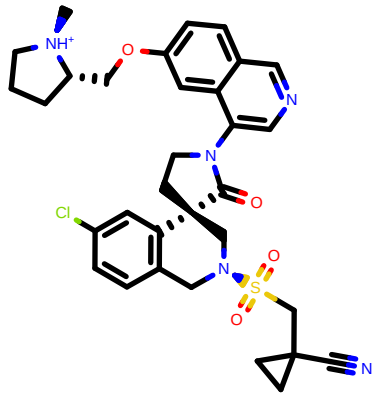
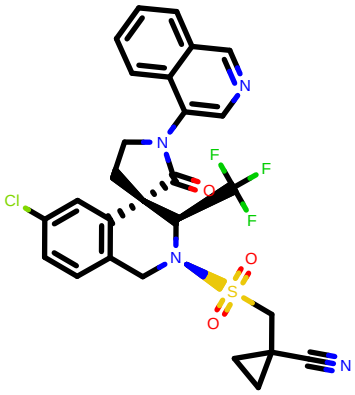
MAT-POS-40ad851a-1_2



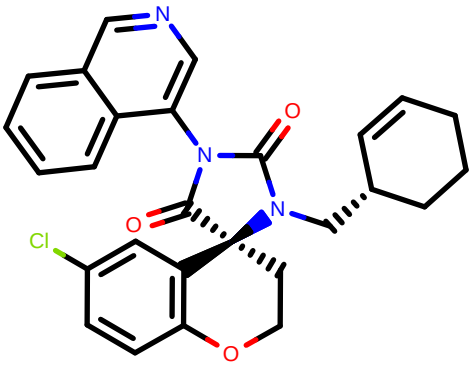
CID:	MAT-POS-40ad851a-1_2
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN660
DDG (kcal/mol):	-3.86
dDDG (kcal/mol):	0.91

VLA-UNK-61877630-9_1



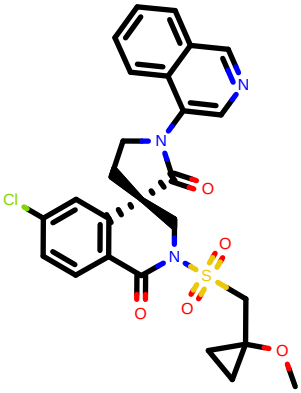
CID:	VLA-UNK-61877630-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)c5cc(ccc5C[N@@]([C@@H]4C(F)(F)F)S(=O)(=O)CC6(CC6)C#N)Cl
RUN:	RUN628
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.31

VLA-UNK-f702bf1c-6_1



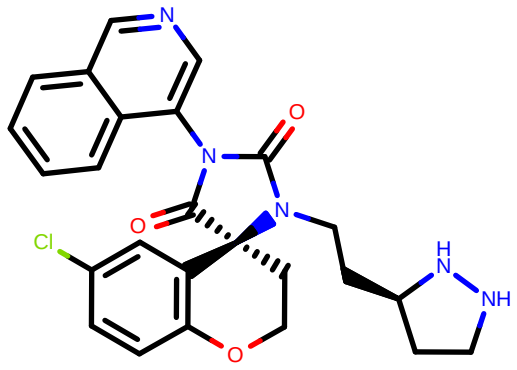
CID:	VLA-UNK-f702bf1c-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN477
DDG (kcal/mol):	-2.95
dDDG (kcal/mol):	0.19

EDJ-MED-9f4ac58c-6_1



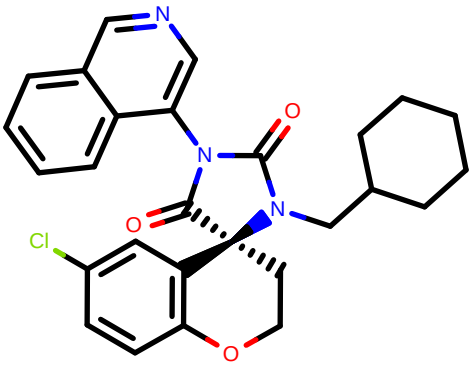
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN545
DDG (kcal/mol):	-2.61
dDDG (kcal/mol):	0.31

