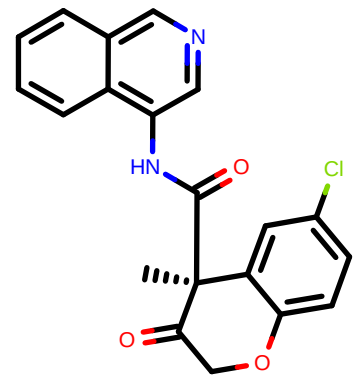
CID:	MAT-POS-b5746674-109_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCC[NH+]3CCOCC3
RUN:	RUN92
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.23

EDJ-MED-670ad2ee-6_2



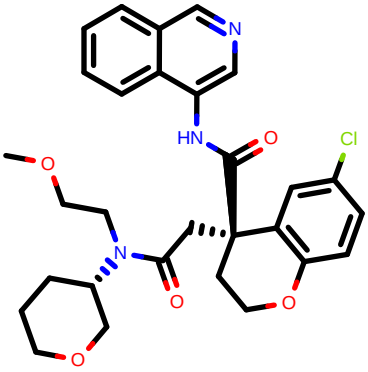
CID:	EDJ-MED-670ad2ee-6_2
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)C5CC5
RUN:	RUN3870
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.22

EDG-MED-ba1ac7b9-28_4



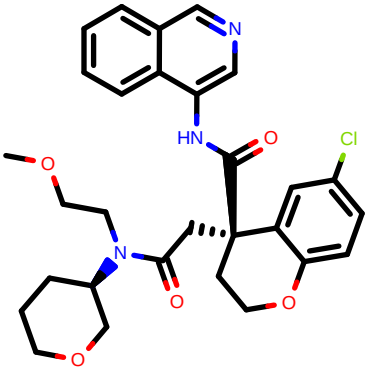
CID:	EDG-MED-ba1ac7b9-28_4
SMILES:	C[N@H+](CCO)C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2735
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.12

ALP-POS-f13221e1-2_1



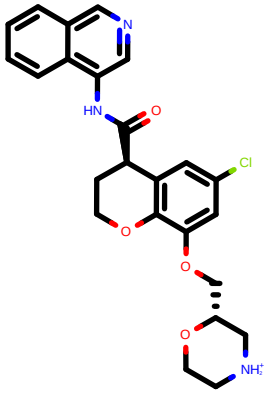
CID:	ALP-POS-f13221e1-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)COc3cccc(c3)Cl
RUN:	RUN183
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.37

MAT-POS-8a69d52e-2_1



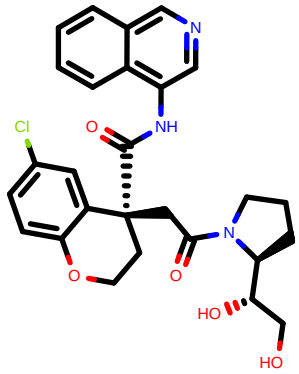
CID:	MAT-POS-8a69d52e-2_1
SMILES:	C[C@@H]1C[C@@H](c2cc(ccc2O1)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN364
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.47

MAT-POS-24589f88-12_2



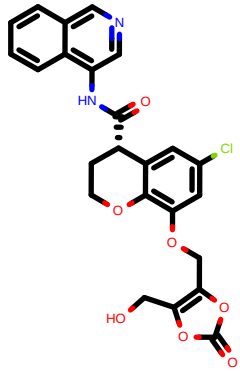
CID:	MAT-POS-24589f88-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5ccc(cc5)S(=O)(=O)N
RUN:	RUN4799
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.21

KAD-UNI-877d7bed-12_1



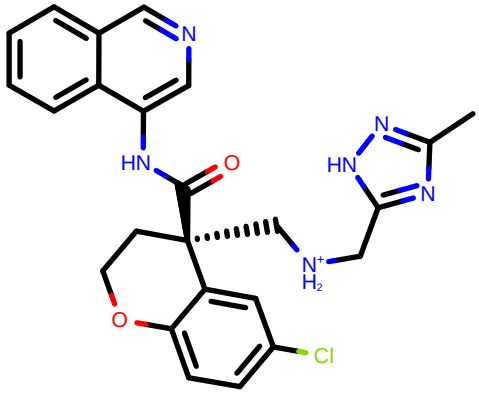
CID:	KAD-UNI-877d7bed-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCC[C@@H]5C(=O)NC(=O)N5)Cl
RUN:	RUN3751
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.24

MIC-UNK-54748b58-2_1



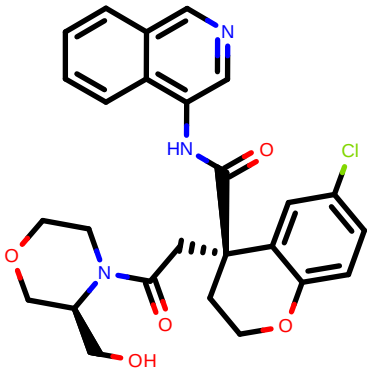
CID:	MIC-UNK-54748b58-2_1
SMILES:	CNC(=O)C[N@@]1C[C@@](c2cc(ccc2S1(=O)=O)Cl)(C(=O)Nc3cncc4c3cccc4)OC
RUN:	RUN4851
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.45

KAD-UNI-8a629cb0-26_1



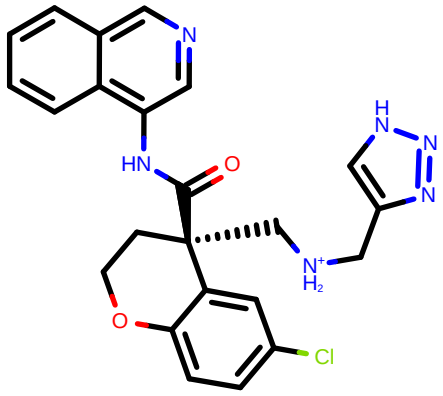
CID:	KAD-UNI-8a629cb0-26_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)N5CC6(C5)CCO6
RUN:	RUN2106
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.34

KAD-UNI-877d7bed-11_2



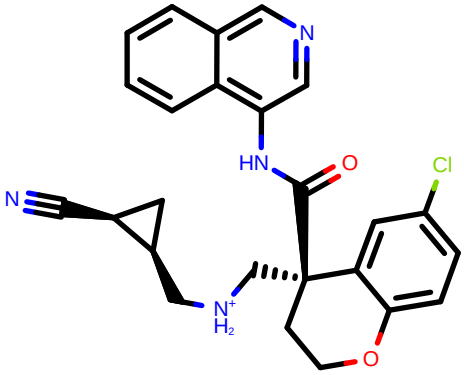
CID:	KAD-UNI-877d7bed-11_2
SMILES:	CC(C)([C@H]1CCN(C1)C(=O)COc2cc(cc3c2OCC[C@@H]3C(=O)Nc4cncc5c4cccc5)Cl)O
RUN:	RUN3748
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.21

ALP-POS-347519b5-3_53



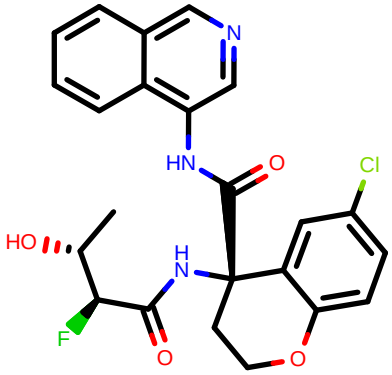
CID:	ALP-POS-347519b5-3_53
SMILES:	CS(=O)(=O)N[C@@]1C[C@@H]2[C@H]3CC[C@@H]([C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4321
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.24

MAT-POS-fc9ede84-1_2



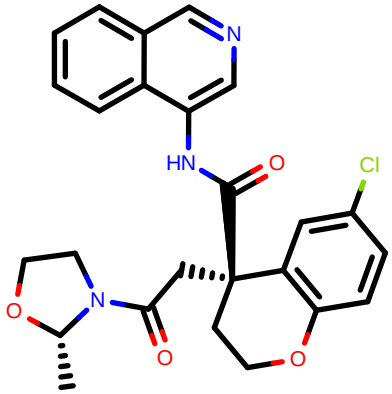
CID:	MAT-POS-fc9ede84-1_2
SMILES:	CN(C)C(=O)COC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4408
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.22

MAT-POS-78e1d523-5_1



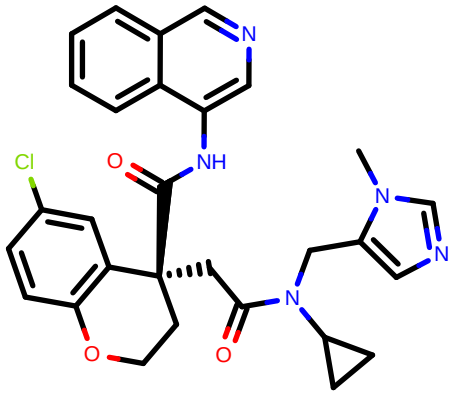
CID:	MAT-POS-78e1d523-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN3282
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.13

MAT-POS-8d5af1ef-1_2



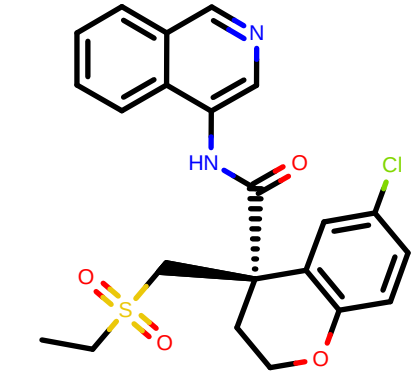
CID:	MAT-POS-8d5af1ef-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC(=O)Nc4c3cc(cc4)Br
RUN:	RUN1129
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.26

ALP-POS-780445ae-2_2



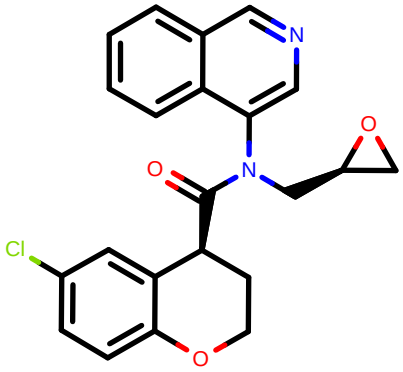
CID:	ALP-POS-780445ae-2_2
SMILES:	CC(C)(C)c1ccc(cc1)N([C@H](c2cncc3c2cccc3)C(=O)NCC[NH+]4CCOCC4)C(=O)c5cocn5
RUN:	RUN1175
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.27

LAU-MED-88a3970a-7_1



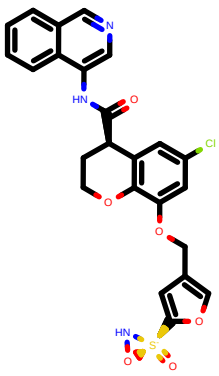
CID:	LAU-MED-88a3970a-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4CCCCO)Cl
RUN:	RUN1502
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.16

LON-WEI-5e7d1b3e-59_2



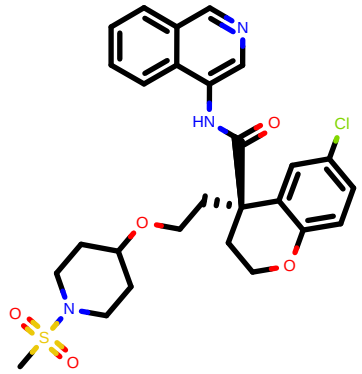
CID:	LON-WEI-5e7d1b3e-59_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)N(Cc3ccco3)C[C@H]4CCCO4
RUN:	RUN1370
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.25

EDJ-MED-fcba3f31-5_1



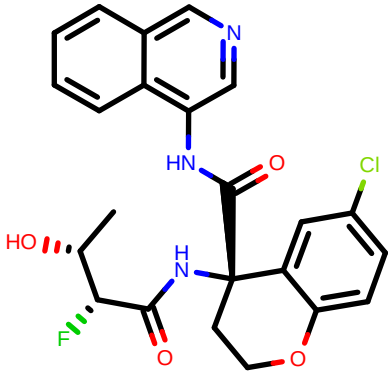
CID:	EDJ-MED-fcba3f31-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)COC[C@H](CO)F
RUN:	RUN2547
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.39

DAR-DIA-0d514e7d-32_8



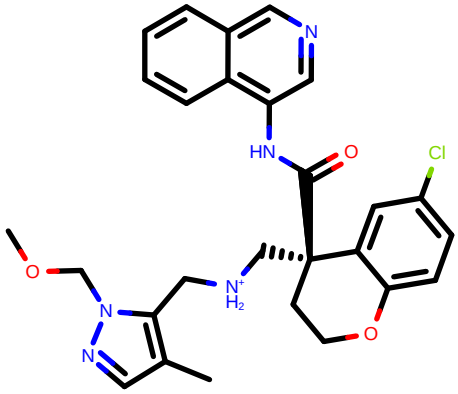
CID:	DAR-DIA-0d514e7d-32_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@H]4C[C@H]4CO[C@@H]5[C@@H]3C=C(C=C5)Cl
RUN:	RUN857
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.35

MAT-POS-fb82b63d-3_3



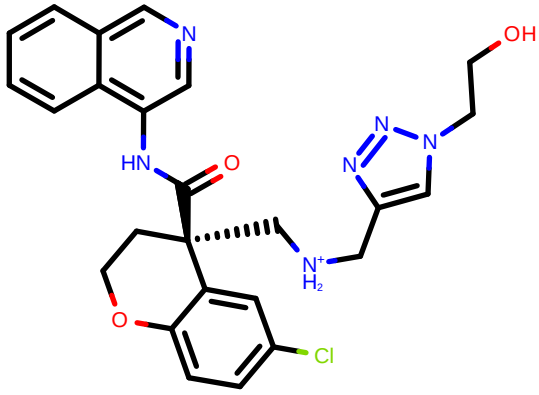
CID:	MAT-POS-fb82b63d-3_3
SMILES:	C[N@@H+]1CCc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3175
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.12

EDJ-MED-93390d0c-2_2



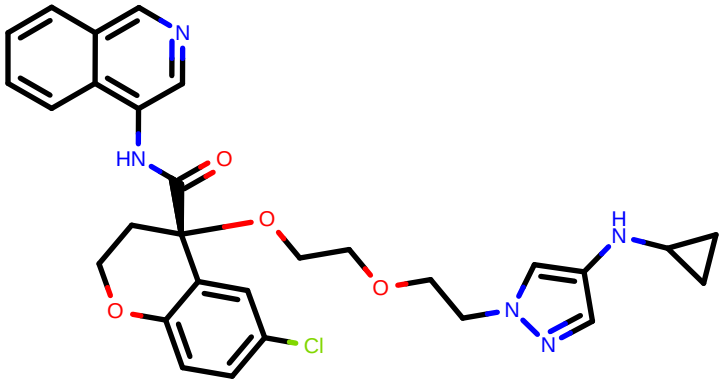
CID:	EDJ-MED-93390d0c-2_2
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2NC(=O)[C@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN4519
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.27

EDJ-MED-c82a5324-2_4



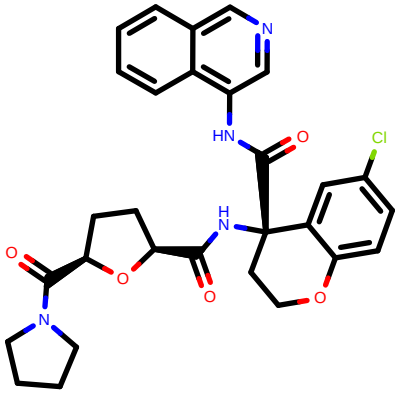
CID:	EDJ-MED-c82a5324-2_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@H+](Cc4c3cc(cc4)Cl)CC(=O)NC5COC5
RUN:	RUN4730
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.25

ALP-POS-fe871b40-7_1



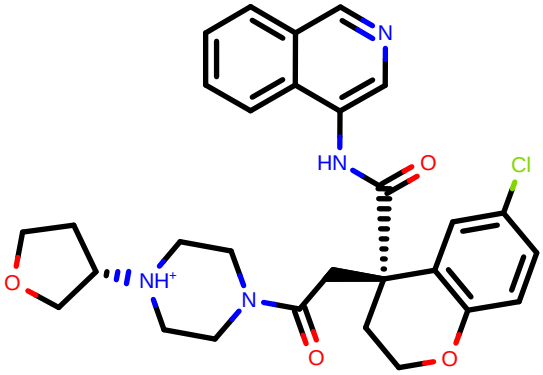
CID:	ALP-POS-fe871b40-7_1
SMILES:	CO[C@@]1(CCOc2c1cc(cn2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3119
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.27

MAT-POS-4223bc15-9_4



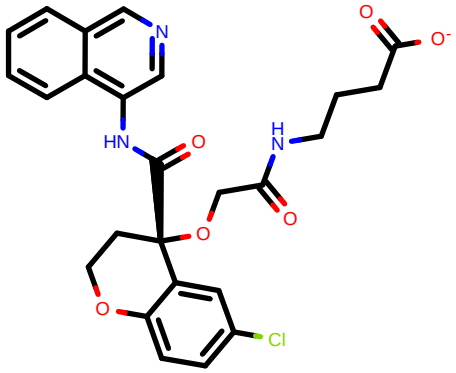
CID:	MAT-POS-4223bc15-9_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)[C@@H]5CCC[C@@H]5O
RUN:	RUN4012
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-20_1



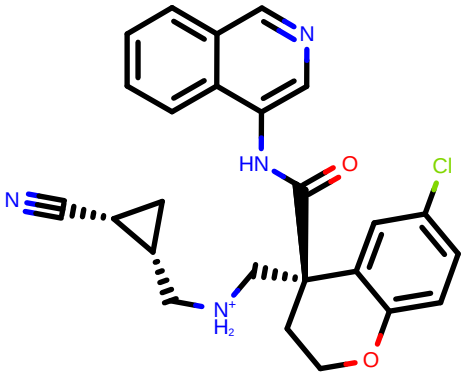
CID:	MAK-UNK-c749d764-20_1
SMILES:	CCCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1007
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.29

ALP-POS-fe871b40-11_2



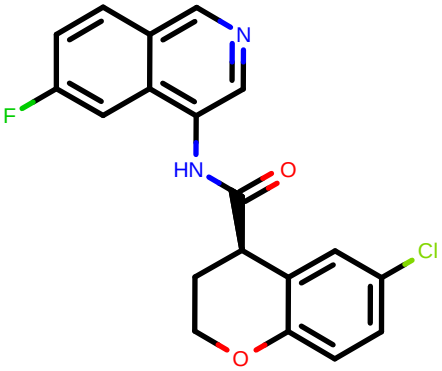
CID:	ALP-POS-fe871b40-11_2
SMILES:	CO[C@]1(CCOc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3130
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.19

EDG-MED-90036822-45_1



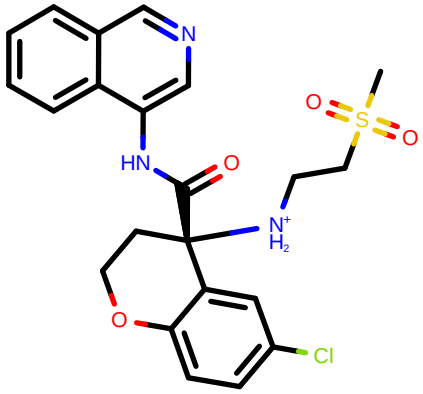
CID:	EDG-MED-90036822-45_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(c5[nH]ccn5)(F)F
RUN:	RUN1723
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.34

DAR-DIA-0f7b7cd9-8_1



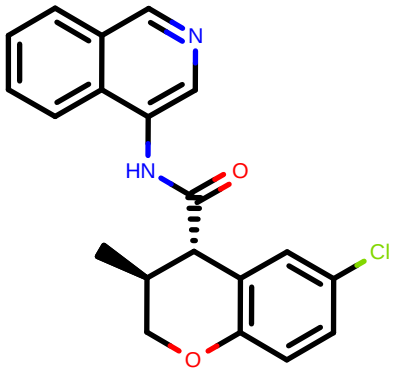
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C(=O)S3
RUN:	RUN3016
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.07

EDG-MED-971238d3-4_1



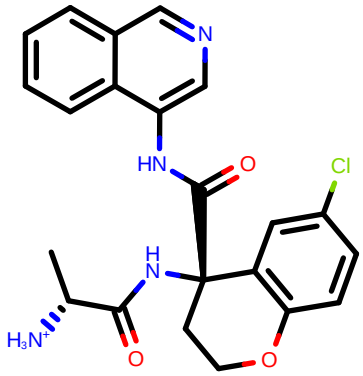
CID:	EDG-MED-971238d3-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[NH3+]
RUN:	RUN1469
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.35

ERI-UCB-ce40166b-5_2



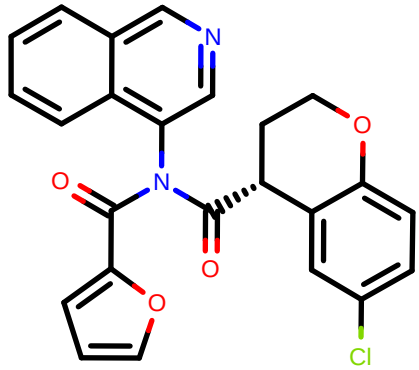
CID:	ERI-UCB-ce40166b-5_2
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Cl)O[C@H]4CC(=O)N4
RUN:	RUN41
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.11

RAL-THA-1d44ff04-11_1



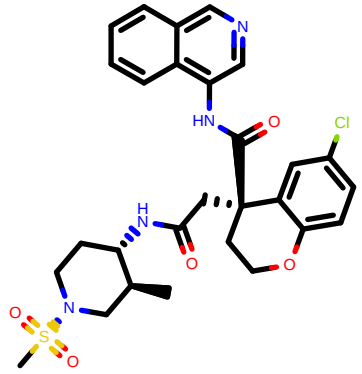
CID:	RAL-THA-1d44ff04-11_1
SMILES:	CNS(=O)(=O)c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN446
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.26

MIC-UNK-9582b2c5-1_1



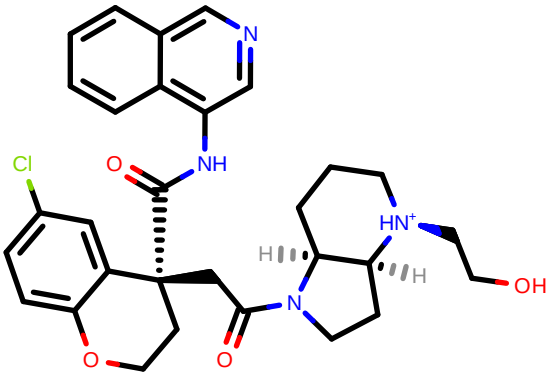
CID:	MIC-UNK-9582b2c5-1_1
SMILES:	CC(=O)N1CC[C@@H]2[C@@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN249
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.27

ALP-POS-a0a4abd7-2_2



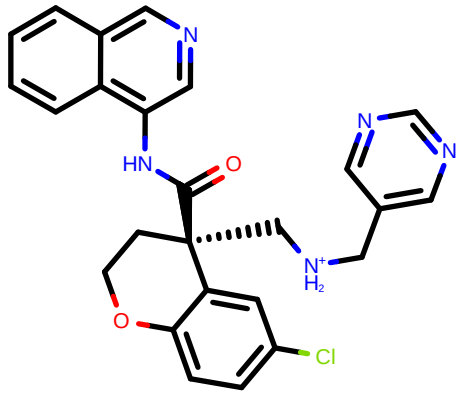
CID:	ALP-POS-a0a4abd7-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3ccc(c4)Cl)CNc5ccc[nH]c5=O
RUN:	RUN3566
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.20

RAL-THA-58fba2bc-1_1



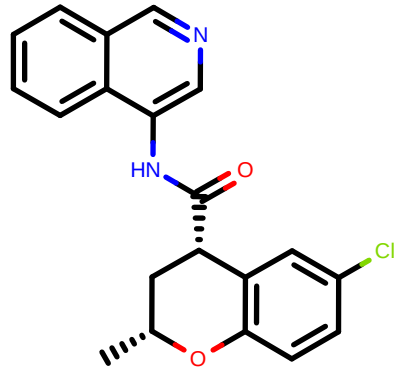
CID:	RAL-THA-58fba2bc-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)[O-]
RUN:	RUN3647
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.37

BEN-DND-d1eb1f41-7_2



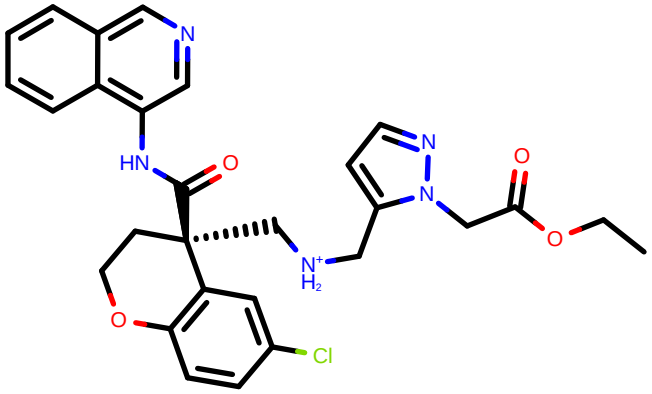
CID:	BEN-DND-d1eb1f41-7_2
SMILES:	C[N@H+]1CCN(C(=O)[C@H]1c2cccc(c2)Cl)c3cncc4c3cccc4
RUN:	RUN4353
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.23

LON-WEI-4d77710c-42_2



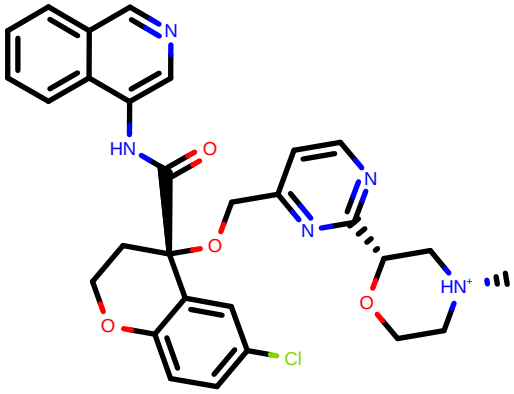
CID:	LON-WEI-4d77710c-42_2
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N[C@H]3CCCc4c3cccc4
RUN:	RUN230
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.12

NIR-THE-590dedc7-1_1



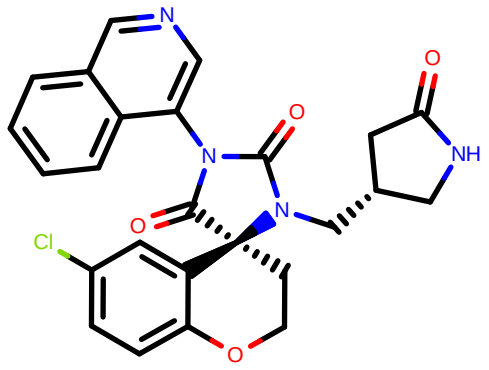
CID:	NIR-THE-590dedc7-1_1
SMILES:	CC(=O)N1CC[NH+](CC1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1940
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.50

MIC-UNK-644c43c7-1_1



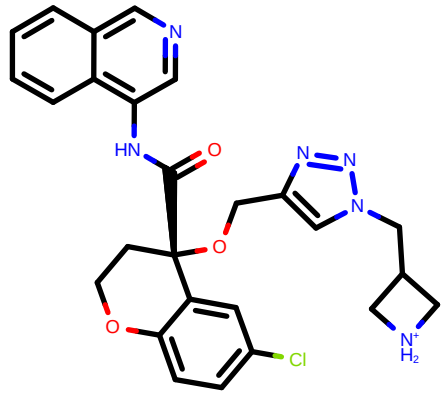
CID:	MIC-UNK-644c43c7-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CCNCC(F)(F)F
RUN:	RUN433
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.33

DAR-DIA-0d514e7d-26_1



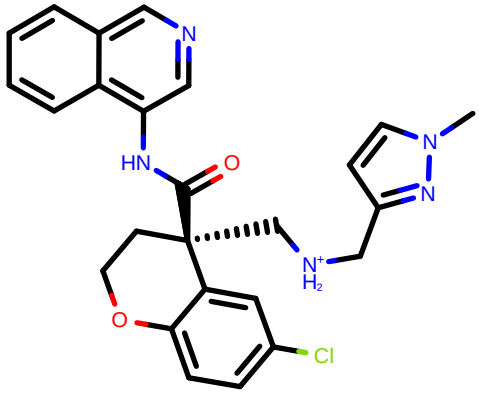
CID:	DAR-DIA-0d514e7d-26_1
SMILES:	C[C@@H]1COc2c(cc(cc2OC)Cl)[C@]1(C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN829
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.23

JAG-UCB-f37eaa14-7_1



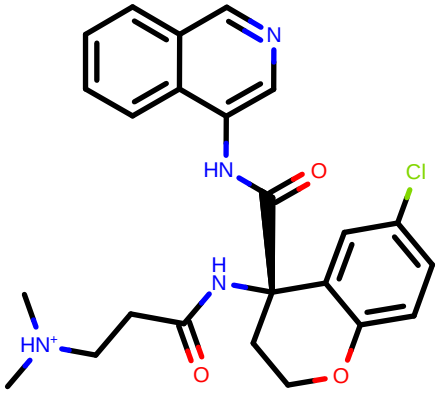
CID:	JAG-UCB-f37eaa14-7_1
SMILES:	CC[C@]1(C[C@@H](C1)[N@]2c3c(cc(cc3)Cl)[C@@]4(C2)C(=O)N(CC4)c5c6c(cnc5)cccc6)O)C
RUN:	RUN3066
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.18

EDJ-MED-c82a5324-2_1



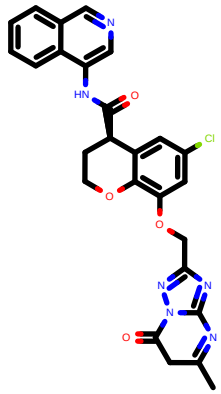
CID:	EDJ-MED-c82a5324-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@H+](Cc4c3cc(cc4)Cl)CC(=O)NC5COC5
RUN:	RUN4727
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.21

MAT-POS-53907a1c-3_2



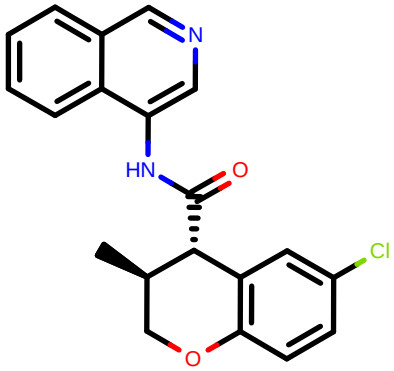
CID:	MAT-POS-53907a1c-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCC3CCCCC3)c4cc(cc(c4)Cl)O[C@H]5CC(=O)N5
RUN:	RUN526
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.43

ALP-POS-e0fe77e5-1_1



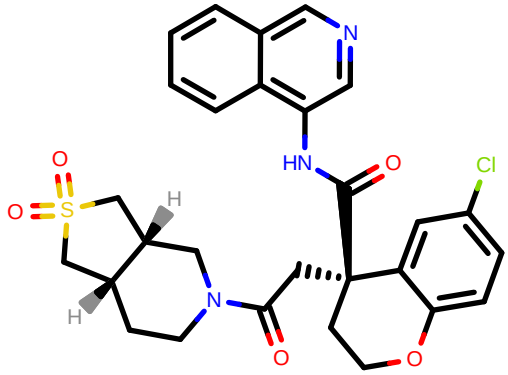
CID:	ALP-POS-e0fe77e5-1_1
SMILES:	c1ccc2c(c1)cncc2N3CCC[C@@H](C3=O)c4ccc(c(c4)Cl)Cl
RUN:	RUN2318
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.48

MAT-POS-b5746674-104_1



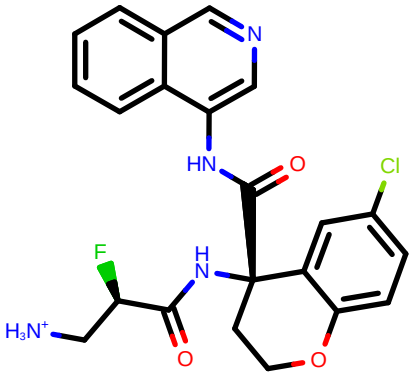
CID:	MAT-POS-b5746674-104_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)N3CCC4(CC3)OCCO4
RUN:	RUN80
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.10

MIC-UNK-0a05c952-1_2



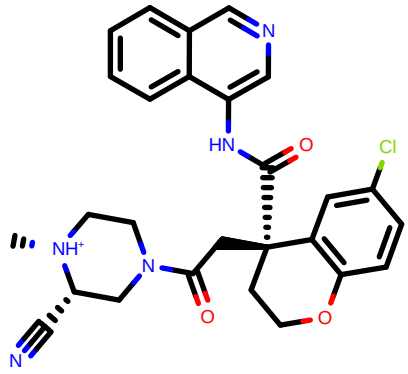
CID:	MIC-UNK-0a05c952-1_2
SMILES:	c1ccc2c(c1)cncc2N3[C@H](C[C@@H](C3=O)c4cccc(c4)Cl)[C@@H]5CO5
RUN:	RUN3497
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.18

RAL-THA-1d44ff04-6_1



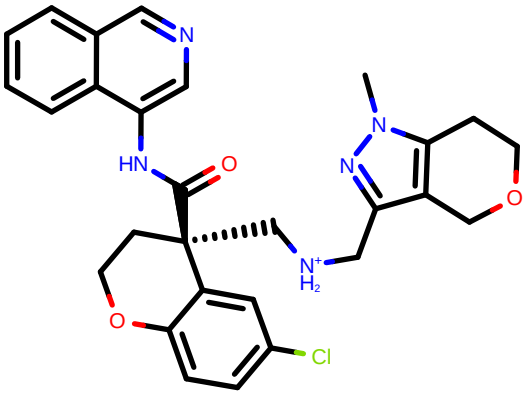
CID:	RAL-THA-1d44ff04-6_1
SMILES:	COC(=O)NCc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN443
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.53

JOH-SUS-a69c159d-5_1



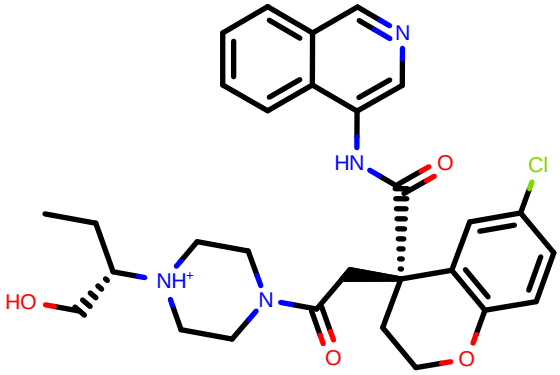
CID:	JOH-SUS-a69c159d-5_1
SMILES:	c1cc2c(cc1F)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1125
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.25

RAL-THA-05e671eb-28_2



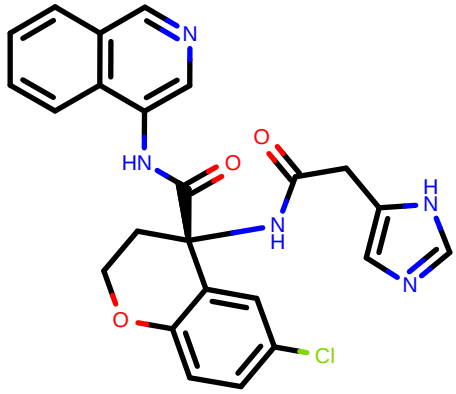
CID:	RAL-THA-05e671eb-28_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3c(c(cc4)Cl)F
RUN:	RUN2061
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.62

RAL-THA-8416115c-2_2



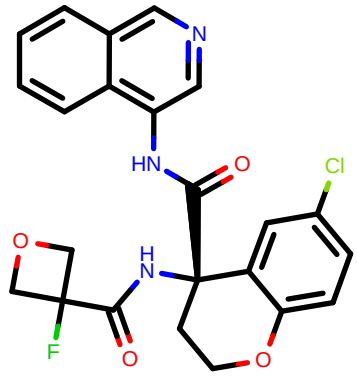
CID:	RAL-THA-8416115c-2_2
SMILES:	CN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1252
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.38

MAK-UNK-8be7dca9-9_1



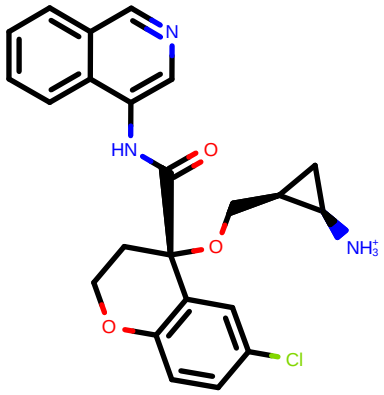
CID:	MAK-UNK-8be7dca9-9_1
SMILES:	c1cc2c(cc1C(=O)[O-])cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN508
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.27

ROB-UNI-322e8f70-1_2



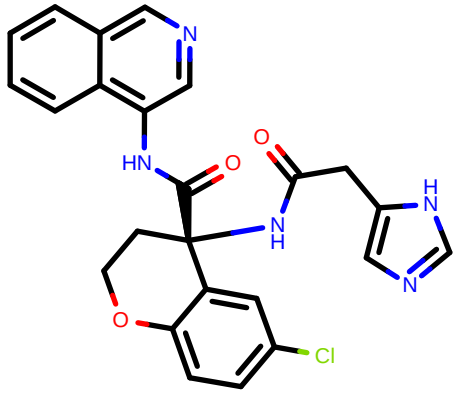
CID:	ROB-UNI-322e8f70-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4NC(=O)N3)Cl
RUN:	RUN3152
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.11

DAR-DIA-23e5a6a0-4_1



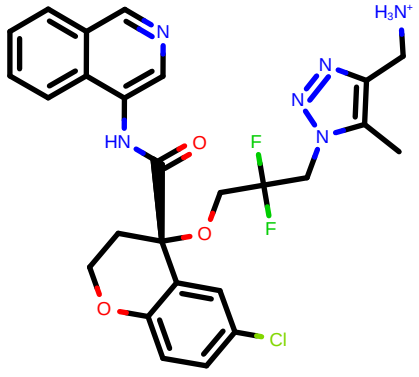
CID:	DAR-DIA-23e5a6a0-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6(CC6)C[NH2+]5)Cl
RUN:	RUN407
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.29

MIC-UNK-02d7a284-3_1



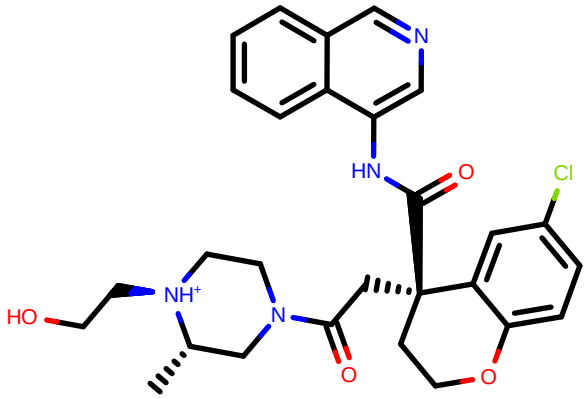
CID:	MIC-UNK-02d7a284-3_1
SMILES:	CC(=O)NC[C@@H]1CN(CC(=O)N1c2cccc(c2)Cl)C(=O)c3cncc4c3cccc4
RUN:	RUN3258
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.14

FRA-DIA-b66f7109-2_1



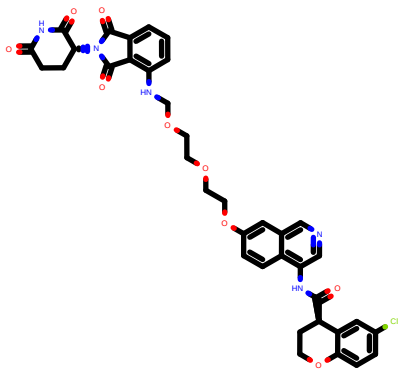
CID:	FRA-DIA-b66f7109-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COc4c3cc(cc4Cl)O[C@@H]5CC(=O)N5
RUN:	RUN393
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.36

MAT-POS-4223bc15-6_4



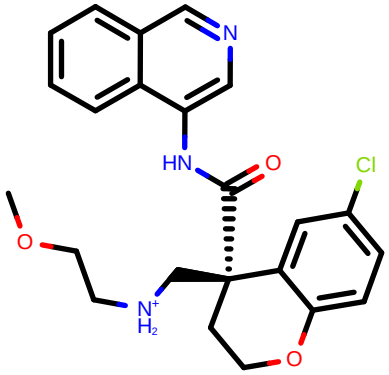
CID:	MAT-POS-4223bc15-6_4
SMILES:	CCS(=O)(=O)[N@]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3995
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.36

MIC-UNK-d854bf4c-1_2



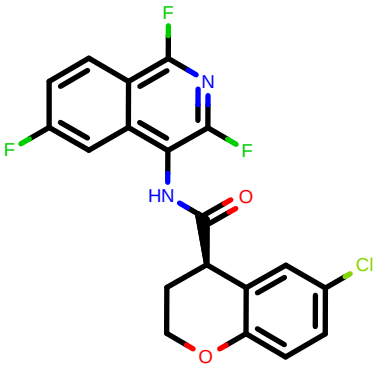
CID:	MIC-UNK-d854bf4c-1_2
SMILES:	CC(=O)N1CCC2(CC1)CN(C(=O)[C@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN3329
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.31

EDG-MED-90036822-55_1



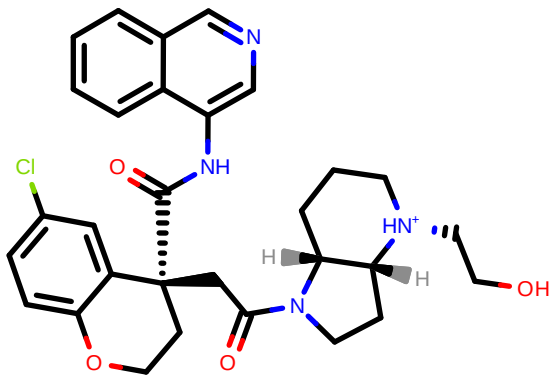
CID:	EDG-MED-90036822-55_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5ccc(nc5)N6CC(C6)[NH3+]
RUN:	RUN1735
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.45

EDJ-MED-8c98ee63-1_1



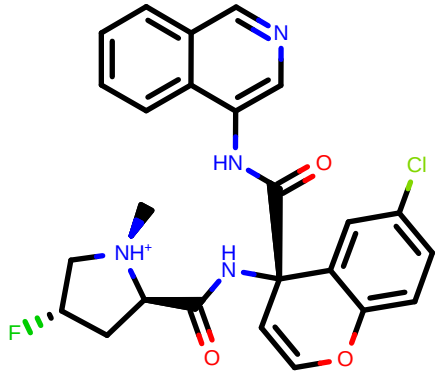
CID:	EDJ-MED-8c98ee63-1_1
SMILES:	COCCC[NH2+]C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2849
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.07

PET-UNK-8c422e11-1_1



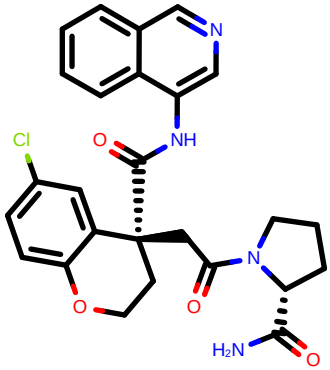
CID:	PET-UNK-8c422e11-1_1
SMILES:	CC(c1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3)(F)F
RUN:	RUN3712
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.45

MIC-UNK-cdc2493e-14_4



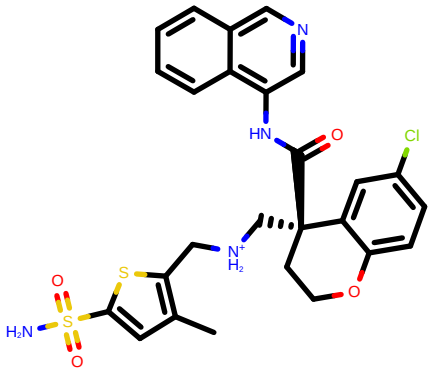
CID:	MIC-UNK-cdc2493e-14_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)[C@H]4CC[C@H](C4)[NH+]5CCCCC5
RUN:	RUN558
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.34

MAK-UNK-c749d764-25_3



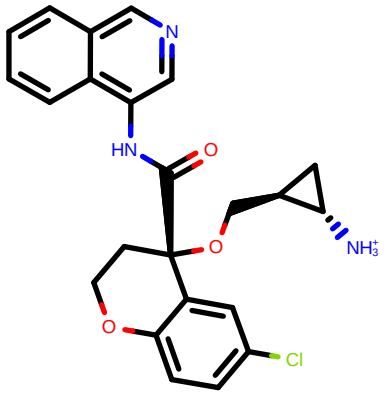
CID:	MAK-UNK-c749d764-25_3
SMILES:	COC(=O)N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1040
DDG (kcal/mol):	-0.54
dDDG (kcal/mol):	0.31

EDJ-MED-1981ceba-4_4



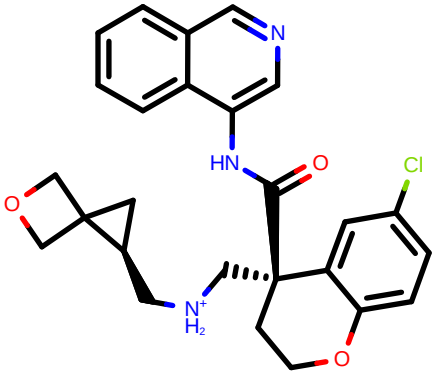
CID:	EDJ-MED-1981ceba-4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@](Cc4c3cc(cc4Cl)S(=O)(=O)N5CC(C5)C#N
RUN:	RUN4695
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.29

ALP-POS-fe871b40-15_1



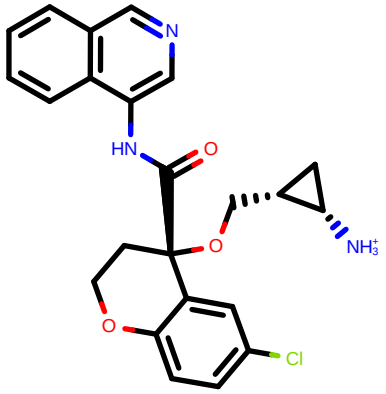
CID:	ALP-POS-fe871b40-15_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(c(c4)F)Cl
RUN:	RUN3135
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.15

RAL-THA-05e671eb-20_2



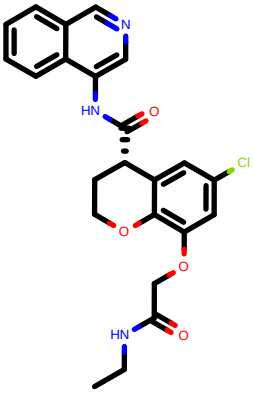
CID:	RAL-THA-05e671eb-20_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4C#N)Cl
RUN:	RUN2045
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.44

PET-UNK-c5865d42-1_2



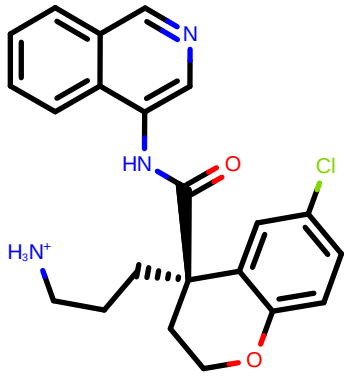
CID:	PET-UNK-c5865d42-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C[C@H]4CC[NH2+]4
RUN:	RUN424
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.31

VLA-UNK-56836b69-1_1



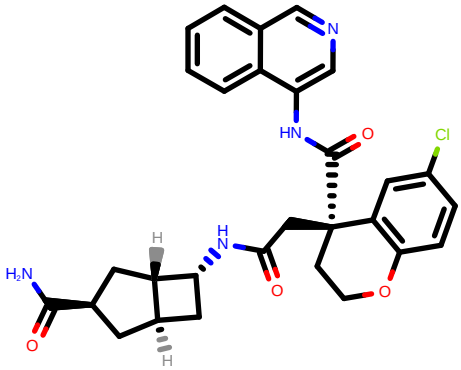
CID:	VLA-UNK-56836b69-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(c(c4)Cl)Cl
RUN:	RUN2300
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.25

ALP-UNI-8e43a71e-5_4



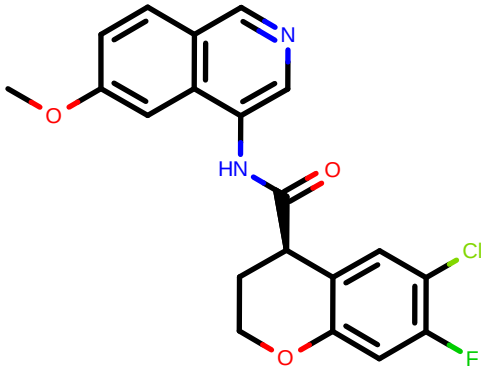
CID:	ALP-UNI-8e43a71e-5_4
SMILES:	C[C@H]1C[N@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2948
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.13

LON-WEI-5e7d1b3e-28_1



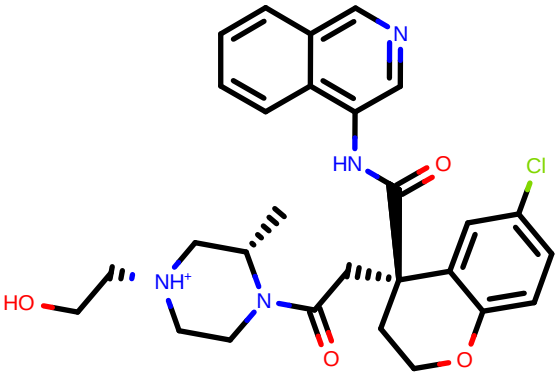
CID:	LON-WEI-5e7d1b3e-28_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCc3cc(ccc3OC)OC
RUN:	RUN1337
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.24

PET-UNK-83d689b6-4_1



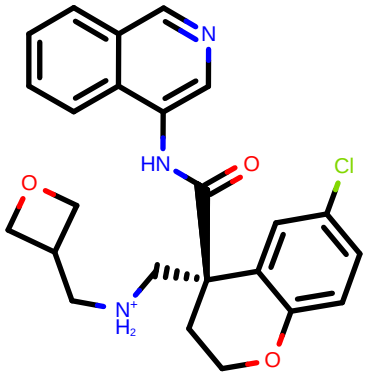
CID:	PET-UNK-83d689b6-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5nncs5
RUN:	RUN4196
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.08

EDJ-MED-670ad2ee-7_2



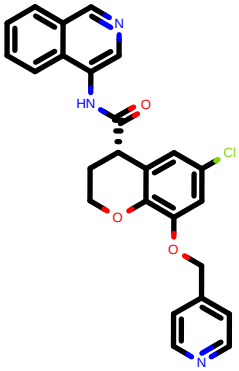
CID:	EDJ-MED-670ad2ee-7_2
SMILES:	CN(C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl
RUN:	RUN3872
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.33

EDG-MED-90036822-90_1



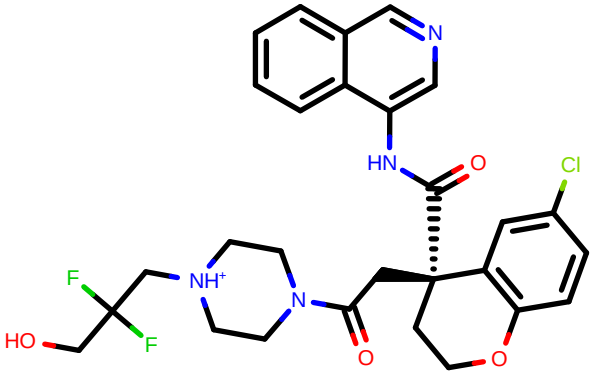
CID:	EDG-MED-90036822-90_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](c5ccccc5F)[NH3+]
RUN:	RUN1795
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.31

EDG-MED-90036822-60_1



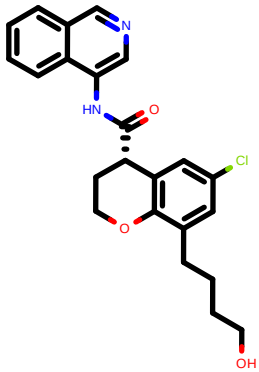
CID:	EDG-MED-90036822-60_1
SMILES:	C[C@@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)n5ccnc5
RUN:	RUN1738
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.24

LON-WEI-5e7d1b3e-33_1



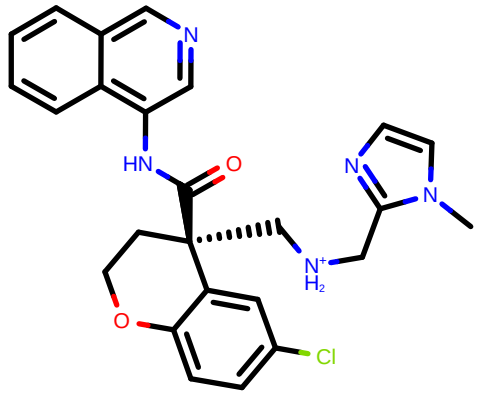
CID:	LON-WEI-5e7d1b3e-33_1
SMILES:	C[C@@H]1c2cc(c(cc2CCN1C(=O)Nc3cn(c(=O)c4c3cccc4)C)OC)OC
RUN:	RUN1334
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.39

ALP-POS-477dc5b7-2_1



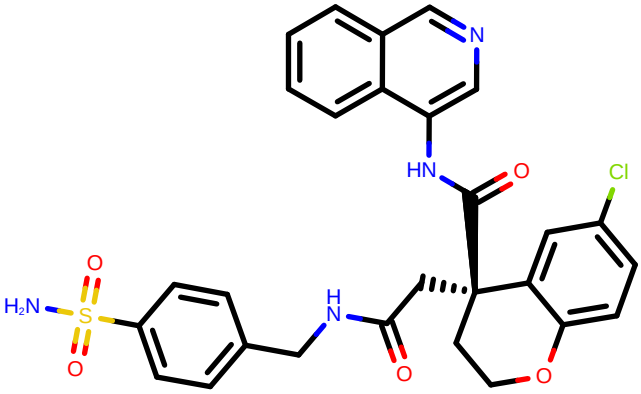
CID:	ALP-POS-477dc5b7-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN299
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.23

EDJ-MED-d1555997-2_1



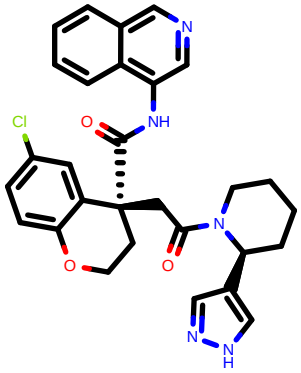
CID:	EDJ-MED-d1555997-2_1
SMILES:	Cc1cccc2c1c(cnc2)NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)C
RUN:	RUN4346
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.27

LAU-MED-88a3970a-16_1



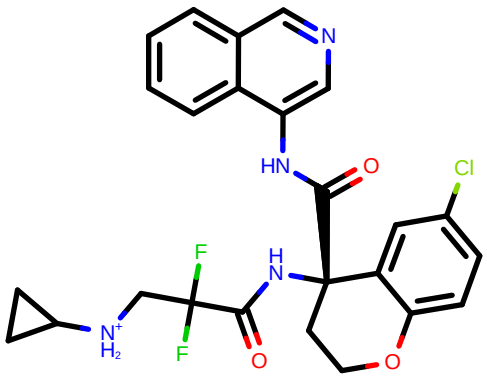
CID:	LAU-MED-88a3970a-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4CCS(=O)(=O)N)Cl
RUN:	RUN1512
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.35

EDJ-MED-841e0cf0-5_4



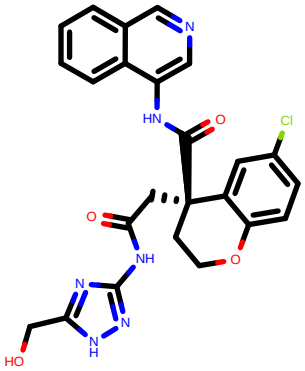
CID:	EDJ-MED-841e0cf0-5_4
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)C5CC5
RUN:	RUN3839
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.21

VLA-UCB-34f3ed0c-20_1



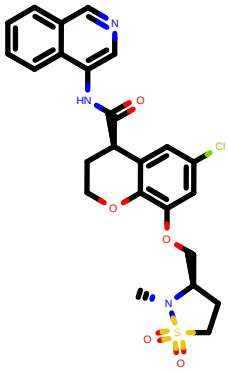
CID:	VLA-UCB-34f3ed0c-20_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)c3cnc[nH]3)C(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN647
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.33

MAK-UNK-c749d764-24_7



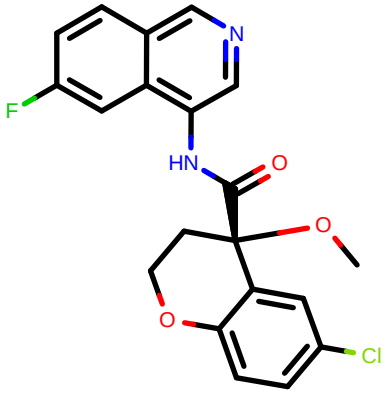
CID:	MAK-UNK-c749d764-24_7
SMILES:	CCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1037
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.40

ALP-UNI-76695c4f-10_1



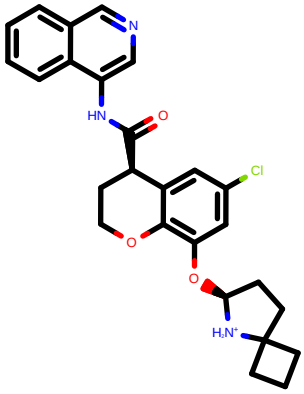
CID:	ALP-UNI-76695c4f-10_1
SMILES:	C[C@]12CN(C[C@]1(C(=O)NC2=O)C)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2174
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.36

PET-UNK-83d689b6-2_1



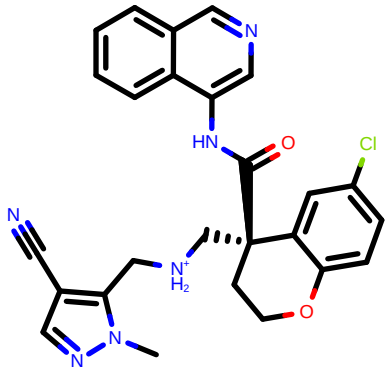
CID:	PET-UNK-83d689b6-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCc5cccnn5
RUN:	RUN4194
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.07

VLA-UCB-1dbca3b4-10_1



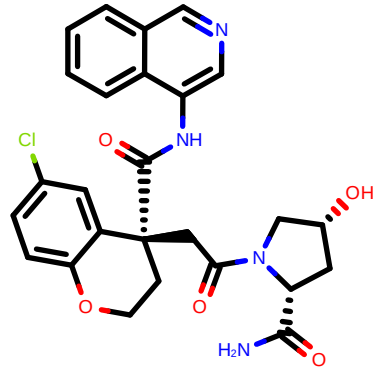
CID:	VLA-UCB-1dbca3b4-10_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CC[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN160
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.44

LEE-CAM-7ab9b158-4_4



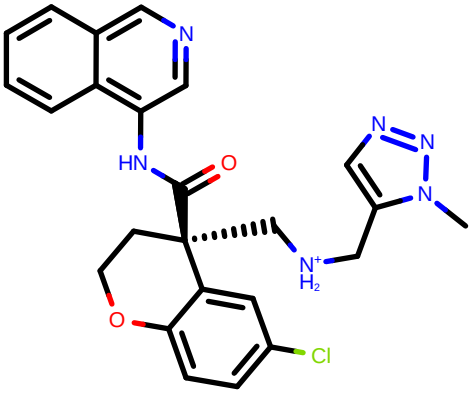
CID:	LEE-CAM-7ab9b158-4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)COC[C@H]5CN6C[C@@H](O5)CCC6=O
RUN:	RUN2213
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.44

ERI-UCB-d6de1f3c-5_2



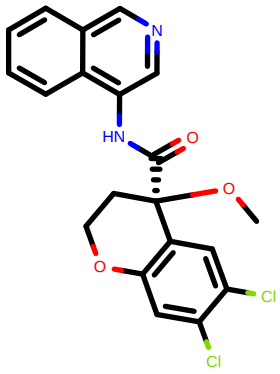
CID:	ERI-UCB-d6de1f3c-5_2
SMILES:	c1ccc2c(c1)cncc2C(=O)N3C[C@H](N(C(=O)C3)c4cccc(c4)Cl)CC5CCCCC5
RUN:	RUN1096
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.33

ALP-POS-347519b5-1_47



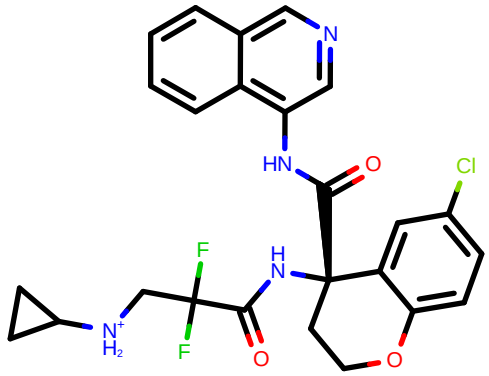
CID:	ALP-POS-347519b5-1_47
SMILES:	CS(=O)(=O)[N@@]1C[C@H]2[C@H]3CC[C@H](C3)[C@@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4253
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.22

DAR-DIA-9e4459de-11_11



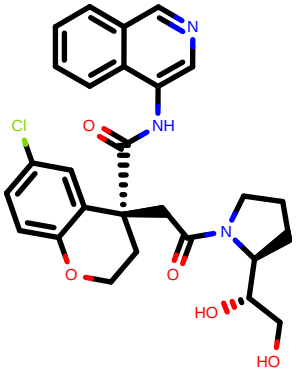
CID:	DAR-DIA-9e4459de-11_11
SMILES:	c1cc2c(c(c1)NCOCCOCCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@@H]7CCC(=O)NC7=O)O
RUN:	RUN1419
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.12

PET-UNK-bb7ffe78-1_1



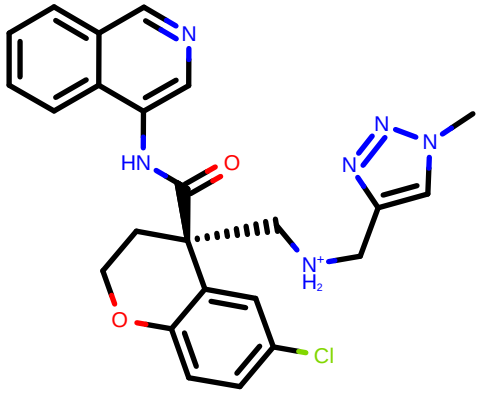
CID:	PET-UNK-bb7ffe78-1_1
SMILES:	CCc1cc(cc(c1)Cl)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN3327
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.18

BEN-BAS-5c03e89e-2_4



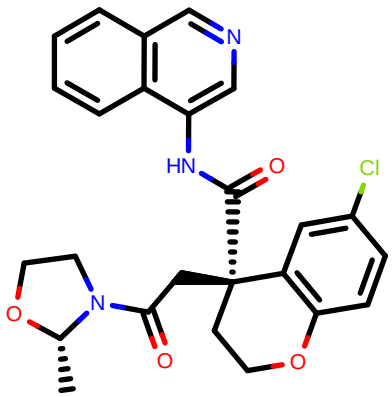
CID:	BEN-BAS-5c03e89e-2_4
SMILES:	CC(C)([C@H]1C=Nc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl)O
RUN:	RUN1146
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.40

RAL-THA-2d450e86-25_1



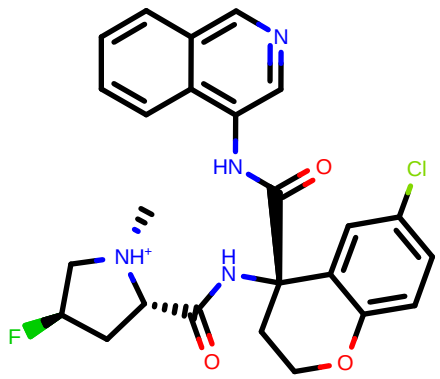
CID:	RAL-THA-2d450e86-25_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(ccc3F)Cl
RUN:	RUN1991
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.40

MIC-UNK-67d4a29a-3_1



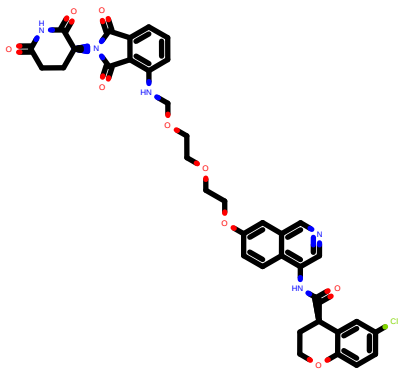
CID:	MIC-UNK-67d4a29a-3_1
SMILES:	Cc1cccc2c1c(cnc2)N(C)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1089
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.20

VLA-UNK-ba665ac8-2_2



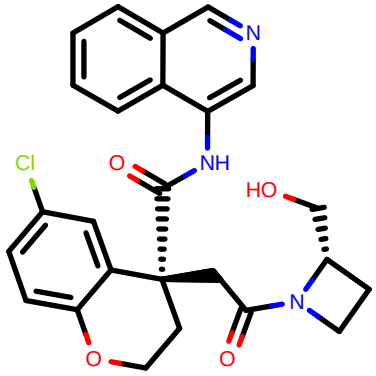
CID:	VLA-UNK-ba665ac8-2_2
SMILES:	C[N@H+]1CC(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN3304
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.22

VLA-UNK-db5e3064-1_1



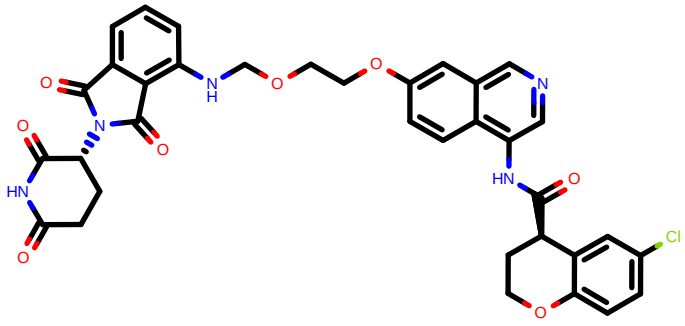
CID:	VLA-UNK-db5e3064-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CO[C@@H](C3=O)c4cccc(c4)Cl
RUN:	RUN3089
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.29

JOH-SUS-a69c159d-4_1



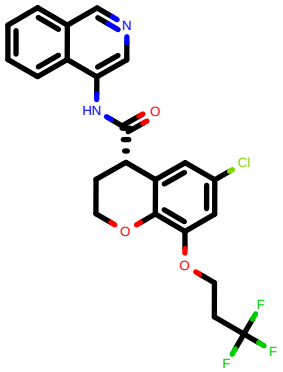
CID:	JOH-SUS-a69c159d-4_1
SMILES:	c1ccc2c(c1)c(cnc2C(F)(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1122
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.27

ALP-UNI-8e43a71e-2_8



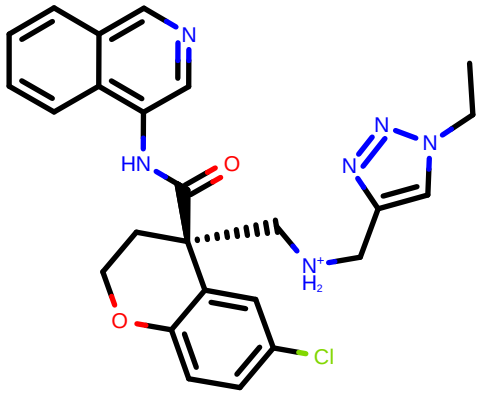
CID:	ALP-UNI-8e43a71e-2_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@H]5CCC[N@@H+]6CCO
RUN:	RUN2930
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.29

EDG-MED-90036822-5_1



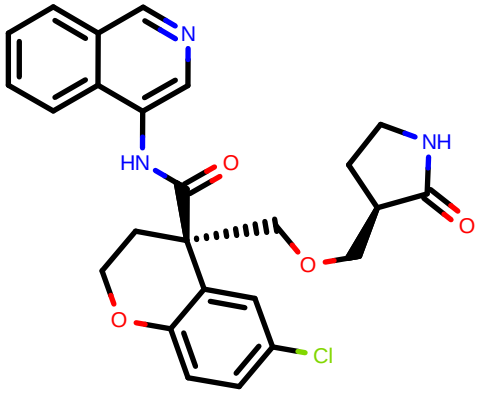
CID:	EDG-MED-90036822-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@@H](CF)[NH3+]
RUN:	RUN1660
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.30

PET-UNK-9b23ef84-11_1



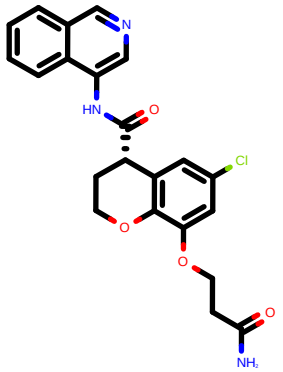
CID:	PET-UNK-9b23ef84-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CN(Cc4c3cc(cc4)Cl)c5ncno5
RUN:	RUN4441
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.25

MAK-UNK-c749d764-20_2



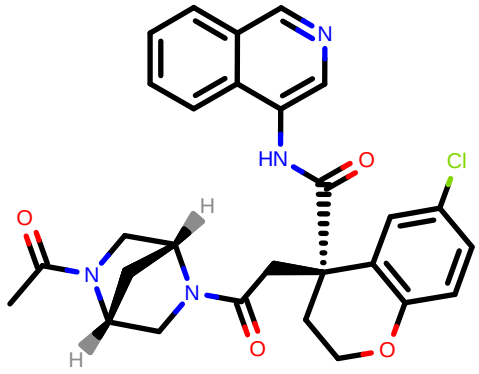
CID:	MAK-UNK-c749d764-20_2
SMILES:	CCCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN1006
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.22

KAD-UNI-80f122c8-5_4



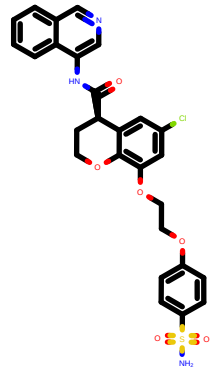
CID:	KAD-UNI-80f122c8-5_4
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2312
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.22

RAL-THA-8416115c-12_2



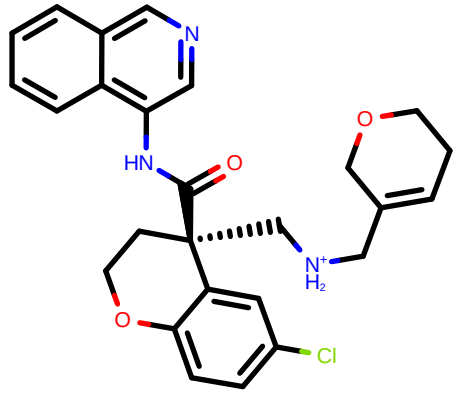
CID:	RAL-THA-8416115c-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5n[n-]nn5
RUN:	RUN1292
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.25

EDG-MED-ba1ac7b9-4_1



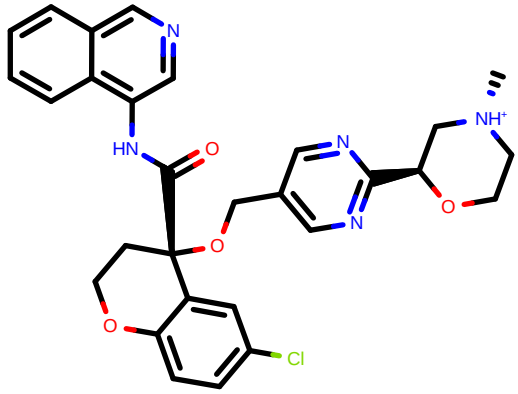
CID:	EDG-MED-ba1ac7b9-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[N@@H+]6CC[C@@H](C6)O
RUN:	RUN2626
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.51

ED_-GRI-5b13fbe2-48_2



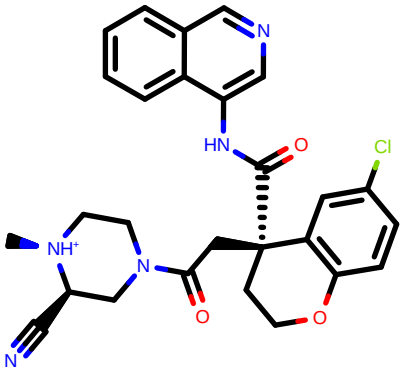
CID:	ED_-GRI-5b13fbe2-48_2
SMILES:	C[C@H](C[NH2+]CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)O
RUN:	RUN1591
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.40

PET-UNK-689df078-1_1



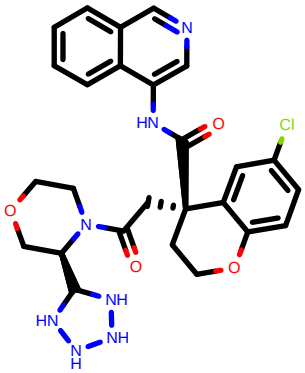
CID:	PET-UNK-689df078-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CC[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN3097
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.21

BEN-BAS-c2bc0d80-1_1



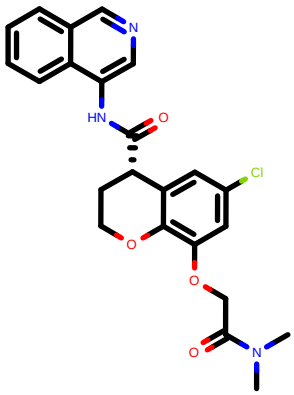
CID:	BEN-BAS-c2bc0d80-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC=Nc4c3cc(cc4)Cl
RUN:	RUN1133
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.26

JOH-SUS-a69c159d-7_1



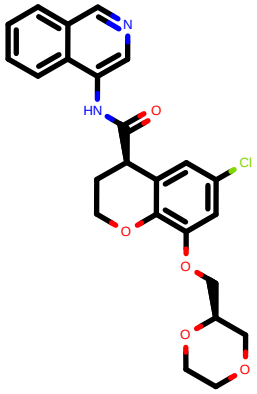
CID:	JOH-SUS-a69c159d-7_1
SMILES:	c1cc2c(cc1F)c(c(nc2F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1130
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.38

VLA-UNK-f702bf1c-4_1



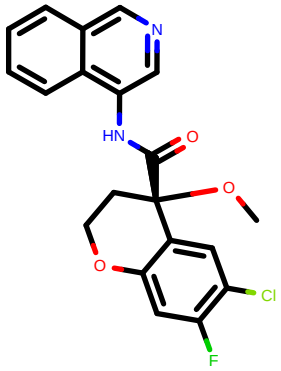
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CC(=O)NC6
RUN:	RUN2313
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.26

PET-UNK-2c6614b6-6_1



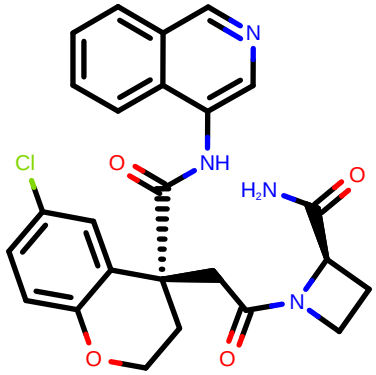
CID:	PET-UNK-2c6614b6-6_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN4811
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.17

MAT-POS-4223bc15-23_3



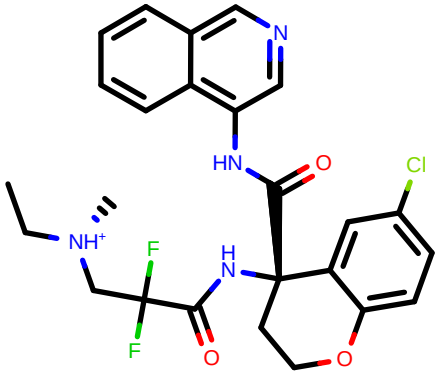
CID:	MAT-POS-4223bc15-23_3
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4108
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.06

BEN-BAS-c2bc0d80-7_1



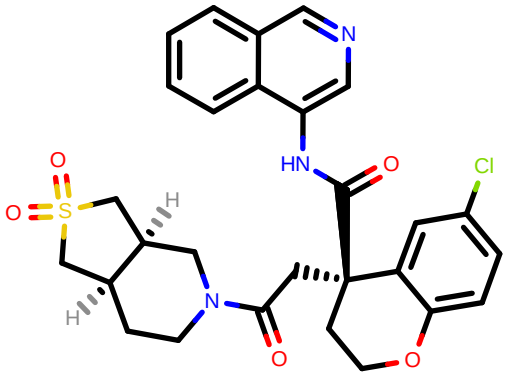
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN1138
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.27

KAD-UNI-877d7bed-16_1



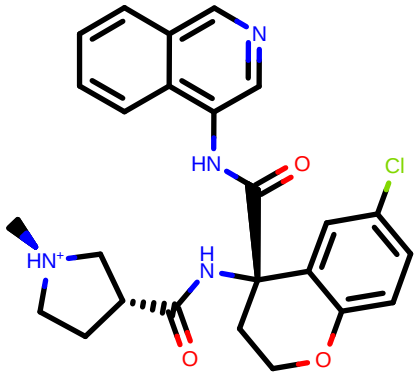
CID:	KAD-UNI-877d7bed-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCCn5c(ccc5O)O)Cl
RUN:	RUN3758
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.17

MIC-UNK-5a93dd5f-12_2



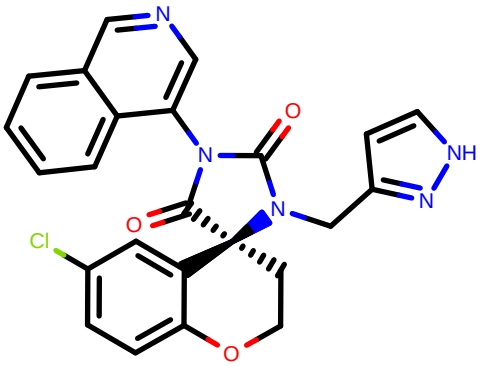
CID:	MIC-UNK-5a93dd5f-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@@]4CC[C@@H](C4)[NH+]5CCCCC5
RUN:	RUN791
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.28

MIC-UNK-b9827f26-1_1



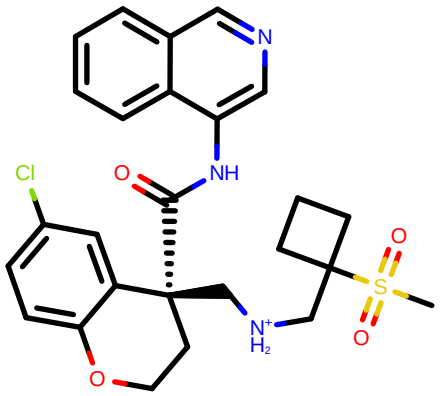
CID:	MIC-UNK-b9827f26-1_1
SMILES:	c1ccc2c(c1)cncc2C(=O)N3CCN(C(=O)C3)c4ccc(c(c4)Cl)Cl
RUN:	RUN3246
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.23

DAR-DIA-0d514e7d-9_1



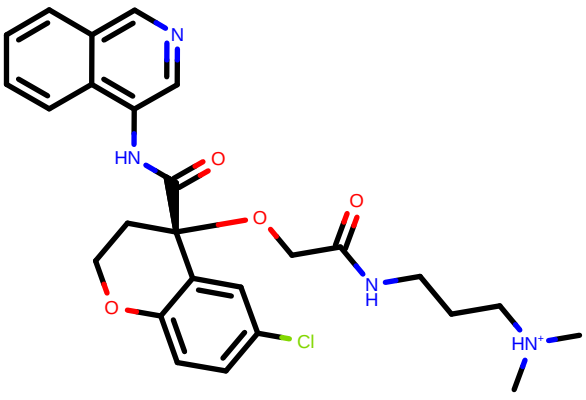
CID:	DAR-DIA-0d514e7d-9_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5ccccc5
RUN:	RUN813
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.20

RAL-THA-2d450e86-4_1



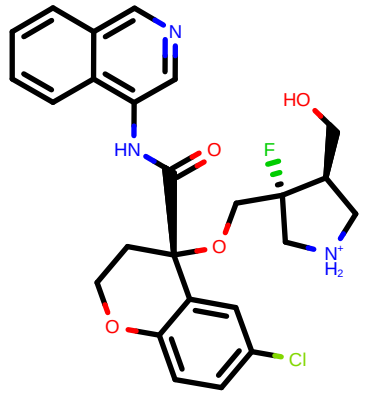
CID:	RAL-THA-2d450e86-4_1
SMILES:	COc1ccc(cc1)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN1969
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.30

EDG-MED-70ae9412-2_1



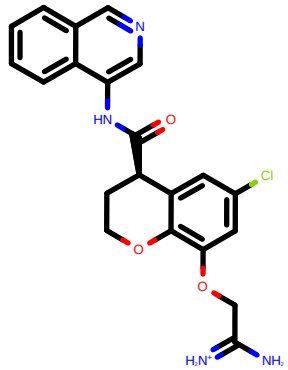
CID:	EDG-MED-70ae9412-2_1
SMILES:	C[NH+](C)CC(=O)NC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3167
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.21

JAG-UCB-f37eaa14-6_1



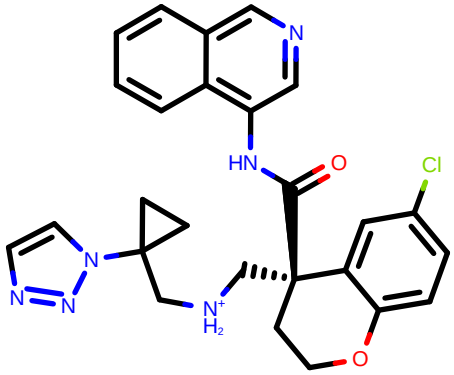
CID:	JAG-UCB-f37eaa14-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](c5c4cc(cc5)Cl)[C@@H]6CC(=O)N6
RUN:	RUN3062
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.21

PET-UNK-1320d94d-3_1



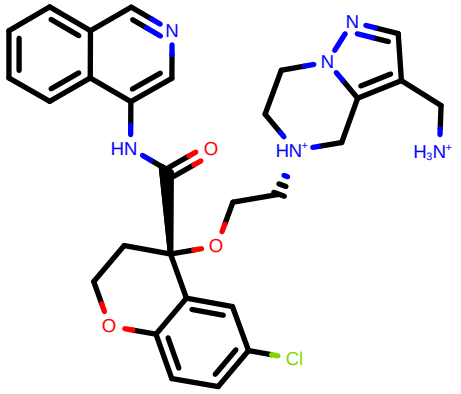
CID:	PET-UNK-1320d94d-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3Cl)NC(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCOCC5
RUN:	RUN4974
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.18

EDJ-MED-1981ceba-3_3



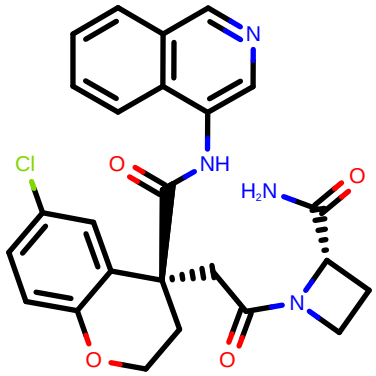
CID:	EDJ-MED-1981ceba-3_3
SMILES:	COC1CN(C1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4691
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.28

DAR-DIA-6a508060-2_1



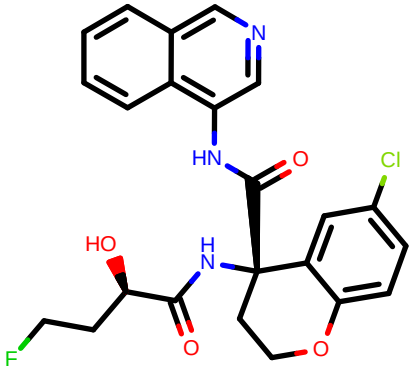
CID:	DAR-DIA-6a508060-2_1
SMILES:	c1ccc2c(c1)cncc2OC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN334
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.70

BEN-BAS-c2bc0d80-4_2



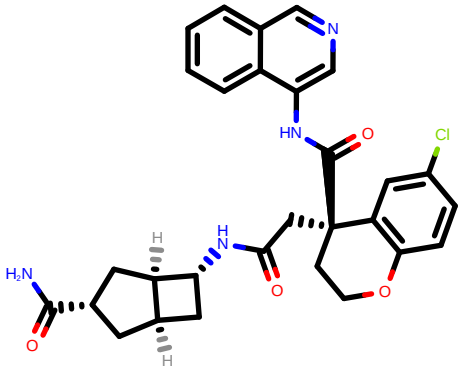
CID:	BEN-BAS-c2bc0d80-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC=Nc4c3[nH]c(cc4=O)Cl
RUN:	RUN1141
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.21

DAR-DIA-0587064e-10_2



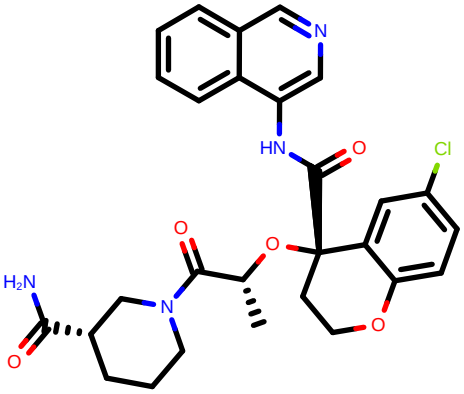
CID:	DAR-DIA-0587064e-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCC(F)(F)F)Cl
RUN:	RUN3358
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.14

LAU-MED-88a3970a-17_1



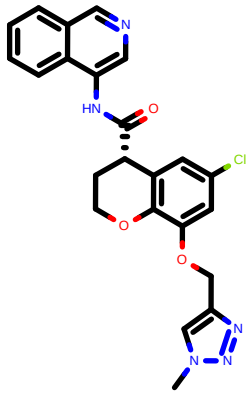
CID:	LAU-MED-88a3970a-17_1
SMILES:	CNC(=O)CCc1cc(cc2c1OCC[C@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN1513
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.56

MIC-UNK-5a93dd5f-2_6



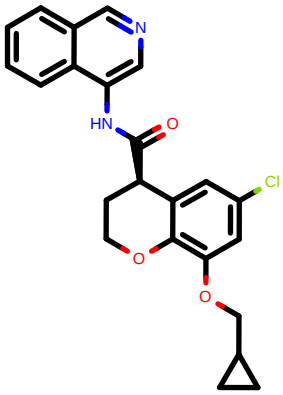
CID:	MIC-UNK-5a93dd5f-2_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[NH+]4C[C@@H]5CCCC[C@H]5C4
RUN:	RUN739
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.29

ALP-POS-5bb456a5-1_2



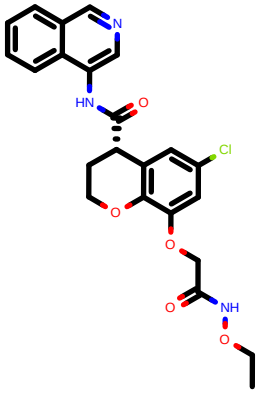
CID:	ALP-POS-5bb456a5-1_2
SMILES:	C[C@H]1C[N@@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2407
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.25

ALP-POS-347519b5-1_61



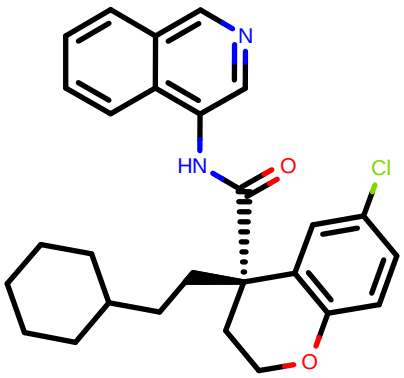
CID:	ALP-POS-347519b5-1_61
SMILES:	CS(=O)(=O)[N@@]1C[C@@H]2[C@H]3CC[C@H](C3)[C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4261
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.13

EDJ-MED-d203f206-10_1



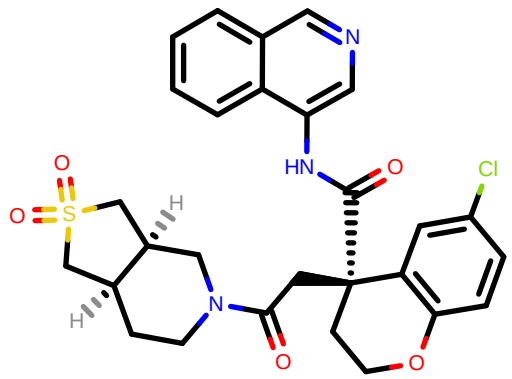
CID:	EDJ-MED-d203f206-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCCC6(C5)[C@@H](C[C@@H]6O)O
RUN:	RUN2572
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.28

ALP-UNI-dbbfd3db-15_2



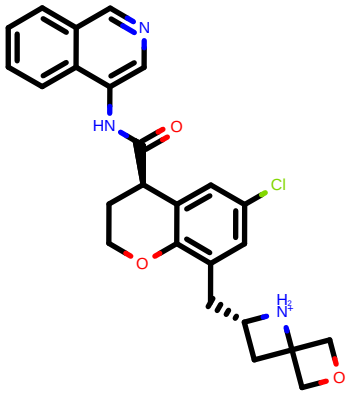
CID:	ALP-UNI-dbbfd3db-15_2
SMILES:	C[C@H](C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)NC(=O)C5CCC5
RUN:	RUN2786
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.29

MAK-UNK-c749d764-21_7



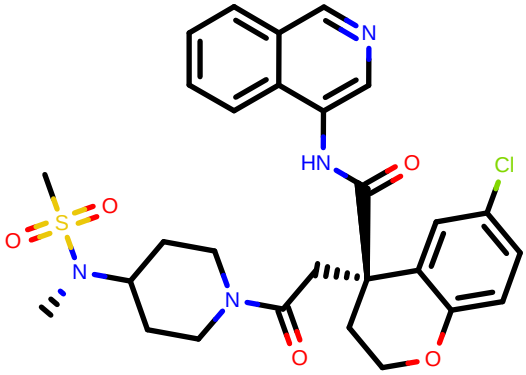
CID:	MAK-UNK-c749d764-21_7
SMILES:	CCCCN(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1021
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.24

DAR-DIA-0cde14eb-58_1



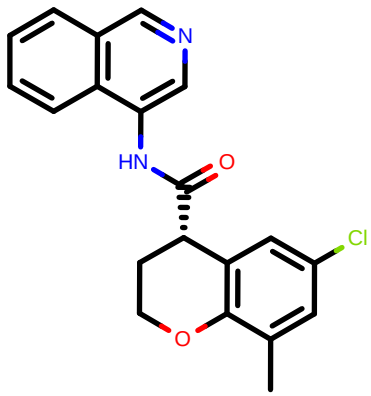
CID:	DAR-DIA-0cde14eb-58_1
SMILES:	C[C@@H](c1cccc(c1)C2(CC2)I)C(=O)Nc3cncc4c3cccc4
RUN:	RUN28
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.45

MIC-UNK-5a93dd5f-9_1



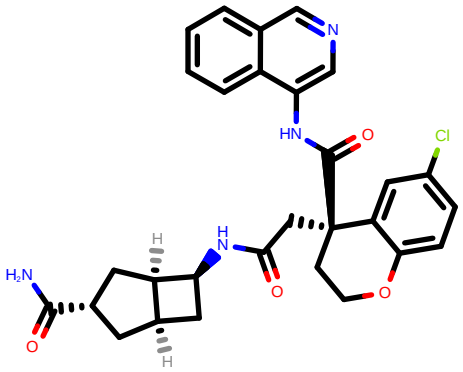
CID:	MIC-UNK-5a93dd5f-9_1
SMILES:	CN(C)[C@@H]1CC[N@@H+](C1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN778
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.29

MAK-UNK-ffc90da7-3_2



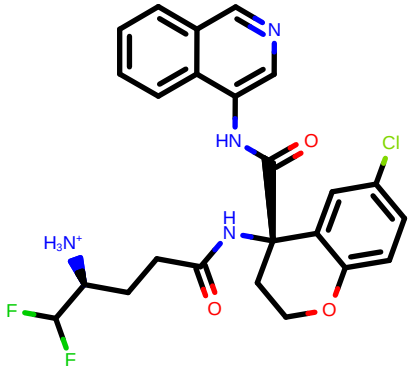
CID:	MAK-UNK-ffc90da7-3_2
SMILES:	CC(C)OC[C@H](c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl)[NH2+]C
RUN:	RUN696
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.12

ALP-POS-ce760d3f-7_1



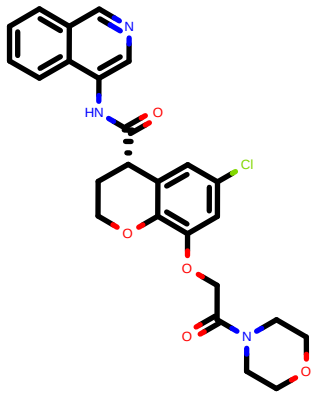
CID:	ALP-POS-ce760d3f-7_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1465
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.39

MIC-UNK-cdc2493e-4_3



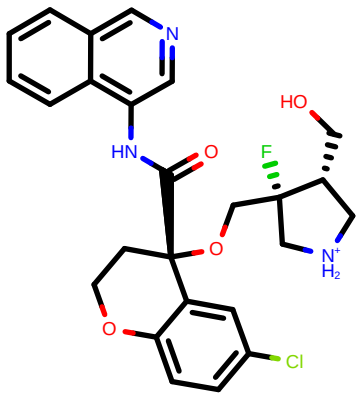
CID:	MIC-UNK-cdc2493e-4_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(c3cccc(c3)Cl)C4C[C@@H]5CCC[C@H]5C4
RUN:	RUN529
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.41

VLA-UNK-f702bf1c-7_1



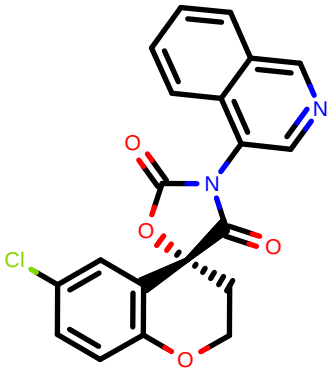
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCN6CC[NH2+]CC6
RUN:	RUN2321
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.31

VLA-UNK-c65c1026-2_1



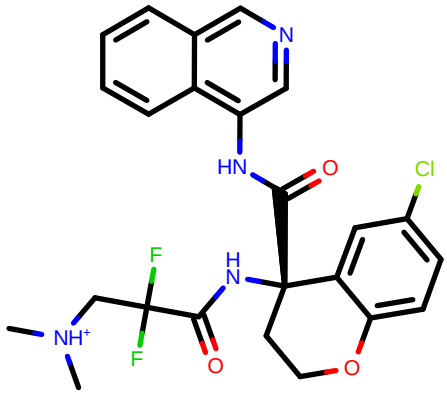
CID:	VLA-UNK-c65c1026-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CC[C@@]4(C3=O)COc5c4cc(cc5)Cl
RUN:	RUN3180
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.19

PET-UNK-acd70dee-2_1



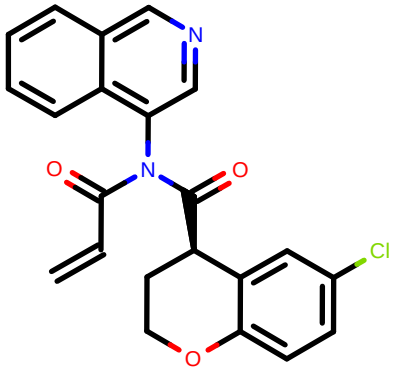
CID:	PET-UNK-acd70dee-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5ncco5
RUN:	RUN4186
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.19

MAT-POS-3b97339c-3_2



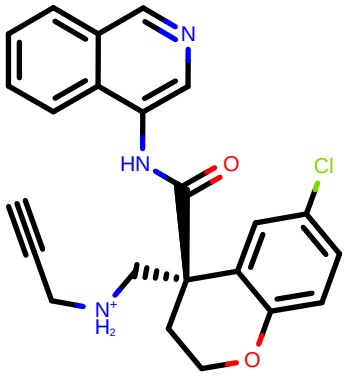
CID:	MAT-POS-3b97339c-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]c5S(=O)(=O)N
RUN:	RUN3308
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.16

EDJ-MED-6d9ff7d0-3_1



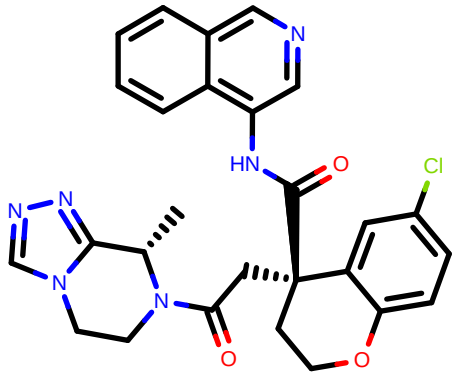
CID:	EDJ-MED-6d9ff7d0-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)[NH2+]Cc5ccn[nH]5
RUN:	RUN3425
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.13

EDG-MED-90036822-99_4



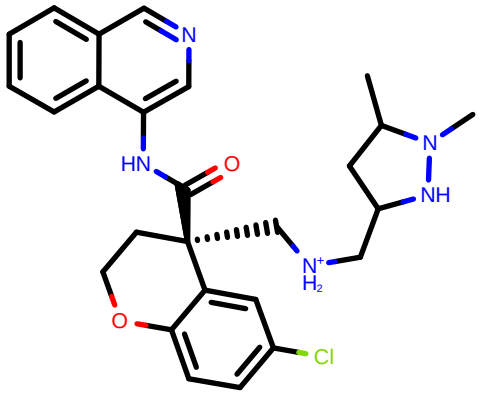
CID:	EDG-MED-90036822-99_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)[C@H]([C@H](C5CCC5)O)F
RUN:	RUN1833
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.34

EDJ-MED-841e0cf0-2_1



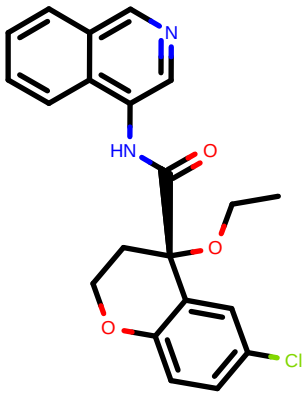
CID:	EDJ-MED-841e0cf0-2_1
SMILES:	CO[C@@]1(C[N@@](Cc2c1cc(c(c2)F)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3830
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.15

EDG-MED-90036822-52_1



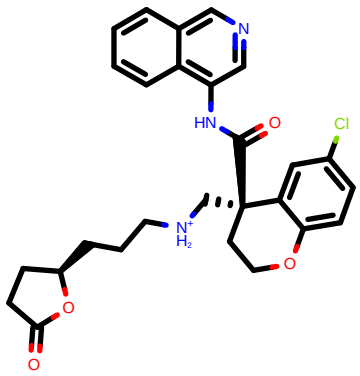
CID:	EDG-MED-90036822-52_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)C(CNCCCO)(F)F
RUN:	RUN1737
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.37

EDJ-MED-923a35c2-4_1



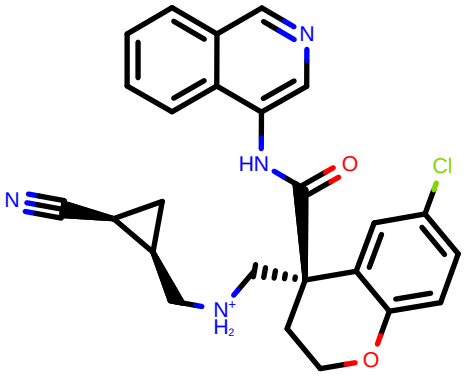
CID:	EDJ-MED-923a35c2-4_1
SMILES:	C[C@@]1(C[N@@](Cc2c1cc(c(c2)F)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cc(cc4)F
RUN:	RUN4222
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.07

MAT-POS-61f37a1a-8_2



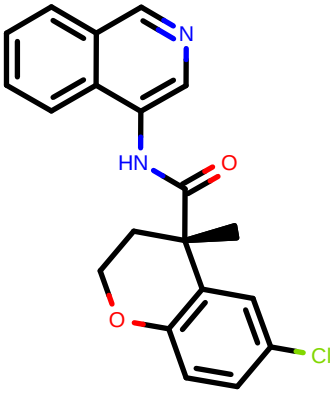
CID:	MAT-POS-61f37a1a-8_2
SMILES:	Cc1c(c(n(n1)C)N2CCOCC2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN4602
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.24

EDG-MED-90036822-38_2



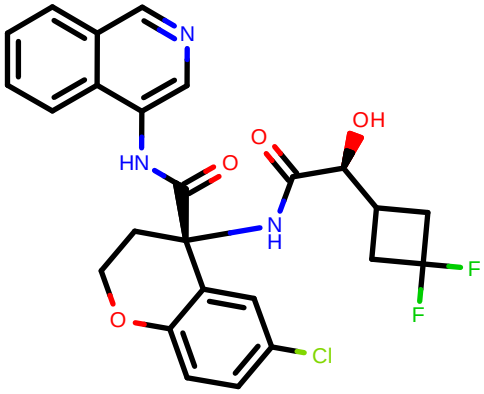
CID:	EDG-MED-90036822-38_2
SMILES:	C[C@H](CNCC(C(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(F)F)O
RUN:	RUN1720
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.42

ERI-UCB-ce40166b-2_1



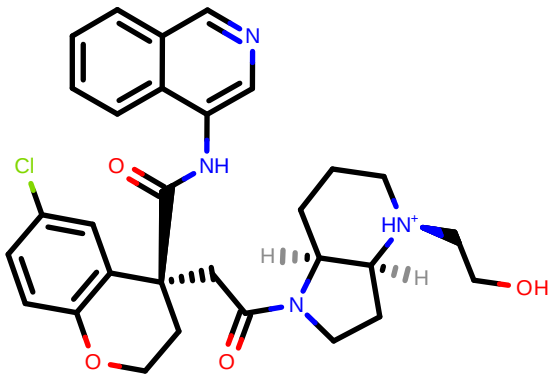
CID:	ERI-UCB-ce40166b-2_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)O[C@@H]4CCC(=O)N4
RUN:	RUN36
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.14

JAG-UCB-706446eb-4_1



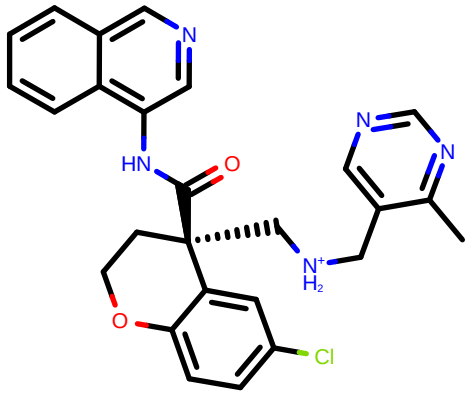
CID:	JAG-UCB-706446eb-4_1
SMILES:	CCOC(=O)CC[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN619
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.26