VLA-UNK-f702bf1c-1_1



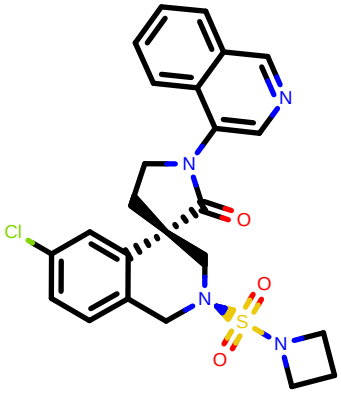
CID:	VLA-UNK-f702bf1c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6ccn[nH]6
RUN:	RUN469
DDG (kcal/mol):	-2.52
dDDG (kcal/mol):	0.16

VLA-UCB-34f3ed0c-14_1



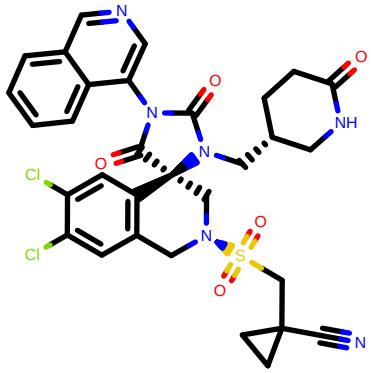
CID:	VLA-UCB-34f3ed0c-14_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN460
DDG (kcal/mol):	-2.47
dDDG (kcal/mol):	0.19

ALP-POS-ecbed2ba-20_1



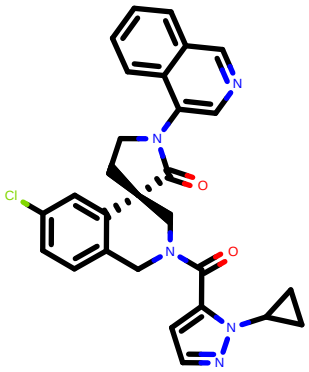
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN448
DDG (kcal/mol):	-2.33
dDDG (kcal/mol):	0.54

JOH-MSK-cef8a2bc-1_1



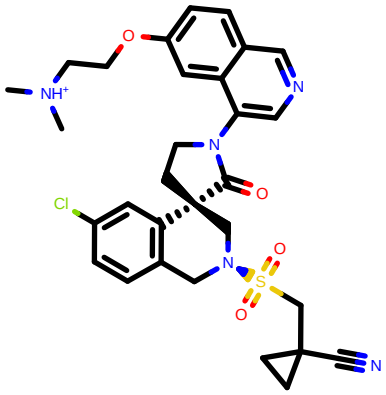
CID:	JOH-MSK-cef8a2bc-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(c(c5)Cl)Cl)S(=O)(=O)CC6(CC6)C#N)N(C3=O)C[C@@H]7CCC(=O)NC7
RUN:	RUN664
DDG (kcal/mol):	-2.21
dDDG (kcal/mol):	0.43

MAT-POS-be048f2c-7_1



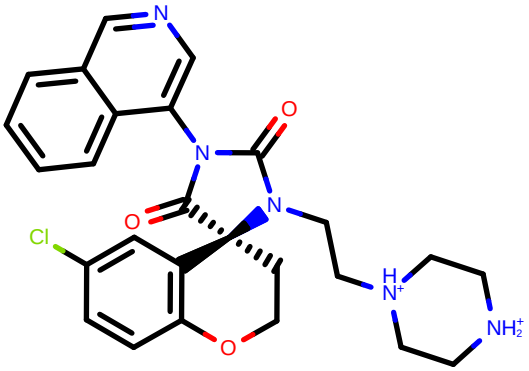
CID:	MAT-POS-be048f2c-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(Cc5c4cc(cc5)Cl)C(=O)c6ccnn6C7CC7
RUN:	RUN578
DDG (kcal/mol):	-2.12
dDDG (kcal/mol):	0.13

LUO-POS-8484f2d3-2_1



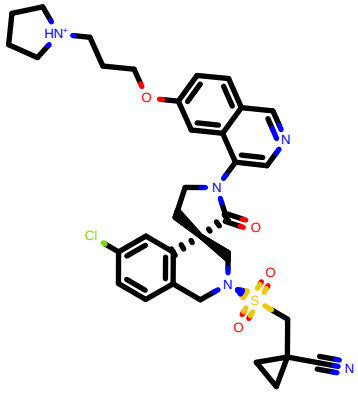
CID:	LUO-POS-8484f2d3-2_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN651
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.51