LON-WEI-5e7d1b3e-50_2



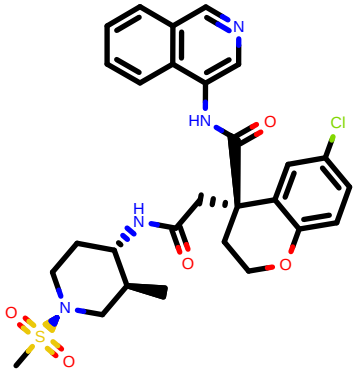
CID:	LON-WEI-5e7d1b3e-50_2
SMILES:	CCCC[N@H+](CCNC(=O)Nc1cn(c(=O)c2c1cccc2)C)Cc3ccco3
RUN:	RUN1365
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.48

EDJ-MED-1b5395f9-5_2



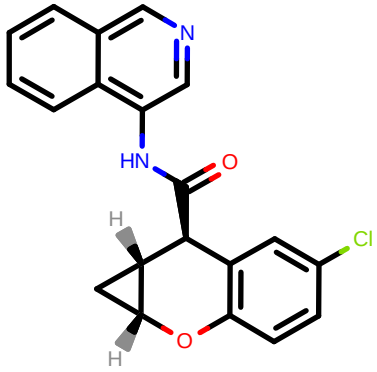
CID:	EDJ-MED-1b5395f9-5_2
SMILES:	CS(=O)(=O)[N@]1Cc2cc(c(cc2[C@@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl)Cl
RUN:	RUN4472
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.24

MAK-UNK-c749d764-25_6



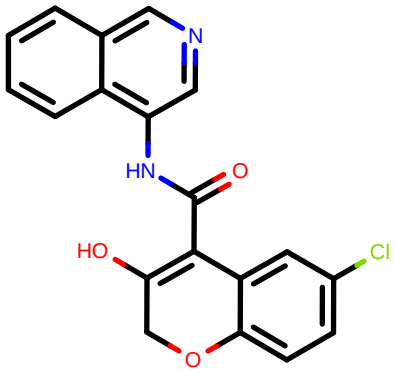
CID:	MAK-UNK-c749d764-25_6
SMILES:	COC(=O)N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1043
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.37

EDJ-MED-ee07cf00-7_2



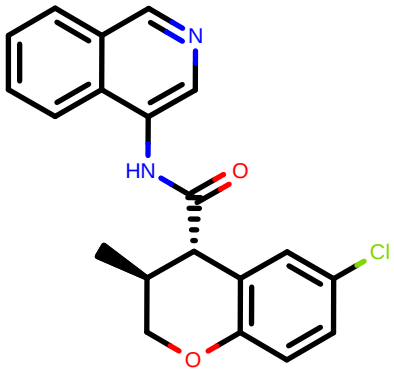
CID:	EDJ-MED-ee07cf00-7_2
SMILES:	Cc1c(c(=O)ccn1CC(=O)N[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4)[O-]
RUN:	RUN2817
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.19

EDG-MED-ba1ac7b9-18_1



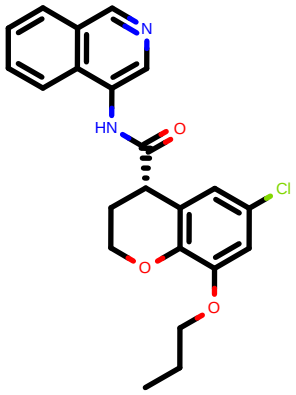
CID:	EDG-MED-ba1ac7b9-18_1
SMILES:	C[C@@H]1Cn2c(ccn2)CN1C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2682
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.23

PET-UNK-7be94445-1_1



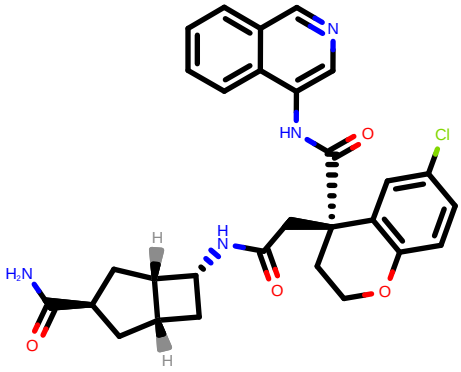
CID:	PET-UNK-7be94445-1_1
SMILES:	c1ccc2c(c1)cncc2N3CCCN(C3=O)c4cccc(c4)Cl
RUN:	RUN132
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.10

EDG-MED-971238d3-6_1



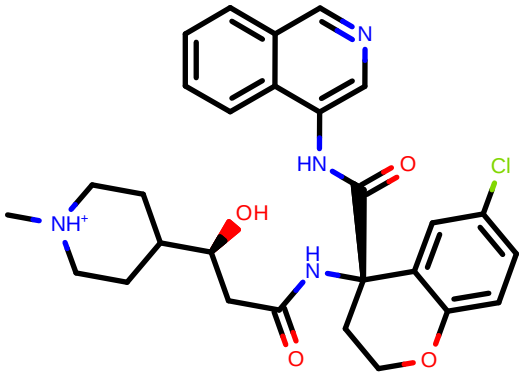
CID:	EDG-MED-971238d3-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC[NH3+]
RUN:	RUN1471
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.26

LON-WEI-5e7d1b3e-35_2



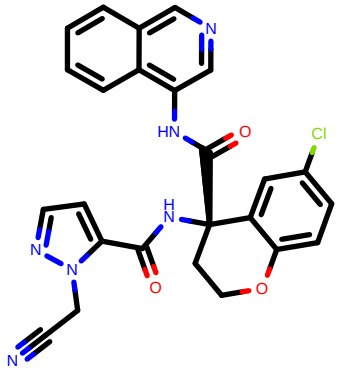
CID:	LON-WEI-5e7d1b3e-35_2
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN1341
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.27

VLA-UCB-34f3ed0c-11_1



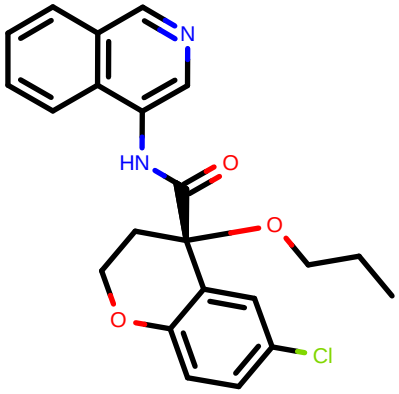
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN631
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.36

KAD-UNI-877d7bed-18_2



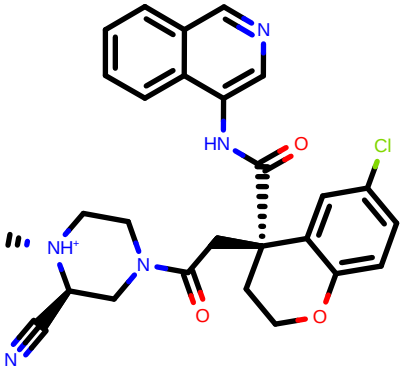
CID:	KAD-UNI-877d7bed-18_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCS(=O)(=O)CCCO)Cl
RUN:	RUN3771
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.14

ALP-POS-347519b5-1_30



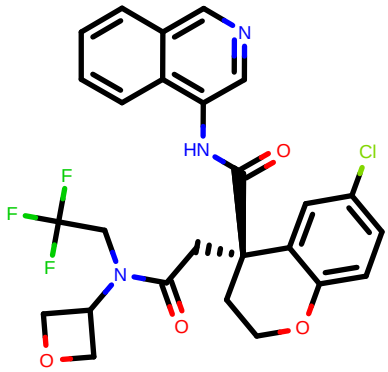
CID:	ALP-POS-347519b5-1_30
SMILES:	CS(=O)(=O)N@]1C[C@@H]2[C@H]3CC[C@H](C3)[C@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4245
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.12

DAR-DIA-076fb6ea-8_1



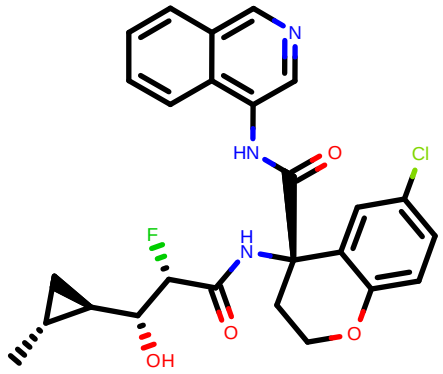
CID:	DAR-DIA-076fb6ea-8_1
SMILES:	C=C=CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1400
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.23

PET-UNK-5d7c542f-1_1



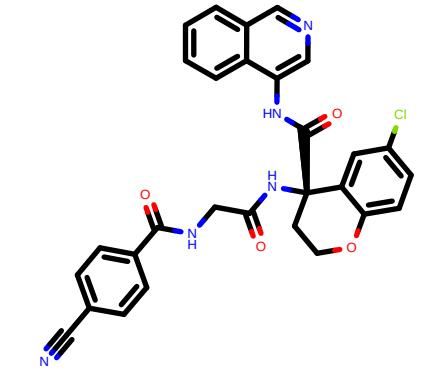
CID:	PET-UNK-5d7c542f-1_1
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc(c4)F
RUN:	RUN3851
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.14

MAT-POS-3b97339c-3_1



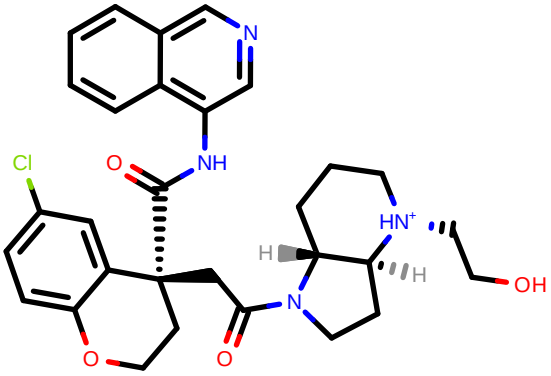
CID:	MAT-POS-3b97339c-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)c5cn[nH]c5S(=O)(=O)N
RUN:	RUN3307
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.18

ALP-POS-966f8da6-1_4



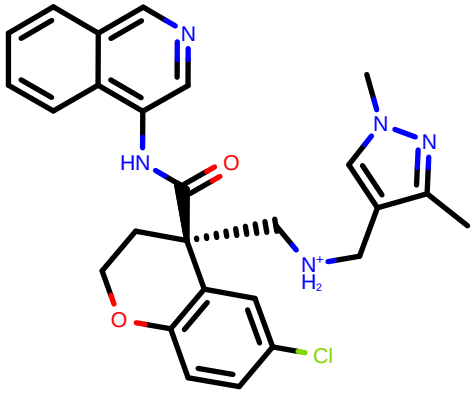
CID:	ALP-POS-966f8da6-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cnc[nH]5
RUN:	RUN1223
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.31

MAT-POS-4223bc15-7_1



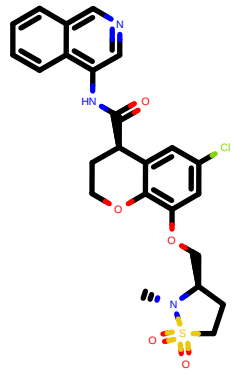
CID:	MAT-POS-4223bc15-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)C5COC5
RUN:	RUN3997
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.35

ED_-GRI-5b13fbe2-74_4



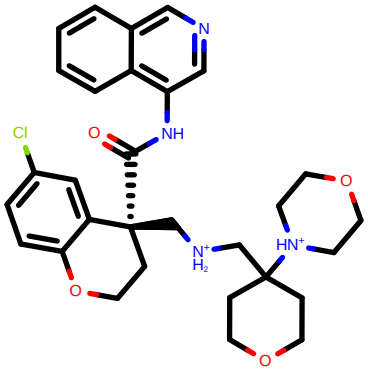
CID:	ED_-GRI-5b13fbe2-74_4
SMILES:	C[N@H+]1CCO[C@H](C1)c2nccc(n2)CO[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN1634
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.51

ALP-POS-67d5babe-1_3



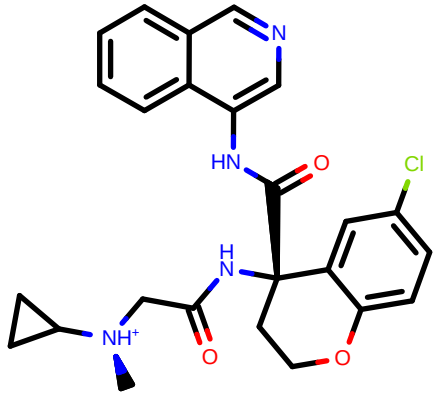
CID:	ALP-POS-67d5babe-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC[N@H+]5CC[C@@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN4868
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.19

MIC-UNK-f792ef5d-1_1



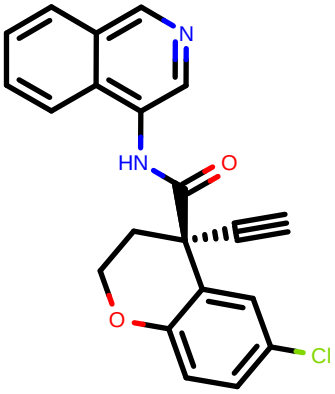
CID:	MIC-UNK-f792ef5d-1_1
SMILES:	C[N@@H+]1C[C@H]2COc3ccc(cc3[C@]2(C1)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4665
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.32

VLA-UCB-34f3ed0c-3_1



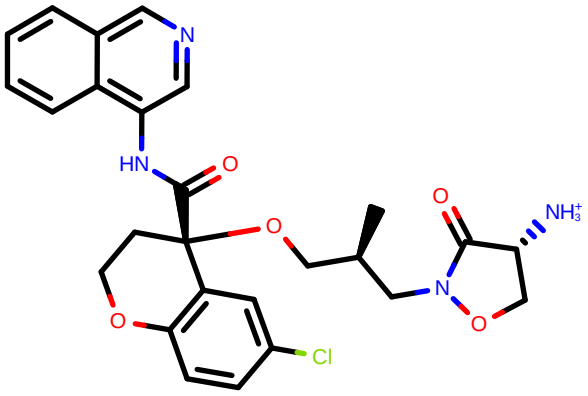
CID:	VLA-UCB-34f3ed0c-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)NCc5ccn[nH]5
RUN:	RUN628
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.31

ALP-UNI-dbbfd3db-13_1



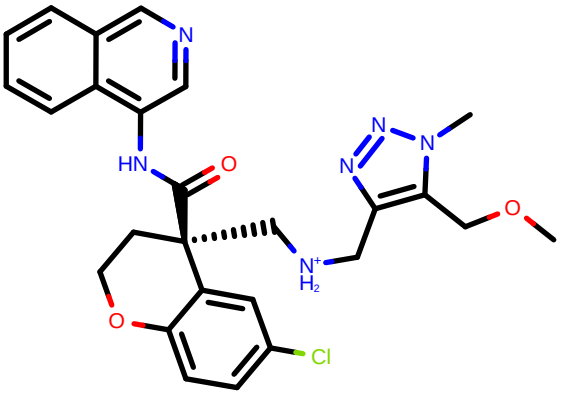
CID:	ALP-UNI-dbbfd3db-13_1
SMILES:	Cn1cc(cn1)C2=NO[C@@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2781
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.08

MIC-UNK-644c43c7-2_1



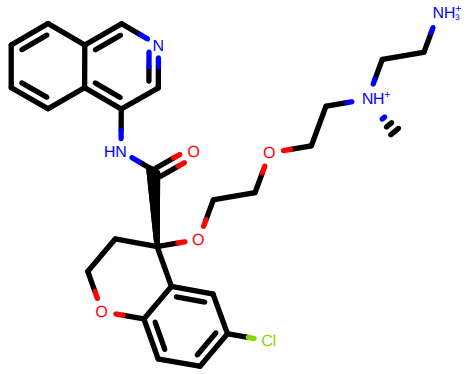
CID:	MIC-UNK-644c43c7-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CCNC(C(F)(F)F)C(F)(F)F
RUN:	RUN435
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.37

EDG-MED-10fcb19e-1_2



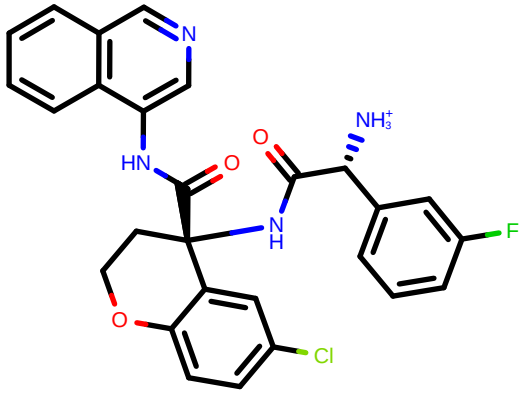
CID:	EDG-MED-10fcb19e-1_2
SMILES:	CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cc(cc4)NS(=O)(=O)C
RUN:	RUN4497
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.27

WIL-UCB-7ba4ac3a-3_1



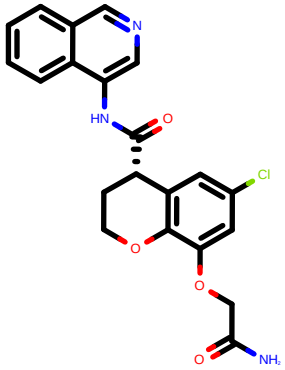
CID:	WIL-UCB-7ba4ac3a-3_1
SMILES:	c1ccc2c(c1)cncc2NS(=O)(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN3020
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.30

MIC-UNK-bcd487e9-1_1



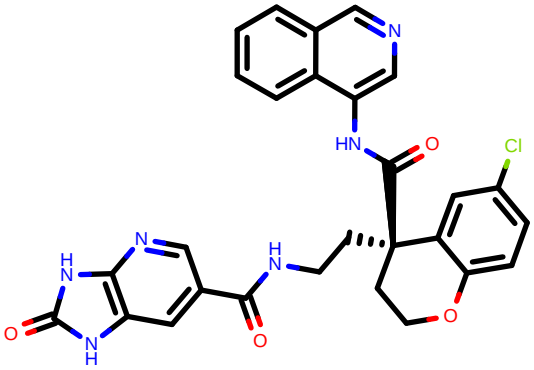
CID:	MIC-UNK-bcd487e9-1_1
SMILES:	c1ccc(cc1)CN(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN586
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.31

VLA-UNK-83c3754c-2_1



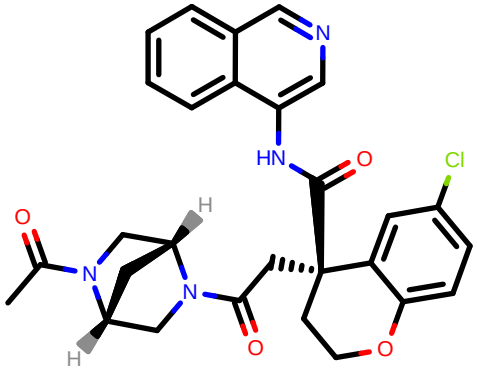
CID:	VLA-UNK-83c3754c-2_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12COc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN2319
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.24

DAR-DIA-0d514e7d-31_16



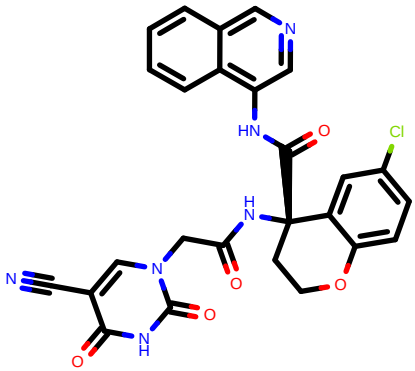
CID:	DAR-DIA-0d514e7d-31_16
SMILES:	C[C@H]1CCO[C@H]2C=CC(=C[C@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN849
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.29

RAL-THA-8416115c-14_4



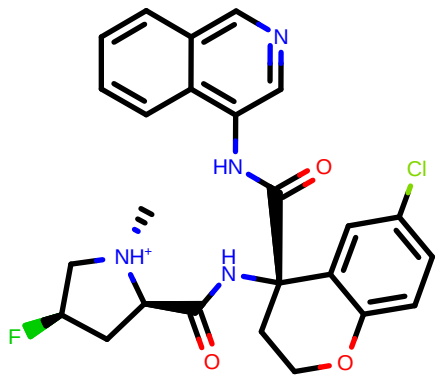
CID:	RAL-THA-8416115c-14_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cn[nH]n5
RUN:	RUN1303
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.32

MAT-POS-4223bc15-14_3



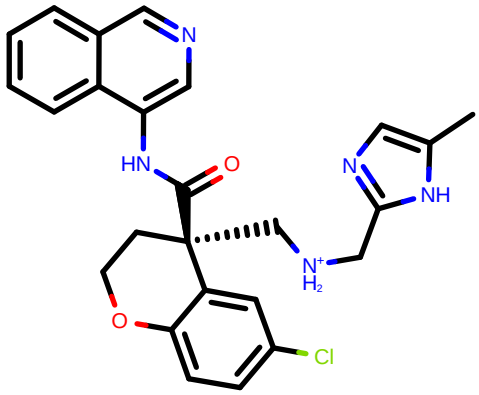
CID:	MAT-POS-4223bc15-14_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5C[NH2+]C5
RUN:	RUN4068
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.16

MIC-UNK-cdc2493e-12_1



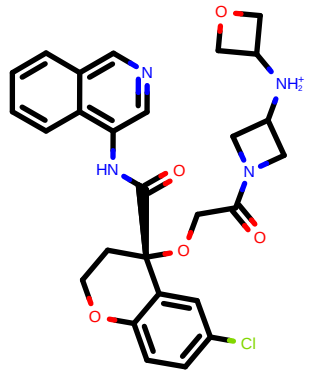
CID:	MIC-UNK-cdc2493e-12_1
SMILES:	C[NH+](C)[C@@H]1CC[C@@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN551
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.31

RAL-THA-05e671eb-16_2



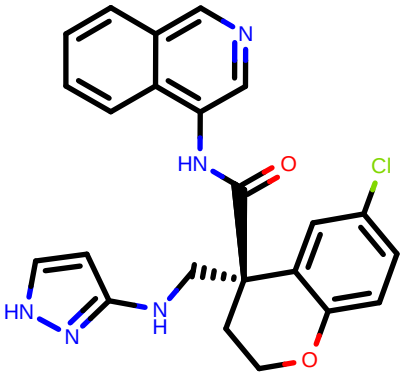
CID:	RAL-THA-05e671eb-16_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4Cl)Cl
RUN:	RUN2037
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.34

EDJ-MED-15e90dfc-7_1



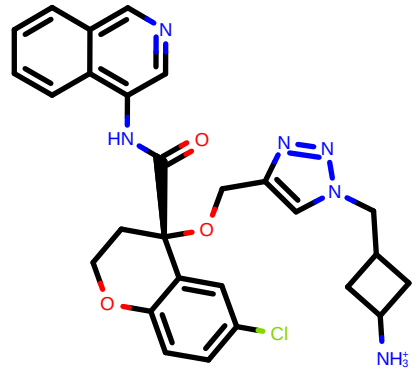
CID:	EDJ-MED-15e90dfc-7_1
SMILES:	CS(=O)(=O)CCNC[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3456
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.24

MAT-POS-4223bc15-34_2



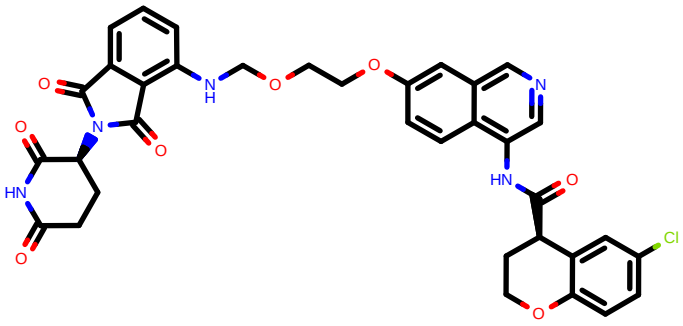
CID:	MAT-POS-4223bc15-34_2
SMILES:	Cn1ccnc1[N@]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4147
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.12

JAG-UCB-f37eaa14-8_2



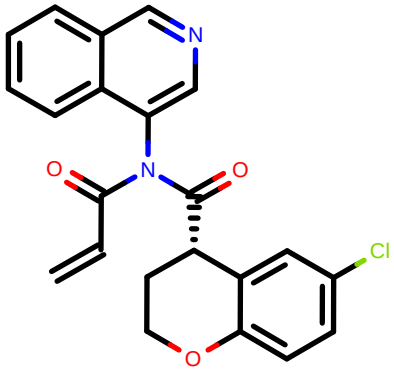
CID:	JAG-UCB-f37eaa14-8_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](c5c4cc(cc5)Cl)CCn6ccnc6
RUN:	RUN3069
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.24

MIC-UNK-25b9c114-1_1



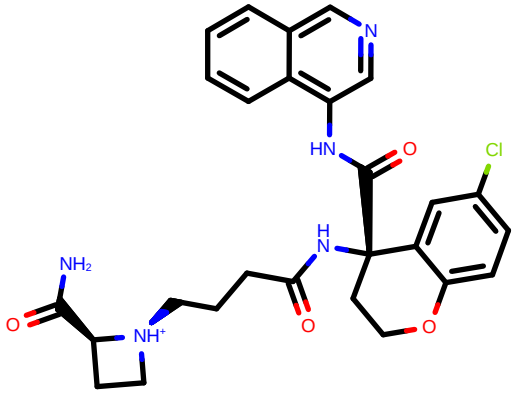
CID:	MIC-UNK-25b9c114-1_1
SMILES:	CS(=O)(=O)NC[C@@H]1CN(C(=O)CN1C(=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN3259
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.28

EDG-MED-ba1ac7b9-25_3



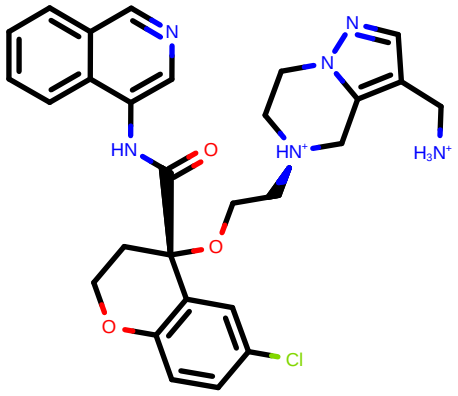
CID:	EDG-MED-ba1ac7b9-25_3
SMILES:	C[C@@H]1CN(CC[NH+]1CCO)C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2715
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.28

EDJ-MED-37aac4bd-3_1



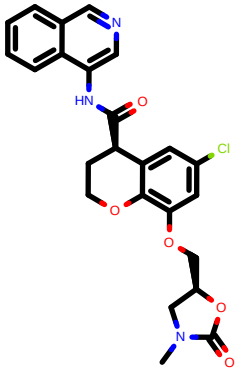
CID:	EDJ-MED-37aac4bd-3_1
SMILES:	COC[C@@]1(CCOc2c1cc(cc2F)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3143
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.22

DAR-DIA-6a508060-2_2



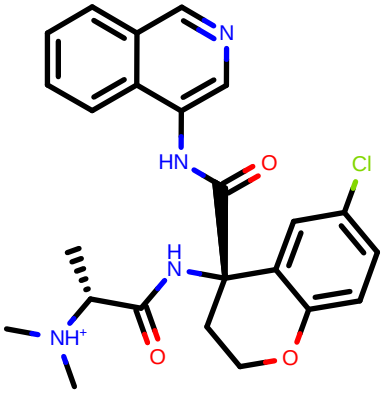
CID:	DAR-DIA-6a508060-2_2
SMILES:	c1ccc2c(c1)cncc2OC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN335
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.57

EDG-MED-ba1ac7b9-4_4



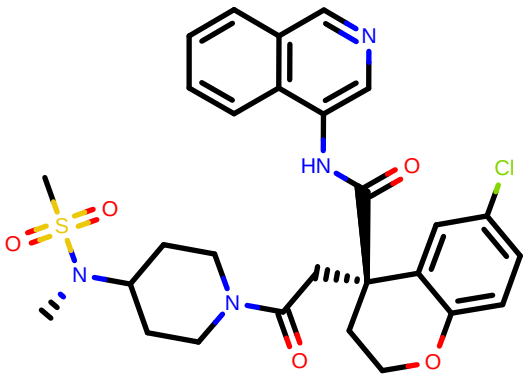
CID:	EDG-MED-ba1ac7b9-4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC(C5)[N@H+]6CC[C@@H](C6)O
RUN:	RUN2629
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.34

MAK-UNK-83e0a0b4-1_1



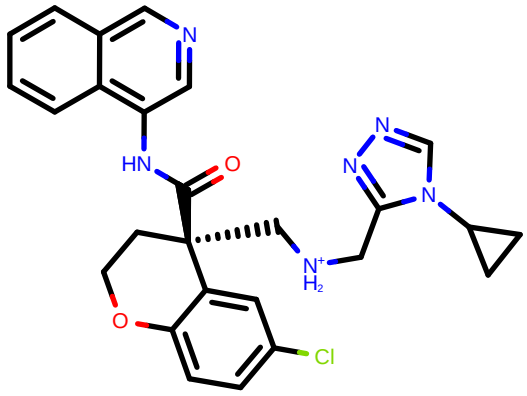
CID:	MAK-UNK-83e0a0b4-1_1
SMILES:	CCCCc1ccc2c(c1)[C@@H](CCO2)C(=O)N(CCNC3C[NH2+]C3)c4cncc5c4ccc(c5)CN6CC[NH2+]CC6
RUN:	RUN727
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.36

LON-WEI-5e7d1b3e-15_1



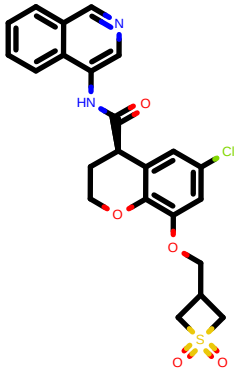
CID:	LON-WEI-5e7d1b3e-15_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCCN3CCCC3=O
RUN:	RUN1325
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.25

EDJ-MED-c82a5324-1_7



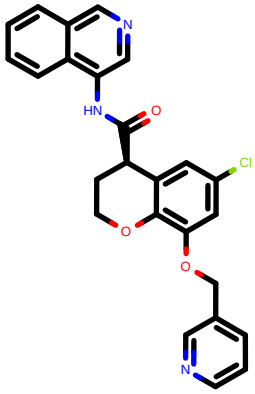
CID:	EDJ-MED-c82a5324-1_7
SMILES:	CNC(=O)[C@@H](CO)[N@H+]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4726
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.22

EDG-MED-5d232de5-3_1



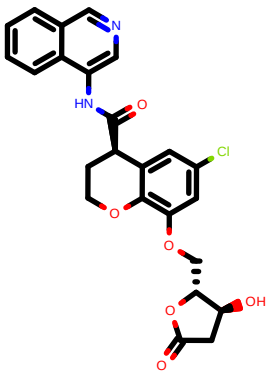
CID:	EDG-MED-5d232de5-3_1
SMILES:	CC(=O)N1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2364
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.47

ALP-POS-347519b5-2_37



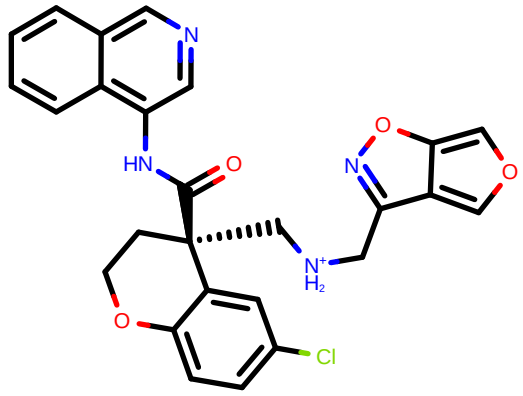
CID:	ALP-POS-347519b5-2_37
SMILES:	CO[C@@]1(C[N@@](C[C@H]2[C@@H]1[C@@H]3CC[C@H]2C3)S(=O)(=O)C)C(=O)Nc4ccc5c4cccc5
RUN:	RUN4284
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.15

ALP-POS-5bb456a5-6_1



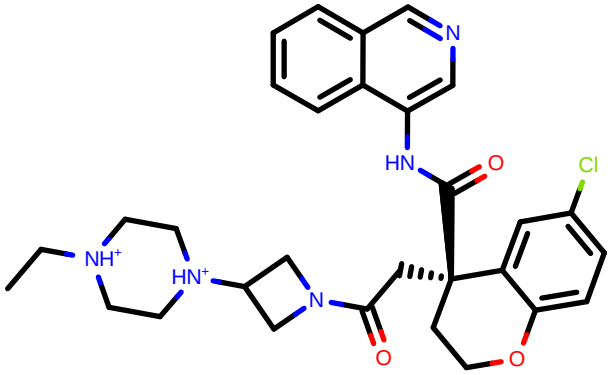
CID:	ALP-POS-5bb456a5-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC(CC5)c6n[n-]nn6
RUN:	RUN2436
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.45

EDJ-MED-139368ae-1_3



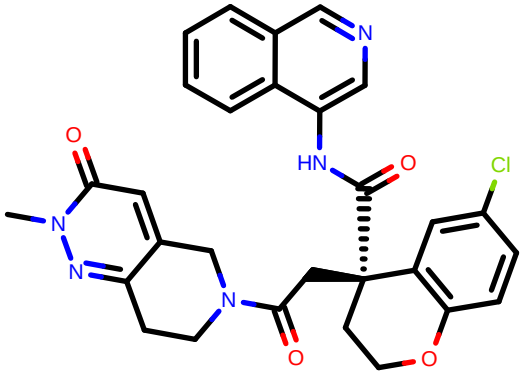
CID:	EDJ-MED-139368ae-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cccc4)S(=O)(=O)N5CCOCC5
RUN:	RUN4534
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.22

MAK-UNK-c749d764-29_6



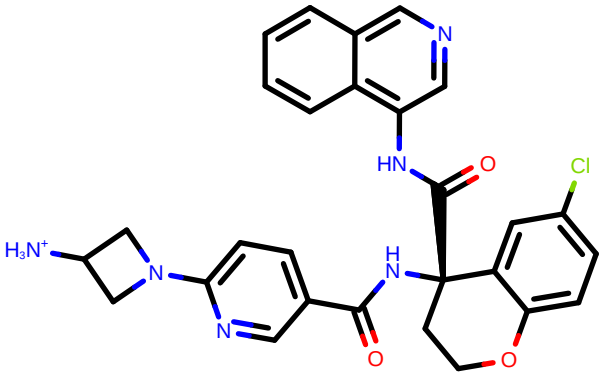
CID:	MAK-UNK-c749d764-29_6
SMILES:	c1ccc2c(c1)cncc2N(C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F)C(=O)ON
RUN:	RUN1067
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.39

LON-WEI-5e7d1b3e-23_1



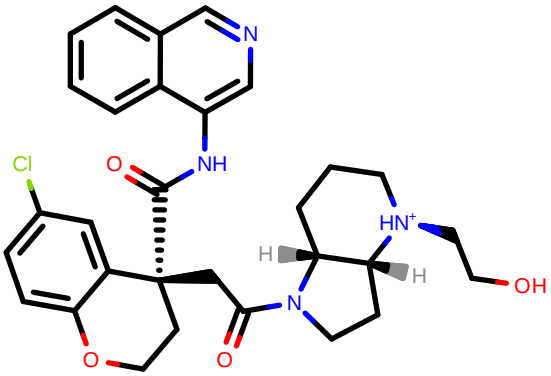
CID:	LON-WEI-5e7d1b3e-23_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3cccc(c3)C(F)(F)F
RUN:	RUN1327
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.29

EDJ-MED-f893e2a1-4_2



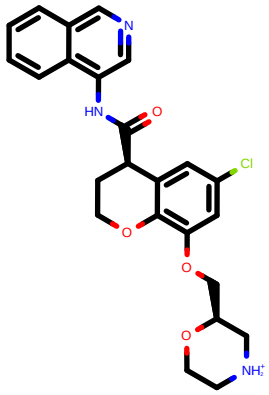
CID:	EDJ-MED-f893e2a1-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@]5(CCSC5)O
RUN:	RUN3199
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.16

MAK-UNK-c749d764-28_7



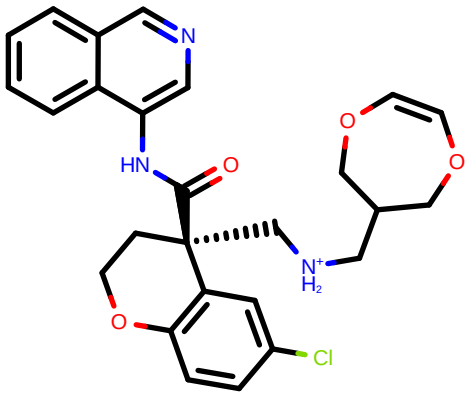
CID:	MAK-UNK-c749d764-28_7
SMILES:	c1ccc2c(c1)cncc2N(C=O)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F
RUN:	RUN1060
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.64

ALF-EVA-07677224-2_2



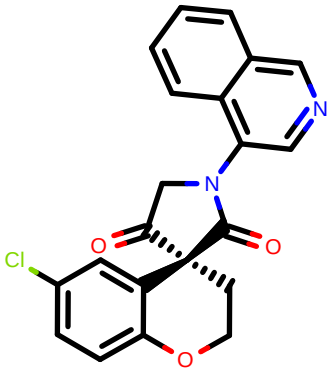
CID:	ALF-EVA-07677224-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)c5ccc(s5)F
RUN:	RUN4901
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.19

JOH-UNI-3fc3434e-10_1



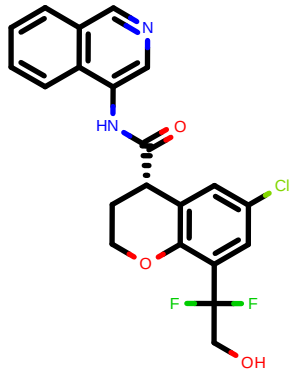
CID:	JOH-UNI-3fc3434e-10_1
SMILES:	CN(c1c2ccccc2cnc1CC(F)(F)F)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1922
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.46

MAT-POS-4223bc15-11_14



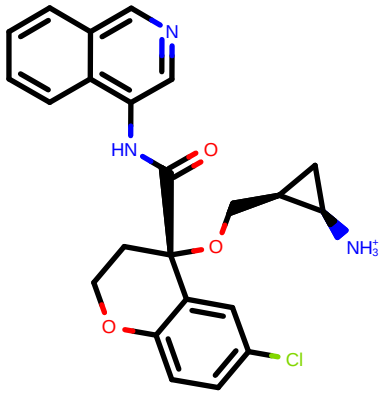
CID:	MAT-POS-4223bc15-11_14
SMILES:	C[C@H]1CC[N@@](C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4044
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.16

VLA-UCB-05e51b3f-11_1



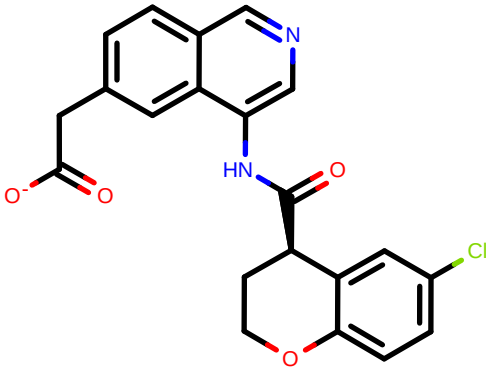
CID:	VLA-UCB-05e51b3f-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4O[C@@H]5CC(=O)N5)Cl
RUN:	RUN319
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.22

VLA-UNK-9a7dc93f-4_2



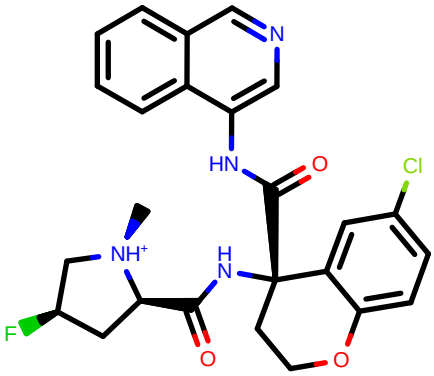
CID:	VLA-UNK-9a7dc93f-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(c(c4F)F)C#N
RUN:	RUN3087
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.20

MAT-POS-b5746674-35_2



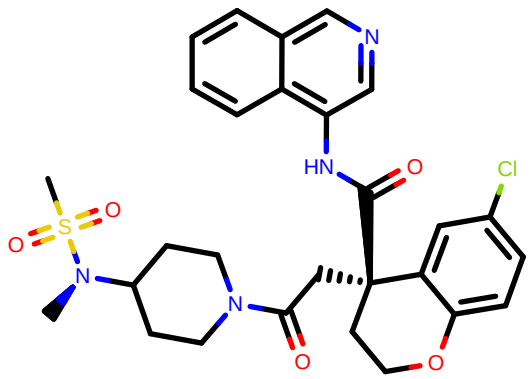
CID:	MAT-POS-b5746674-35_2
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCC[N@H+](Cc3ccco3)C4CCCC4
RUN:	RUN70
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.23

MIC-UNK-cdc2493e-12_3



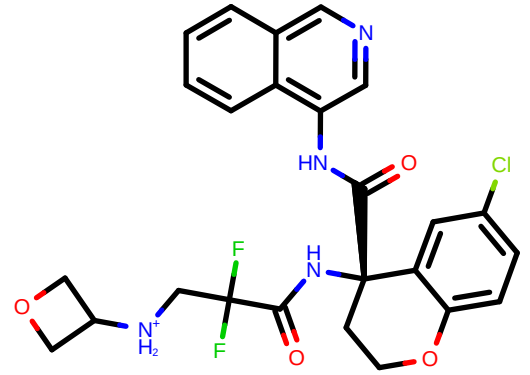
CID:	MIC-UNK-cdc2493e-12_3
SMILES:	C[NH+](C)[C@@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN552
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.28

MIC-UNK-0a05c952-4_6



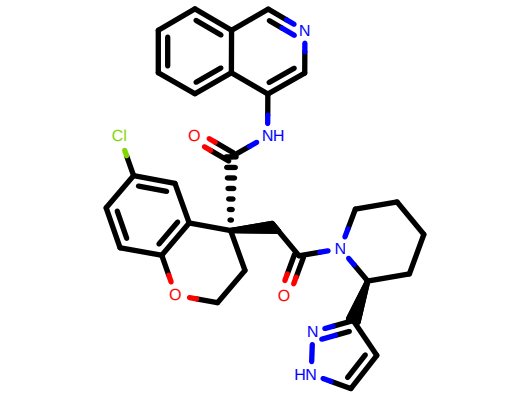
CID:	MIC-UNK-0a05c952-4_6
SMILES:	c1ccc2c(c1)cncc2N3[C@H](CC[C@@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@H]5CO5
RUN:	RUN3526
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.16

EDJ-MED-f893e2a1-4_1



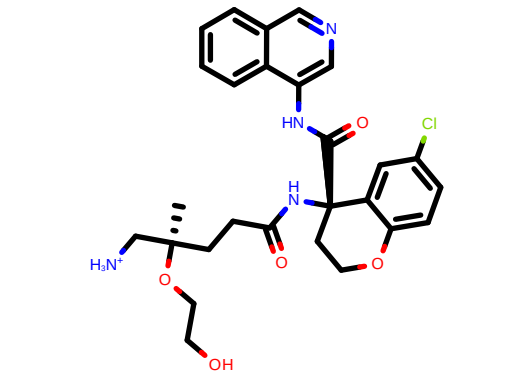
CID:	EDJ-MED-f893e2a1-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@]5(CCSC5)O
RUN:	RUN3196
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.19

BEN-BAS-c2bc0d80-4_1



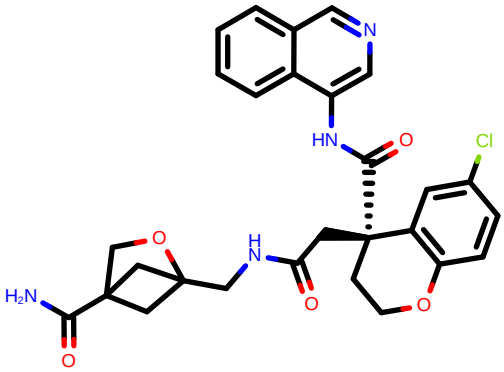
CID:	BEN-BAS-c2bc0d80-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC=Nc4c3[nH]c(cc4=O)Cl
RUN:	RUN1139
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.32

MIC-UNK-91acba05-6_4



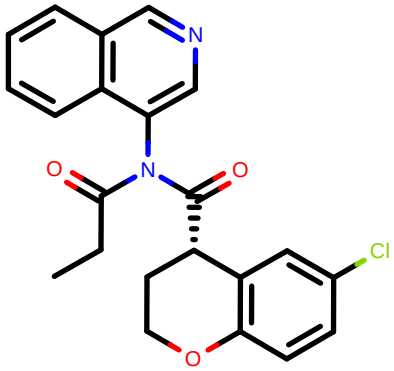
CID:	MIC-UNK-91acba05-6_4
SMILES:	CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN482
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.62

MAK-UNK-c749d764-1_4



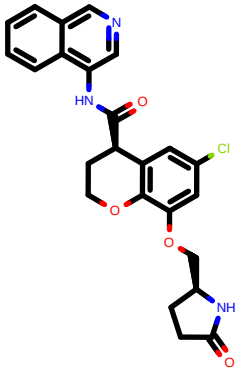
CID:	MAK-UNK-c749d764-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@H]([C@@H]3O)C4CC4
RUN:	RUN892
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.26

ERI-UCB-ce40166b-1_1



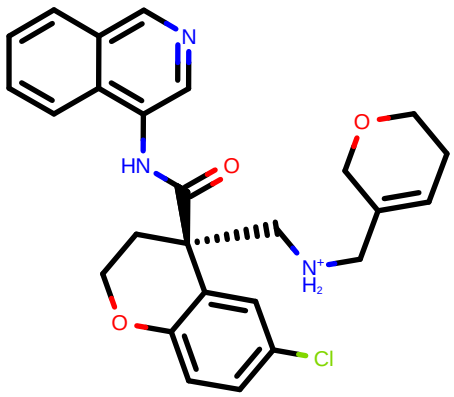
CID:	ERI-UCB-ce40166b-1_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)O[C@@H]4CC(=O)N4
RUN:	RUN33
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.20

MAT-POS-a3f7f96a-7_4



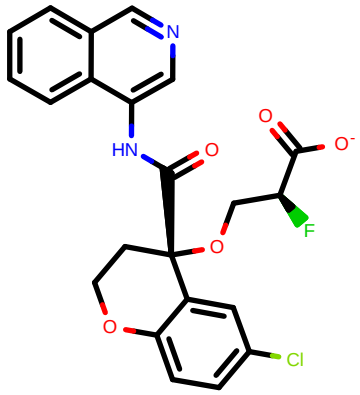
CID:	MAT-POS-a3f7f96a-7_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cnn(c5)[C@H]6CCS(=O)(=O)C6
RUN:	RUN5045
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.20

ALP-POS-347519b5-2_35



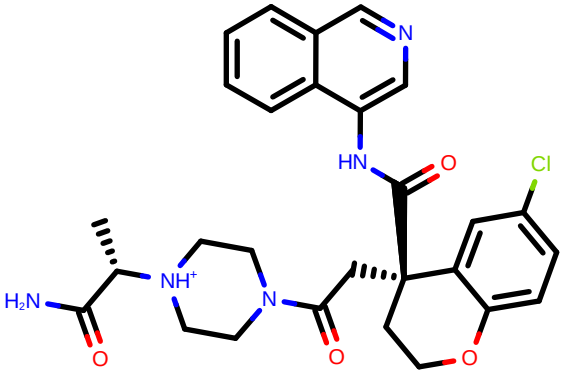
CID:	ALP-POS-347519b5-2_35
SMILES:	CO[C@@]1(C[N@](C[C@@H]2[C@@H]1[C@@H]3CC[C@H]2C3)S(=O)(=O)C)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4282
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.18

PET-UNK-c5865d42-2_1



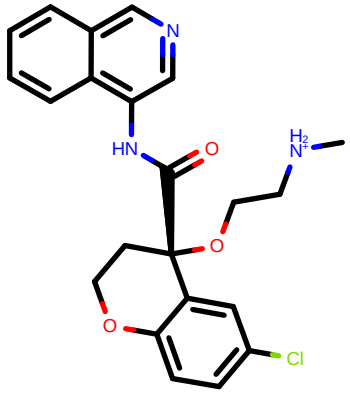
CID:	PET-UNK-c5865d42-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)C([C@@H]4CCN4)(F)F
RUN:	RUN427
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.29

MIC-UNK-5a93dd5f-1_1



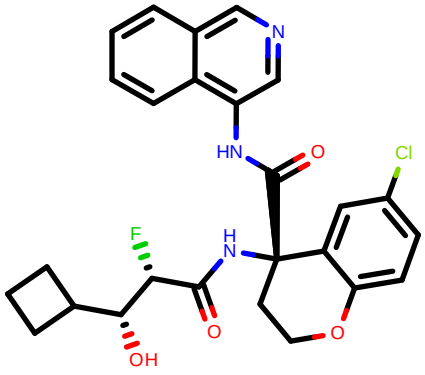
CID:	MIC-UNK-5a93dd5f-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)[NH+]4C[C@H]5CCC[C@H]5C4
RUN:	RUN721
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.35

DAR-DIA-0f2f46c9-4_3



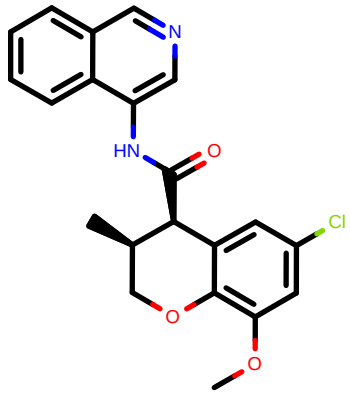
CID:	DAR-DIA-0f2f46c9-4_3
SMILES:	CS(=O)(=O)[N@@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3228
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.30

RAL-THA-e002e396-5_2



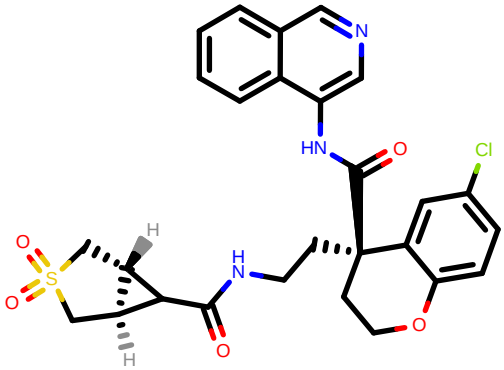
CID:	RAL-THA-e002e396-5_2
SMILES:	CNS(=O)(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3462
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.19

MAT-POS-3b92565d-3_1



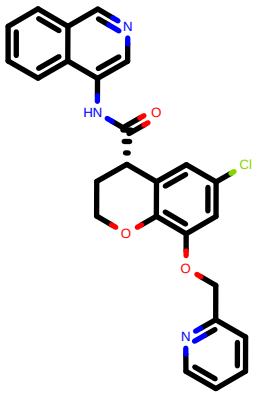
CID:	MAT-POS-3b92565d-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CC(=O)N4
RUN:	RUN111
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.26

MIC-UNK-5a93dd5f-8_2



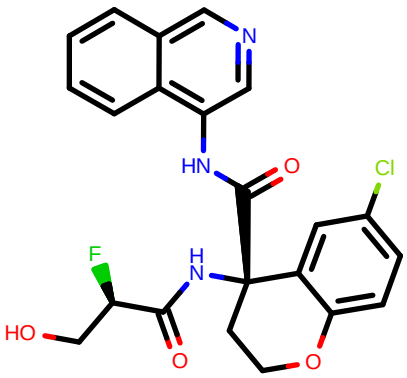
CID:	MIC-UNK-5a93dd5f-8_2
SMILES:	C[NH+](C)C1CC[NH+](CC1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN775
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.29

ED_-GRI-5b13fbe2-17_1



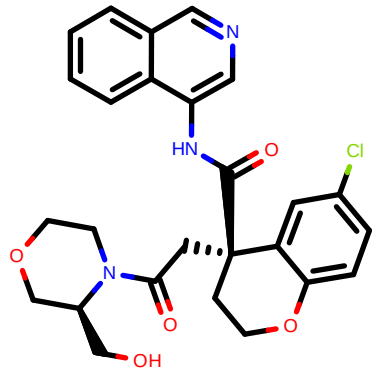
CID:	ED_-GRI-5b13fbe2-17_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](c5cn(nn5)CC6CC6)[NH3+]
RUN:	RUN1549
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.26

EDJ-MED-424a8a89-2_1



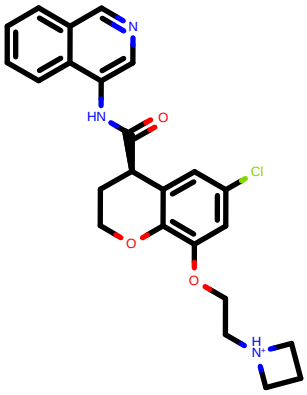
CID:	EDJ-MED-424a8a89-2_1
SMILES:	CC(C)[NH2+]C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3216
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.12

MAK-UNK-c749d764-31_3



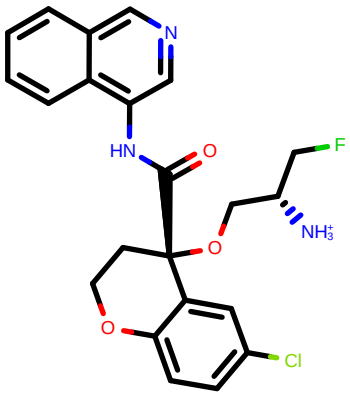
CID:	MAK-UNK-c749d764-31_3
SMILES:	CC/C=C(/c1cncc2c1cccc2)\C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1072
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.34

ALF-EVA-5b152d2f-1_1



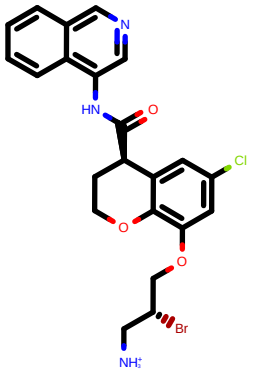
CID:	ALF-EVA-5b152d2f-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCCOc4c3cc(cc4)Cl
RUN:	RUN2353
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.53

VLA-UNK-9a7dc93f-2_1



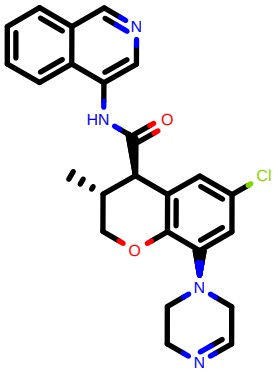
CID:	VLA-UNK-9a7dc93f-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(c(c(c3)F)F)C#N
RUN:	RUN3081
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.41

ALP-POS-67d5babe-1_6



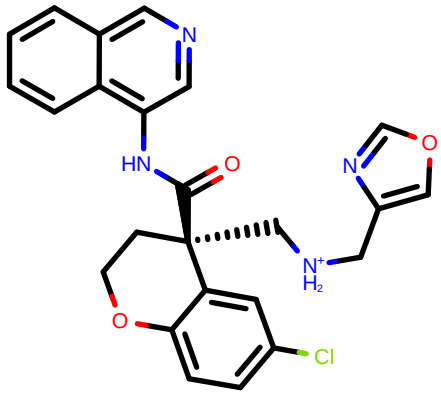
CID:	ALP-POS-67d5babe-1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC[N@@H+]5CC[C@H]6CS(=O)(=O)C[C@@H]6C5
RUN:	RUN4870
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.25

MAT-POS-9ff17035-1_1



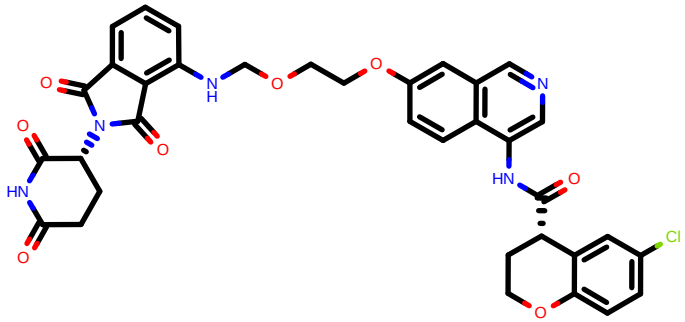
CID:	MAT-POS-9ff17035-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)O[C@@H]4CCC(=O)N4
RUN:	RUN146
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.31

MAT-POS-5f1400cf-1_2



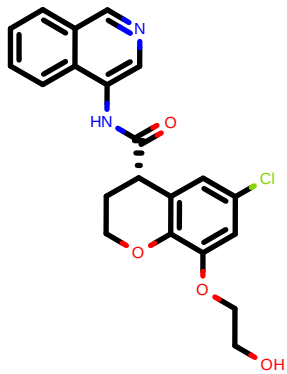
CID:	MAT-POS-5f1400cf-1_2
SMILES:	Cn1cc(cn1)N2CC[C@@H](C2)C[NH2+]C[C@@]3(COCc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN4507
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.32

MIC-UNK-9582b2c5-2_8



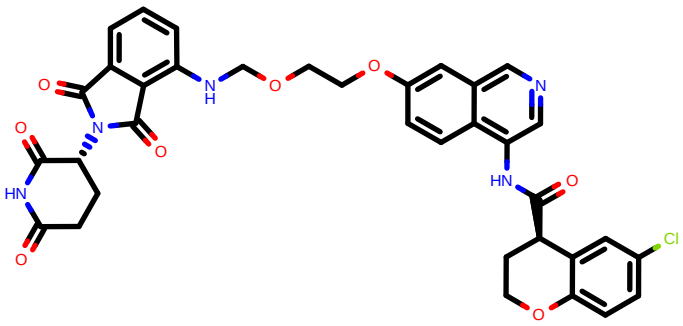
CID:	MIC-UNK-9582b2c5-2_8
SMILES:	CC(=O)N1CC[C@H]2[C@H](C1)C[C@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN268
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.36

ALP-POS-5bb456a5-1_14



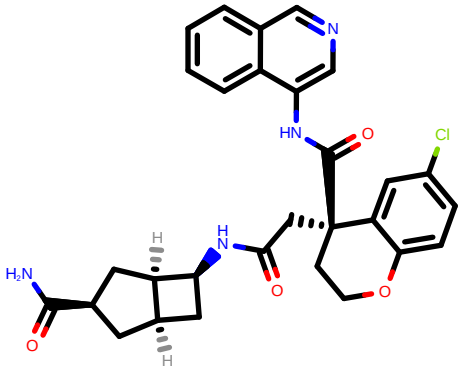
CID:	ALP-POS-5bb456a5-1_14
SMILES:	C[C@H]1C[N@@](CC[C@H]1NC(=O)C[C@]2(COCc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2419
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.23

DAR-DIA-0f2f46c9-4_1



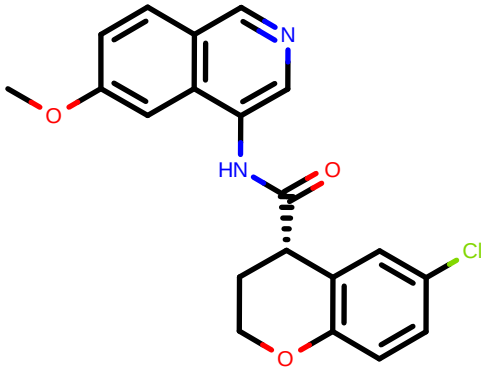
CID:	DAR-DIA-0f2f46c9-4_1
SMILES:	CS(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3226
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.28

DAR-DIA-56cf811e-3_1



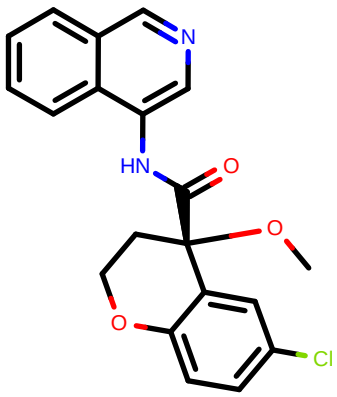
CID:	DAR-DIA-56cf811e-3_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)/C=C/C#N
RUN:	RUN1521
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.42

DAR-DIA-0d514e7d-32_20



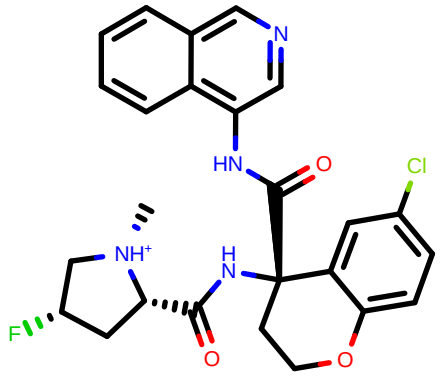
CID:	DAR-DIA-0d514e7d-32_20
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@H]4C[C@@H]4CO[C@@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN868
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.10

ALP-UNI-dbbfd3db-13_2



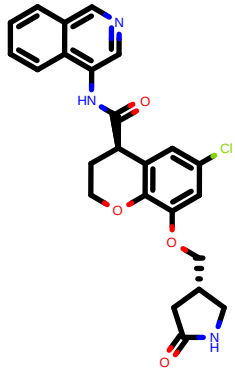
CID:	ALP-UNI-dbbfd3db-13_2
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2782
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.07

DAR-DIA-0f2f46c9-6_1



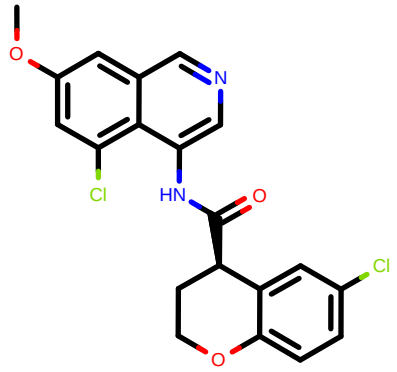
CID:	DAR-DIA-0f2f46c9-6_1
SMILES:	CS(=O)(=O)[N@@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3232
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.16

MIC-UNK-54748b58-1_1



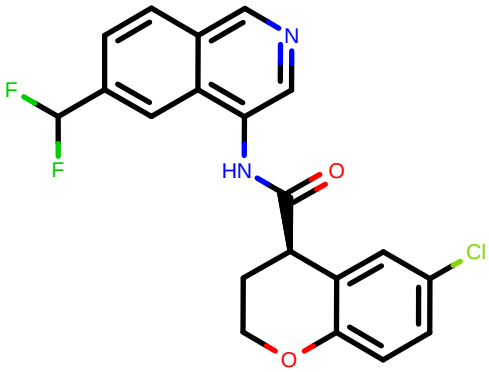
CID:	MIC-UNK-54748b58-1_1
SMILES:	CNC(=O)C[N@@]1C[C@@H](c2cc(ccc2S1(=O)=O)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4847
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.17

RAL-THA-6e4c80cf-4_2



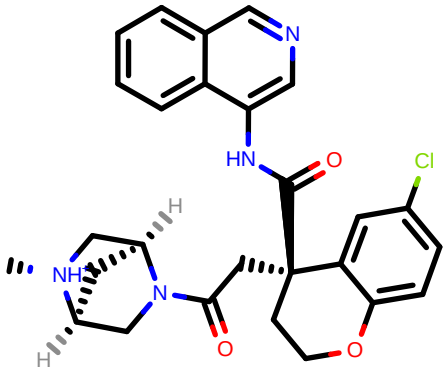
CID:	RAL-THA-6e4c80cf-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CN(Cc4c3cc(cc4)Cl)C(=O)OCc5ccccn5
RUN:	RUN3903
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.09

DAR-DIA-ecdbc7dd-10_2



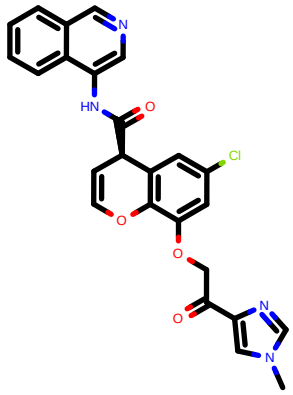
CID:	DAR-DIA-ecdbc7dd-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCNc4c3cc(cc4)Cl)C[NH+]5CCOCC5
RUN:	RUN2895
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.08

JOH-SUS-a69c159d-3_1



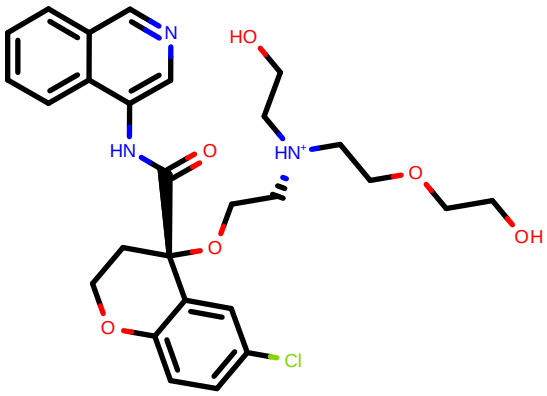
CID:	JOH-SUS-a69c159d-3_1
SMILES:	c1ccc2c(c1)c(cnc2C(F)F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1120
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.36

MAT-POS-e9e99895-12_2



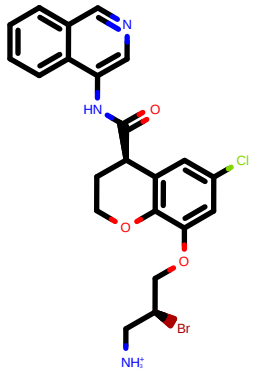
CID:	MAT-POS-e9e99895-12_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)CC[NH+](C)C
RUN:	RUN2266
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.40

DAR-DIA-6a508060-11_1



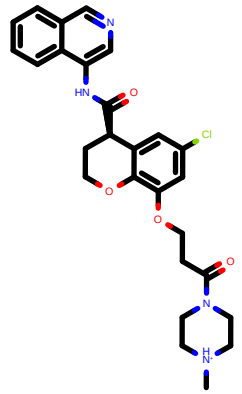
CID:	DAR-DIA-6a508060-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)C3CC(C3)[C@@H]4C[C@@H]4Cl
RUN:	RUN346
DDG (kcal/mol):	-0.36
dDDG (kcal/mol):	0.96

MAT-POS-24589f88-6_2



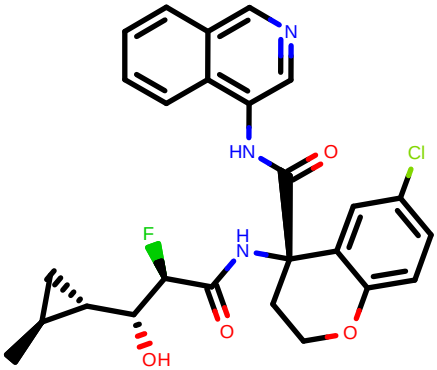
CID:	MAT-POS-24589f88-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5c(nc6ccccn6c5=O)N7CCOCC7
RUN:	RUN4777
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.31

EDG-MED-ba1ac7b9-5_3



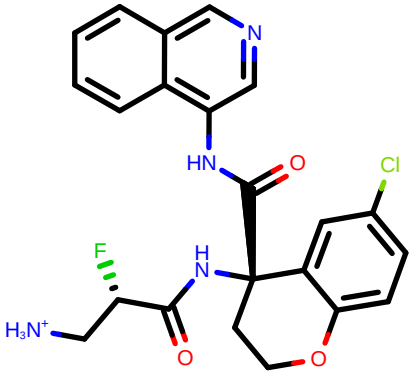
CID:	EDG-MED-ba1ac7b9-5_3
SMILES:	CC[C@@H](CO)[NH+]1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2638
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.45

RAL-THA-e002e396-7_2



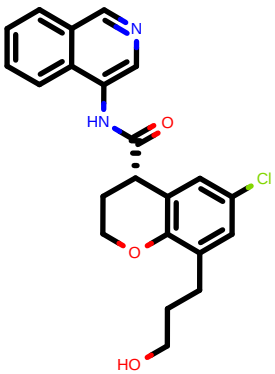
CID:	RAL-THA-e002e396-7_2
SMILES:	CN(C)S(=O)(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3466
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.15

LON-WEI-9739a092-1_1



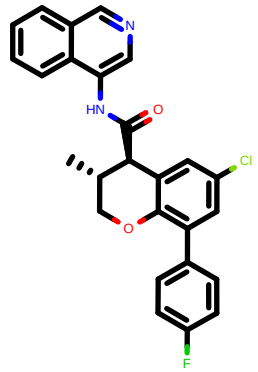
CID:	LON-WEI-9739a092-1_1
SMILES:	COc1cc(nc(n1)Nc2cc(cc(c2)Cl)CC(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3265
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.50

MAT-POS-8e4737f4-1_1



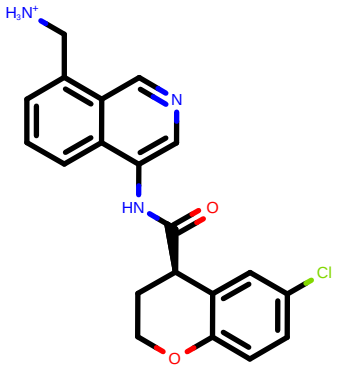
CID:	MAT-POS-8e4737f4-1_1
SMILES:	C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN309
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.21

LON-WEI-4d77710c-35_2



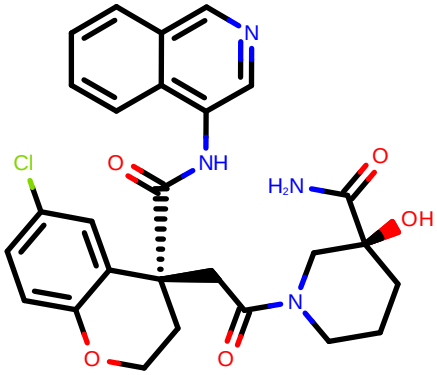
CID:	LON-WEI-4d77710c-35_2
SMILES:	Cc1ccc(cc1)C[N@H+]2CC[C@@H](C2)CNC(=O)Nc3cn(c(=O)c4c3cccc4)CC(C)C
RUN:	RUN223
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.31

ERI-UCB-ce40166b-11_1



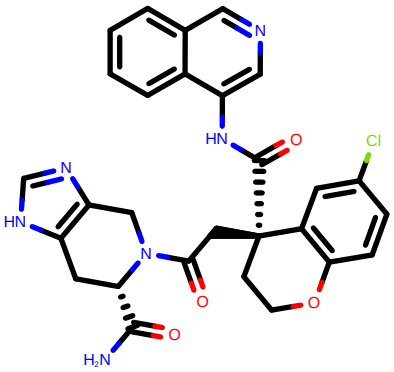
CID:	ERI-UCB-ce40166b-11_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Oc4cccc(=O)[nH]4)C#N
RUN:	RUN50
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.25

KAD-UNI-877d7bed-13_2



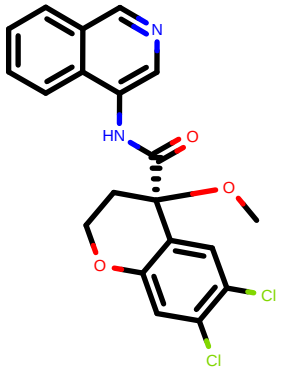
CID:	KAD-UNI-877d7bed-13_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCC(=O)c5ccc(cc5)S(=O)(=O)N)Cl
RUN:	RUN3756
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.21

RAL-THA-4aa06b95-6_1



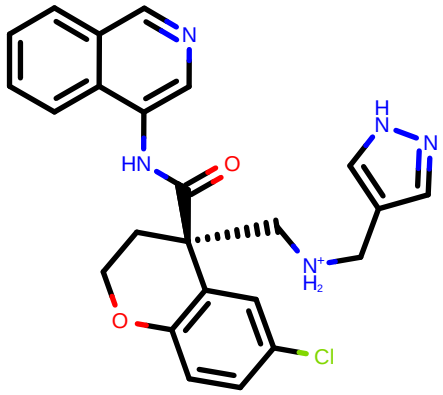
CID:	RAL-THA-4aa06b95-6_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCN(c4c3cc(cc4)Cl)CCO
RUN:	RUN1239
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.25

DAR-DIA-0d514e7d-31_9



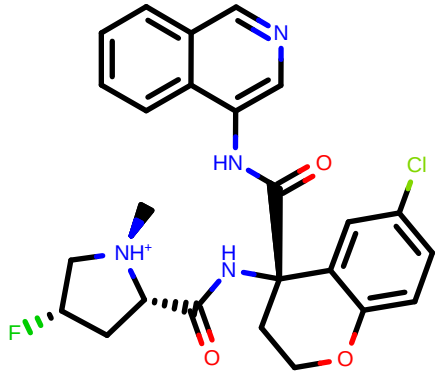
CID:	DAR-DIA-0d514e7d-31_9
SMILES:	C[C@@H]1CCO[C@@H]2C=CC(=C[C@@H]2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN843
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.12

KAD-UNI-8a629cb0-34_1



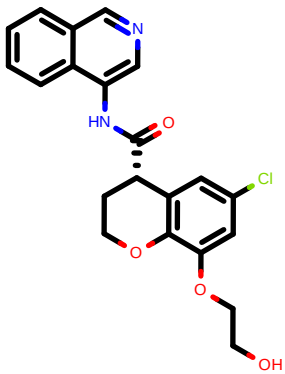
CID:	KAD-UNI-8a629cb0-34_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC[=O][C@@H]5[C@@H]6[C@@H]5COCC6
RUN:	RUN2116
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.37

DAR-DIA-0f2f46c9-5_1



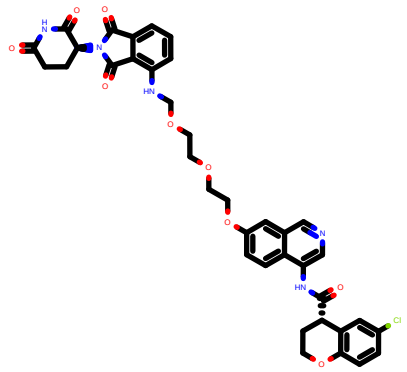
CID:	DAR-DIA-0f2f46c9-5_1
SMILES:	CS(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3230
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.17

VLA-UCB-05e51b3f-9_1



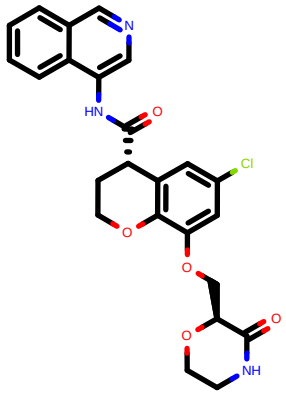
CID:	VLA-UCB-05e51b3f-9_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)CCl)C(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN317
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.21

BRU-THA-01b12488-1_1



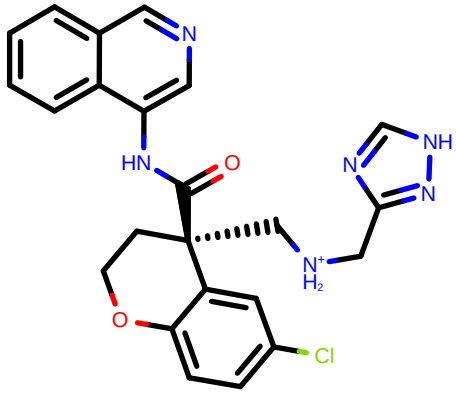
CID:	BRU-THA-01b12488-1_1
SMILES:	C[C@@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN383
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.46

ALP-POS-5bb456a5-2_7



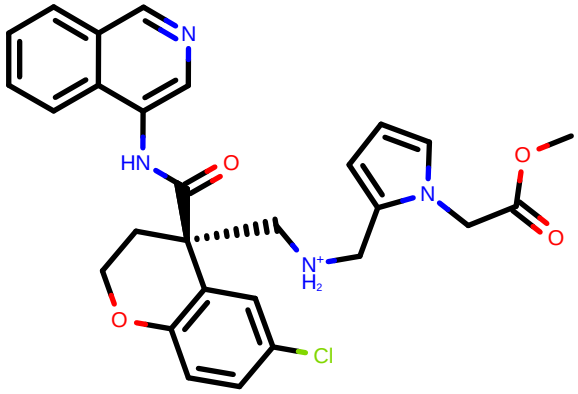
CID:	ALP-POS-5bb456a5-2_7
SMILES:	C[C@@H]1C[N@](CC[C@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2428
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.28

KAD-UNI-8a629cb0-32_1



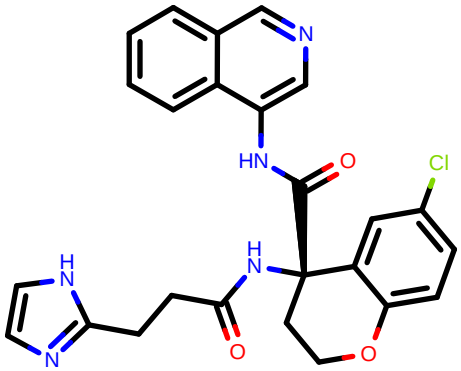
CID:	KAD-UNI-8a629cb0-32_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)C5[C@@H]6[C@@H]5CS(=O)(=O)C6
RUN:	RUN2115
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.35

ED_-GRI-5b13fbe2-60_2



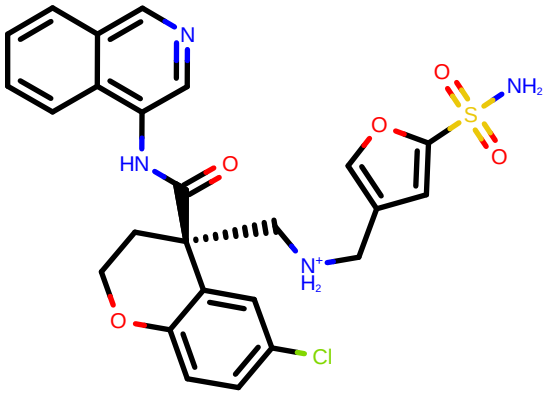
CID:	ED_-GRI-5b13fbe2-60_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cc6c(n5)CC[C@H](C6)[NH3+]
RUN:	RUN1607
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.50

NAU-LAT-a5c7d7cb-8_1



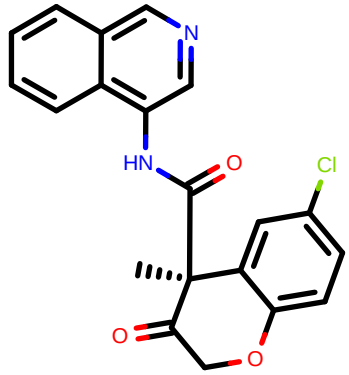
CID:	NAU-LAT-a5c7d7cb-8_1
SMILES:	c1ccc2c(c1)cncc2CNC(=O)COc3cccc(c3)Cl
RUN:	RUN578
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.32

MAT-POS-64942dd0-1_4



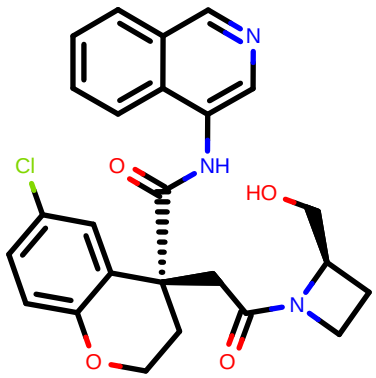
CID:	MAT-POS-64942dd0-1_4
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@H]3C[N@](Cc4c3cc(c(c4)F)Cl)S(=O)(=O)C
RUN:	RUN4384
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.33

EDG-MED-ba1ac7b9-32_1



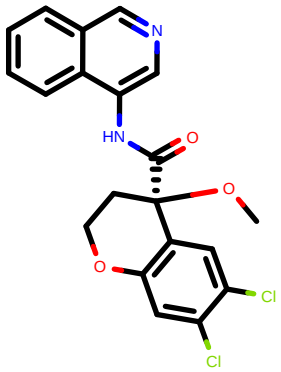
CID:	EDG-MED-ba1ac7b9-32_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)C6CCOCC6
RUN:	RUN2744
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.12

MIC-UNK-67d4a29a-1_1



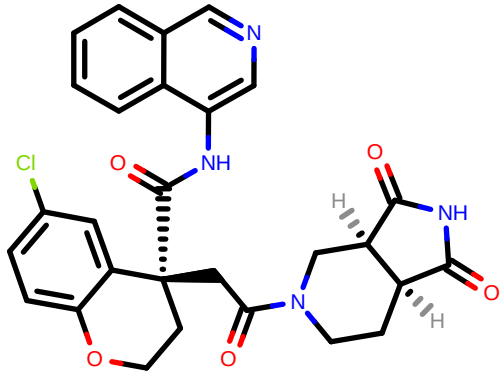
CID:	MIC-UNK-67d4a29a-1_1
SMILES:	CN(c1cncc2c1c(ccc2)Cl)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1086
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.31

DAR-DIA-5ff57136-17_1



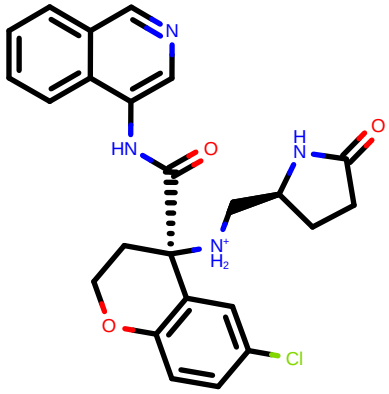
CID:	DAR-DIA-5ff57136-17_1
SMILES:	c1ccc2c(c1)cncc2N(CC#CBr)C(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1390
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.13

MAK-UNK-c749d764-28_4



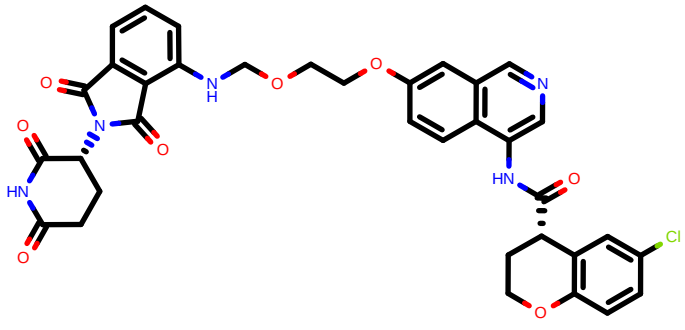
CID:	MAK-UNK-c749d764-28_4
SMILES:	c1ccc2c(c1)cncc2N(C=O)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F
RUN:	RUN1057
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.32

ED_-GRI-5b13fbe2-7_2



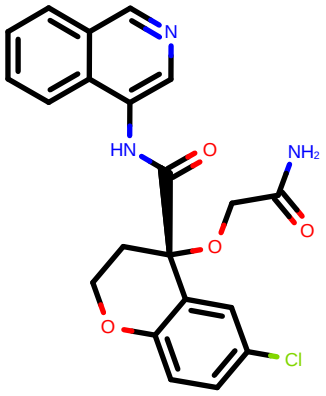
CID:	ED_-GRI-5b13fbe2-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCc5cn(nn5)C[C@H]6C[NH2+]CCO6
RUN:	RUN1532
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.30

DAR-DIA-23e5a6a0-2_1



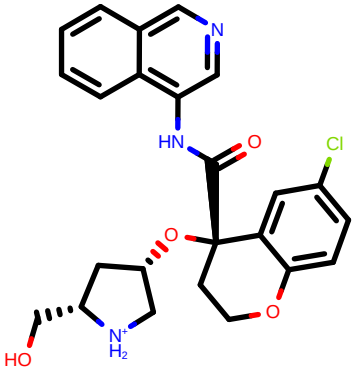
CID:	DAR-DIA-23e5a6a0-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O[C@@H]5CC6([NH2+]5)CCC6)Cl
RUN:	RUN403
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.42

ALP-POS-7c6e02c7-3_1



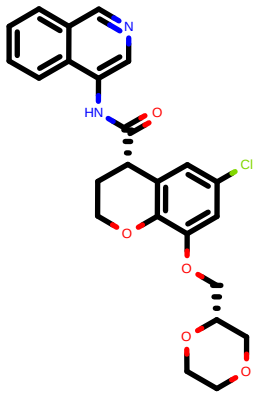
CID:	ALP-POS-7c6e02c7-3_1
SMILES:	CN(C)c1ccc(nc1)N(Cc2ccc(c(c2)Cl)F)C(=O)Cc3cncc4c3cccc4
RUN:	RUN3100
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.11

DAR-DIA-0f2f46c9-2_2



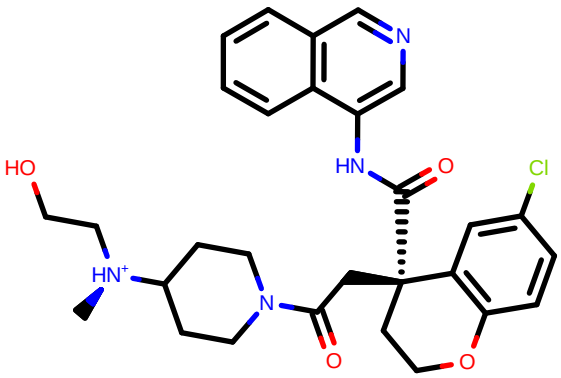
CID:	DAR-DIA-0f2f46c9-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC[N@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3223
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.23

KAD-UNI-8a629cb0-19_1



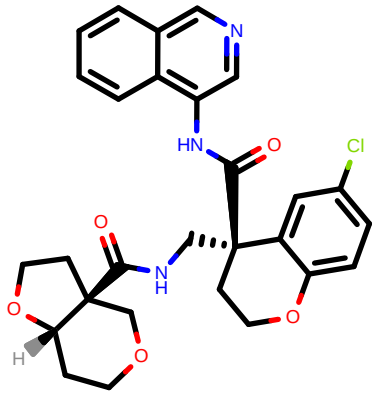
CID:	KAD-UNI-8a629cb0-19_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCNC(=O)c5ccnc6c5CC(=O)N6
RUN:	RUN2100
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.27

BEN-DND-f2e727cd-4_2



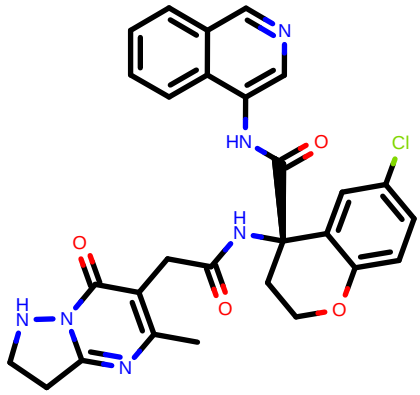
CID:	BEN-DND-f2e727cd-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3COCc4c3cc(cc4)Cl
RUN:	RUN1194
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.48

KAD-UNI-cb0f2bbc-10_1



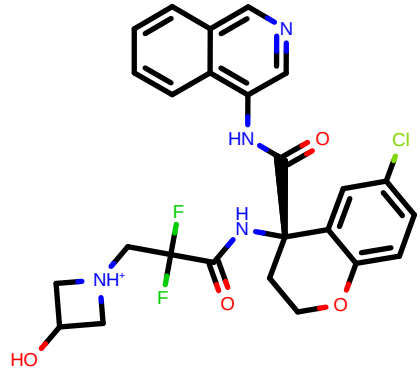
CID:	KAD-UNI-cb0f2bbc-10_1
SMILES:	CC(C)(C)OC(=O)N[C@@H](CCO)C[NH2+]C[C@]1(CCOc2c1cc(cc2Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3695
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.13

RAL-THA-c11c1343-1_1



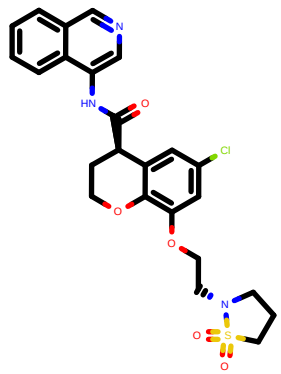
CID:	RAL-THA-c11c1343-1_1
SMILES:	CC(=O)N1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1227
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.29

EDJ-MED-946e547c-1_1



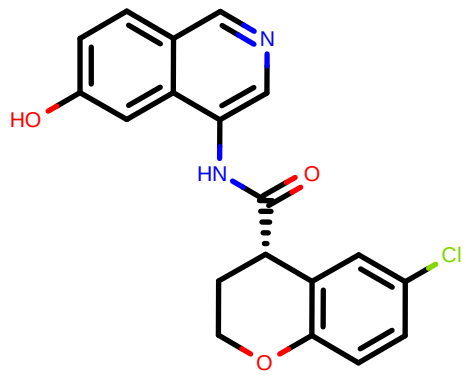
CID:	EDJ-MED-946e547c-1_1
SMILES:	CO[C@@]1(CCNc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cc(cc4)S(=O)(=O)C
RUN:	RUN3316
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.17

ALP-POS-5bb456a5-8_2



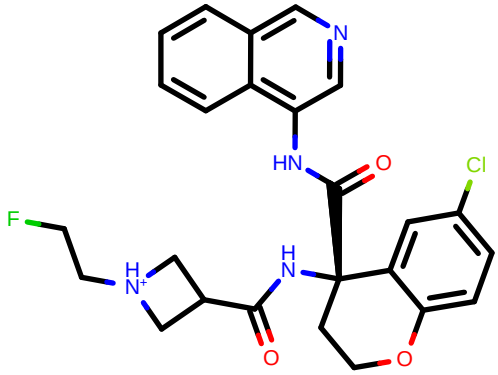
CID:	ALP-POS-5bb456a5-8_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@H]6CCOC6
RUN:	RUN2441
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.39

LON-WEI-4d77710c-39_2



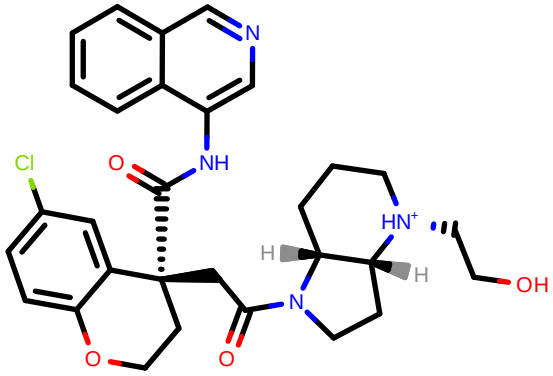
CID:	LON-WEI-4d77710c-39_2
SMILES:	C[C@H](CCc1ccco1)NC(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN228
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.11

EDJ-MED-424a8a89-2_2



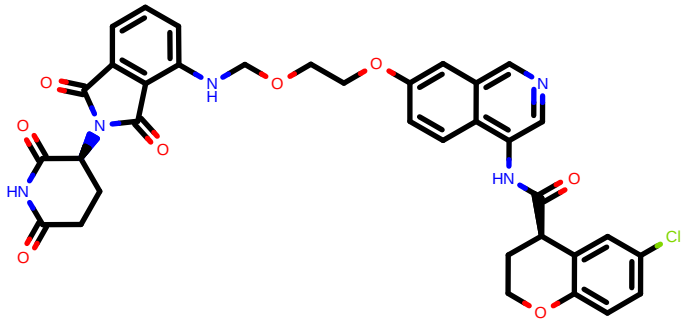
CID:	EDJ-MED-424a8a89-2_2
SMILES:	CC(C)[NH2+]C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3217
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.21

MAK-UNK-c749d764-15_10



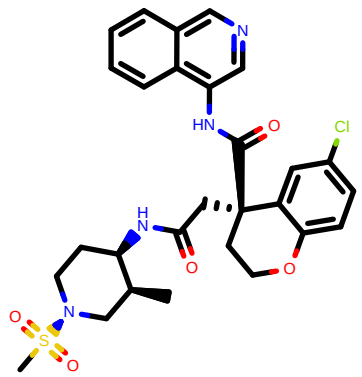
CID:	MAK-UNK-c749d764-15_10
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN970
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.56

ERI-UCB-b3e6b0c2-3_1



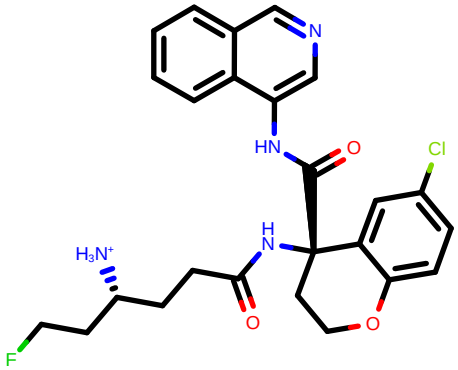
CID:	ERI-UCB-b3e6b0c2-3_1
SMILES:	C[N@@]1C[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cc(cc4)C[NH3+]
RUN:	RUN3034
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.24

MAT-POS-4223bc15-9_2



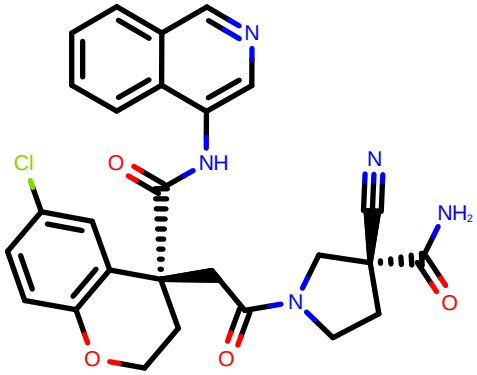
CID:	MAT-POS-4223bc15-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)[C@@H]5CCC[C@@H]5O
RUN:	RUN4010
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.25

MAK-UNK-c749d764-12_4



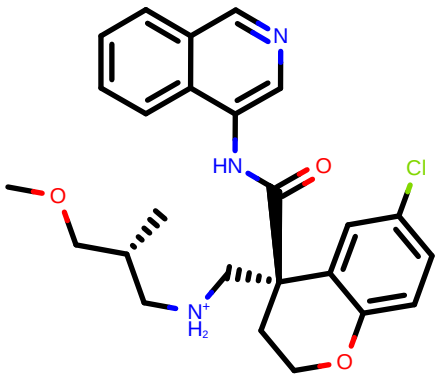
CID:	MAK-UNK-c749d764-12_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@H]([C@@H]3O)Cl
RUN:	RUN953
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.31

MAK-UNK-c749d764-28_5



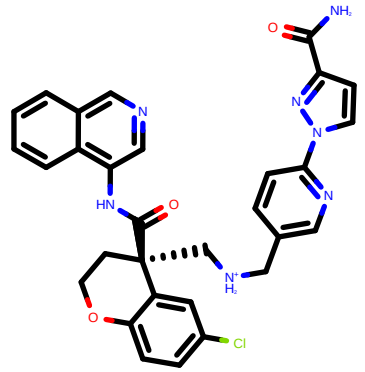
CID:	MAK-UNK-c749d764-28_5
SMILES:	c1ccc2c(c1)cncc2N(C=O)C(=O)C[C@@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1058
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.22

MAT-POS-de59a476-1_2



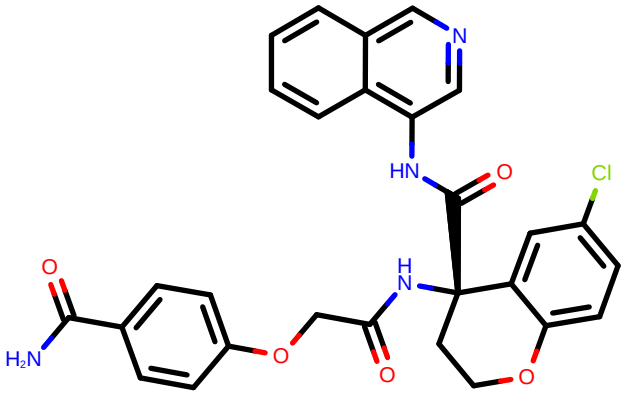
CID:	MAT-POS-de59a476-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)O
RUN:	RUN2214
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.46

PET-UNK-0cc03aae-3_1



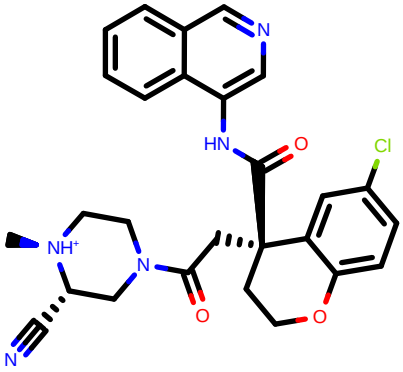
CID:	PET-UNK-0cc03aae-3_1
SMILES:	CS(=O)(=O)NCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4478
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.27

MAT-POS-e6dd326d-10_1



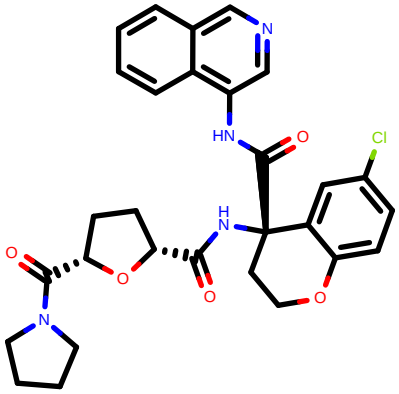
CID:	MAT-POS-e6dd326d-10_1
SMILES:	COC(=O)C[NH2+]C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3955
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.16

JOH-SUS-a69c159d-5_2



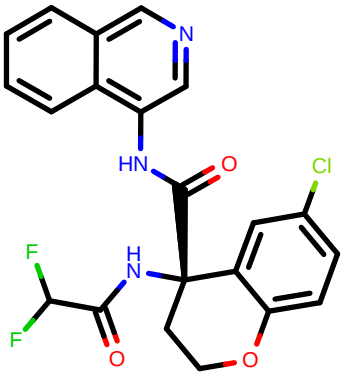
CID:	JOH-SUS-a69c159d-5_2
SMILES:	c1cc2c(cc1F)c(cnc2F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1124
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.33

MAT-POS-4223bc15-9_9



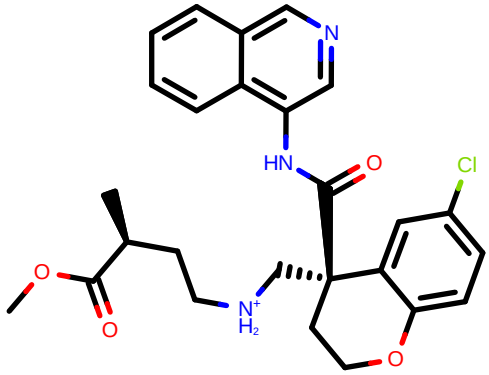
CID:	MAT-POS-4223bc15-9_9
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)[C@@H]5CCC[C@H]5O
RUN:	RUN4017
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.18

EDJ-MED-f893e2a1-6_3



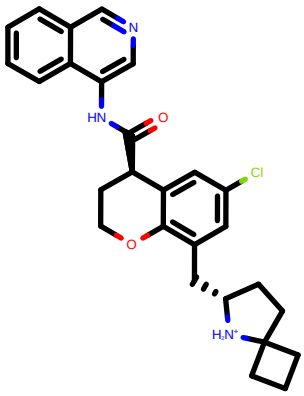
CID:	EDJ-MED-f893e2a1-6_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@H]5CC(=O)NC5
RUN:	RUN3205
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.08

ALP-UNI-dbb9503d-1_2



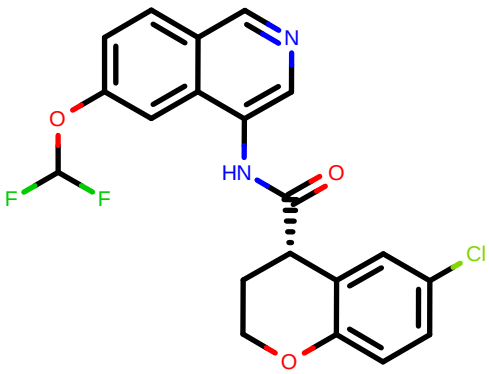
CID:	ALP-UNI-dbb9503d-1_2
SMILES:	CO[C@]1(CCN(C1=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN4329
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.23

ERI-UCB-ce40166b-3_1



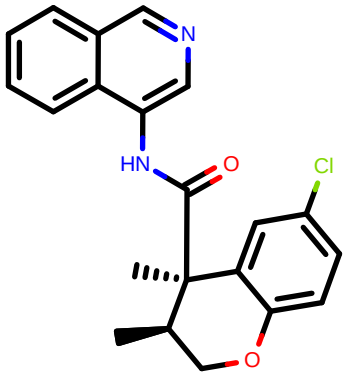
CID:	ERI-UCB-ce40166b-3_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cccc(c3)Oc4cccc(=O)[nH]4
RUN:	RUN38
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.38

LON-WEI-4d77710c-20_1



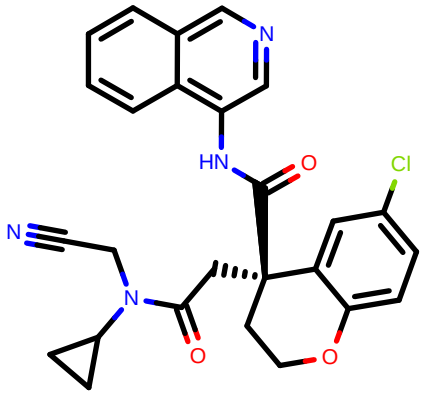
CID:	LON-WEI-4d77710c-20_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCCc3c[nH]c4c3cccc4
RUN:	RUN208
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.11

EDJ-MED-ee07cf00-6_4



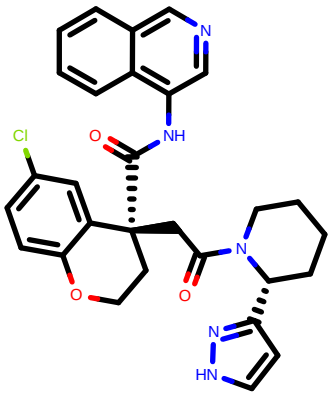
CID:	EDJ-MED-ee07cf00-6_4
SMILES:	Cn1cc(cn1)C2=NO[C@H](C2)C(=O)N[C@H](c3cccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2819
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.07

KAD-UNI-b13decd3-1_4



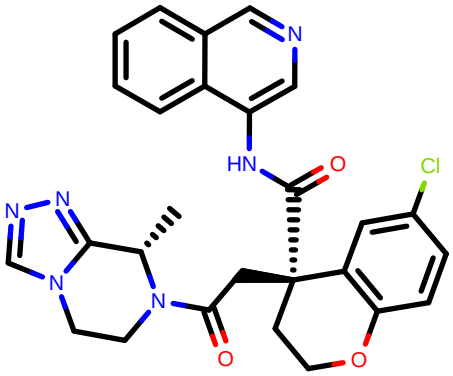
CID:	KAD-UNI-b13decd3-1_4
SMILES:	Cn1cc(cn1)N2CC[C@H](C2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3782
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.12

KAD-UNI-b13decd3-10_1



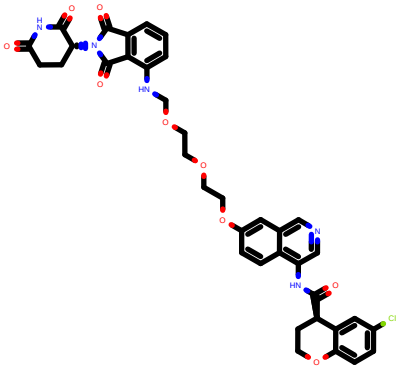
CID:	KAD-UNI-b13decd3-10_1
SMILES:	COc1nc2ncc(cn2n1)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3791
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.15