VLA-UNK-f702bf1c-7_1



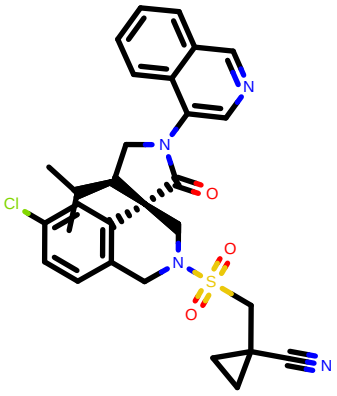
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCN6CC[NH2+]CC6
RUN:	RUN509
DDG (kcal/mol):	-1.75
dDDG (kcal/mol):	0.20

MAT-POS-40ad851a-5_1



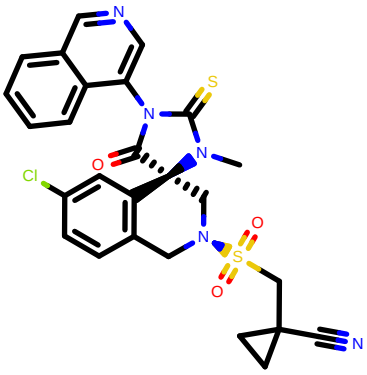
CID:	MAT-POS-40ad851a-5_1
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN673
DDG (kcal/mol):	-1.72
dDDG (kcal/mol):	0.46

MAT-POS-50a80394-3_2



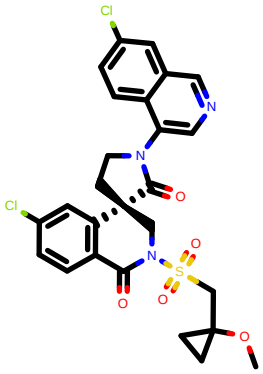
CID:	MAT-POS-50a80394-3_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN619
DDG (kcal/mol):	-1.69
dDDG (kcal/mol):	0.36

MAT-POS-c2d406ed-4_1



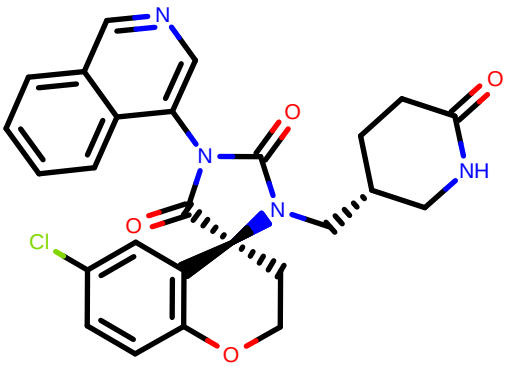
CID:	MAT-POS-c2d406ed-4_1
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN593
DDG (kcal/mol):	-1.67
dDDG (kcal/mol):	0.24

EDJ-MED-9f4ac58c-5_1



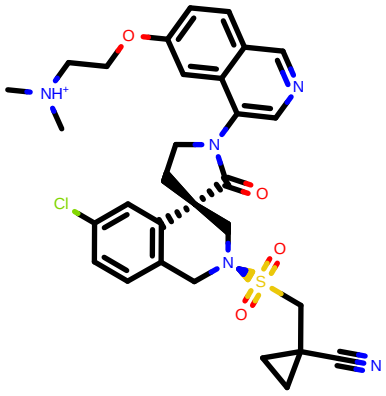
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl
RUN:	RUN594
DDG (kcal/mol):	-1.66
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-5_1



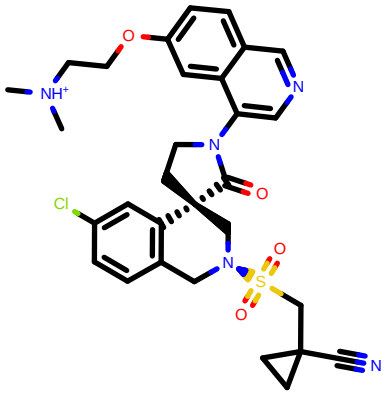
CID:	VLA-UNK-f702bf1c-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6
RUN:	RUN504
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.19