BEN-BAS-c2bc0d80-5_2



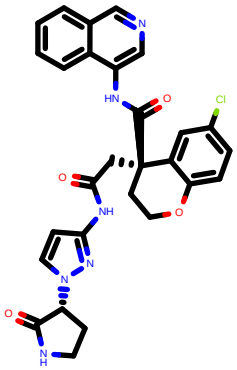
CID:	BEN-BAS-c2bc0d80-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3[nH]c(cc4=O)Cl
RUN:	RUN1142
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.24

ALP-UNI-8e43a71e-9_3



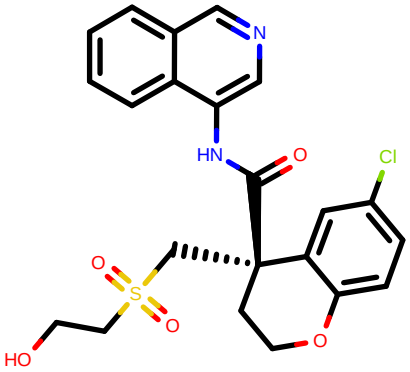
CID:	ALP-UNI-8e43a71e-9_3
SMILES:	C[N@@](C1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2969
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.36

MAK-UNK-c749d764-16_15



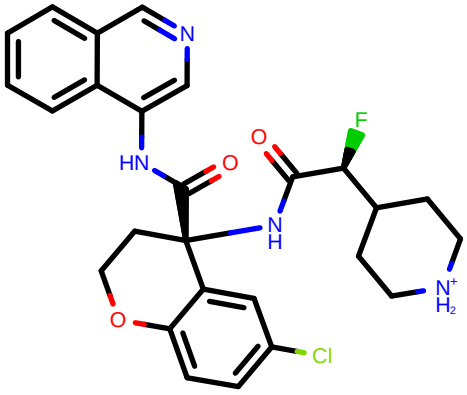
CID:	MAK-UNK-c749d764-16_15
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F)O
RUN:	RUN988
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.47

EDG-MED-90036822-12_1



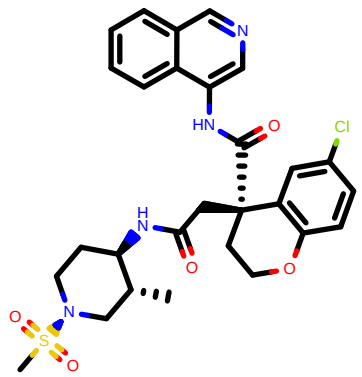
CID:	EDG-MED-90036822-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)/C=C/C[N@@H+]5CC[C@@H]5C(=O)N
RUN:	RUN1671
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.40

JAG-UCB-706446eb-3_1



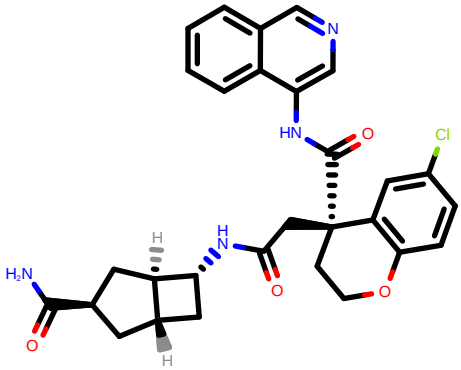
CID:	JAG-UCB-706446eb-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CCC(=O)[O-]
RUN:	RUN617
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.30

DAR-DIA-0d514e7d-33_2



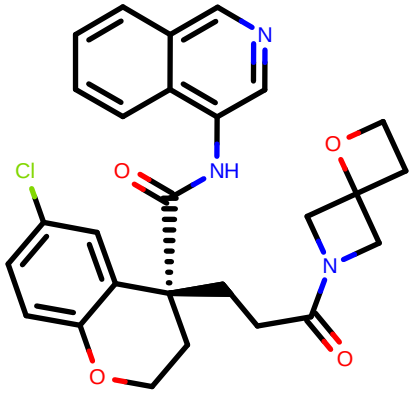
CID:	DAR-DIA-0d514e7d-33_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4O[C@H]5[C@@H]3C5)Cl
RUN:	RUN883
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.29

ED_-GRI-5b13fbe2-58_2



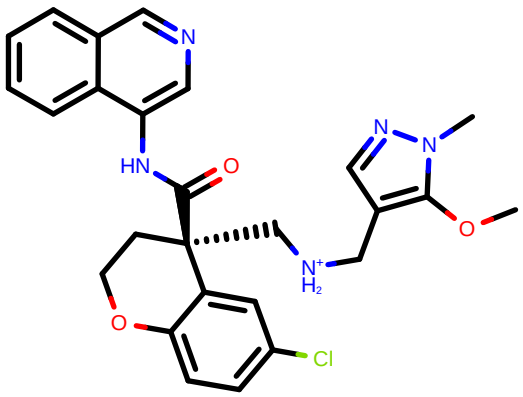
CID:	ED_-GRI-5b13fbe2-58_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCn5cc(nn5)[C@H]6CCC[NH2+]6
RUN:	RUN1608
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.27

DAR-DIA-f6ee7aeb-4_2



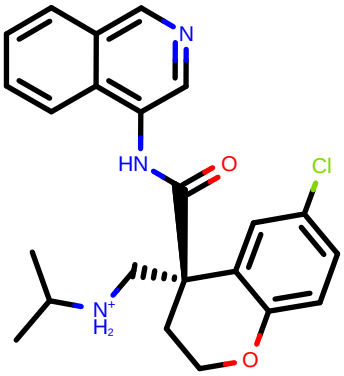
CID:	DAR-DIA-f6ee7aeb-4_2
SMILES:	c1ccc2c(c1)cncc2N3C[C@H]([C@@H](CC3=O)c4cc(cc(c4)Cl)OCCC(F)(F)F)c5c[nH]c(=O)[nH]c5=O
RUN:	RUN3413
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.16

RAL-THA-2d450e86-12_1



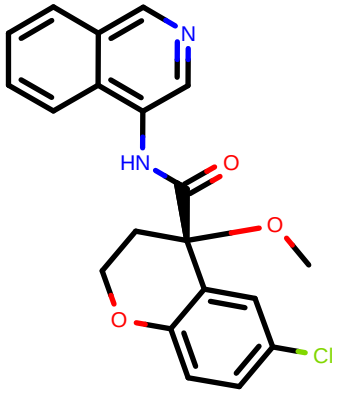
CID:	RAL-THA-2d450e86-12_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)C#N
RUN:	RUN1978
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.48

MAT-POS-4223bc15-19_2



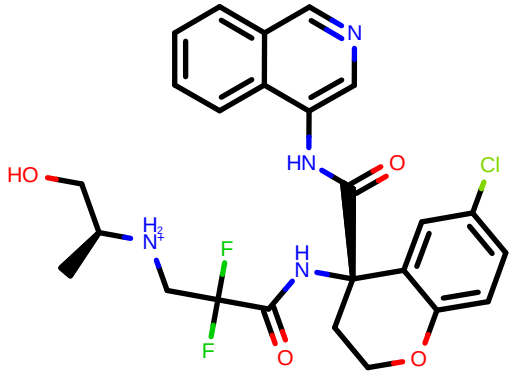
CID:	MAT-POS-4223bc15-19_2
SMILES:	COC(=O)N1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4094
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.16

MAT-POS-932d1078-3_1



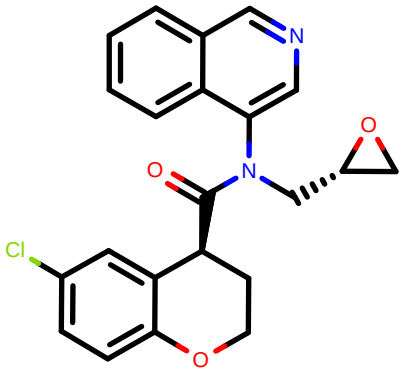
CID:	MAT-POS-932d1078-3_1
SMILES:	CO[C@]1(CCOc2c1cc(cc2F)F)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3595
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.06

MAK-UNK-ffc90da7-4_1



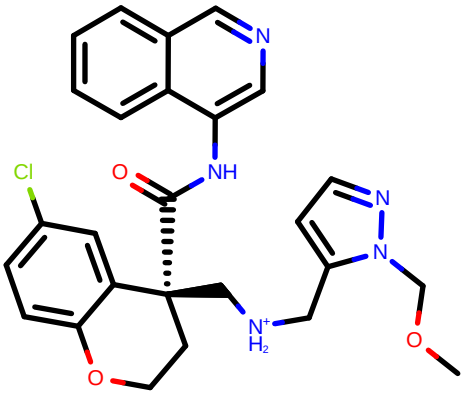
CID:	MAK-UNK-ffc90da7-4_1
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN693
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.39

DAR-DIA-5ff57136-5_1



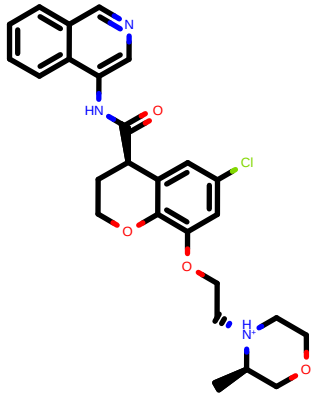
CID:	DAR-DIA-5ff57136-5_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)C3=CCCc4c3cc(cc4)Cl
RUN:	RUN1375
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.25

RAL-THA-05e671eb-29_2



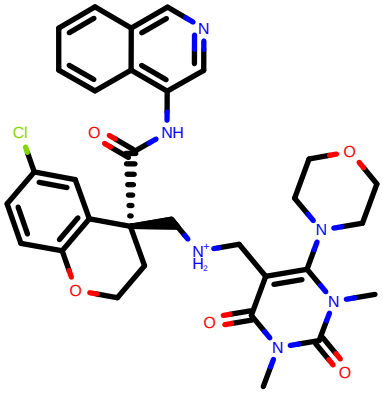
CID:	RAL-THA-05e671eb-29_2
SMILES:	Cc1c(ccc2c1[C@H](CCO2)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN2063
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.43

EDJ-MED-fcba3f31-7_1



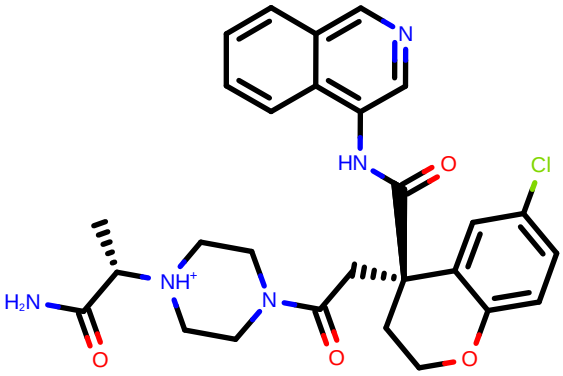
CID:	EDJ-MED-fcba3f31-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CO[C@H]5CCNC5=O
RUN:	RUN2543
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.48

EDG-MED-90036822-41_1



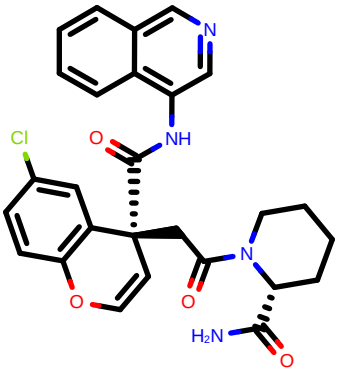
CID:	EDG-MED-90036822-41_1
SMILES:	Cn1ccnc1CC(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1715
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.66

EDJ-MED-15e90dfc-6_4



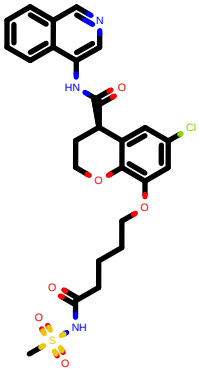
CID:	EDJ-MED-15e90dfc-6_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH2+]C[C@H]5CCC(=O)N5
RUN:	RUN3450
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.23

KAD-UNI-877d7bed-7_2



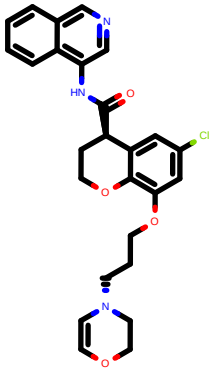
CID:	KAD-UNI-877d7bed-7_2
SMILES:	Cc1cc(=O)n2c(n1)nc([nH]2)COc3cc(cc4c3OCC[C@H]4C(=O)Nc5cncc6c5cccc6)Cl
RUN:	RUN3734
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.17

ALP-POS-2da19ca7-7_6



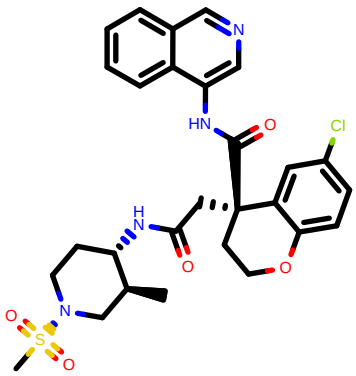
CID:	ALP-POS-2da19ca7-7_6
SMILES:	C[C@H]1C[N@@]([CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2387
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.62

PET-UNK-1320d94d-23_1



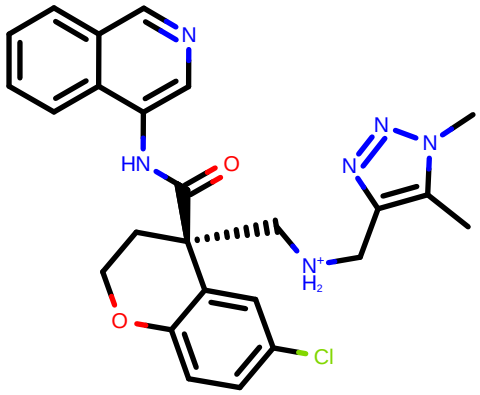
CID:	PET-UNK-1320d94d-23_1
SMILES:	CN[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)C(=O)[C@@H]4CC[C@@H](O4)C(=O)N5CCOCC5
RUN:	RUN4994
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.35

MAK-UNK-c749d764-1_6



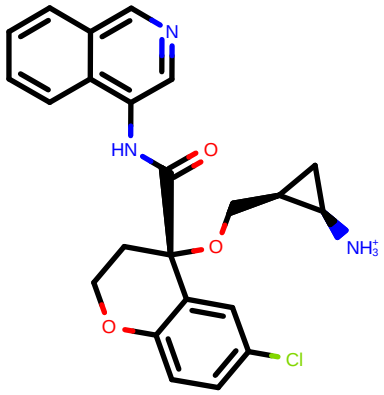
CID:	MAK-UNK-c749d764-1_6
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@@H]([C@H]3O)C4CC4
RUN:	RUN894
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.34

EDG-MED-90036822-96_2



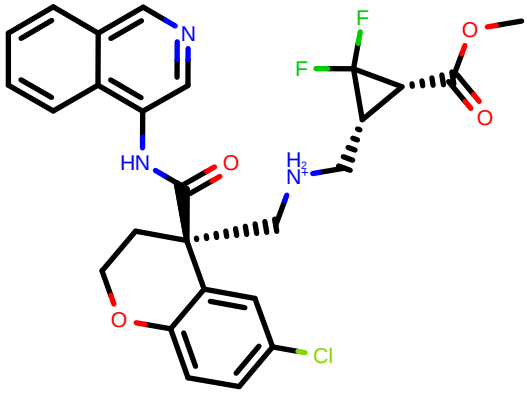
CID:	EDG-MED-90036822-96_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC[C@H](CCF)[NH3+]
RUN:	RUN1824
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.36

VLA-UNK-9a7dc93f-1_1



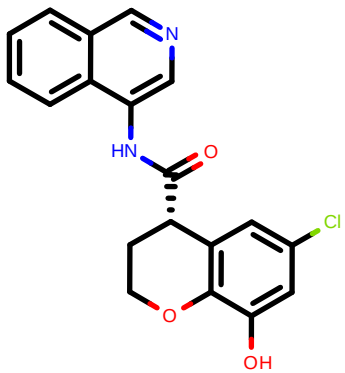
CID:	VLA-UNK-9a7dc93f-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(c(c(c3)Cl)F)F
RUN:	RUN3082
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.19

ALP-POS-347519b5-3_5



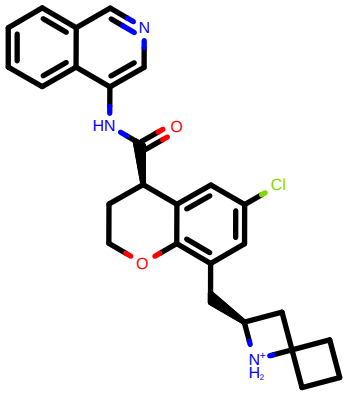
CID:	ALP-POS-347519b5-3_5
SMILES:	CS(=O)(=O)N@@1C[C@@H]2[C@H]3CC[C@@H]([C@@H]2[C@@H](C1)C(=O)Nc4ncc5c4cccc5)O3
RUN:	RUN4296
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.27

MIC-UNK-9582b2c5-2_6



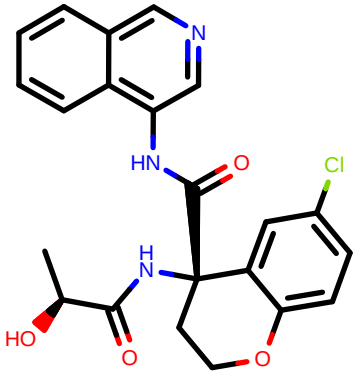
CID:	MIC-UNK-9582b2c5-2_6
SMILES:	CC(=O)N1CC[C@H]2[C@@H](C1)C[C@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN267
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.17

MIC-UNK-9582b2c5-1_3



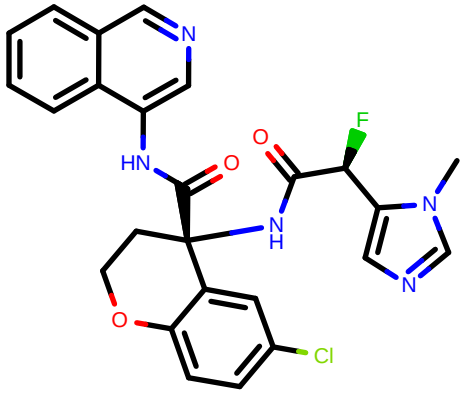
CID:	MIC-UNK-9582b2c5-1_3
SMILES:	CC(=O)N1CC[C@@H]2[C@H](C1)CN(C(=O)[C@@H]2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN256
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.36

VLA-UNK-b9c208fe-1_1



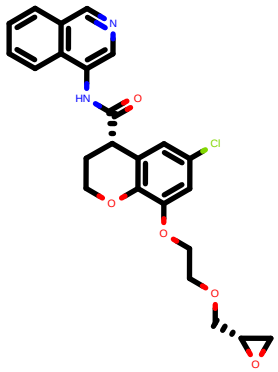
CID:	VLA-UNK-b9c208fe-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(c(c(c3)Cl)F)C#N
RUN:	RUN3157
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.10

MAK-UNK-8be7dca9-10_4



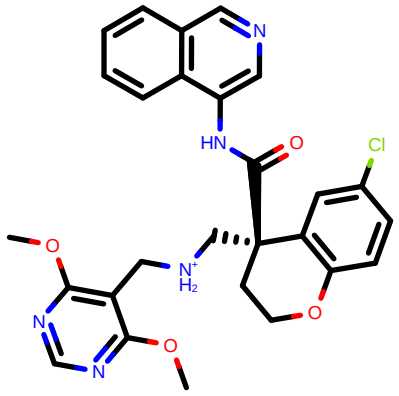
CID:	MAK-UNK-8be7dca9-10_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[C@H](Oc4c3cc(cc4)Cl)C(=O)[O-]
RUN:	RUN514
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.29

MAT-POS-f9802937-6_1



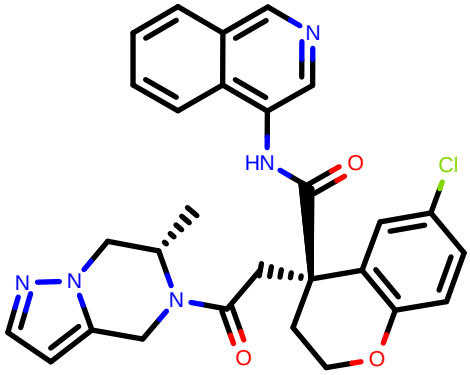
CID:	MAT-POS-f9802937-6_1
SMILES:	CNC(=O)C[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2399
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.29

ED_-GRI-5b13fbe2-29_1



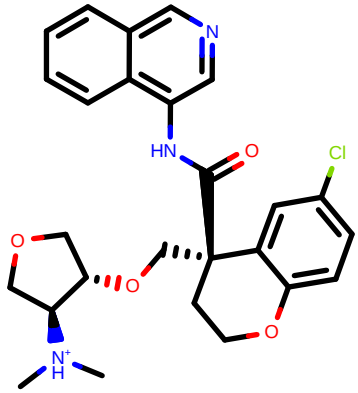
CID:	ED_-GRI-5b13fbe2-29_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCOCCOCC[NH3+]
RUN:	RUN1564
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.45

EDJ-MED-eff36d94-1_1



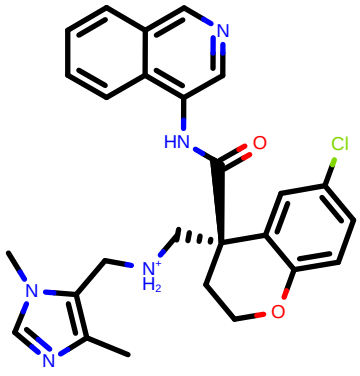
CID:	EDJ-MED-eff36d94-1_1
SMILES:	c1ccc2c(c1)cn(=O)cc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1215
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.24

MIC-UNK-0a05c952-2_3



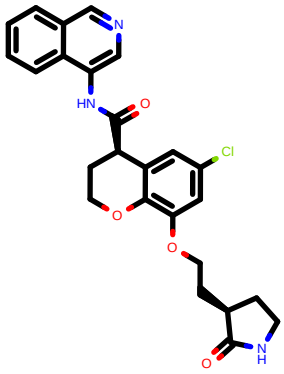
CID:	MIC-UNK-0a05c952-2_3
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](CC[C@H](C3=O)c4cccc(c4)Cl)[C@@H]5CO5
RUN:	RUN3507
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.13

EDG-MED-90036822-106_1



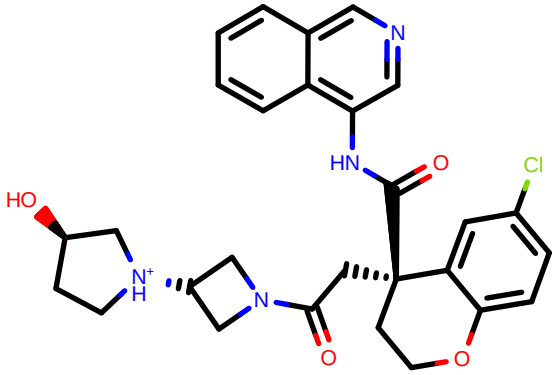
CID:	EDG-MED-90036822-106_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CC(C[NH3+])(F)F
RUN:	RUN1843
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.50

KAD-UNI-8a629cb0-47_1



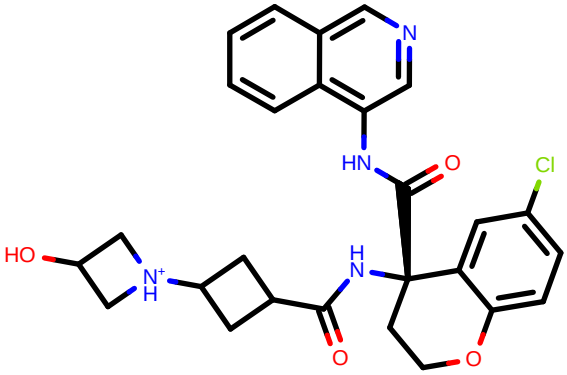
CID:	KAD-UNI-8a629cb0-47_1
SMILES:	Cn1cc(nn1)CC(=O)NCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2139
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.45

KAD-UNI-877d7bed-19_1



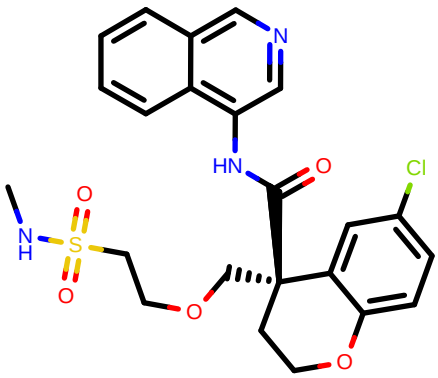
CID:	KAD-UNI-877d7bed-19_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4OCc5cc(on5)S(=O)(=O)N)Cl
RUN:	RUN3765
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.20

VLA-UNK-c65c1026-5_1



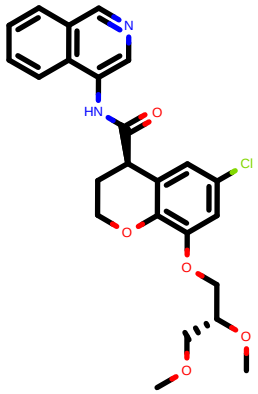
CID:	VLA-UNK-c65c1026-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[NH2+][C@@]4(C3=O)COc5c4cc(cc5)Cl
RUN:	RUN3186
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.18

PET-UNK-d9de6a0b-2_1



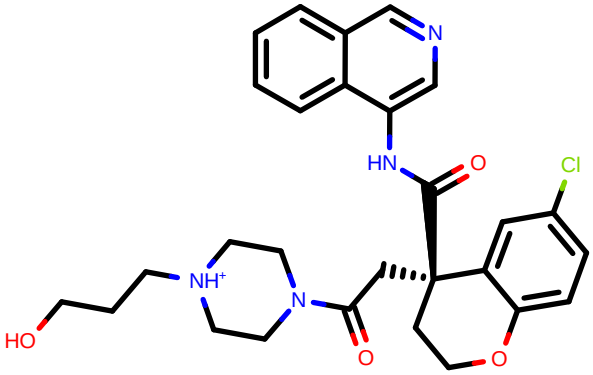
CID:	PET-UNK-d9de6a0b-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC5CS(=O)(=O)C5
RUN:	RUN4235
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.16

PET-UNK-ab76d8f6-1_1



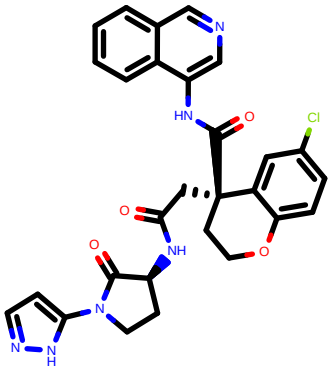
CID:	PET-UNK-ab76d8f6-1_1
SMILES:	CO[C@]1(CCS(=O)(=O)c2c1cc(cc2)Cl)C(=O)Nc3cncc4c3ccc(c4)C#N
RUN:	RUN5033
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.20

ED_-GRI-5b13fbe2-1_1



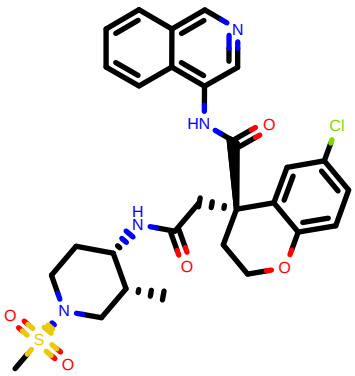
CID:	ED_-GRI-5b13fbe2-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC[NH2+]Cc5cc(no5)C(=O)[O-]
RUN:	RUN1526
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.51

MIC-UNK-45817b9b-1_2



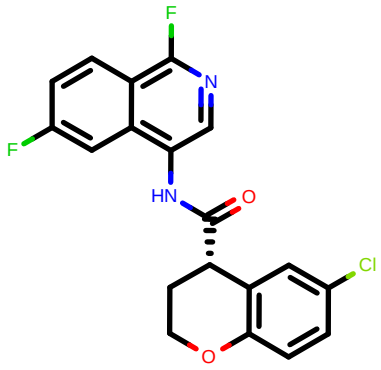
CID:	MIC-UNK-45817b9b-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC(=O)Nc4c3cc(cc4)Cl
RUN:	RUN1304
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.47

MAT-POS-4223bc15-4_1



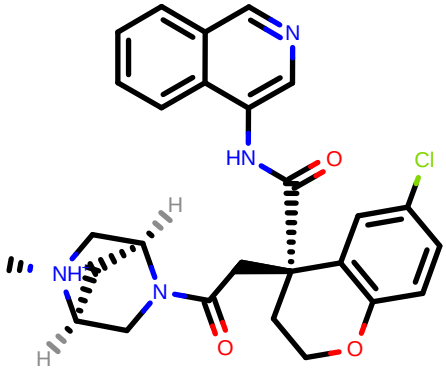
CID:	MAT-POS-4223bc15-4_1
SMILES:	COCCS(=O)(=O)[N@@]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3986
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.24

LON-WEI-4d77710c-44_1



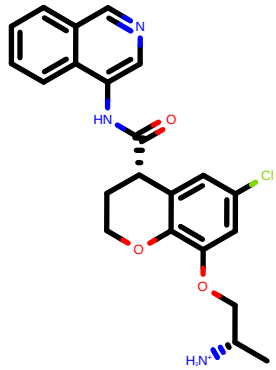
CID:	LON-WEI-4d77710c-44_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCc3ccco3
RUN:	RUN234
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.12

JOH-SUS-a69c159d-2_1



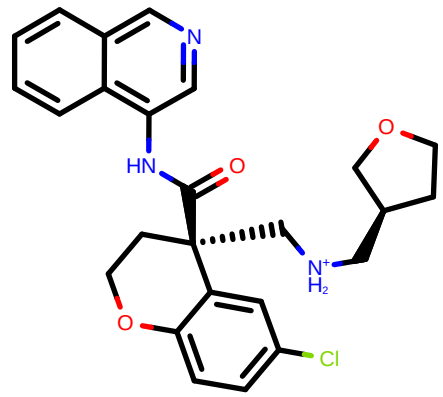
CID:	JOH-SUS-a69c159d-2_1
SMILES:	c1ccc2c(c1)c(cnc2F)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1118
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.25

MAT-POS-e9e99895-7_2



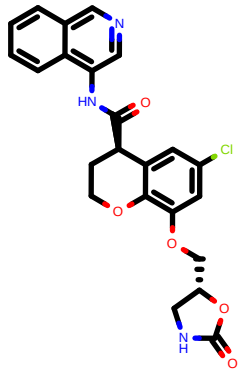
CID:	MAT-POS-e9e99895-7_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)Cc4ccc(cc4)n5cnnn5
RUN:	RUN2254
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.29

PET-UNK-9b23ef84-7_1



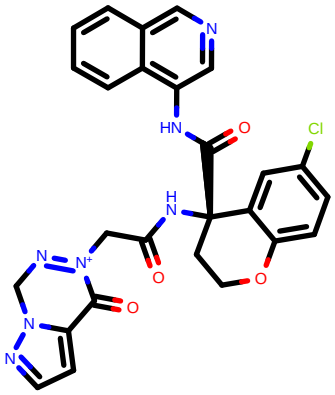
CID:	PET-UNK-9b23ef84-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CN(Cc4c3cc(c(c4)F)Cl)c5nnco5
RUN:	RUN4433
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.21

MIC-UNK-06e5f114-2_1



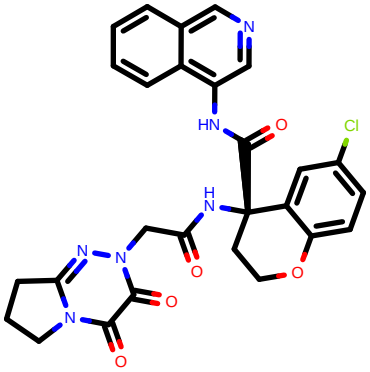
CID:	MIC-UNK-06e5f114-2_1
SMILES:	CS(=O)(=O)c1cccc(c1)NCc2ccc(cc2CC(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN5061
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.19

MIC-UNK-d58dbb53-1_1



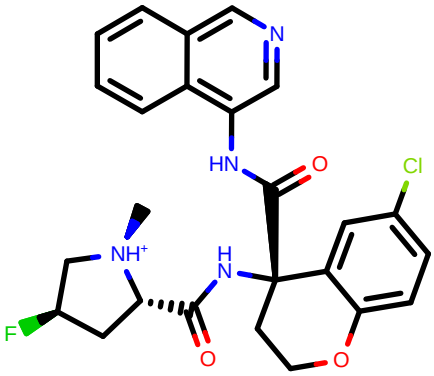
CID:	MIC-UNK-d58dbb53-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)OC[C@@H]5CCCS5(=O)=O
RUN:	RUN3676
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.19

DAR-DIA-076fb6ea-1_1



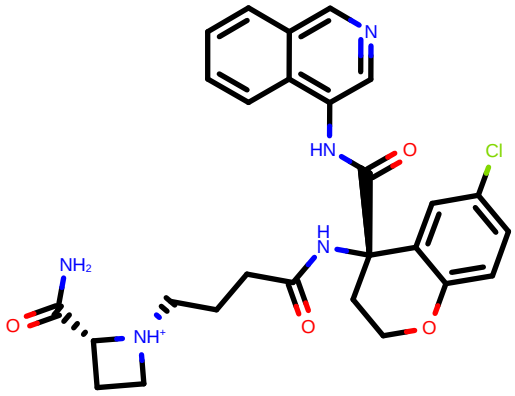
CID:	DAR-DIA-076fb6ea-1_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1397
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.40

DAR-DIA-0f2f46c9-7_3



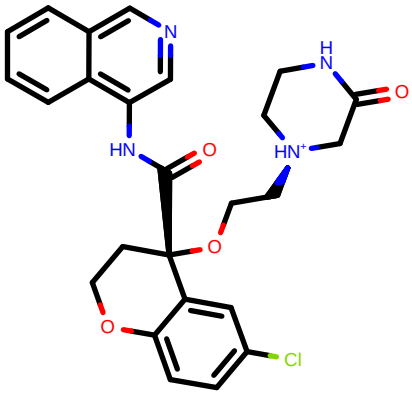
CID:	DAR-DIA-0f2f46c9-7_3
SMILES:	CNS(=O)(=O)[N@@]1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3236
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.16

NIR-THE-47736cde-1_1



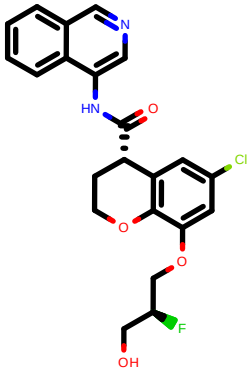
CID:	NIR-THE-47736cde-1_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN3325
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.20

PET-UNK-689df078-2_1



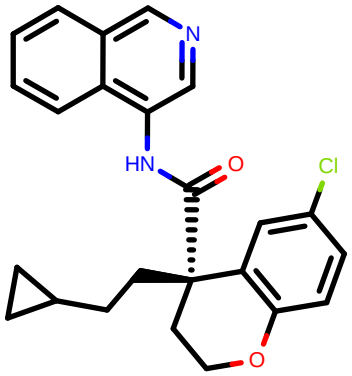
CID:	PET-UNK-689df078-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)CO[C@H](C3=O)c4cccc(c4)Cl
RUN:	RUN3098
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.33

MAT-POS-1f3f1a6f-2_2



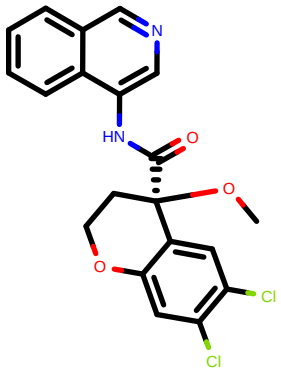
CID:	MAT-POS-1f3f1a6f-2_2
SMILES:	C[NH+](C)[C@H](c1ccc(c(c1)Cl)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN2278
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.27

EDG-MED-ba1ac7b9-19_2



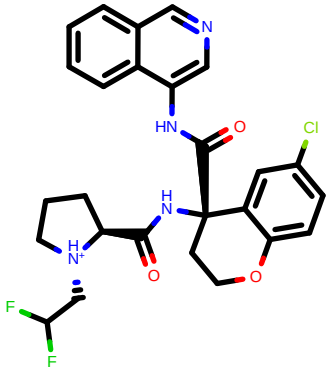
CID:	EDG-MED-ba1ac7b9-19_2
SMILES:	C[C@H]1c2nncn2CCN1C(=O)C[C@@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2691
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.26

DAR-DIA-0d514e7d-32_22



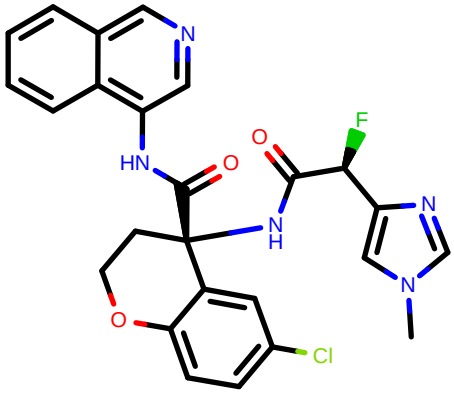
CID:	DAR-DIA-0d514e7d-32_22
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3[C@@H]4C[C@H]4CO[C@@H]5[C@H]3C=C(C=C5)Cl
RUN:	RUN871
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.13

MAK-UNK-83e0a0b4-3_2



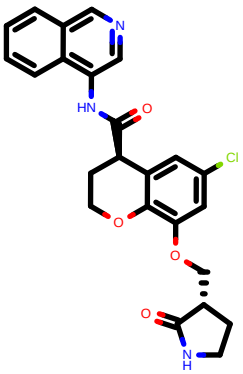
CID:	MAK-UNK-83e0a0b4-3_2
SMILES:	c1ccc2c(c1)cncc2N(CCNC3C[NH2+]C3)C(=O)[C@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN722
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.32

MAT-POS-3b97339c-1_4



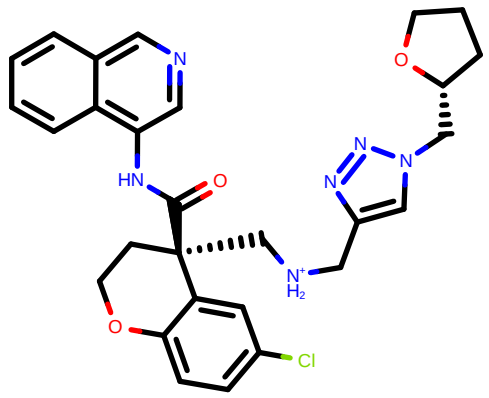
CID:	MAT-POS-3b97339c-1_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@]5(CCSC5)O
RUN:	RUN3300
DDG (kcal/mol):	-0.25
dDDG (kcal/mol):	0.16

MAT-POS-8293a91a-4_2



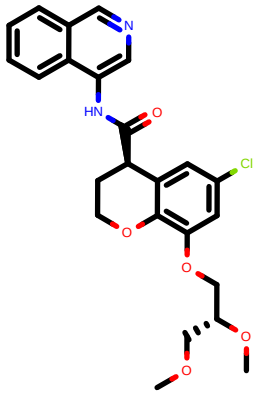
CID:	MAT-POS-8293a91a-4_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN5083
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.19

ALP-POS-e6e0c683-4_1



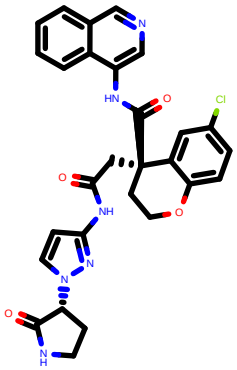
CID:	ALP-POS-e6e0c683-4_1
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CS(=O)(=O)Cc4c3cc(cc4)Cl
RUN:	RUN4528
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.33

EDJ-MED-9e38fd34-5_1



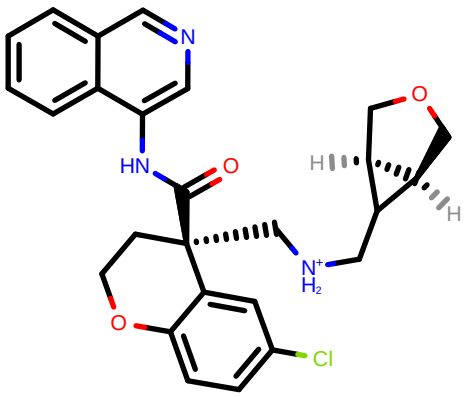
CID:	EDJ-MED-9e38fd34-5_1
SMILES:	C[C@]1(c2cc(c(cc2NC1=O)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2351
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.40

ED_-GRI-5b13fbe2-40_1



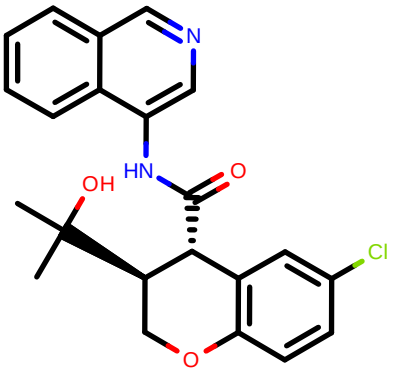
CID:	ED_-GRI-5b13fbe2-40_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@H](C[NH3+])F
RUN:	RUN1574
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.42

EDJ-MED-92e193ae-2_1



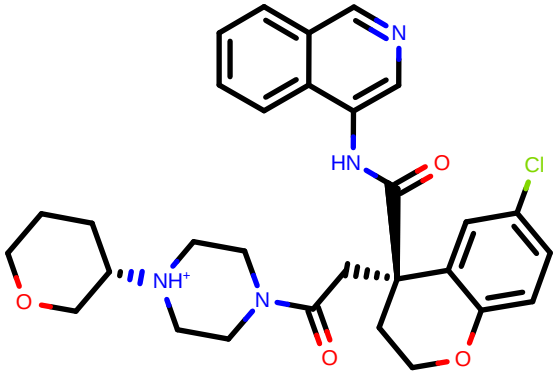
CID:	EDJ-MED-92e193ae-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCNc4c3cc(cc4)Cl
RUN:	RUN1853
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.39

MAT-POS-f7918075-1_1



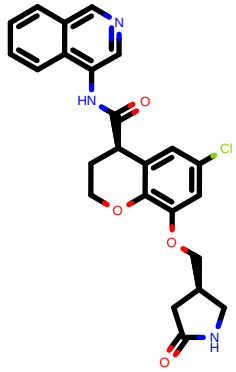
CID:	MAT-POS-f7918075-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN187
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.15

BEN-DND-c852c98b-2_2



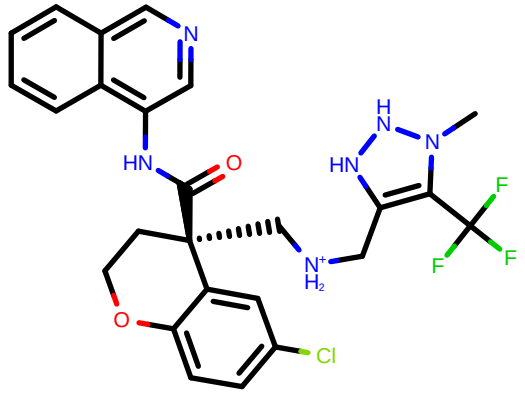
CID:	BEN-DND-c852c98b-2_2
SMILES:	c1cc2cncc(c2cc1OC(F)(F)F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1206
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.37

ALF-EVA-82cf4849-10_1



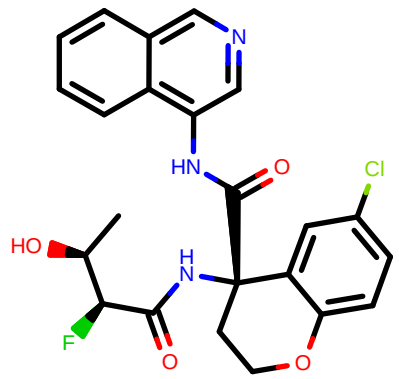
CID:	ALF-EVA-82cf4849-10_1
SMILES:	c1cc2cncc(c2cc1C[NH3+])NC(=O)[C@@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN4837
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.20

EDJ-MED-1981ceba-5_2



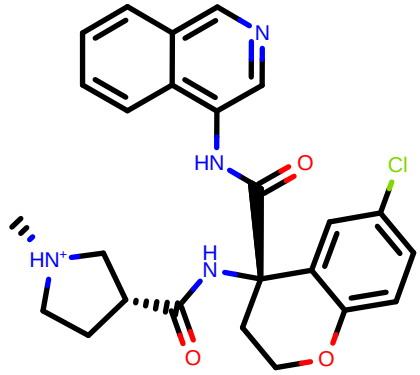
CID:	EDJ-MED-1981ceba-5_2
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4698
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.29

MAT-POS-fb82b63d-4_2



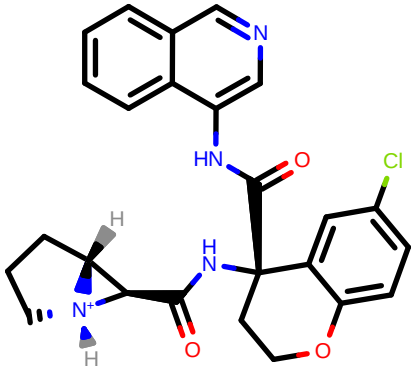
CID:	MAT-POS-fb82b63d-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4CC[N@@H+]3CC5CC5)Cl
RUN:	RUN3181
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.14

MIC-UNK-0a05c952-2_1



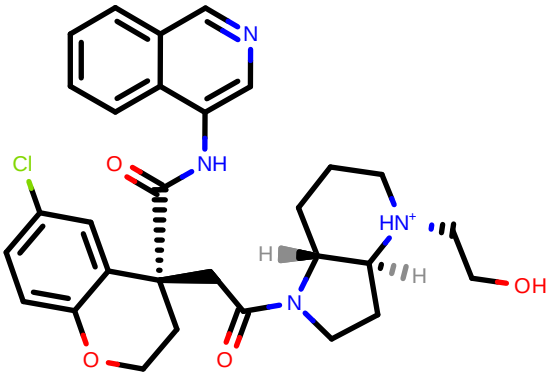
CID:	MIC-UNK-0a05c952-2_1
SMILES:	c1ccc2c(c1)cncc2N3[C@@H](CC[C@@H](C3=O)c4cccc(c4)Cl)[C@@H]5CO5
RUN:	RUN3505
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.18

MIC-UNK-cdc2493e-16_1



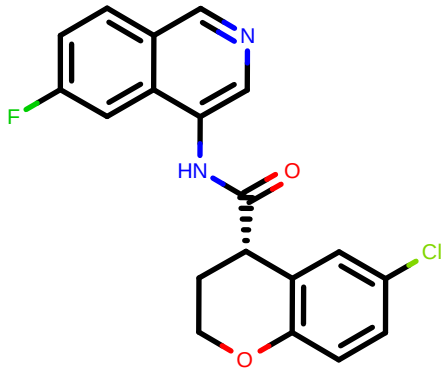
CID:	MIC-UNK-cdc2493e-16_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CCc3ccco3)c4cccc(c4)Cl
RUN:	RUN561
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.29

MIC-UNK-c5a20098-2_1



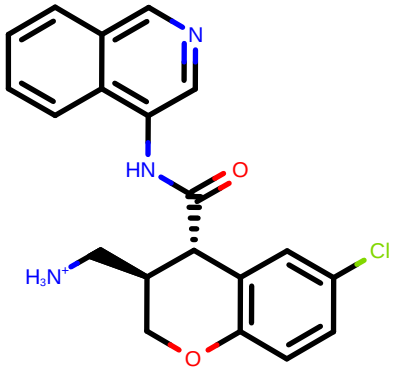
CID:	MIC-UNK-c5a20098-2_1
SMILES:	c1ccc2c(c1)cncc2C(=O)C(C3CN(C3)c4cccc(c4)Cl)(F)F
RUN:	RUN1306
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.49

MAK-UNK-c749d764-15_6



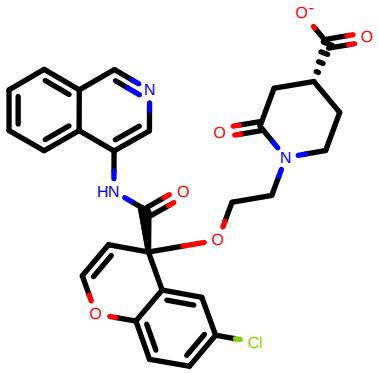
CID:	MAK-UNK-c749d764-15_6
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN963
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.10

ERI-UCB-ce40166b-6_1



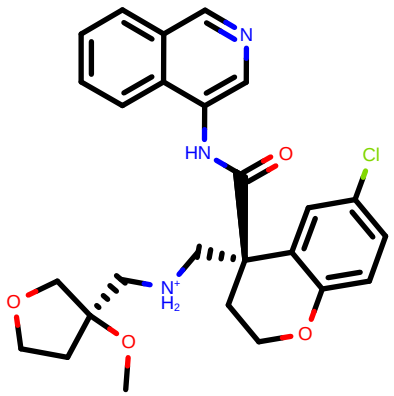
CID:	ERI-UCB-ce40166b-6_1
SMILES:	c1ccc2c(c1)cncc2CC(=O)Nc3cc(cc(c3)Cl)O[C@@H]4CCC(=O)N4
RUN:	RUN42
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.20

MIC-UNK-cdc2493e-12_4



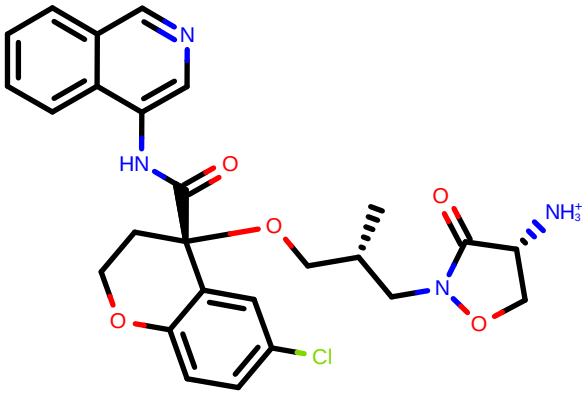
CID:	MIC-UNK-cdc2493e-12_4
SMILES:	C[NH+](C)[C@H]1CC[C@H](C1)N(c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN553
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.34

EDG-MED-90036822-27_2



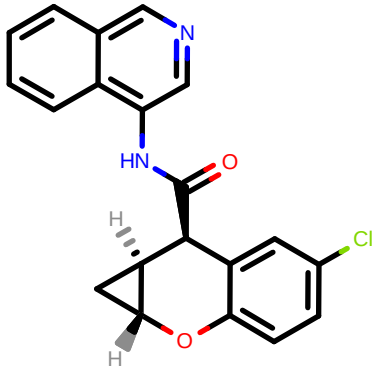
CID:	EDG-MED-90036822-27_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)CO[C@H](CN)C(F)(F)F
RUN:	RUN1702
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.57

ALP-POS-fe871b40-1_1



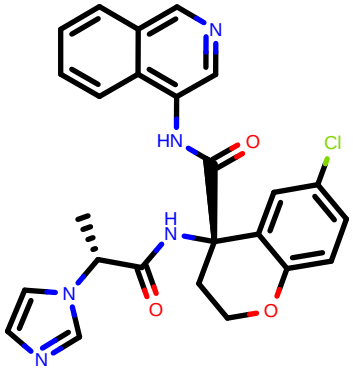
CID:	ALP-POS-fe871b40-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C#N)Cl
RUN:	RUN3109
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.21