MAT-POS-853c0ffa-9_1



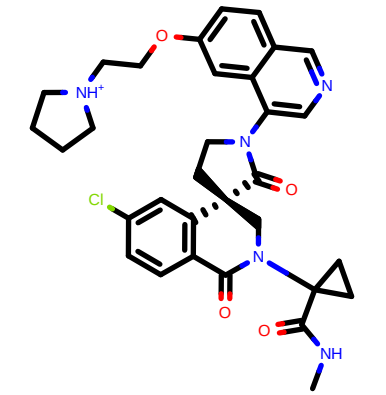
CID:	MAT-POS-853c0ffa-9_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN646
DDG (kcal/mol):	-1.59
dDDG (kcal/mol):	0.58

LUO-POS-8484f2d3-1_1



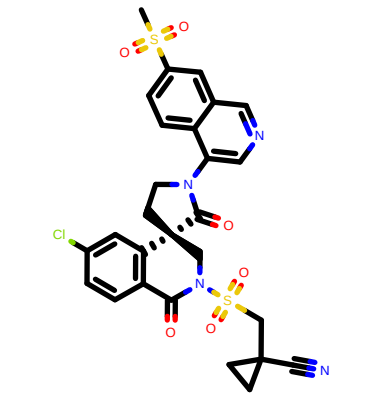
CID:	LUO-POS-8484f2d3-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN655
DDG (kcal/mol):	-1.50
dDDG (kcal/mol):	0.53

EDJ-MED-dfa1d800-1_1



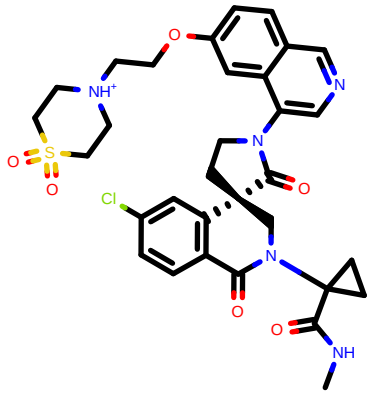
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN648
DDG (kcal/mol):	-1.45
dDDG (kcal/mol):	0.29

EDJ-MED-9f4ac58c-4_1



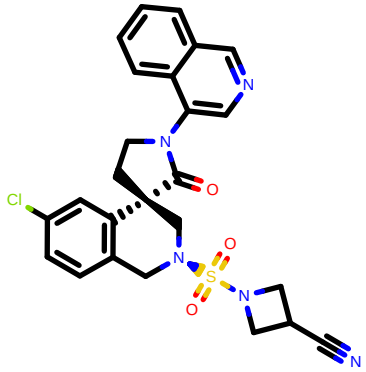
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN623
DDG (kcal/mol):	-1.44
dDDG (kcal/mol):	0.48

EDJ-MED-dfa1d800-3_1



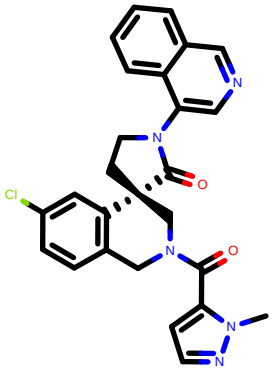
CID:	EDJ-MED-dfa1d800-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CCS(=O)(=O)CC6)c7cc(ccc7C2=O)Cl
RUN:	RUN661
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.29

ALP-POS-ecbed2ba-9_1



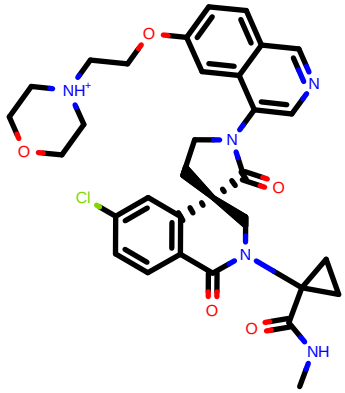
CID:	ALP-POS-ecbed2ba-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN518
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.34