EDJ-MED-ee07cf00-8_1



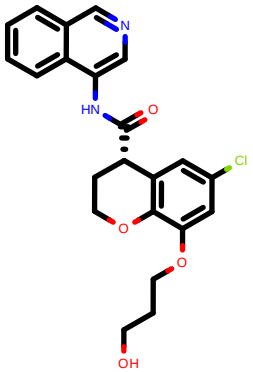
CID:	EDJ-MED-ee07cf00-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H](c3cccc(c3)Cl)NC(=O)Cn4cc(c(=O)[nH]c4=O)C#N
RUN:	RUN2818
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.19

DAR-DIA-0f2f46c9-4_2



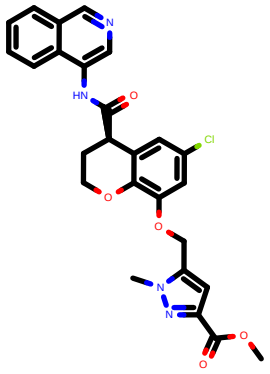
CID:	DAR-DIA-0f2f46c9-4_2
SMILES:	CS(=O)(=O)[N@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3225
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.14

DAR-DIA-23e5a6a0-9_2



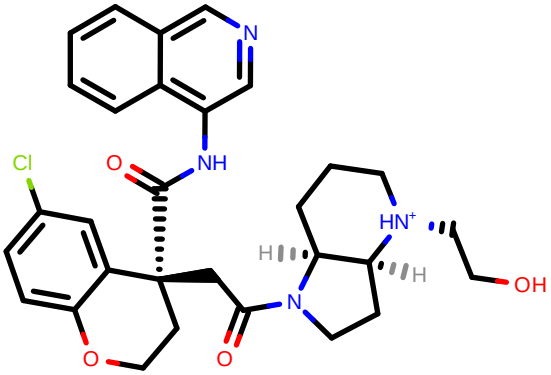
CID:	DAR-DIA-23e5a6a0-9_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CC6(CC6)C[NH2+]5)Cl
RUN:	RUN419
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.23

EDJ-MED-d203f206-36_1



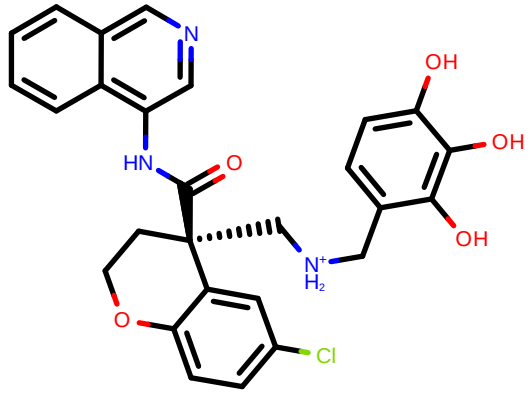
CID:	EDJ-MED-d203f206-36_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@@](C5)(C#N)C(=O)N
RUN:	RUN2598
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.39

MAT-POS-e6dd326d-11_1



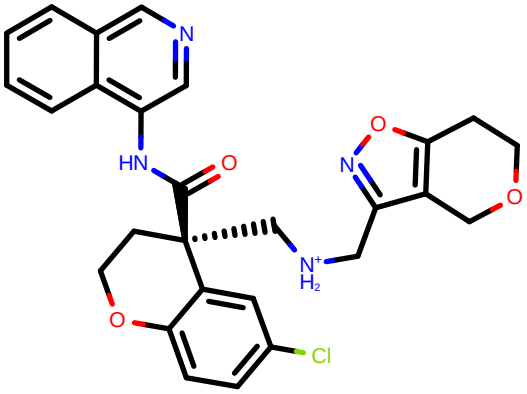
CID:	MAT-POS-e6dd326d-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]CC(=O)[O-]
RUN:	RUN3956
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.33

ED_-GRI-5b13fbe2-34_2



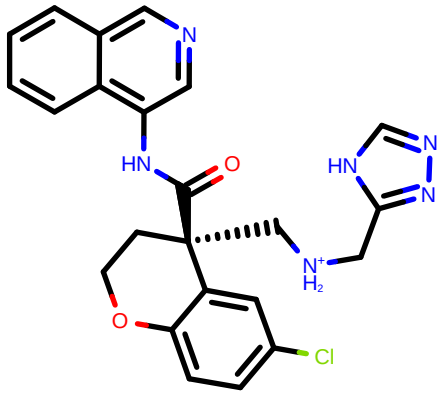
CID:	ED_-GRI-5b13fbe2-34_2
SMILES:	C[N@@](CCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)CC(C(=O)N)(F)F
RUN:	RUN1568
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.53

KAD-UNI-8a629cb0-1_1



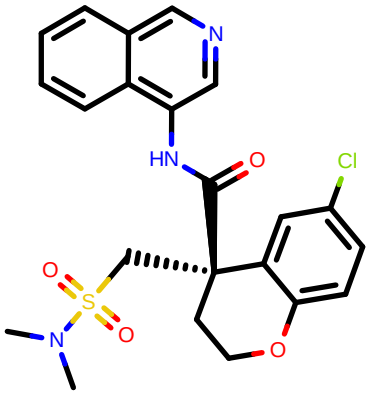
CID:	KAD-UNI-8a629cb0-1_1
SMILES:	CS(=O)(=O)[N@@]1CC[C@H](C1)COCC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2086
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.40

EDJ-MED-139368ae-5_2



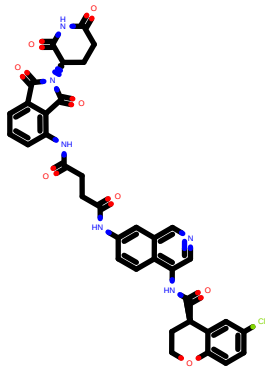
CID:	EDJ-MED-139368ae-5_2
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccccc3[C@@H](C2)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4549
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.22

JOH-UNI-21fd6073-1_2



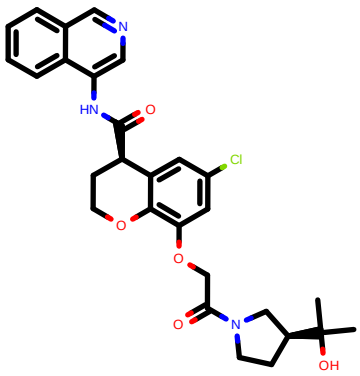
CID:	JOH-UNI-21fd6073-1_2
SMILES:	c1ccc(cc1)S(=O)(=O)N(CC#N)C(=O)CN(c2cncc3c2cccc3)C(=O)[C@H]4COc5c4cc(cc5)Cl
RUN:	RUN4183
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.12

JAG-UCB-f37eaa14-4_2



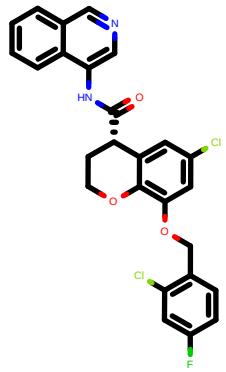
CID:	JAG-UCB-f37eaa14-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](c5c4cc(cc5)Cl)CC[NH2+]C6CC6
RUN:	RUN3061
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.22

ALF-EVA-07677224-1_3



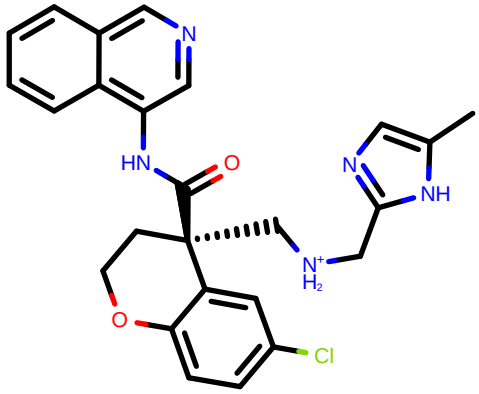
CID:	ALF-EVA-07677224-1_3
SMILES:	Cc1nc(ns1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@H](C2)C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN4898
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.20

ALP-POS-ce760d3f-1_1



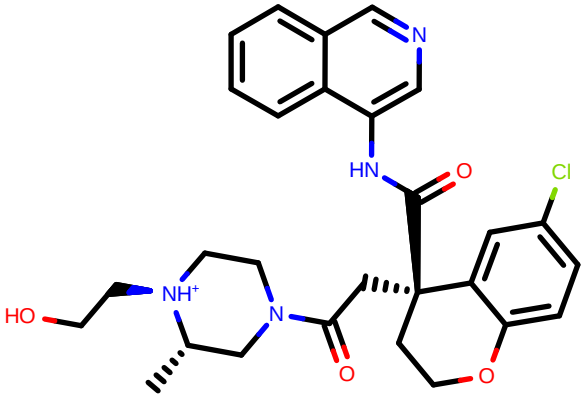
CID:	ALP-POS-ce760d3f-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4O)Cl
RUN:	RUN1461
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.26

MAT-POS-dc2604c4-3_1



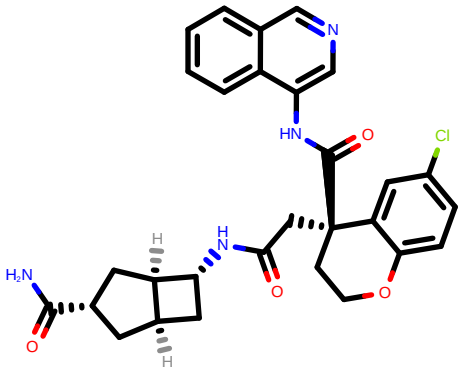
CID:	MAT-POS-dc2604c4-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5(CNC5)C#N
RUN:	RUN4711
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.18

RAL-THA-8416115c-14_2



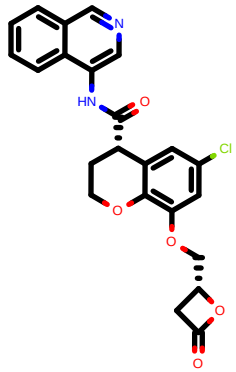
CID:	RAL-THA-8416115c-14_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5cn[nH]n5
RUN:	RUN1300
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.46

RAL-THA-8416115c-13_2



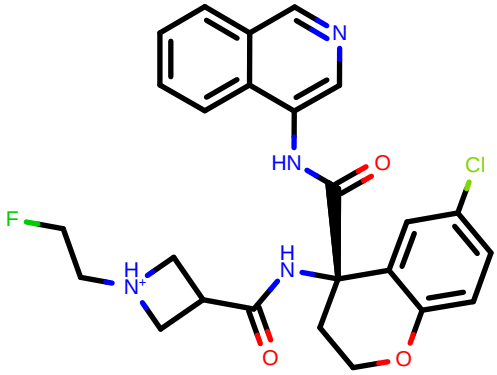
CID:	RAL-THA-8416115c-13_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)Cc5[nH]ncn5
RUN:	RUN1296
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.46

DAR-DIA-6be260fc-4_1



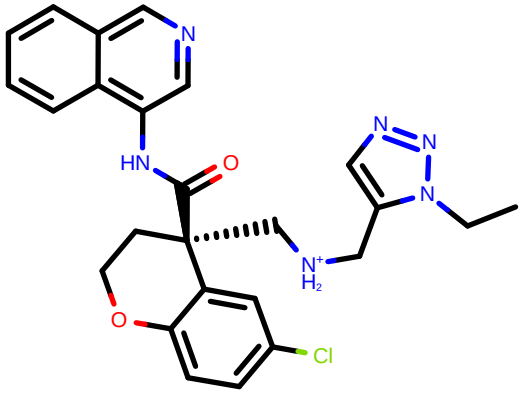
CID:	DAR-DIA-6be260fc-4_1
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12CNc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN2135
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.27

DAR-DIA-0d514e7d-17_1



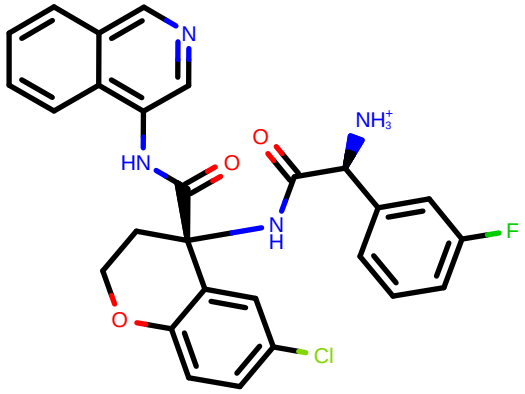
CID:	DAR-DIA-0d514e7d-17_1
SMILES:	C[C@H]1COc2c(cc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)c5cc(cc(c5)F)F
RUN:	RUN820
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.40

EDJ-MED-1981ceba-4_1



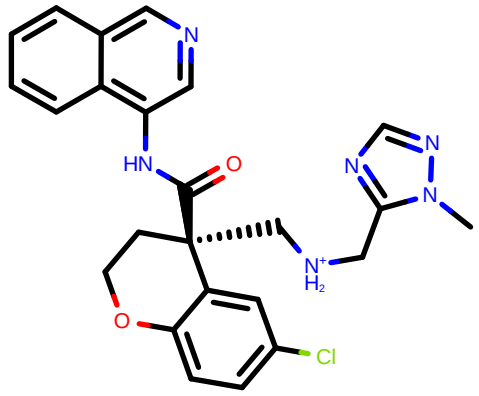
CID:	EDJ-MED-1981ceba-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)N5CC(C5)C#N
RUN:	RUN4693
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.20

MIC-UNK-25b9c114-2_2



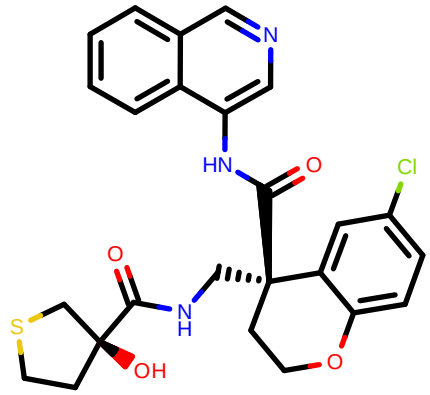
CID:	MIC-UNK-25b9c114-2_2
SMILES:	c1ccc2c(c1)cncc2C(=O)N3CC(=O)N(C[C@H]3CNS(=O)(=O)N)c4cccc(c4)Cl
RUN:	RUN3264
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.17

ALP-POS-347519b5-3_9



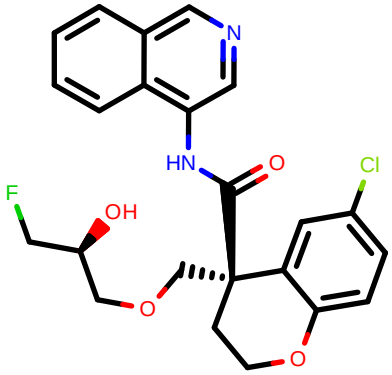
CID:	ALP-POS-347519b5-3_9
SMILES:	CS(=O)(=O)N@@]1C[C@@H]2[C@@H]3CC[C@H]([C@@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4300
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.25

KAD-UNI-cb0f2bbc-5_1



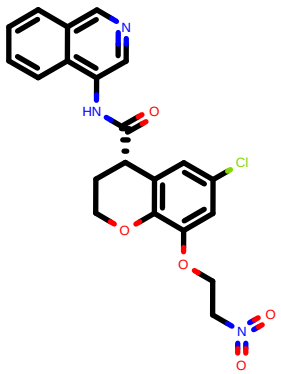
CID:	KAD-UNI-cb0f2bbc-5_1
SMILES:	CNC(=O)COc1ccc(cc1OC)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3688
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.14

KAD-UNI-cb0f2bbc-20_3



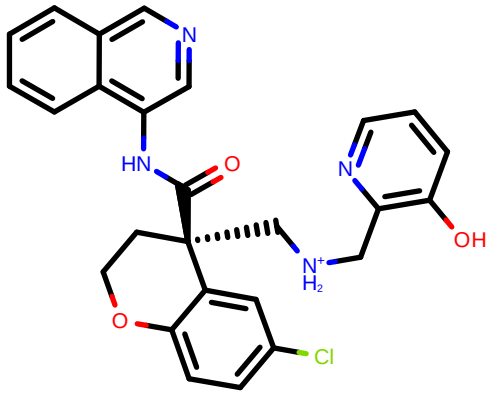
CID:	KAD-UNI-cb0f2bbc-20_3
SMILES:	Cn1cc(cn1)N2CC[C@H](C2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3709
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.14

ALF-EVA-07677224-10_2



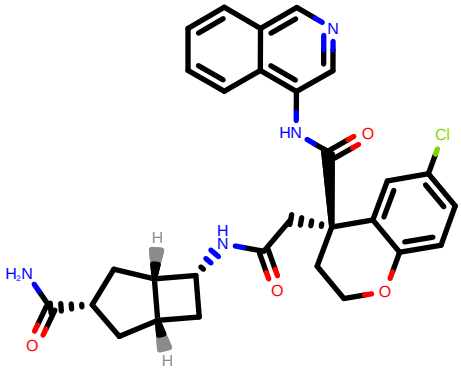
CID:	ALF-EVA-07677224-10_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)c5[nH]ncn5
RUN:	RUN4945
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.31

ALP-POS-347519b5-3_28



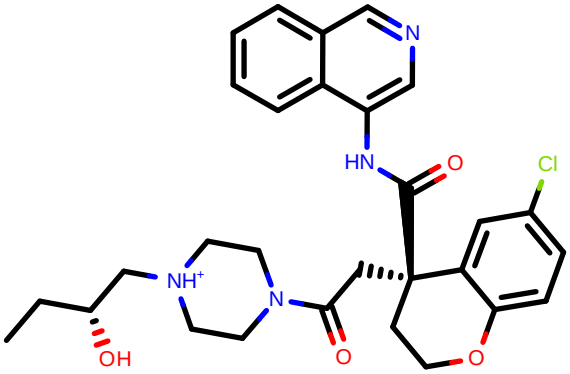
CID:	ALP-POS-347519b5-3_28
SMILES:	CS(=O)(=O)[N@]1C[C@H]2[C@@H]3CC[C@H][C@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4311
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.32

KAD-UNI-cb0f2bbc-20_2



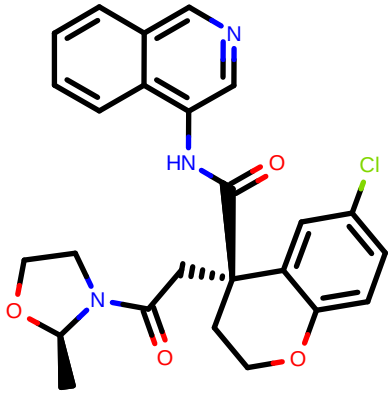
CID:	KAD-UNI-cb0f2bbc-20_2
SMILES:	Cn1cc(cn1)N2CC[C@@H](C2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3706
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.24

MIC-UNK-5a93dd5f-3_12



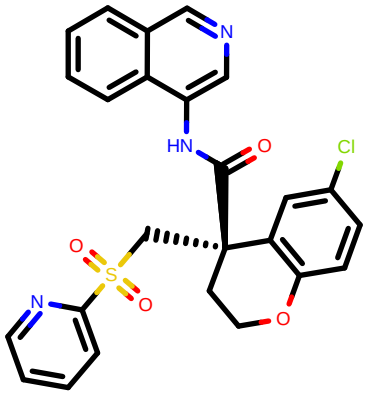
CID:	MIC-UNK-5a93dd5f-3_12
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3cccc(c3)Cl)[N@H+]4CC[C@@H]5CCCC[C@H]5C4
RUN:	RUN751
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.49

KAD-UNI-b13decd3-1_2



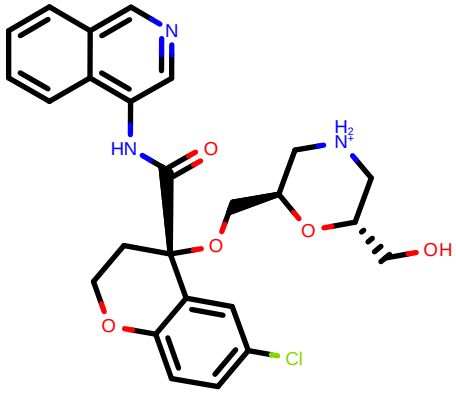
CID:	KAD-UNI-b13decd3-1_2
SMILES:	Cn1cc(cn1)N2CC[C@@H](C2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN3779
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.10

PET-UNK-12d8d43f-1_1



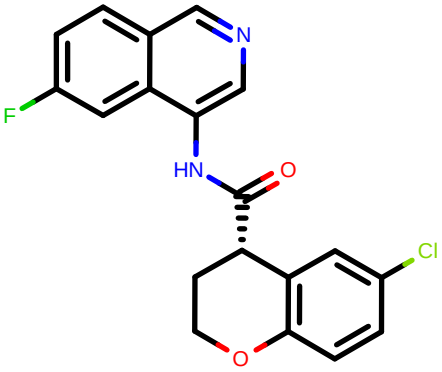
CID:	PET-UNK-12d8d43f-1_1
SMILES:	c1ccc2c(c1)cncc2N(C=O)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1495
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.32

DAR-DIA-0f7b7cd9-10_1



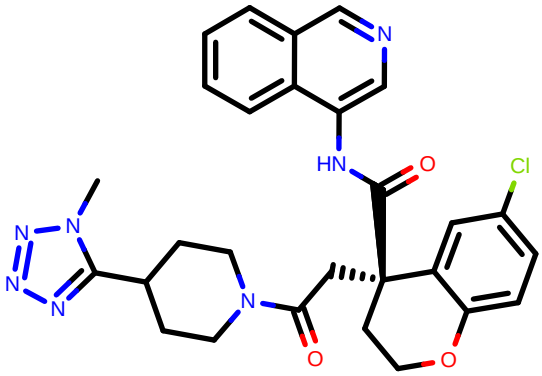
CID:	DAR-DIA-0f7b7cd9-10_1
SMILES:	c1ccc2c(c1)cncc2N3CCC(=O)N(C3=O)c4ccccc4Cl
RUN:	RUN3019
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.25

MIC-UNK-9582b2c5-3_4



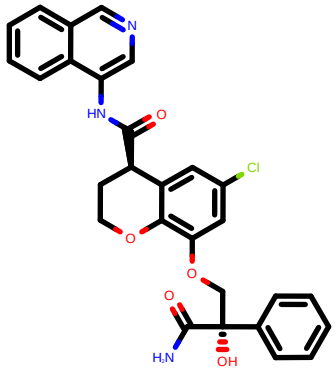
CID:	MIC-UNK-9582b2c5-3_4
SMILES:	CC(=O)N1CC[C@H]2[C@H](C1)CN(C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN272
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.11

MIC-UNK-5a93dd5f-5_8



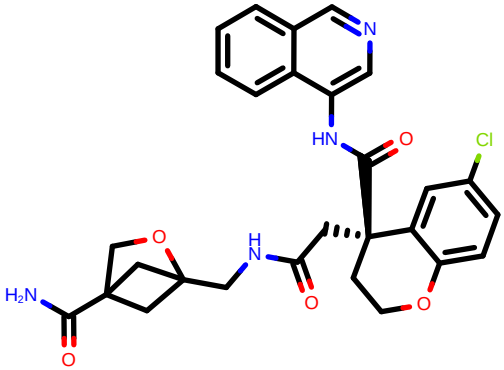
CID:	MIC-UNK-5a93dd5f-5_8
SMILES:	CC(=O)N[C@H]1CC[N@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN764
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.32

MAT-POS-e9e99895-3_2



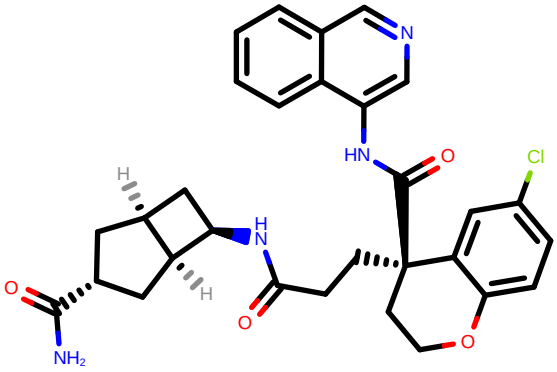
CID:	MAT-POS-e9e99895-3_2
SMILES:	C[C@](c1ccc(c(c1)Cl)Cl)(C(=O)Nc2cncc3c2cccc3)NC(=O)[C@@H]4CCC(=O)NC4
RUN:	RUN2244
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.46

MIC-UNK-5a93dd5f-5_7



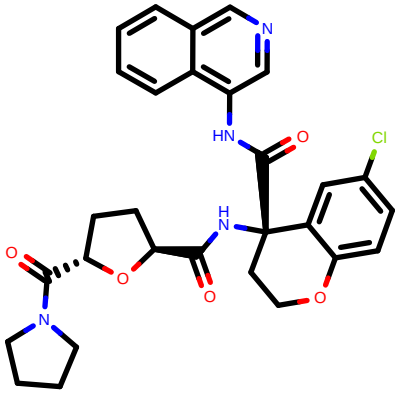
CID:	MIC-UNK-5a93dd5f-5_7
SMILES:	CC(=O)N[C@@H]1CC[N@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN765
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.31

MIC-UNK-5a93dd5f-9_6



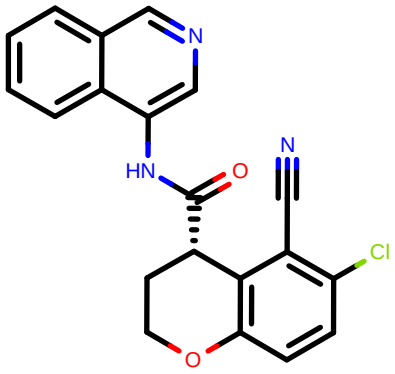
CID:	MIC-UNK-5a93dd5f-9_6
SMILES:	CN(C)[C@H]1CC[N@@H+](C1)[C@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN783
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.28

RAL-THA-6e4c80cf-2_2



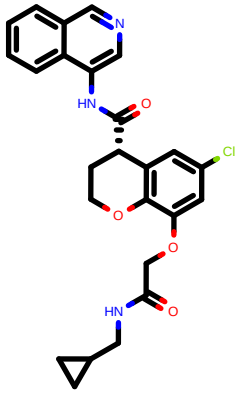
CID:	RAL-THA-6e4c80cf-2_2
SMILES:	CCOC(=O)N1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN3897
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.17

MAK-UNK-ffc90da7-1_4



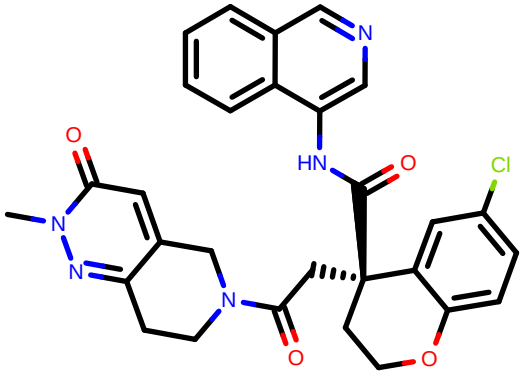
CID:	MAK-UNK-ffc90da7-1_4
SMILES:	C[C@H](C[NH2+]CCCO)[C@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN690
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.10

EDJ-MED-6864a934-8_1



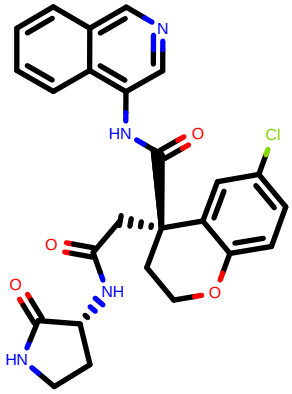
CID:	EDJ-MED-6864a934-8_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)c5cccc6n5nnc6
RUN:	RUN2613
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.32

MAK-UNK-c749d764-18_2



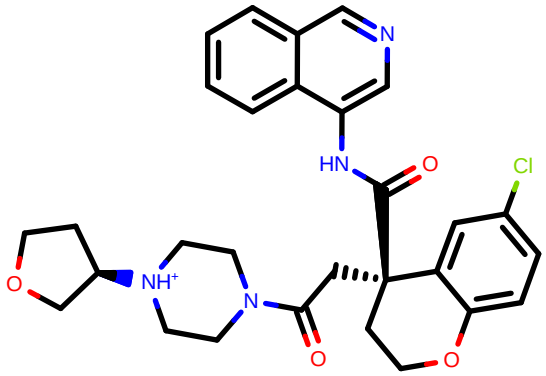
CID:	MAK-UNK-c749d764-18_2
SMILES:	CC(C)SCN(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN991
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.31

KAD-UNI-877d7bed-8_1



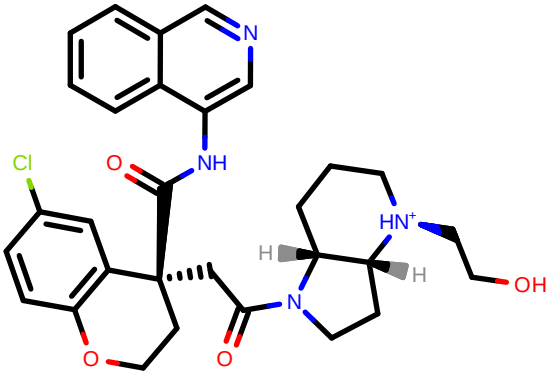
CID:	KAD-UNI-877d7bed-8_1
SMILES:	CC(=O)N1CCN(CC1)C(=O)COc2cc(cc3c2OCC[C@@H]3C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3735
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.15

MAK-UNK-c749d764-5_1



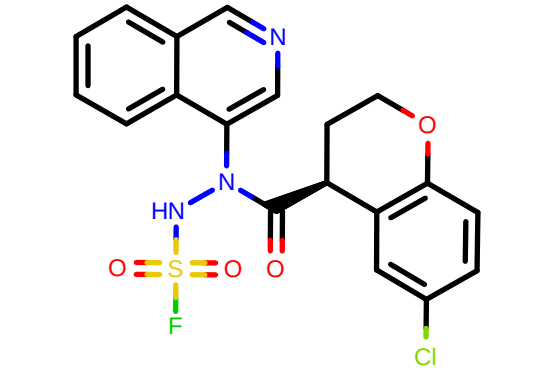
CID:	MAK-UNK-c749d764-5_1
SMILES:	c1ccc2c(c1)cncc2N(CO)C(=O)C[C@@H]3CCC[C@@H]([C@@H]3O)C(F)F
RUN:	RUN921
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.38

DAR-DIA-9e4459de-13_8



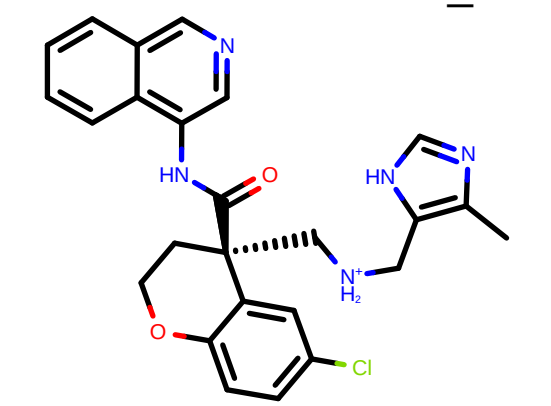
CID:	DAR-DIA-9e4459de-13_8
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1432
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.52

MAK-UNK-c749d764-15_7



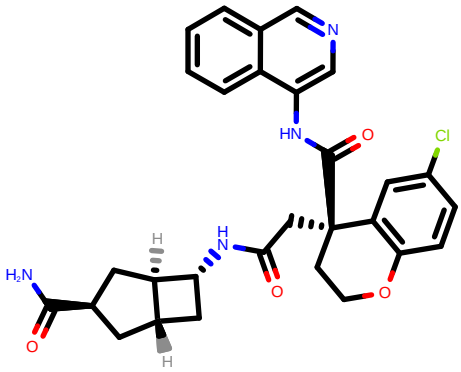
CID:	MAK-UNK-c749d764-15_7
SMILES:	C[C@@H](N(c1cncc2c1cccc2)C(=O)C[C@H]3CCC[C@H]([C@@H]3O)C(F)F)OCC4CCCCC4
RUN:	RUN964
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.24

RAL-THA-b9d6aec1-2_1



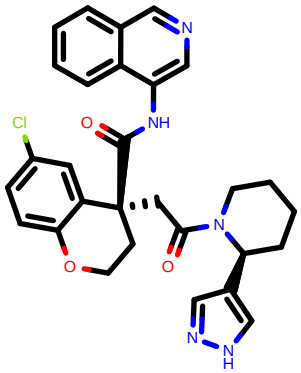
CID:	RAL-THA-b9d6aec1-2_1
SMILES:	CNS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN4490
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.33

NAU-LAT-4ce8bf23-3_1



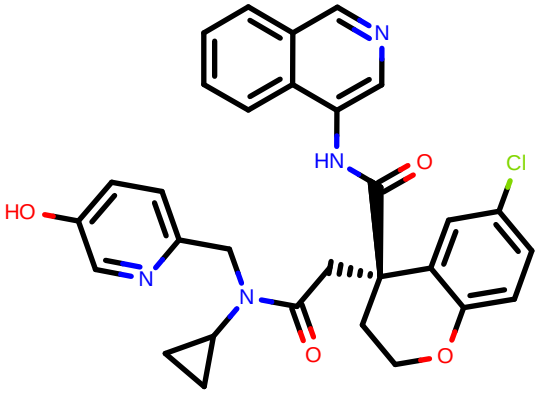
CID:	NAU-LAT-4ce8bf23-3_1
SMILES:	CC(=O)N[C@@H](c1cncc2c1cccc2)C(=O)Nc3cccc(c3)Cl
RUN:	RUN1393
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.38

BEN-DND-c852c98b-1_2



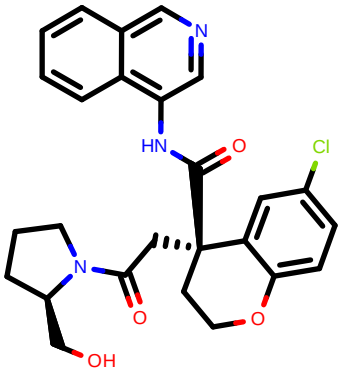
CID:	BEN-DND-c852c98b-1_2
SMILES:	c1cc2cncc(c2cc1C#N)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1203
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.18

RAL-THA-8416115c-1_3



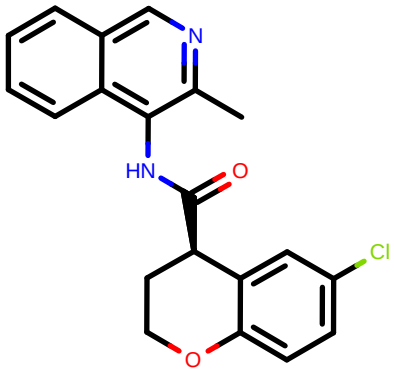
CID:	RAL-THA-8416115c-1_3
SMILES:	c1ccc(cc1)CN2CC[C@H](c3c2ccc(c3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN1249
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.56

DAR-DIA-4987d2cd-4_4



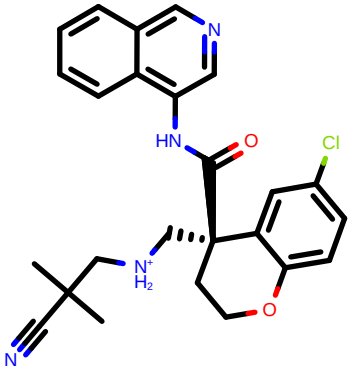
CID:	DAR-DIA-4987d2cd-4_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3c4cc(ccc4CN3c5c(c(=O)c5=O)[O-])Cl
RUN:	RUN3817
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.16

ALP-UNI-dbbfd3db-10_1



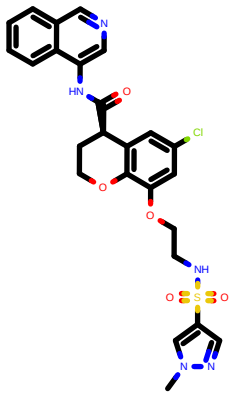
CID:	ALP-UNI-dbbfd3db-10_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)NC(=O)Cn5cc(c(=O)[nH]c5=O)Cl
RUN:	RUN2778
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.11

MAT-POS-4223bc15-22_2



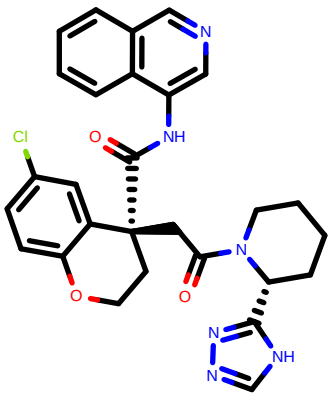
CID:	MAT-POS-4223bc15-22_2
SMILES:	COC(=O)C[N@H+]1Cc2ccc(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4102
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.20

EDG-MED-ba1ac7b9-14_5



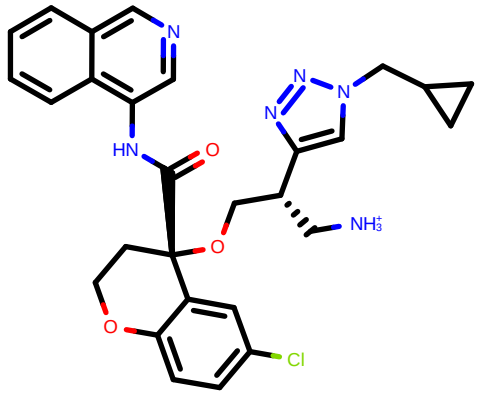
CID:	EDG-MED-ba1ac7b9-14_5
SMILES:	C[N@@]1CCN(C[C@@H]1C#N)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN2670
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.53

RAL-THA-4aa06b95-1_2



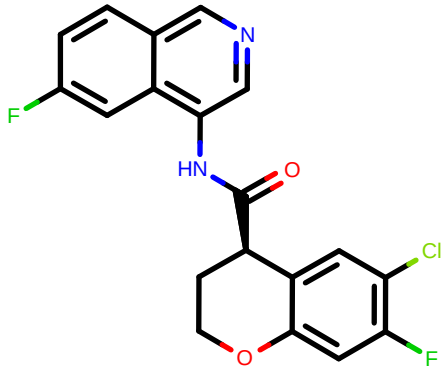
CID:	RAL-THA-4aa06b95-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCN(c4c3cc(cc4)Cl)C(=O)N
RUN:	RUN1230
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.37

DAR-DIA-0f2f46c9-13_1



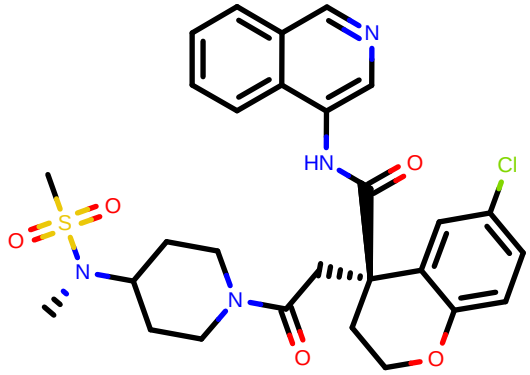
CID:	DAR-DIA-0f2f46c9-13_1
SMILES:	CN(C)S(=O)(=O)[N@@]1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3250
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.21

ALP-POS-347519b5-3_40



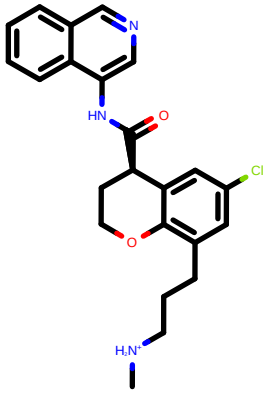
CID:	ALP-POS-347519b5-3_40
SMILES:	CS(=O)(=O)[N@]1C[C@H]2[C@H]3CC[C@@H][C@@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4315
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.08

MIC-UNK-5a93dd5f-8_1



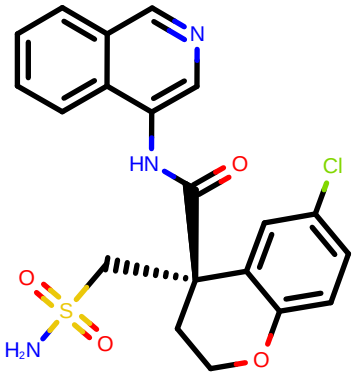
CID:	MIC-UNK-5a93dd5f-8_1
SMILES:	C[NH+](C)C1CC[NH+](CC1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN776
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.28

ALP-UNI-8e43a71e-12_4



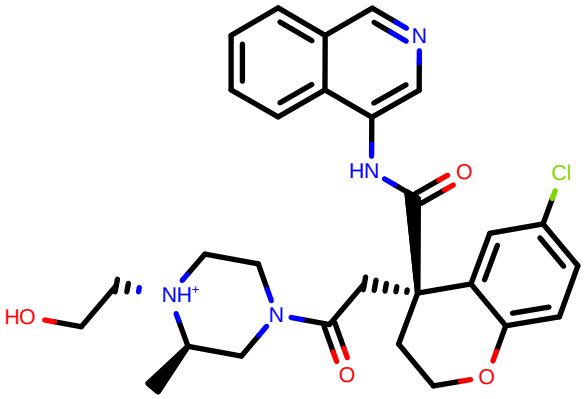
CID:	ALP-UNI-8e43a71e-12_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)Nc5ccn(n5)[C@H]6CCNC6=O
RUN:	RUN2978
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.22

JOH-UNI-a38a7bdd-6_3



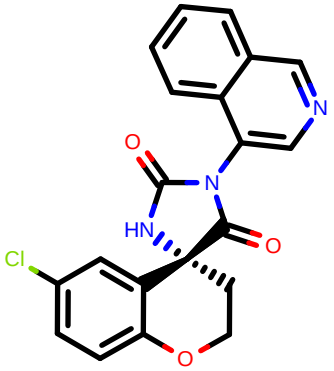
CID:	JOH-UNI-a38a7bdd-6_3
SMILES:	c1ccc2c(c1)cncc2N(C(=O)Cc3cccc(c3)Cl)C(=O)[C@@H]4C[C@H]4C(F)(F)F
RUN:	RUN1492
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.22

ALP-POS-c3a96089-2_1



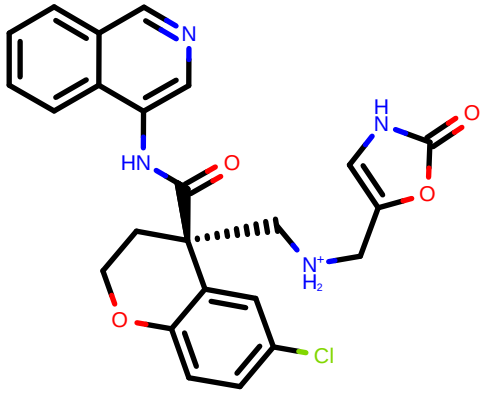
CID:	ALP-POS-c3a96089-2_1
SMILES:	Cc1ccc(nc1)N(Cc2cscn2)C(=O)Cc3cncc4c3cccc4
RUN:	RUN1182
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.58

MAK-UNK-c749d764-1_7



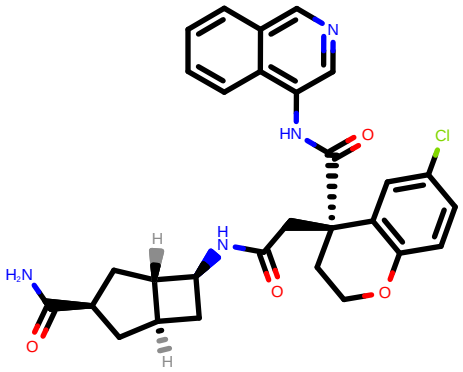
CID:	MAK-UNK-c749d764-1_7
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@H]([C@H]3O)C4CC4
RUN:	RUN895
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.17

DAR-DIA-9e4459de-13_14



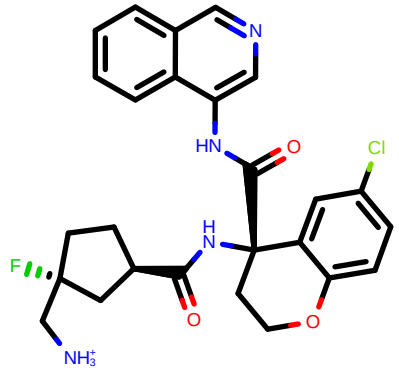
CID:	DAR-DIA-9e4459de-13_14
SMILES:	c1cc2c(c(c1)NCOCCOc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1437
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.37

ED_-GRI-5b13fbe2-5_1



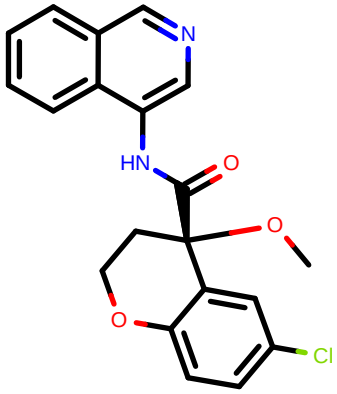
CID:	ED_-GRI-5b13fbe2-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OC[C@@H](c5n[n-]nn5)[NH3+]
RUN:	RUN1527
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.24

MAK-UNK-ffc90da7-8_1



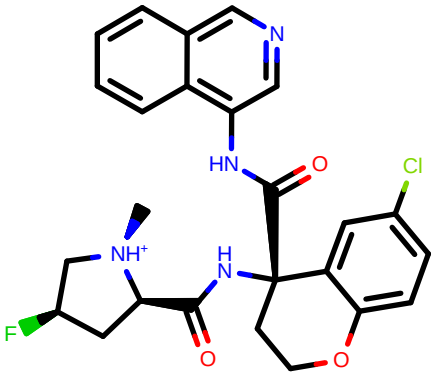
CID:	MAK-UNK-ffc90da7-8_1
SMILES:	CC(C)OCCCc1ccc2c(c1)cncc2NC(=O)Cc3cccc(c3)Cl
RUN:	RUN711
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.42

MIC-UNK-0a05c952-3_8



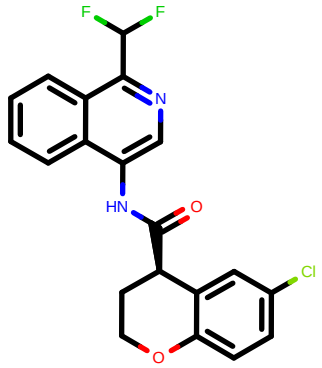
CID:	MIC-UNK-0a05c952-3_8
SMILES:	c1ccc2c(c1)cncc2N3[C@H](C[C@H](C3=O)c4ccc(c(c4)Cl)Cl)[C@H]5CO5
RUN:	RUN3518
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.06

PET-UNK-824b5c6a-2_1



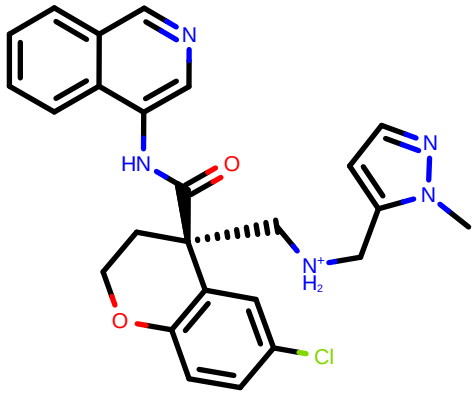
CID:	PET-UNK-824b5c6a-2_1
SMILES:	CCCO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3288
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.15

LON-WEI-4d77710c-6_1



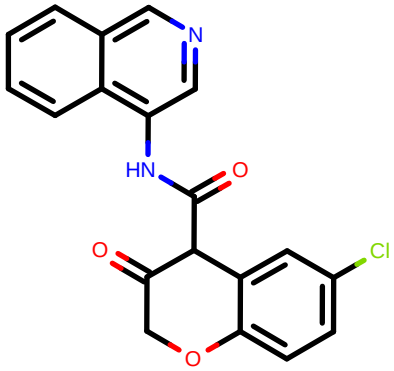
CID:	LON-WEI-4d77710c-6_1
SMILES:	CC(=O)c1cccc(c1)NC(=O)Nc2cn(c(=O)c3c2cccc3)C
RUN:	RUN196
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.27

ED_-GRI-5b13fbe2-38_1



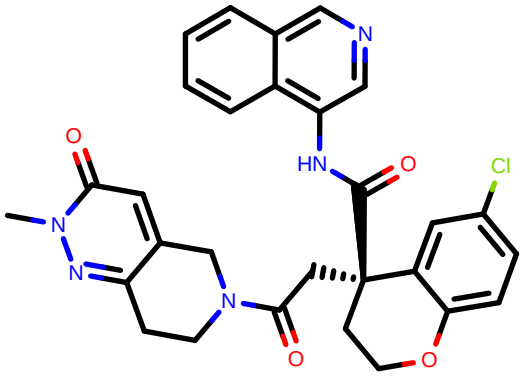
CID:	ED_-GRI-5b13fbe2-38_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCC[N@@H+]5CCn6c(c(cn6)C[NH3+])C5
RUN:	RUN1572
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.52

EDG-MED-ba1ac7b9-15_3



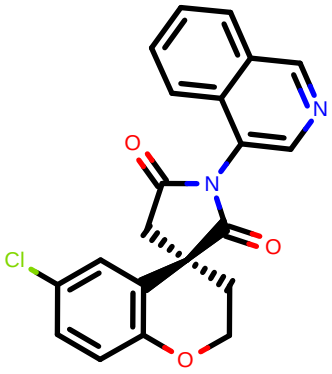
CID:	EDG-MED-ba1ac7b9-15_3
SMILES:	C[C@@H]1C[N@H+](CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2676
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.21

JOH-UNI-21fd6073-4_2



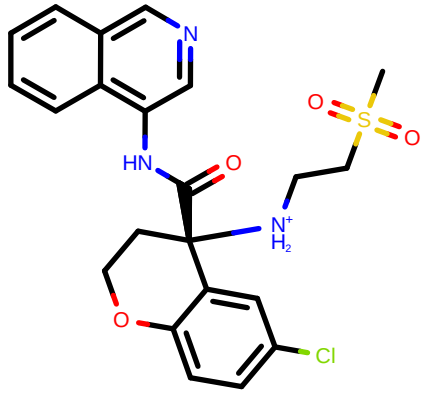
CID:	JOH-UNI-21fd6073-4_2
SMILES:	c1ccc2c(c1)cncc2N(CC(=O)On3c(ccc3O)O)C(=O)[C@H]4COc5c4cc(cc5)Cl
RUN:	RUN4184
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.16

EDG-MED-ba1ac7b9-15_4



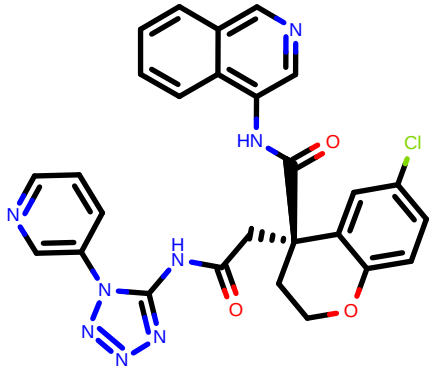
CID:	EDG-MED-ba1ac7b9-15_4
SMILES:	C[C@H]1C[N@H+](CCN1C(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)C
RUN:	RUN2677
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.18

EDJ-MED-923a35c2-5_3



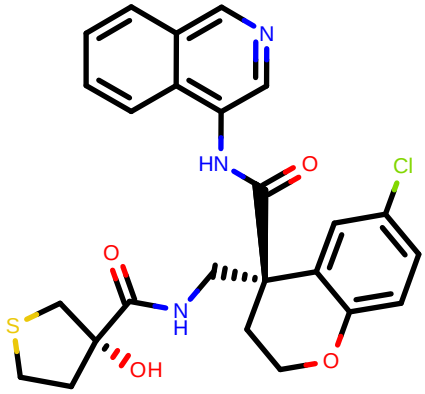
CID:	EDJ-MED-923a35c2-5_3
SMILES:	CO[C@@]1(C[N@](Cc2c1cc(cc2)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cc(cc4)F
RUN:	RUN4228
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.17

KAD-UNI-877d7bed-1_2



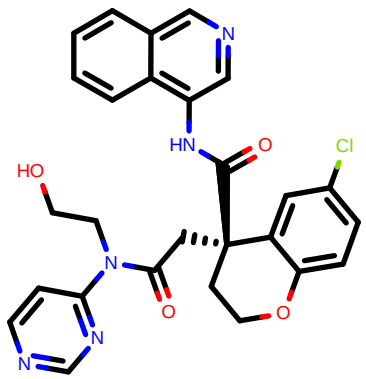
CID:	KAD-UNI-877d7bed-1_2
SMILES:	c1ccc(cc1)[C@](COc2cc(cc3c2OCC[C@@H]3C(=O)Nc4cncc5c4cccc5)Cl)(C(=O)N)O
RUN:	RUN3720
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.17

KAD-UNI-877d7bed-2_2



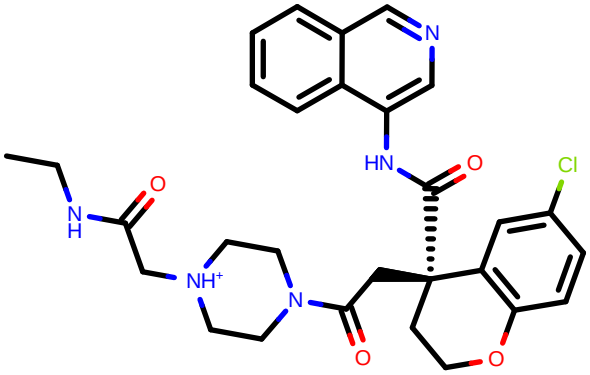
CID:	KAD-UNI-877d7bed-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cc(cc4OCCOc5ccc(cc5)S(=O)(=O)N)Cl
RUN:	RUN3726
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.13

KAD-UNI-cb0f2bbc-18_1



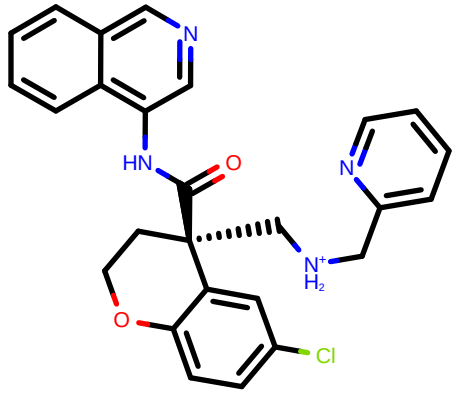
CID:	KAD-UNI-cb0f2bbc-18_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cnc(nc5)N6CCOCC6
RUN:	RUN3703
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.22

MAK-UNK-c749d764-19_6



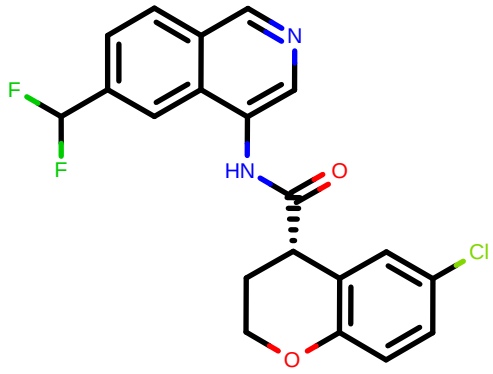
CID:	MAK-UNK-c749d764-19_6
SMILES:	c1ccc2c(c1)cncc2N(C[NH3+])C(=O)C[C@H]3CCC[C@@H]([C@H]3O)C(F)F
RUN:	RUN1003
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.31

MAT-POS-4223bc15-35_2



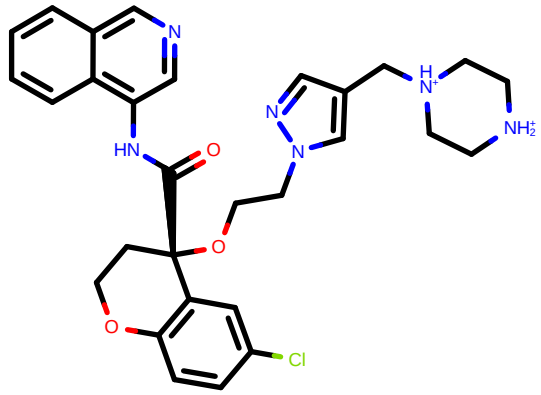
CID:	MAT-POS-4223bc15-35_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CN(Cc4c3cc(cc4)Cl)C(=O)CCO
RUN:	RUN4152
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.22

LON-WEI-4d77710c-16_1



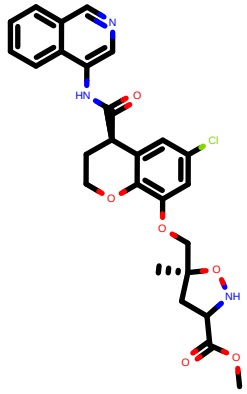
CID:	LON-WEI-4d77710c-16_1
SMILES:	CC(C)Cn1cc(c2ccccc2c1=O)NC(=O)NCC[NH+]3CCOCC3
RUN:	RUN204
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.11

VLA-UNK-9a7dc93f-7_1



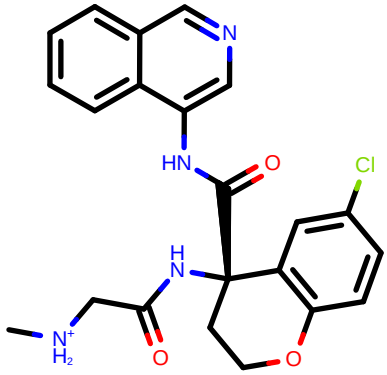
CID:	VLA-UNK-9a7dc93f-7_1
SMILES:	CO[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN3093
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.27

EDJ-MED-d203f206-40_1



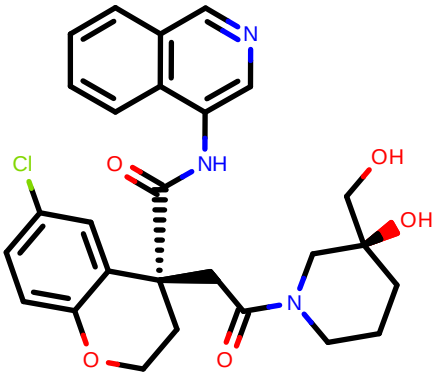
CID:	EDJ-MED-d203f206-40_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]([C@@H](C5)CO)O
RUN:	RUN2603
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.51

MIC-UNK-91acba05-1_2



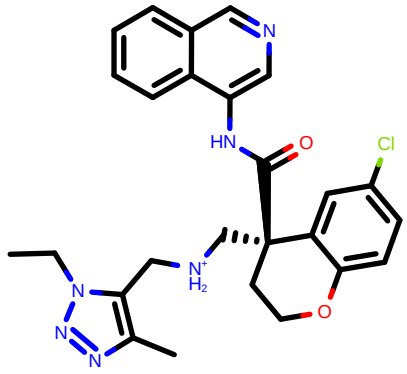
CID:	MIC-UNK-91acba05-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CNC(=O)c4c3cc(cc4)Cl
RUN:	RUN468
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.25

EDJ-MED-009f762b-1_2



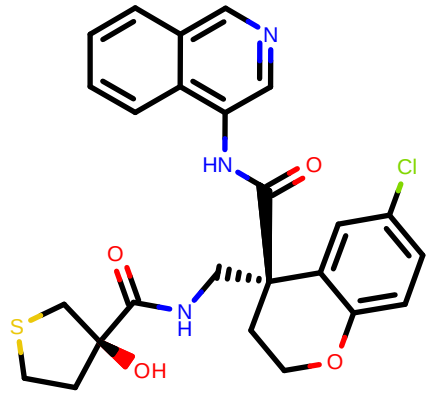
CID:	EDJ-MED-009f762b-1_2
SMILES:	Cn1ccc(n1)C[N@H+]2Cc3ccc(cc3[C@@H](C2)C(=O)Nc4cncc5c4cc(cc5)F)Cl
RUN:	RUN3907
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.24

RAL-THA-05e671eb-24_2



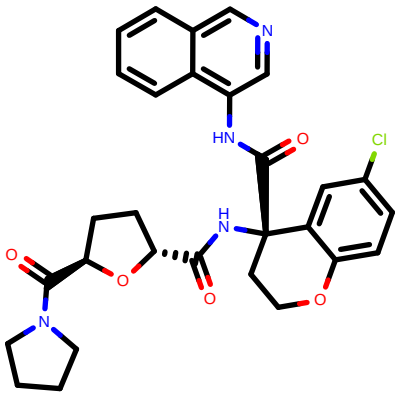
CID:	RAL-THA-05e671eb-24_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CCOc4c3cccc4C#N
RUN:	RUN2053
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.36

MIC-UNK-d854bf4c-6_2



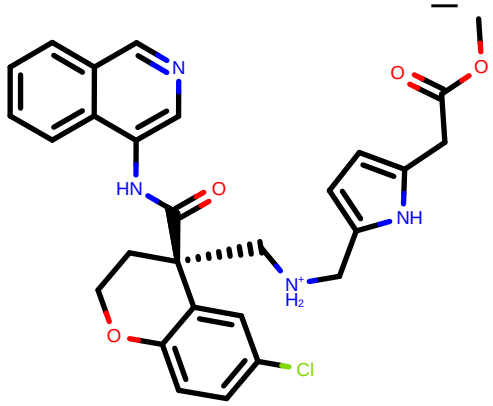
CID:	MIC-UNK-d854bf4c-6_2
SMILES:	CS(=O)(=O)N1CCC2(CC1)CN(C(=O)[C@H]2c3ccc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN3341
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.14

MAT-POS-4223bc15-5_4



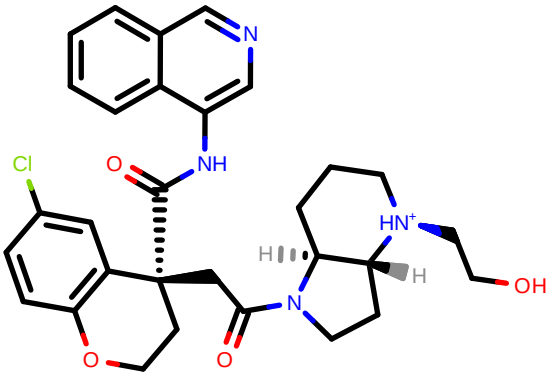
CID:	MAT-POS-4223bc15-5_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)CCO
RUN:	RUN3992
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.19

JOH-UNI-ee5ed7c8-10_1



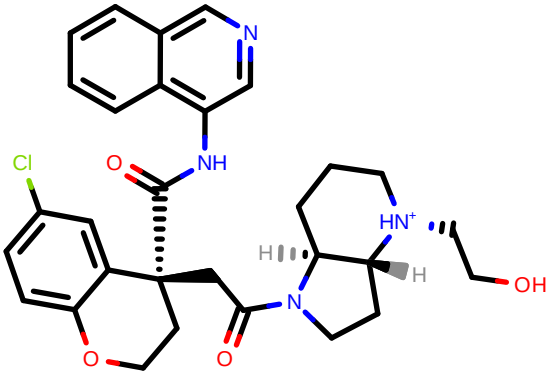
CID:	JOH-UNI-ee5ed7c8-10_1
SMILES:	CN(c1c2ccccc2cnc1CC(F)(F)F)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1909
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.37

PET-UNK-9bf1291a-5_2



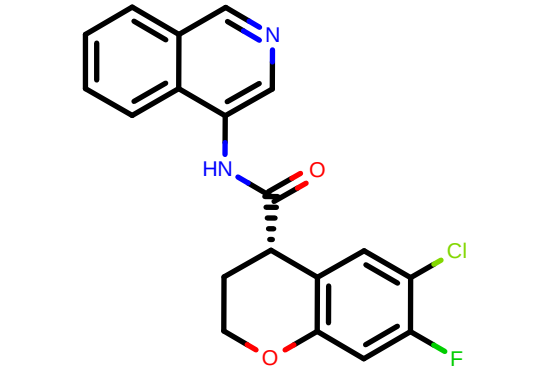
CID:	PET-UNK-9bf1291a-5_2
SMILES:	CO[C@]1(C[N@](Cc2c1cc(cc2)Cl)CC#N)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3970
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.31

RAL-THA-58fba2bc-2_1



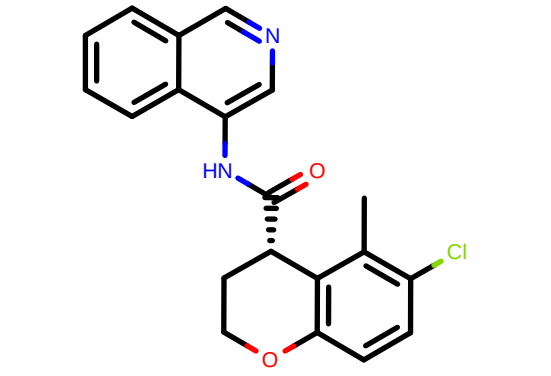
CID:	RAL-THA-58fba2bc-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)[O-]
RUN:	RUN3651
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.44

LAU-MED-88a3970a-15_1



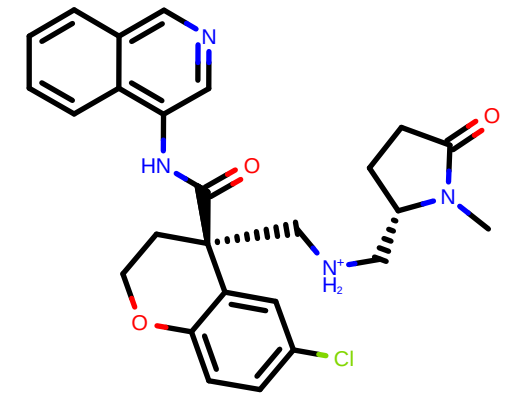
CID:	LAU-MED-88a3970a-15_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4CCS(=O)(=O)N)Cl
RUN:	RUN1511
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.10

MAK-UNK-ffc90da7-2_5



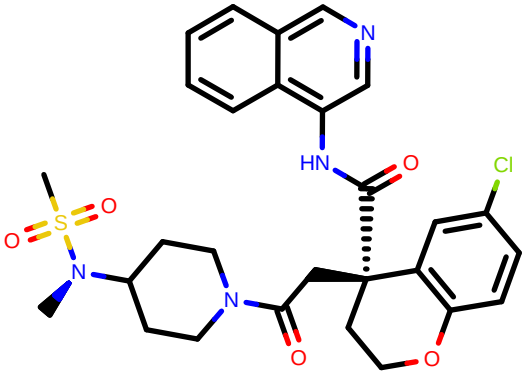
CID:	MAK-UNK-ffc90da7-2_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@@H]([C@H]3O)Cl
RUN:	RUN685
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.09

EDJ-MED-1b5395f9-2_2



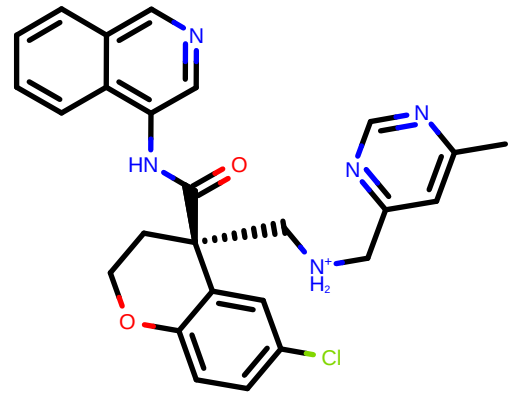
CID:	EDJ-MED-1b5395f9-2_2
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@@H]3C[N@](Cc4c3cc(c(c4)Cl)Cl)S(=O)(=O)C
RUN:	RUN4464
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.23

MAT-POS-4223bc15-7_3



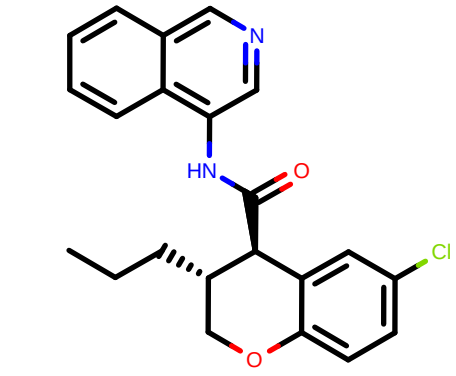
CID:	MAT-POS-4223bc15-7_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)C5COC5
RUN:	RUN3999
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.28

ALP-UNI-dbb9503d-2_2



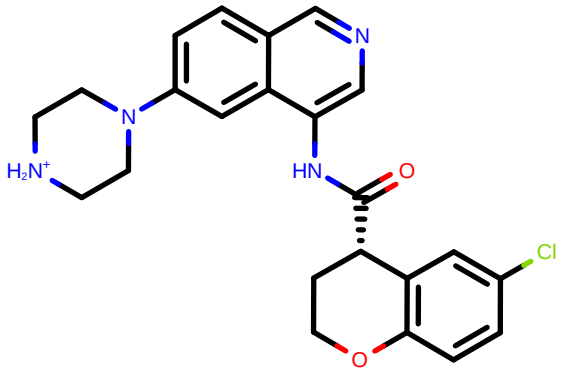
CID:	ALP-UNI-dbb9503d-2_2
SMILES:	CO[C@]1(CCCN(C1=O)c2cncc3c2cccc3)c4cccc(c4)Cl
RUN:	RUN4331
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.21

EDG-MED-ba1ac7b9-20_3



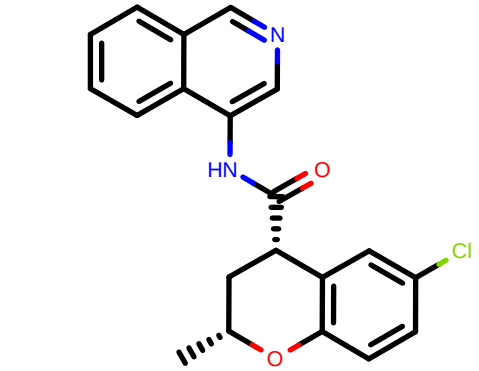
CID:	EDG-MED-ba1ac7b9-20_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCOC[C@H]5CC(F)F
RUN:	RUN2696
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.09

EDJ-MED-ee07cf00-4_1



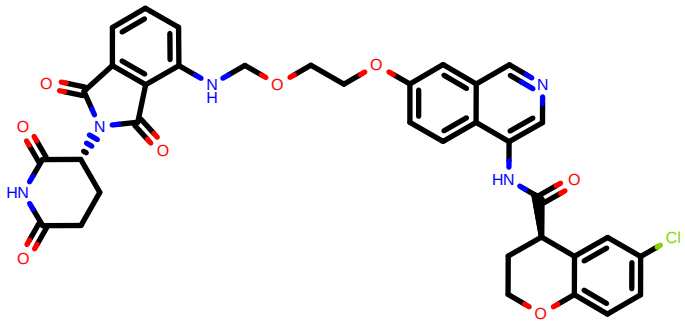
CID:	EDJ-MED-ee07cf00-4_1
SMILES:	C[C@@H](C(=O)N[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3)NC(=O)C4CCC4
RUN:	RUN2807
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.22

MIC-UNK-d36ab305-1_1



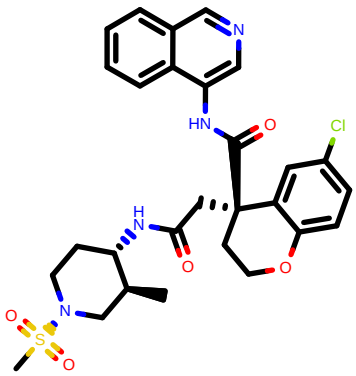
CID:	MIC-UNK-d36ab305-1_1
SMILES:	CC(=O)Nc1ccc(cc1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN151
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.12

ALP-UNI-8e43a71e-2_16



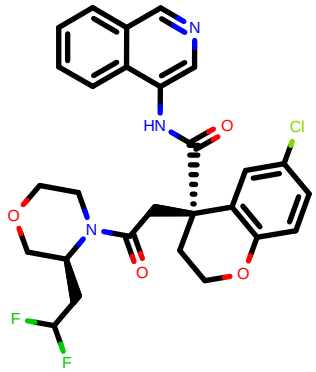
CID:	ALP-UNI-8e43a71e-2_16
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6[C@H]5CCC[N@H+]6CCO
RUN:	RUN2938
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.29

MAK-UNK-c749d764-16_14



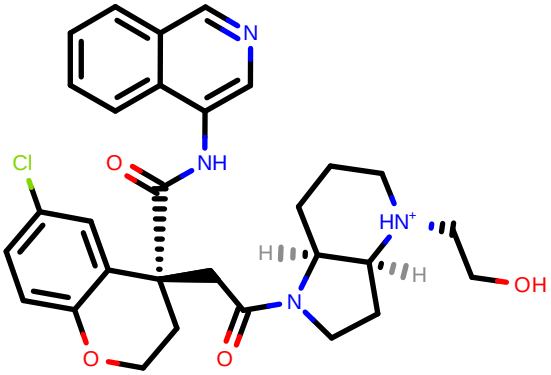
CID:	MAK-UNK-c749d764-16_14
SMILES:	C[C@H](N(c1cncc2c1cccc2)C(=O)C[C@@H]3CCC[C@H]([C@H]3O)C(F)F)O
RUN:	RUN987
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.40

JOH-UNI-f51e3bbc-4_1



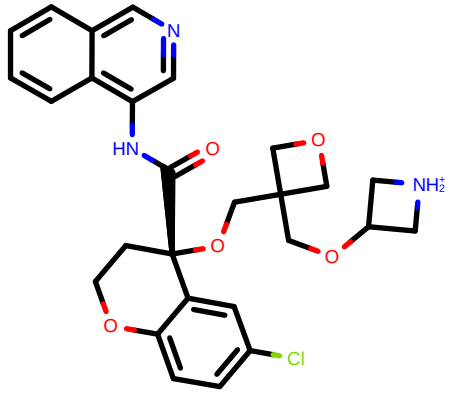
CID:	JOH-UNI-f51e3bbc-4_1
SMILES:	COc1c(c2ccccc2cn1)NC(=O)[C@@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1164
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.20

MAK-UNK-c749d764-29_8



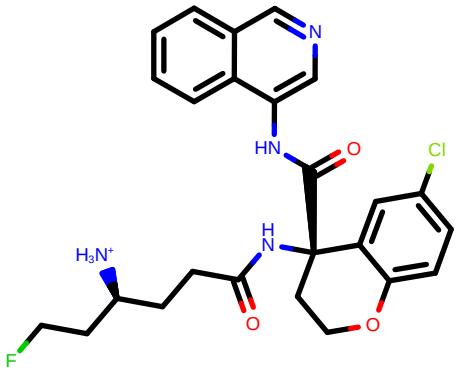
CID:	MAK-UNK-c749d764-29_8
SMILES:	c1ccc2c(c1)cncc2N(C(=O)C[C@H]3CCC[C@H]([C@H]3O)C(F)F)C(=O)ON
RUN:	RUN1070
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.45

DAR-DIA-0f2f46c9-1_3



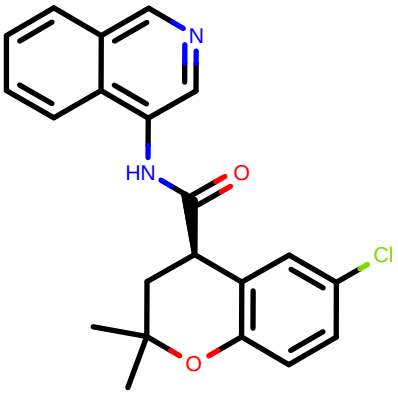
CID:	DAR-DIA-0f2f46c9-1_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC[N@](c4c3cc(cc4)Cl)S(=O)(=O)N
RUN:	RUN3220
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.24

MAK-UNK-c749d764-3_3



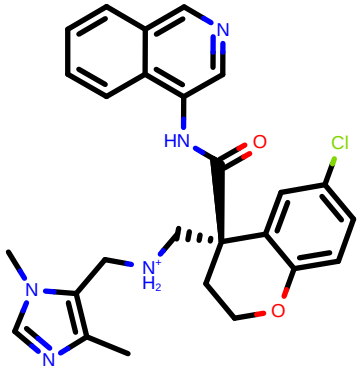
CID:	MAK-UNK-c749d764-3_3
SMILES:	CC1(C[NH2+]C1)OCN(c2cncc3c2cccc3)C(=O)C[C@@H]4CCC[C@H]([C@@H]4O)C(F)F
RUN:	RUN907
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.33

EDG-MED-ba1ac7b9-33_2



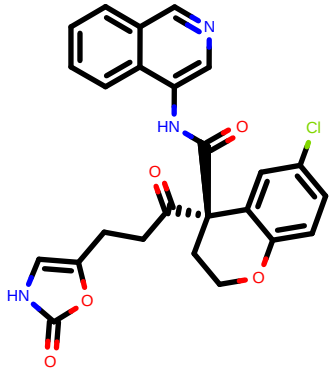
CID:	EDG-MED-ba1ac7b9-33_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@@H]6CCOC6
RUN:	RUN2749
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.07

EDJ-MED-93390d0c-1_1



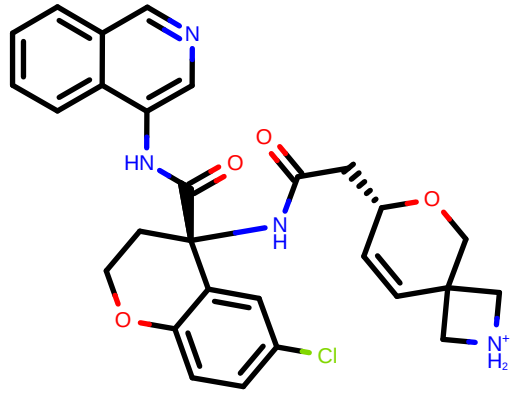
CID:	EDJ-MED-93390d0c-1_1
SMILES:	CS(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@@H]3CCS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN4516
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.26

MAR-TRE-a3327163-39_1



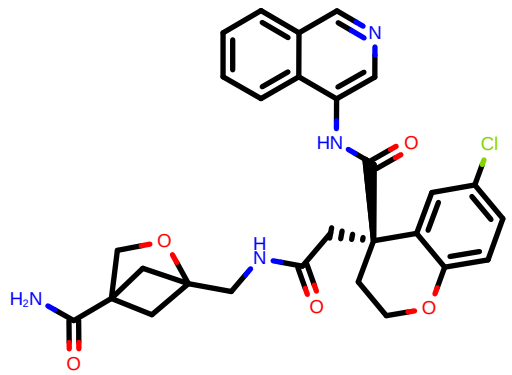
CID:	MAR-TRE-a3327163-39_1
SMILES:	CCc1c2cc(c(cc2c(c(n1)C)C#N)OC)OC
RUN:	RUN103
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.28

MIC-UNK-bcd487e9-2_1



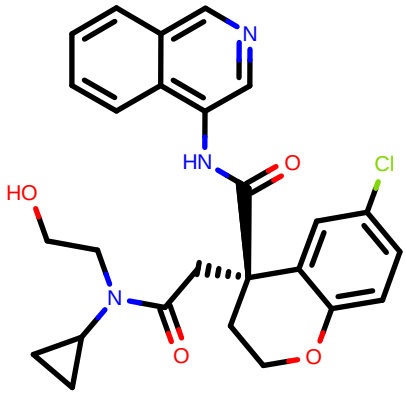
CID:	MIC-UNK-bcd487e9-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(CC3CCCCC3)c4cccc(c4)Cl
RUN:	RUN587
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.31

MIC-UNK-5a93dd5f-6_1



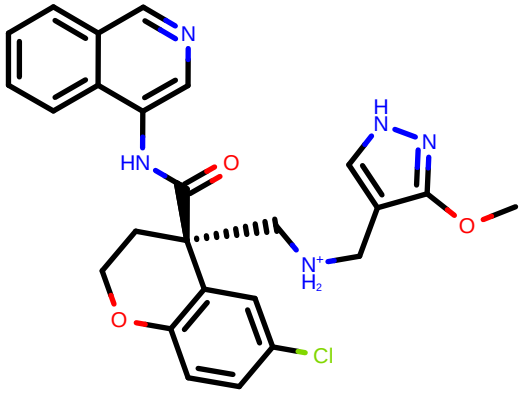
CID:	MIC-UNK-5a93dd5f-6_1
SMILES:	CC(=O)N(C)C1CC[NH+](CC1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN766
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.49

EDJ-MED-841e0cf0-7_3



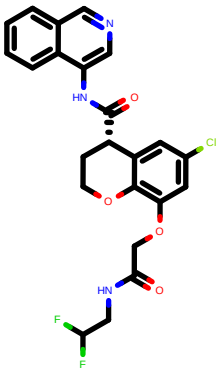
CID:	EDJ-MED-841e0cf0-7_3
SMILES:	CNS(=O)(=O)[N@@]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl
RUN:	RUN3846
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.15

JOH-UNI-ee5ed7c8-13_1



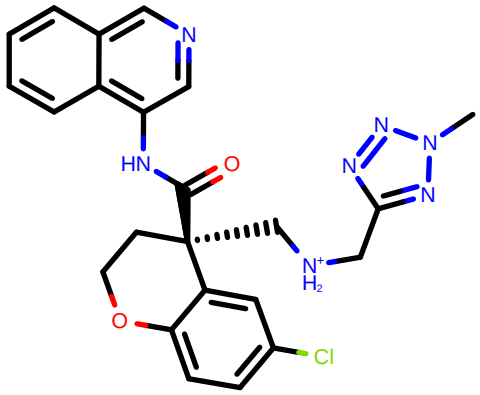
CID:	JOH-UNI-ee5ed7c8-13_1
SMILES:	CN(c1cncc2c1c(ccc2)CC(F)(F)F)C(=O)Cc3cccc(c3)Cl
RUN:	RUN1911
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.37

MAT-POS-f39f51fd-1_1



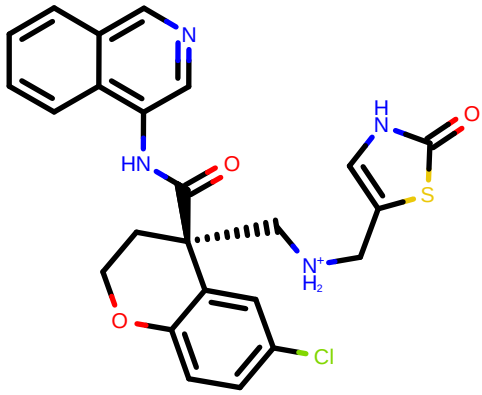
CID:	MAT-POS-f39f51fd-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CC(=O)Nc4c3cc(cc4Cl)Cl
RUN:	RUN2404
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.29

ALP-POS-347519b5-3_54



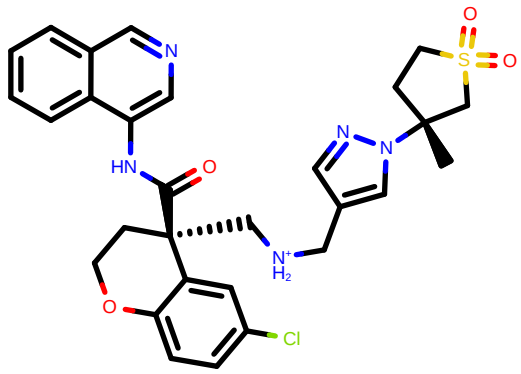
CID:	ALP-POS-347519b5-3_54
SMILES:	CS(=O)(=O)[N@]1C[C@@H]2[C@H]3CC[C@@H]([C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4320
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

ALP-POS-347519b5-3_10



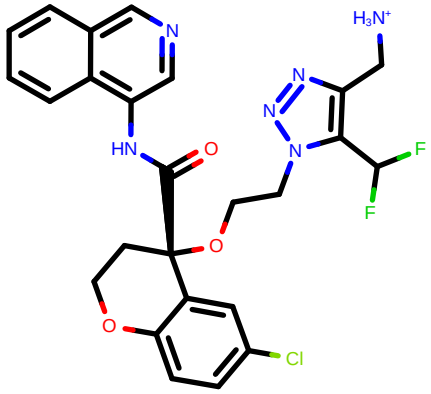
CID:	ALP-POS-347519b5-3_10
SMILES:	CS(=O)(=O)[N@]1C[C@@H]2[C@@H]3CC[C@H]([C@@H]2[C@@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4302
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

MAT-POS-64942dd0-2_3



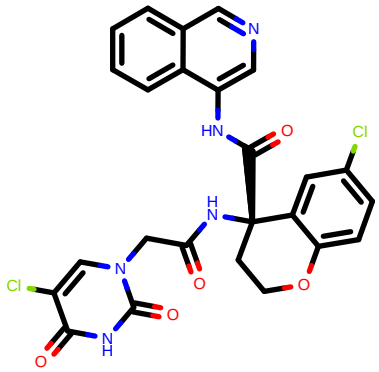
CID:	MAT-POS-64942dd0-2_3
SMILES:	CS(=O)(=O)[N@@]1Cc2cc(c(cc2[C@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl)F
RUN:	RUN4387
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.29

ERI-UCB-b3e6b0c2-15_1



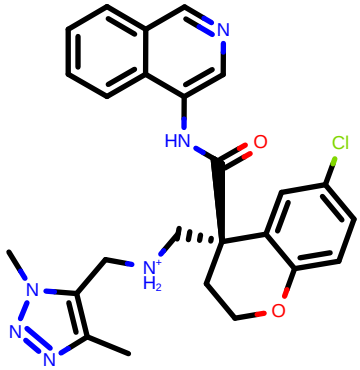
CID:	ERI-UCB-b3e6b0c2-15_1
SMILES:	COCCOc1ccc2c(c1)cncc2NC(=O)[C@@H]3COc4c3cc(cc4)Cl
RUN:	RUN3050
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.22

RAL-THA-4aa06b95-7_2



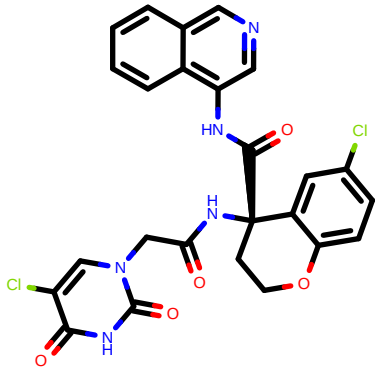
CID:	RAL-THA-4aa06b95-7_2
SMILES:	COCCN1CC[C@@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1244
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.36

MAT-POS-61f37a1a-4_1



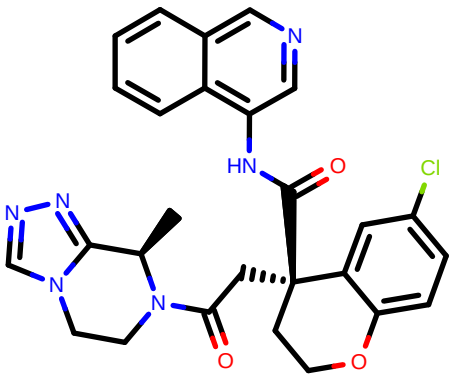
CID:	MAT-POS-61f37a1a-4_1
SMILES:	CC(C)(C)OC(=O)NCc1c(n(nn1)C)C[NH2+][C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4593
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.24

DAR-DIA-f6ee7aeb-6_4



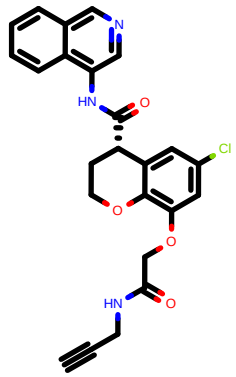
CID:	DAR-DIA-f6ee7aeb-6_4
SMILES:	c1ccc2c(c1)cncc2N3C[C@H]([C@H](CC3=O)c4cccc(c4)Cl)c5c[nH]c(=O)[nH]c5=O
RUN:	RUN3422
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.15

EDJ-MED-841e0cf0-2_2



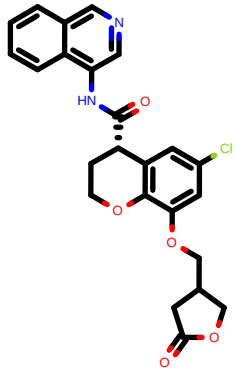
CID:	EDJ-MED-841e0cf0-2_2
SMILES:	CO[C@@]1(C[N@](Cc2c1cc(c(c2)F)Cl)S(=O)(=O)C)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3831
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.17

MAT-POS-d8472c4f-5_1



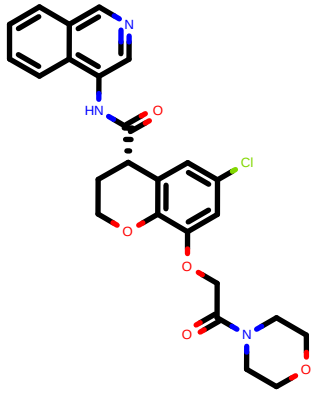
CID:	MAT-POS-d8472c4f-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[NH2+]Cc4c3cc(cc4)Cl
RUN:	RUN5018
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.38

ALP-POS-2da19ca7-2_2



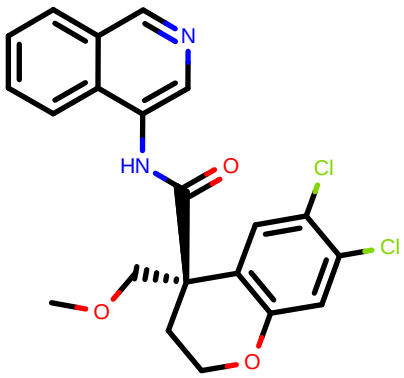
CID:	ALP-POS-2da19ca7-2_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[NH+](CC5)[C@H]6CCOC6
RUN:	RUN2376
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.23

ALP-POS-67d5babe-4_2



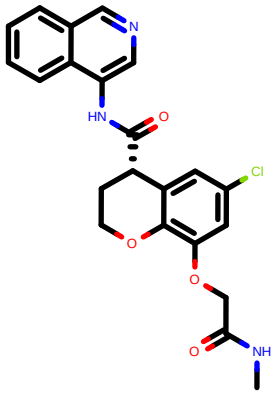
CID:	ALP-POS-67d5babe-4_2
SMILES:	CS(=O)(=O)CC1CCN(CC1)C(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN4892
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.32

EDG-MED-4c68219f-11_1



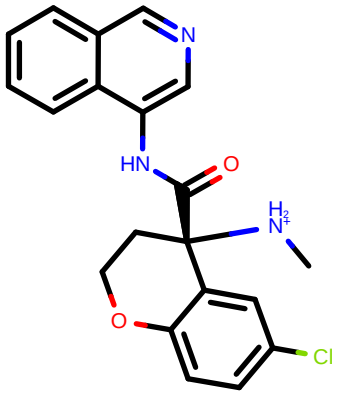
CID:	EDG-MED-4c68219f-11_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCC(=O)NCCCC(=O)[O-]
RUN:	RUN1655
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.13

EDG-MED-5d232de5-6_2



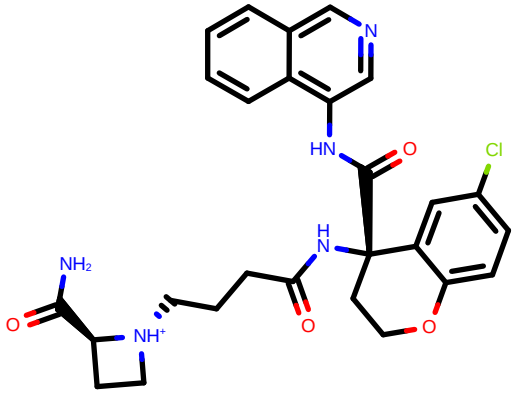
CID:	EDG-MED-5d232de5-6_2
SMILES:	CN1CC[C@H](c2c1ccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2372
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.23

MAK-UNK-c749d764-1_2



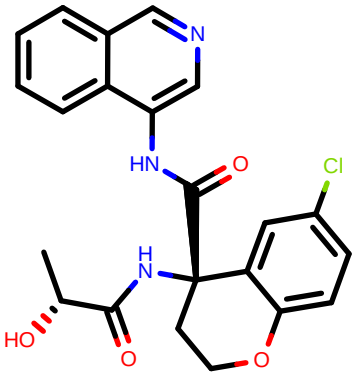
CID:	MAK-UNK-c749d764-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@H]3CCC[C@@H]([C@@H]3O)C4CC4
RUN:	RUN889
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.31

EDJ-MED-37aac4bd-1_2



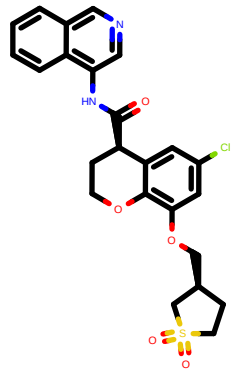
CID:	EDJ-MED-37aac4bd-1_2
SMILES:	CO[C@]1(CCOc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3140
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.21

VLA-UNK-b9c208fe-2_1



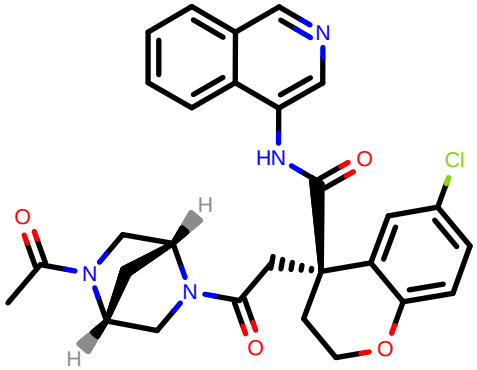
CID:	VLA-UNK-b9c208fe-2_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(c(c(c3)Cl)F)Cl
RUN:	RUN3158
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.12

MIC-UNK-37660950-3_2



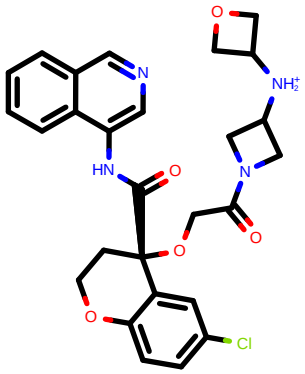
CID:	MIC-UNK-37660950-3_2
SMILES:	CS(=O)(=O)[N@]1CCC[C@@H](C1)CNc2ccc(cc2CC(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN5113
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.20

MAK-UNK-c749d764-22_1



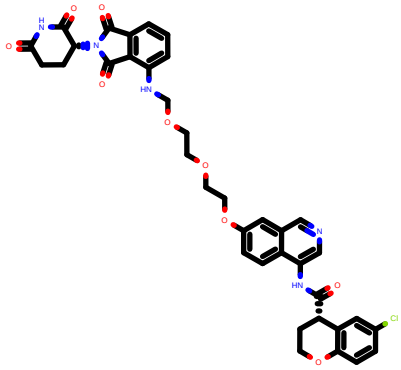
CID:	MAK-UNK-c749d764-22_1
SMILES:	C[C@@H](C[NH2+]C[C@@H]1CCCO1)[C@@H](c2cccc(c2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN1022
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.32

JAG-UCB-706446eb-7_2



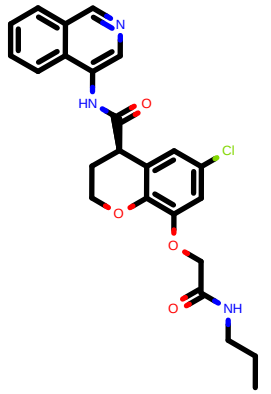
CID:	JAG-UCB-706446eb-7_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@H]5CCCOC5
RUN:	RUN624
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.44

MAT-POS-8a69d52e-4_3



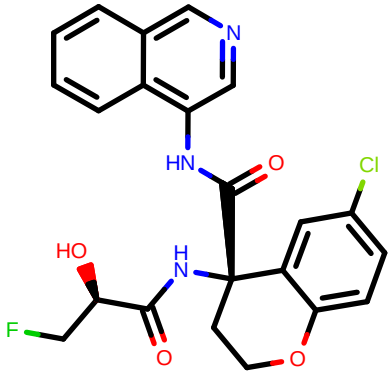
CID:	MAT-POS-8a69d52e-4_3
SMILES:	C[C@@H]1COc2ccc(cc2[C@H]1C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN368
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.38

MAT-POS-a3f7f96a-9_1



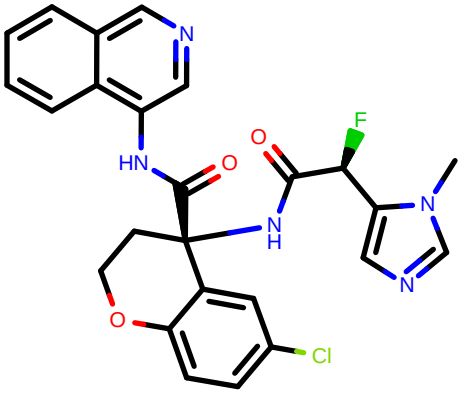
CID:	MAT-POS-a3f7f96a-9_1
SMILES:	COc1ccc(cc1OCC(=O)N)C[NH2+]C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN5058
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.18

ALP-POS-fe871b40-15_2



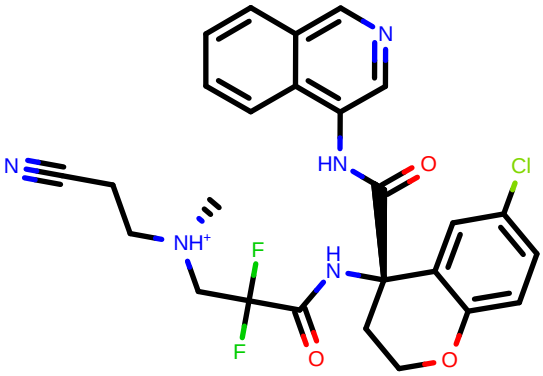
CID:	ALP-POS-fe871b40-15_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CC(=O)Nc4c3cc(c(c4)F)Cl
RUN:	RUN3137
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.16

EDJ-MED-4f704dc9-2_1



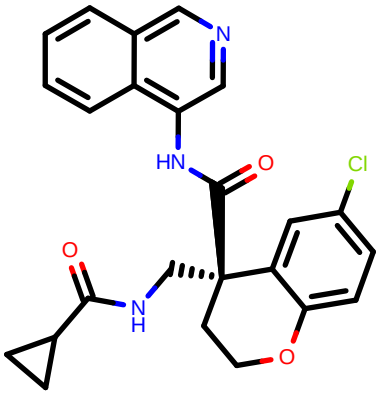
CID:	EDJ-MED-4f704dc9-2_1
SMILES:	COC[C@@]1(CC(=O)Nc2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3161
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.16

MAT-POS-78e1d523-1_1



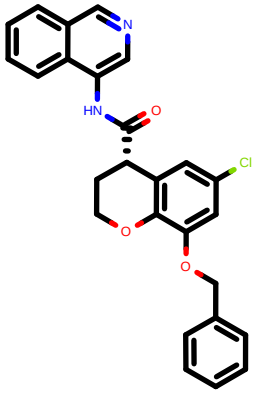
CID:	MAT-POS-78e1d523-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCSc4c3cc(cc4)Cl
RUN:	RUN3277
DDG (kcal/mol):	-0.08
dDDG (kcal/mol):	0.20

MAT-POS-e6dd326d-3_1



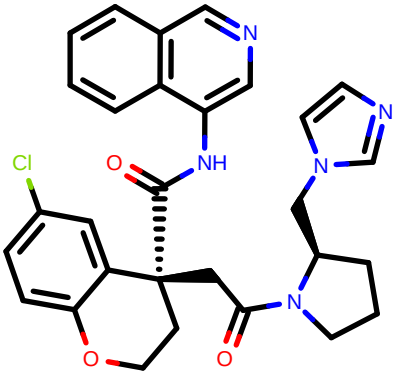
CID:	MAT-POS-e6dd326d-3_1
SMILES:	C[NH+](C)C[C@@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3941
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.10

DAR-DIA-9e4459de-15_5



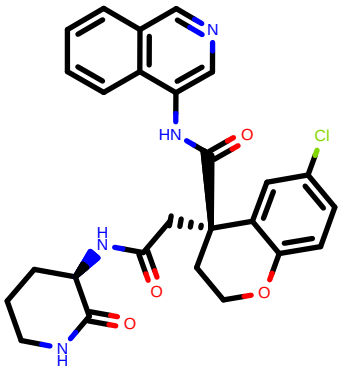
CID:	DAR-DIA-9e4459de-15_5
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1447
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.24

JOH-UNI-6fede743-5_1



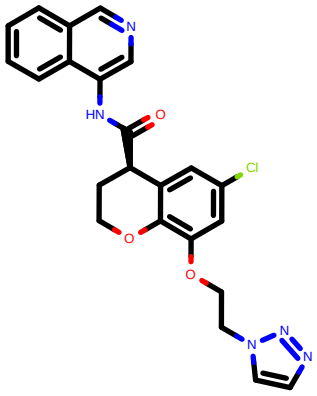
CID:	JOH-UNI-6fede743-5_1
SMILES:	c1cc(cc(c1)Cl)CC(=O)Nc2c3cc(ccc3cnc2C(F)F)F
RUN:	RUN1171
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.47

KAD-UNI-b13decd3-5_2



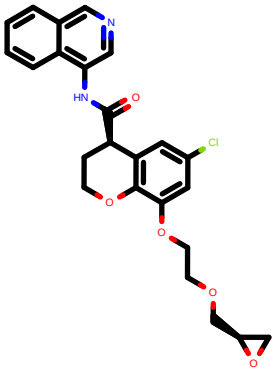
CID:	KAD-UNI-b13decd3-5_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5cn(nn5)C[C@H]6CCCO6
RUN:	RUN3786
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.17

MAT-POS-a3f7f96a-6_4



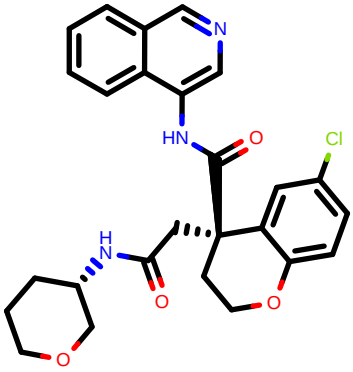
CID:	MAT-POS-a3f7f96a-6_4
SMILES:	C[C@]1(CCS(=O)(=O)C1)n2cc(cn2)C[NH2+]C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN5044
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.20

BEN-DND-11faade0-1_2



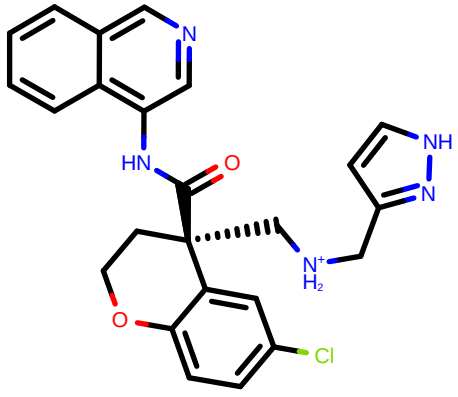
CID:	BEN-DND-11faade0-1_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CNS(=O)(=O)c4c3cccc4
RUN:	RUN5075
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.20

LON-WEI-4d77710c-49_1



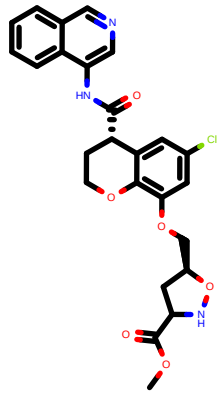
CID:	LON-WEI-4d77710c-49_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)NCc3ccccn3
RUN:	RUN238
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.38

EDJ-MED-1b5395f9-5_1



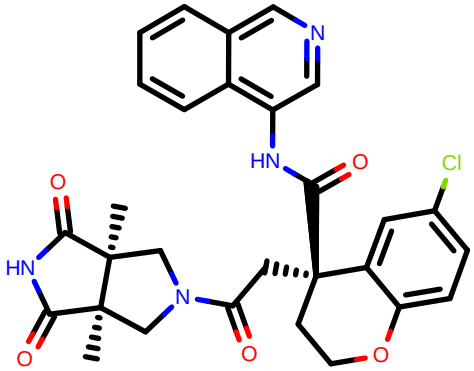
CID:	EDJ-MED-1b5395f9-5_1
SMILES:	CS(=O)(=O)[N@@]1Cc2cc(c(cc2[C@@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl)Cl
RUN:	RUN4471
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.22

EDJ-MED-40433386-3_1



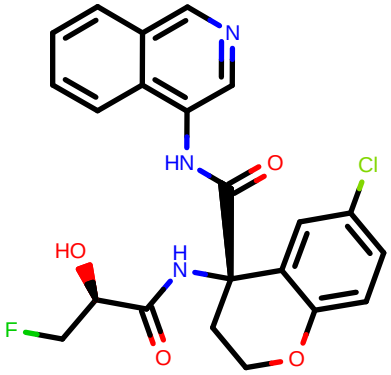
CID:	EDJ-MED-40433386-3_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)CNC(=O)[C@@]5(CCSC5)O
RUN:	RUN2552
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.37

EDJ-MED-611d11e7-5_1



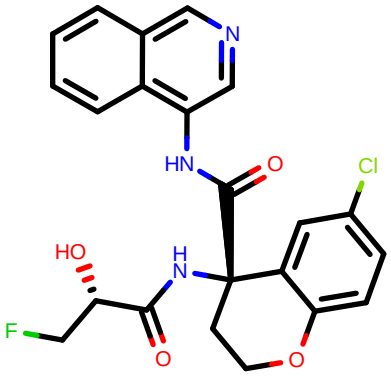
CID:	EDJ-MED-611d11e7-5_1
SMILES:	c1cc2cncc(c2cc1F)NC(=O)[C@@H]3CCNc4c3cc(c(c4)Cl)Cl
RUN:	RUN3488
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.19

EDJ-MED-37aac4bd-5_1



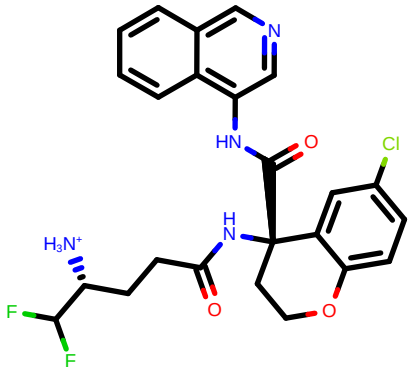
CID:	EDJ-MED-37aac4bd-5_1
SMILES:	CO[C@@]1(CCOc2c1cc(cn2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3147
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.16

EDJ-MED-60df06f3-1_1



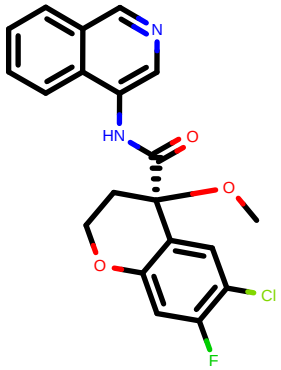
CID:	EDJ-MED-60df06f3-1_1
SMILES:	Cn1cnnc1COC[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3170
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.13

DAR-DIA-0587064e-20_2



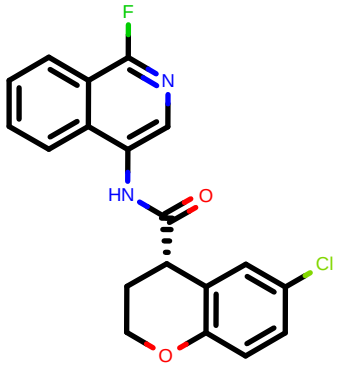
CID:	DAR-DIA-0587064e-20_2
SMILES:	c1ccc(cc1)CCOc2cc(cc3c2OCC[C@H]3C(=O)Nc4cncc5c4cccc5)Cl
RUN:	RUN3378
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.24

DAR-DIA-5ff57136-18_1



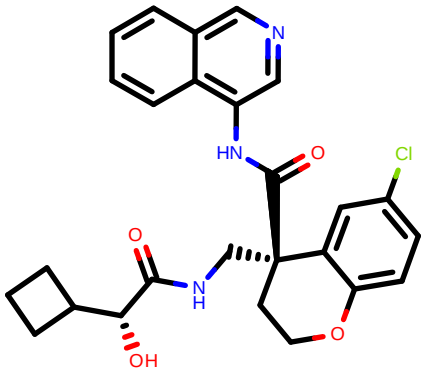
CID:	DAR-DIA-5ff57136-18_1
SMILES:	c1ccc2c(c1)cncc2N(C(=O)[C@@H]3CCOc4c3cc(cc4)Cl)N=C=S
RUN:	RUN1391
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.05

ALP-POS-6747fa38-1_1



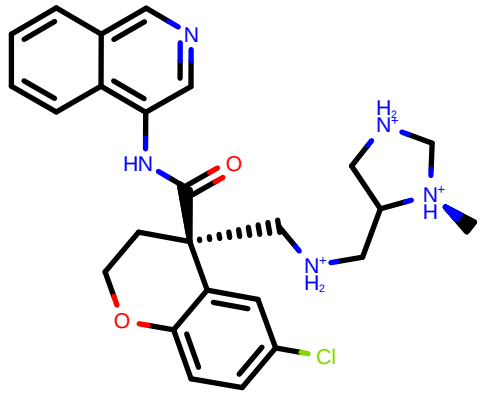
CID:	ALP-POS-6747fa38-1_1
SMILES:	CC(=O)N1CC[NH+](CC1)CC(=O)Nc2cncc3c2cccc3
RUN:	RUN188
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.10

KAD-UNI-cb0f2bbc-9_1



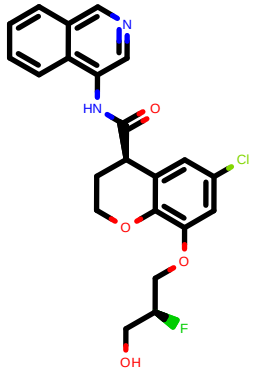
CID:	KAD-UNI-cb0f2bbc-9_1
SMILES:	COc1ccc(cc1OCC(=O)N)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3692
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.12

BEN-DND-d1eb1f41-15_2



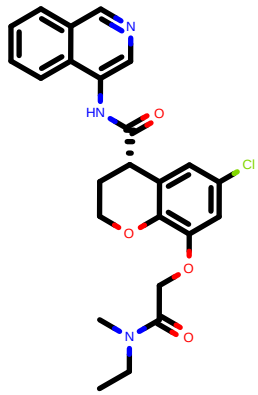
CID:	BEN-DND-d1eb1f41-15_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@H](C3=O)c4ccc(c(c4)Cl)F
RUN:	RUN4361
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.21

ALF-EVA-a24cc7ce-2_2



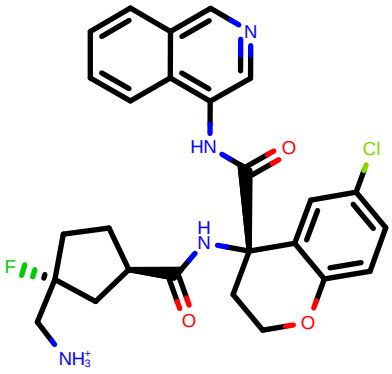
CID:	ALF-EVA-a24cc7ce-2_2
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@H]3COc4c3cc(cc4)Cl
RUN:	RUN4956
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.22

EDJ-MED-9e38fd34-4_2



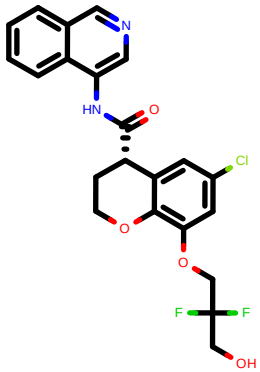
CID:	EDJ-MED-9e38fd34-4_2
SMILES:	C[C@]1(c2cc(c(cc2NC1=O)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN2350
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.28

MIC-UNK-02d7a284-3_2



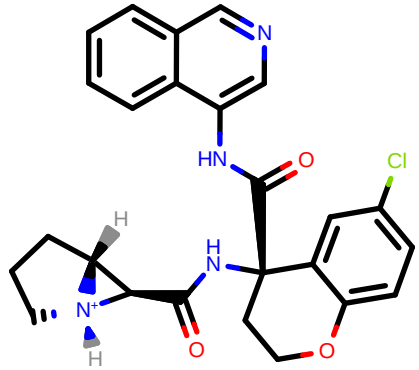
CID:	MIC-UNK-02d7a284-3_2
SMILES:	CC(=O)NC[C@H]1CN(CC(=O)N1c2cccc(c2)Cl)C(=O)c3cncc4c3cccc4
RUN:	RUN3257
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.22

VLA-UNK-f702bf1c-8_1



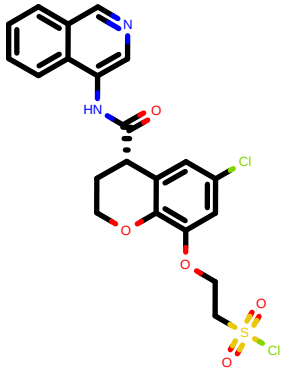
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncn6
RUN:	RUN2322
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.28

NAU-LAT-0543f7f2-10_1



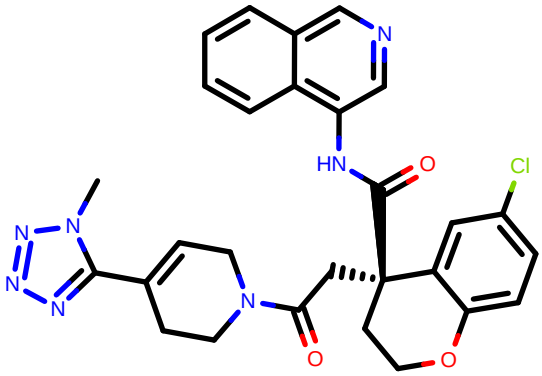
CID:	NAU-LAT-0543f7f2-10_1
SMILES:	CC(=O)NCCOc1cc(cc2c1OCC[C@@H]2C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN659
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

KAD-UNI-80f122c8-3_8



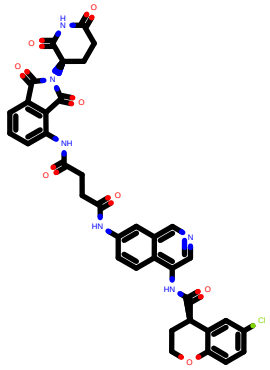
CID:	KAD-UNI-80f122c8-3_8
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CC[C@H]6CS(=O)(=O)C[C@H]6C5
RUN:	RUN2296
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

PET-UNK-3bb57da2-2_1



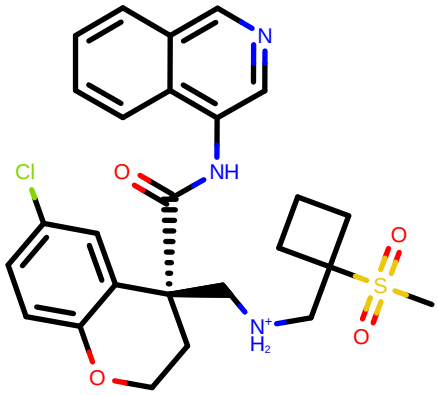
CID:	PET-UNK-3bb57da2-2_1
SMILES:	CN(C)S(=O)(=O)CO[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3648
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.20

MAR-UCB-6ab2ec87-3_1



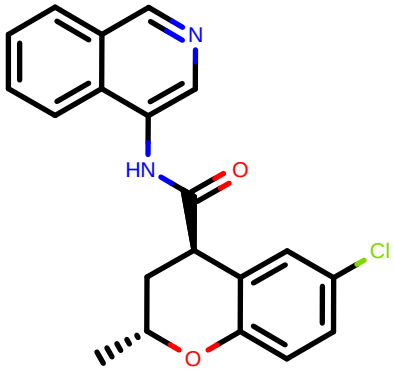
CID:	MAR-UCB-6ab2ec87-3_1
SMILES:	CO[C@]1(COc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3023
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.23

MIC-UNK-ea4eb352-5_1



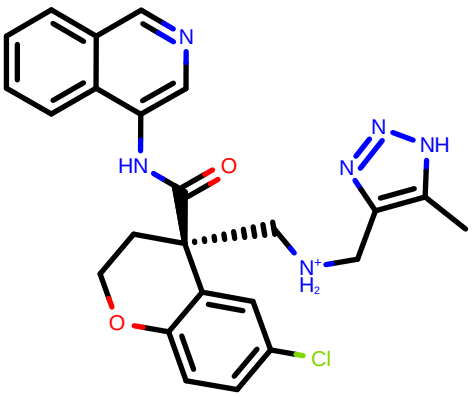
CID:	MIC-UNK-ea4eb352-5_1
SMILES:	CO[C@@]1(CCS(=O)(=O)c2c1cc(c(c2)Cl)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN4642
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.27

EDG-MED-ba1ac7b9-17_2



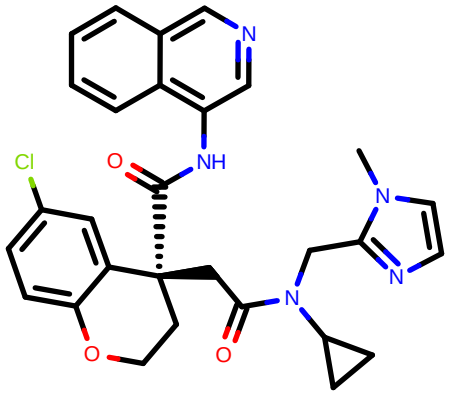
CID:	EDG-MED-ba1ac7b9-17_2
SMILES:	Cn1ccnc1CN(C2CC2)C(=O)C[C@]3(CCOc4c3cc(cc4)Cl)C(=O)Nc5cncc6c5cccc6
RUN:	RUN2689
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.08

EDJ-MED-1b5395f9-1_1



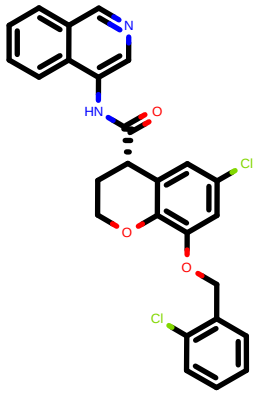
CID:	EDJ-MED-1b5395f9-1_1
SMILES:	COc1ccc2cncc(c2c1)NC(=O)[C@@H]3C[N@@](Cc4c3cc(c(c4)Cl)Cl)S(=O)(=O)C
RUN:	RUN4458
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.26

VLA-UNK-8e76d113-3_1



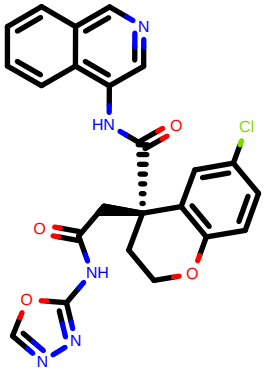
CID:	VLA-UNK-8e76d113-3_1
SMILES:	CO[C@]1(CCNc2c1cc(c(c2C#N)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3854
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.23

DAR-DIA-9e4459de-15_14



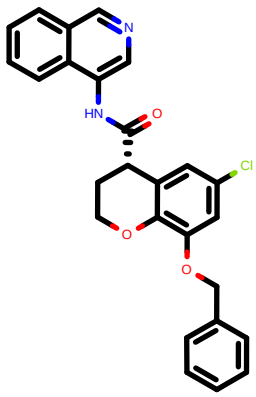
CID:	DAR-DIA-9e4459de-15_14
SMILES:	c1cc2c(c(c1)NC(=O)CCC(=O)Nc3ccc4c(c3)cncc4NC(=O)[C@H]5CCOc6c5cc(cc6)Cl)c(n(c2O)[C@H]7CCC(=O)NC7=O)O
RUN:	RUN1454
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.28

MAT-POS-dd3ad2b5-3_2



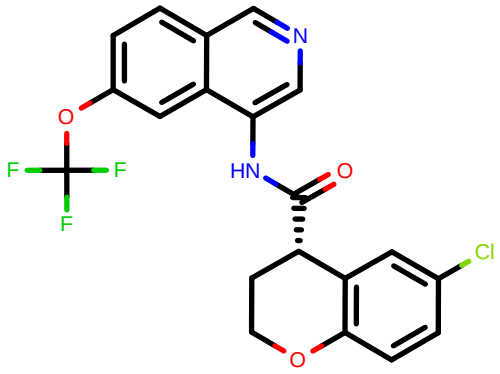
CID:	MAT-POS-dd3ad2b5-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3CN(Cc4c3cc(cc4)Cl)C(=O)N
RUN:	RUN3536
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.34

ED_-GRI-5b13fbe2-72_1



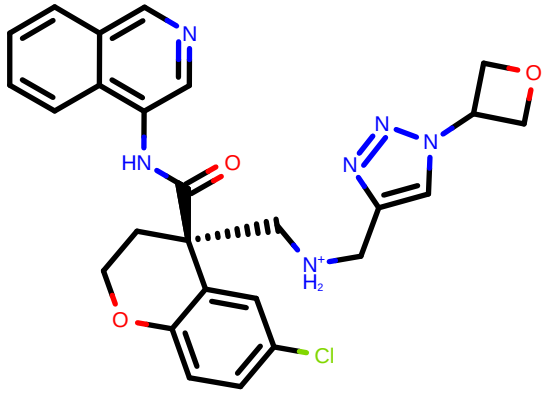
CID:	ED_-GRI-5b13fbe2-72_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCO
RUN:	RUN1629
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.24

LON-WEI-4d77710c-5_1



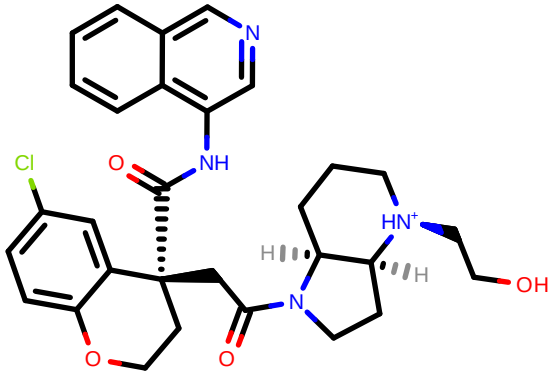
CID:	LON-WEI-4d77710c-5_1
SMILES:	Cn1cc(c2ccccc2c1=O)NC(=O)Nc3ccc(c(c3)OC)OC
RUN:	RUN195
DDG (kcal/mol):	-0.04
dDDG (kcal/mol):	0.12

ALP-POS-a577c8a2-3_3



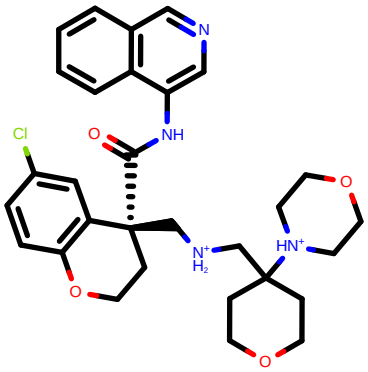
CID:	ALP-POS-a577c8a2-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@][S(=O)(=O)c4c3cc(cc4)Cl)Cc5[nH]ccn5
RUN:	RUN4632
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.24

MAT-POS-4223bc15-12_2



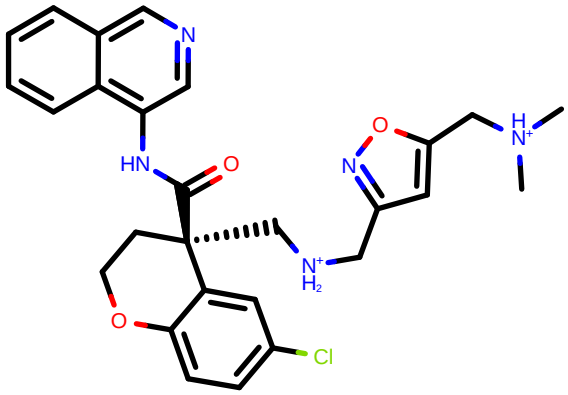
CID:	MAT-POS-4223bc15-12_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H]3C[N@@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5(CCC5)C#N
RUN:	RUN4046
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.34

EDG-MED-90036822-94_10



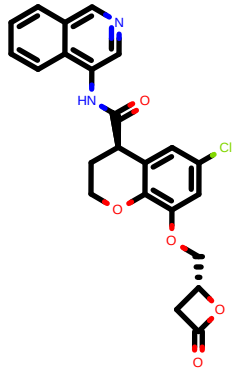
CID:	EDG-MED-90036822-94_10
SMILES:	C[C@H]1C[C@@H]1C@@H][C@H](C(=O)N[C@]2(CCOc3c2ccc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F)O
RUN:	RUN1814
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.52

ALP-POS-347519b5-3_55



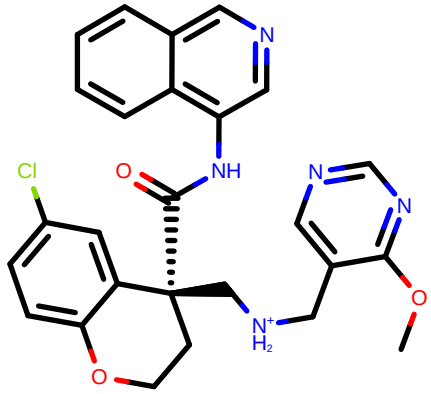
CID:	ALP-POS-347519b5-3_55
SMILES:	CS(=O)(=O)[N@@]1C[C@H]2[C@H]3CC[C@@H]([C@H]2[C@H](C1)C(=O)Nc4cncc5c4cccc5)O3
RUN:	RUN4322
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.24

PET-UNK-b566c0b0-9_1



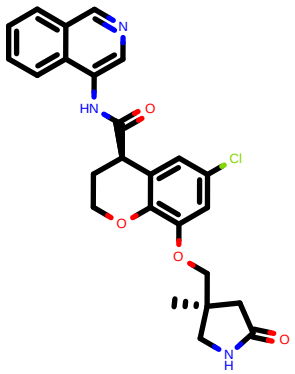
CID:	PET-UNK-b566c0b0-9_1
SMILES:	CN(C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@@](C1)(C(=O)Nc3cncc4c3ccc(c4)F)OC)Cl
RUN:	RUN4755
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.18

PET-UNK-022eab87-1_1



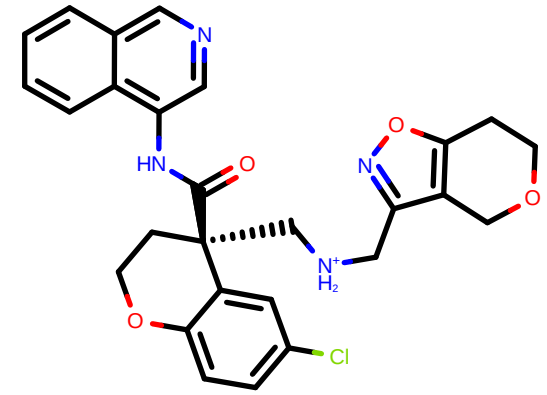
CID:	PET-UNK-022eab87-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CS(=O)(=O)c4c3cc(cc4)Cl
RUN:	RUN4701
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.24

ALP-POS-5bb456a5-2_4



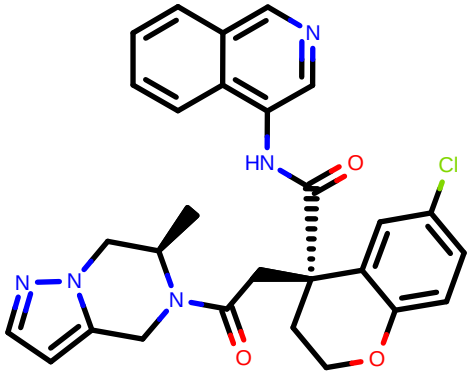
CID:	ALP-POS-5bb456a5-2_4
SMILES:	C[C@H]1C[N@](CC[C@@H]1NC(=O)C[C@@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)S(=O)(=O)C
RUN:	RUN2423
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.31

RAL-THA-b9d6aec1-1_2



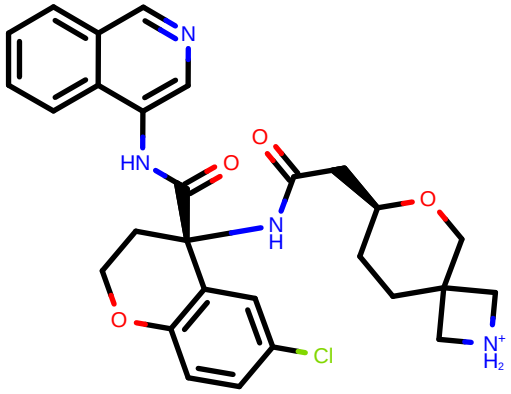
CID:	RAL-THA-b9d6aec1-1_2
SMILES:	CN(C)S(=O)(=O)c1ccc2cncc(c2c1)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN4493
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.25

NIR-THE-1e03c142-1_1



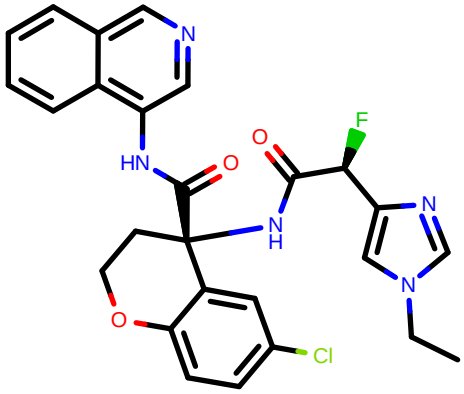
CID:	NIR-THE-1e03c142-1_1
SMILES:	c1ccc2c(c1)cncc2C3=CCC[C@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1187
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.23

MAK-UNK-ffc90da7-1_2



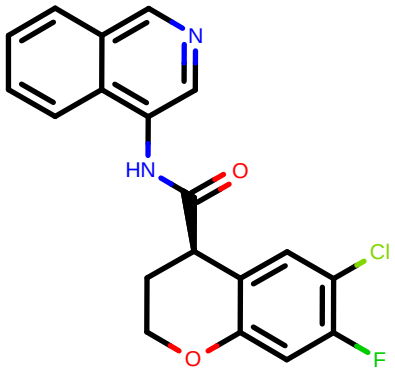
CID:	MAK-UNK-ffc90da7-1_2
SMILES:	C[C@H](C[NH2+]CCCO)[C@@H](c1cccc(c1)Cl)C(=O)Nc2cncc3c2cccc3
RUN:	RUN687
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.35

EDJ-MED-f893e2a1-7_1



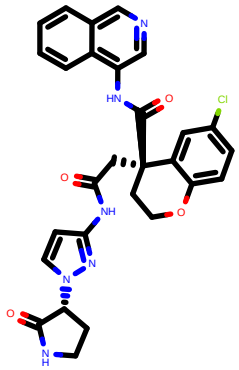
CID:	EDJ-MED-f893e2a1-7_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)C[NH2+]Cc5c[nH]c(=O)o5
RUN:	RUN3206
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.18

NIR-THE-5be8b355-1_1



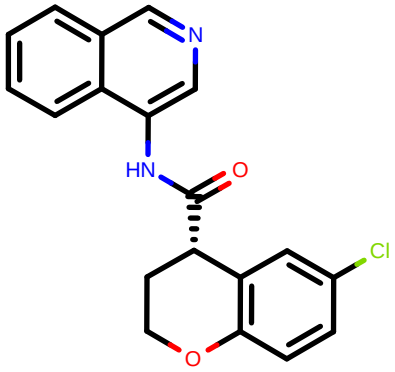
CID:	NIR-THE-5be8b355-1_1
SMILES:	c1ccc2c(c1)cncc2N(CCc3c[nH]c(=O)[nH]c3=O)C(=O)[C@@H]4CCOc5c4ccc(c5)Cl
RUN:	RUN3423
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.07

BEN-DND-a02b439d-3_2



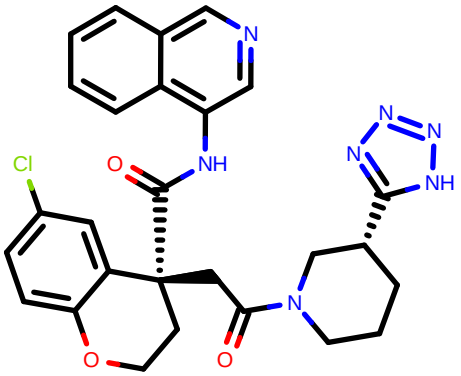
CID:	BEN-DND-a02b439d-3_2
SMILES:	COCC[N@H+]1Cc2cc(c(cc2[C@@H](C1)C(=O)Nc3cncc4c3cccc4)Cl)Cl
RUN:	RUN3664
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.20

DAR-DIA-0cde14eb-54_1



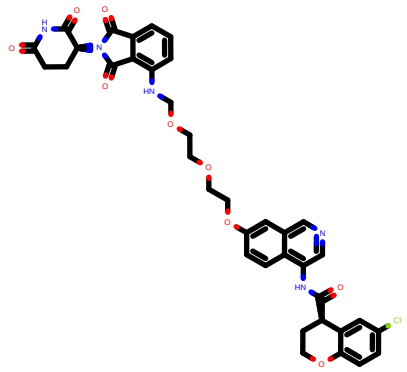
CID:	DAR-DIA-0cde14eb-54_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Nc3cccc(c3)C4(CC4)C#N
RUN:	RUN19
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.09

MAT-POS-4223bc15-28_4



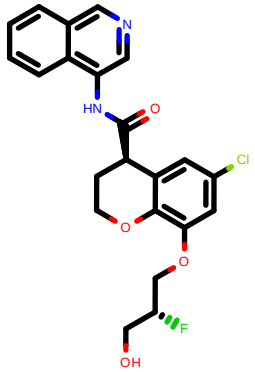
CID:	MAT-POS-4223bc15-28_4
SMILES:	COCC[N@H+]1Cc2ccc(cc2[C@H](C1)C(=O)Nc3cncc4c3cccc4)Cl
RUN:	RUN4128
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.27

ALP-UNI-8e43a71e-15_18



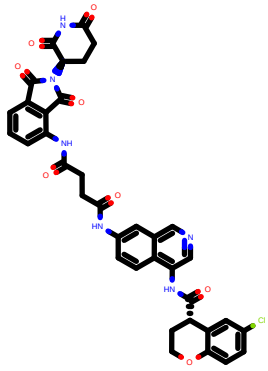
CID:	ALP-UNI-8e43a71e-15_18
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N[C@@H]5C[C@@H]6[C@@H]5C[C@H](C6)C(=O)N
RUN:	RUN3000
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.33

EDJ-MED-e9a22d5d-2_2



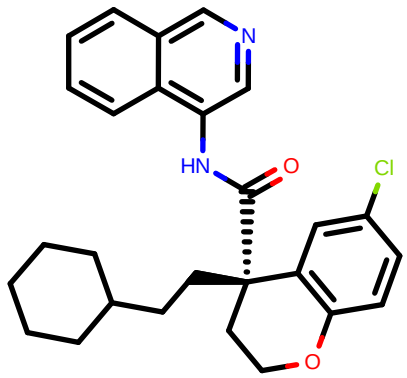
CID:	EDJ-MED-e9a22d5d-2_2
SMILES:	CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@@](C1)(C(=O)Nc3cncc4c3cccc4)OCC#C)Cl
RUN:	RUN4957
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.20

ALP-POS-7c6e02c7-1_1



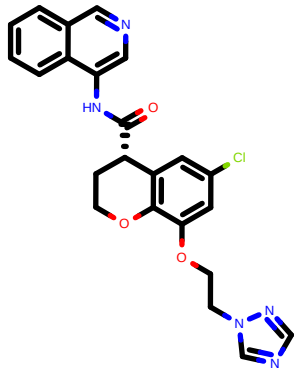
CID:	ALP-POS-7c6e02c7-1_1
SMILES:	CN(C)c1cnc(nc1)N(Cc2ccc(c(c2)Cl)Cl)C(=O)Cc3cncc4c3cccc4
RUN:	RUN3099
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.42

EDG-MED-ba1ac7b9-21_4



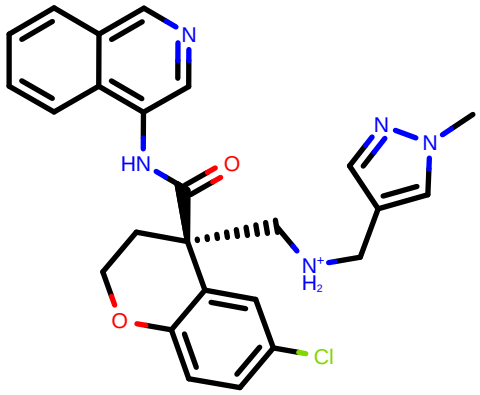
CID:	EDG-MED-ba1ac7b9-21_4
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)CC(=O)N5CCC[C@H]5Cn6ccnc6
RUN:	RUN2701
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.27

ALP-POS-5bb456a5-1_13



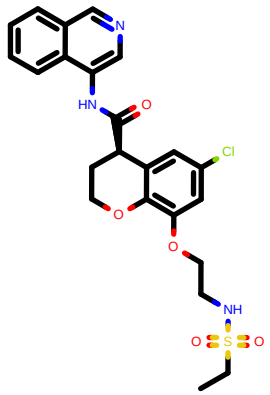
CID:	ALP-POS-5bb456a5-1_13
SMILES:	C[C@@H]1C[N@@](CC[C@H]1NC(=O)C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4ccc5c4cccc5)S(=O)(=O)C
RUN:	RUN2417
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.25

RAL-THA-eb6cb89c-1_1



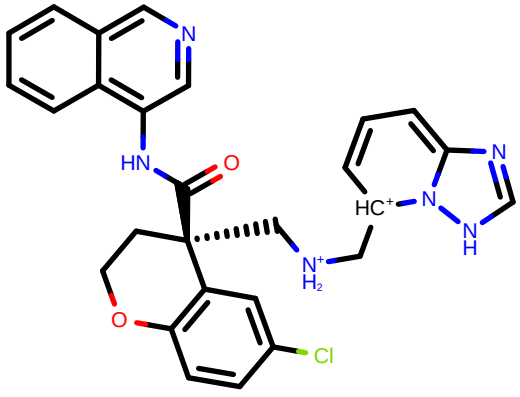
CID:	RAL-THA-eb6cb89c-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]34CC[C@@H](O3)c5c4cccc5
RUN:	RUN4340
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.22

MAT-POS-de59a476-3_2



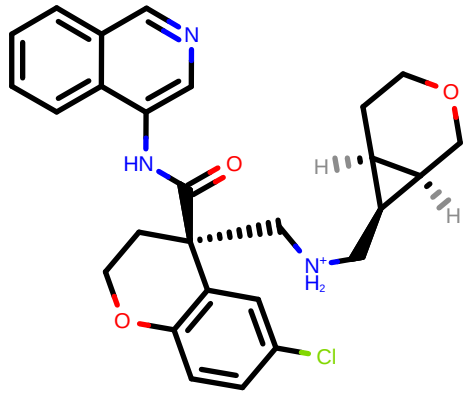
CID:	MAT-POS-de59a476-3_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@H](c3ccc(c(c3)Cl)Cl)OCCN4CCOCC4=O
RUN:	RUN2223
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.38

ED_-GRI-5b13fbe2-54_1



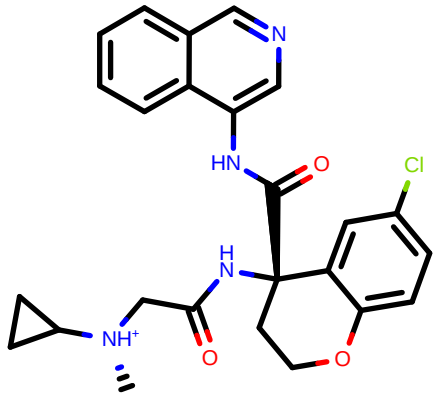
CID:	ED_-GRI-5b13fbe2-54_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)OCCCn5c(c(nn5)C[NH3+])C(F)F
RUN:	RUN1599
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.41

PET-UNK-b87f07d0-4_1



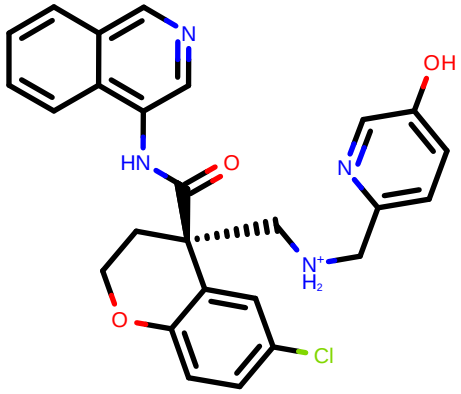
CID:	PET-UNK-b87f07d0-4_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)Cc3cc(cc(c3)Cl)CCCNc4nnco4
RUN:	RUN1901
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.40

MIC-UNK-bcd487e9-5_1



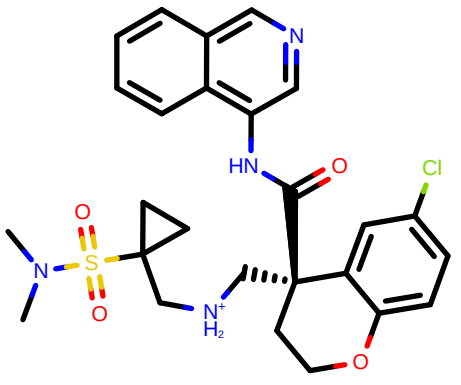
CID:	MIC-UNK-bcd487e9-5_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)N(Cc3ccco3)c4cccc(c4)Cl
RUN:	RUN591
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.39

EDJ-MED-1b5395f9-6_2



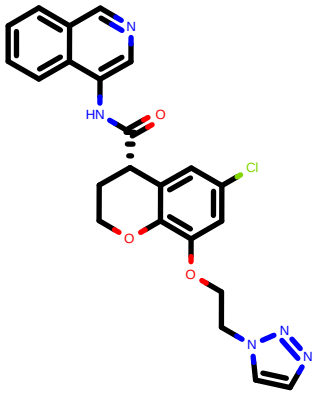
CID:	EDJ-MED-1b5395f9-6_2
SMILES:	CS(=O)(=O)[N@]1Cc2cc(c(cc2[C@H](C1)C(=O)Nc3cncc4c3cc(cc4)F)Cl)Cl
RUN:	RUN4474
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.23

MAT-POS-ec6d90b7-2_1



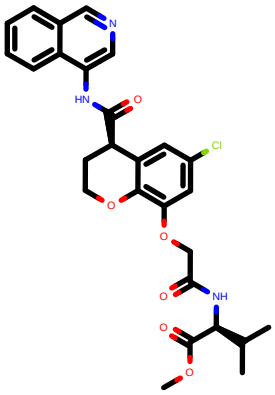
CID:	MAT-POS-ec6d90b7-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN4452
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.45

ALF-EVA-5b152d2f-7_1



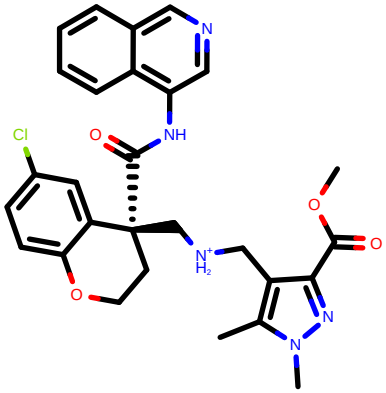
CID:	ALF-EVA-5b152d2f-7_1
SMILES:	c1cc2cncc(c2cc1C3CCC3)NC(=O)[C@@H]4CCOc5c4cc(cc5)Cl
RUN:	RUN2361
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.27

MAT-POS-2905de8c-1_1



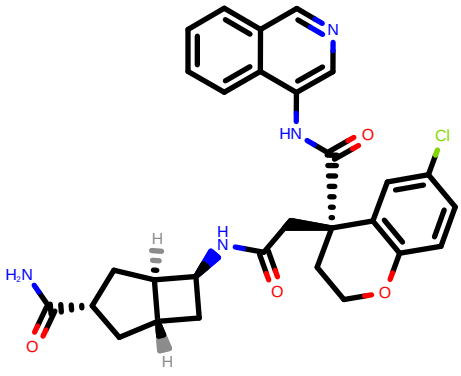
CID:	MAT-POS-2905de8c-1_1
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@]3(CCOc4c3cc(cc4)Cl)[NH3+]
RUN:	RUN2225
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.36

EDG-MED-90036822-22_1



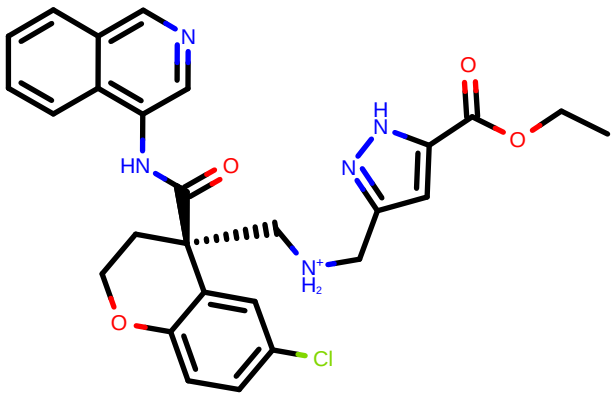
CID:	EDG-MED-90036822-22_1
SMILES:	C[C@@](CCC(=O)N[C@]1(CCOc2c1cc(cc2)Cl)C(=O)Nc3cncc4c3cccc4)(C[NH3+])OCCO
RUN:	RUN1691
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.46

DAR-DIA-5ff57136-7_1



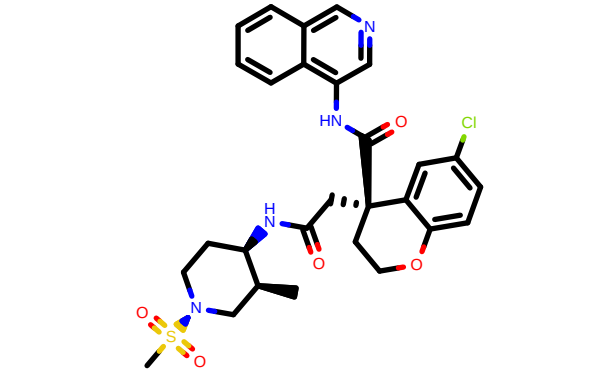
CID:	DAR-DIA-5ff57136-7_1
SMILES:	C=CC(=O)N(c1cncc2c1cccc2)C(=O)C3=CCOc4c3cc(cc4)Cl
RUN:	RUN1376
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.24

MAT-POS-dc2604c4-3_3



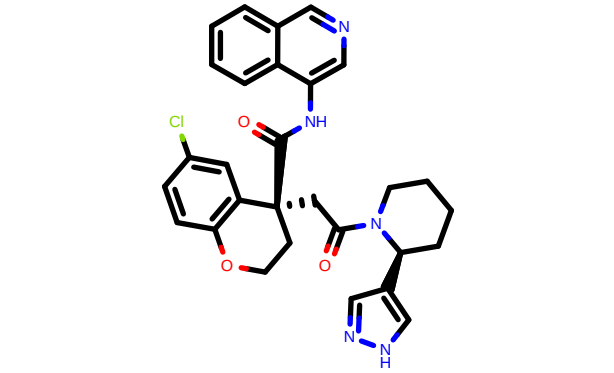
CID:	MAT-POS-dc2604c4-3_3
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3C[N@](Cc4c3cc(cc4)Cl)S(=O)(=O)CC5(CNC5)C#N
RUN:	RUN4714
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.25

MAT-POS-993cdc78-1_1



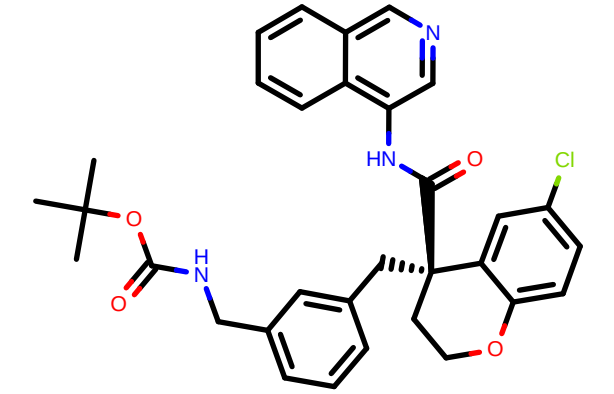
CID:	MAT-POS-993cdc78-1_1
SMILES:	CO[C@@]1(CCOc2c1cc(c(c2)F)Cl)C(=O)Nc3cncc4c3cccc4
RUN:	RUN3659
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.18

KAD-UNI-b13decd3-11_1



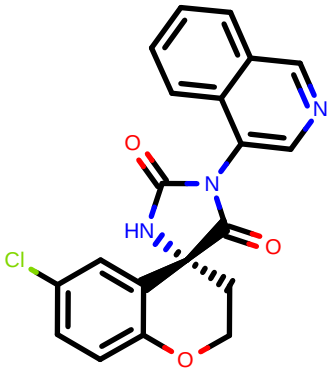
CID:	KAD-UNI-b13decd3-11_1
SMILES:	CS(=O)(=O)CCn1cc(cn1)C[NH2+]C[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5
RUN:	RUN3799
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.24

DAR-DIA-ecdbc7dd-4_2



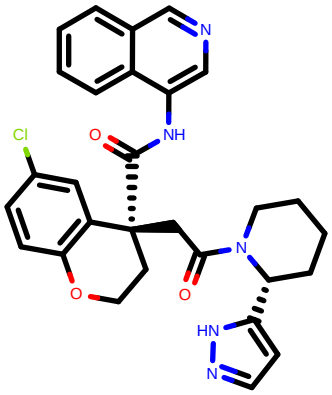
CID:	DAR-DIA-ecdbc7dd-4_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@]3(CCOc4c3cc(cc4)Cl)C[NH+]5CCC5
RUN:	RUN2882
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.16

MIC-UNK-9582b2c5-2_2



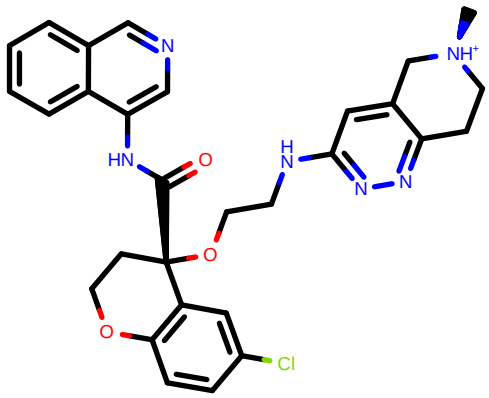
CID:	MIC-UNK-9582b2c5-2_2
SMILES:	CC(=O)N1CC[C@H]2[C@@H](C1)C[C@@H](C(=O)N2c3cccc(c3)Cl)c4cncc5c4cccc5
RUN:	RUN263
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.17

JOH-SUS-a69c159d-2_2



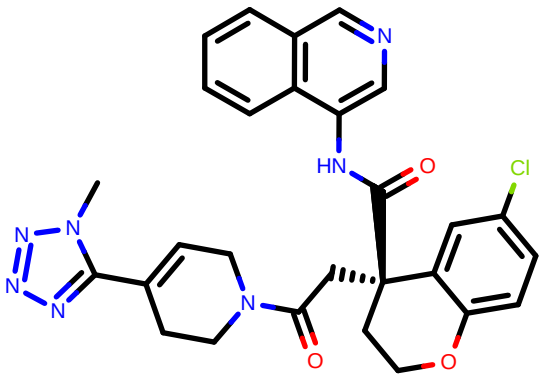
CID:	JOH-SUS-a69c159d-2_2
SMILES:	c1ccc2c(c1)c(cnc2F)NC(=O)[C@H]3CCOc4c3cc(cc4)Cl
RUN:	RUN1119
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.28

DAR-DIA-23e5a6a0-6_2



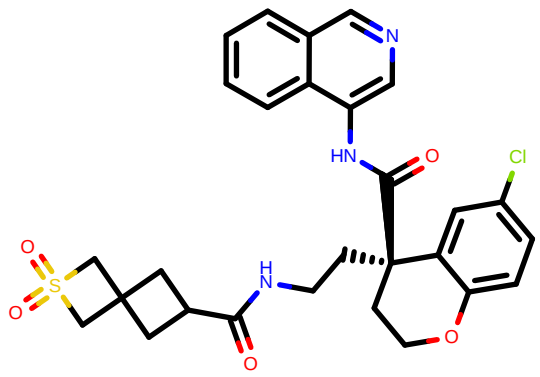
CID:	DAR-DIA-23e5a6a0-6_2
SMILES:	c1ccc2c(c1)cncc2NC(=O)[C@@H]3CCOc4c3cc(cc4C[C@H]5CCC6([NH2+]5)CCC6)Cl
RUN:	RUN412
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.41

MAK-UNK-c749d764-12_5



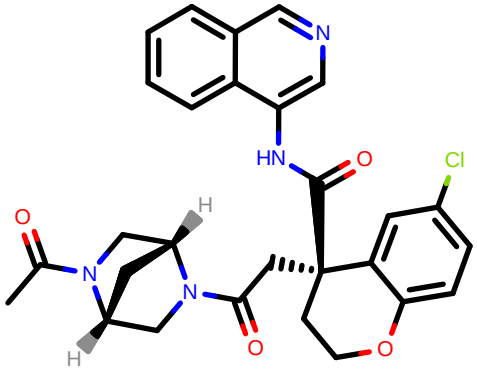
CID:	MAK-UNK-c749d764-12_5
SMILES:	c1ccc2c(c1)cncc2NC(=O)C[C@@H]3CCC[C@@H]([C@H]3O)Cl
RUN:	RUN954
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.29

MAK-UNK-3875bbc8-3_2



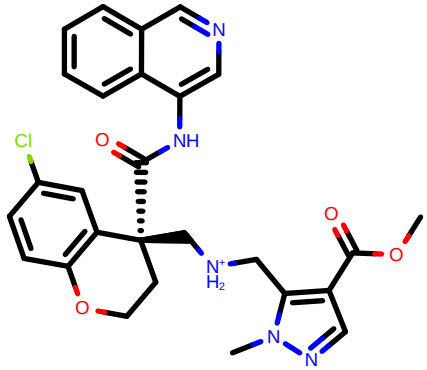
CID:	MAK-UNK-3875bbc8-3_2
SMILES:	CN(c1cncc2c1cccc2)C(=O)[C@H]3CCOc4c3cccc4
RUN:	RUN803
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.24

DAR-DIA-0d514e7d-3_1



CID:	DAR-DIA-0d514e7d-3_1
SMILES:	CC1(COc2ccc(cc2[C@@H]1C(=O)Nc3cncc4c3cccc4)Cl)C
RUN:	RUN805
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.27

EDG-MED-90036822-74_5



CID:	EDG-MED-90036822-74_5
SMILES:	C[N@@H+]1C[C@@H](C[C@H]1C(=O)N[C@]2(CCOc3c2cc(cc3)Cl)C(=O)Nc4cncc5c4cccc5)F
RUN:	RUN1766
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.54