EDJ-MED-cc48ee33-3_1



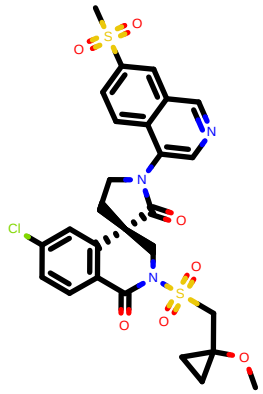
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN496
DDG (kcal/mol):	-1.31
dDDG (kcal/mol):	0.10

EDJ-MED-dfa1d800-2_1



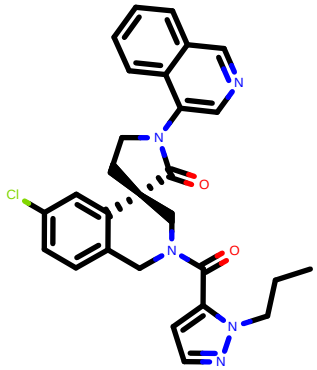
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCOCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN672
DDG (kcal/mol):	-1.27
dDDG (kcal/mol):	0.45

EDJ-MED-9f4ac58c-8_1



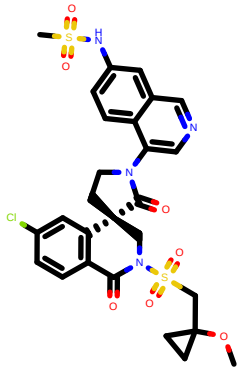
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN637
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.47

MAT-POS-be048f2c-8_1



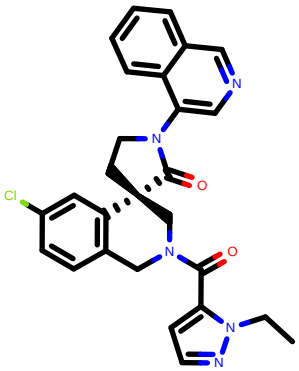
CID:	MAT-POS-be048f2c-8_1
SMILES:	CCCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN570
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.15

EDJ-MED-9f4ac58c-7_1



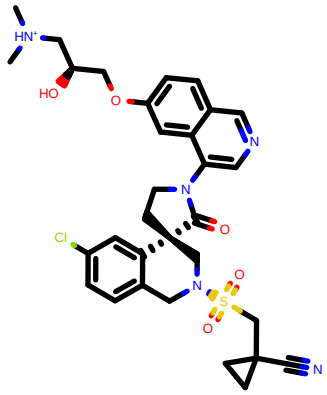
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN645
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.31

MAT-POS-be048f2c-5_1



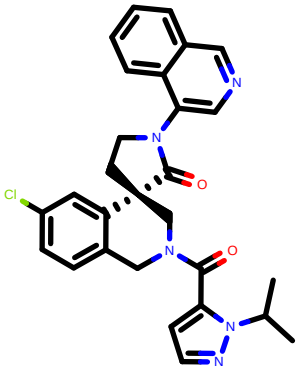
CID:	MAT-POS-be048f2c-5_1
SMILES:	CCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN547
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.13

EDJ-MED-ee81482e-3_1



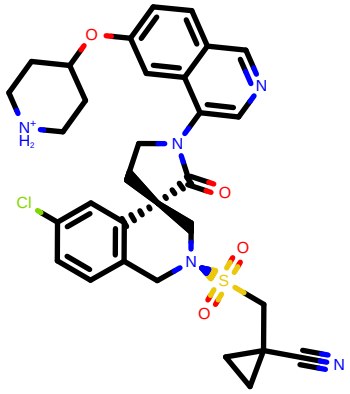
CID:	EDJ-MED-ee81482e-3_1
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN662
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.62

MAT-POS-be048f2c-6_1



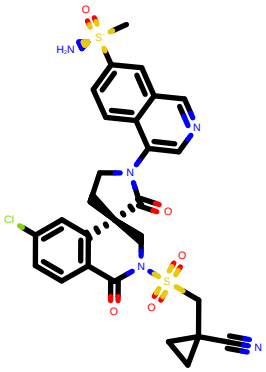
CID:	MAT-POS-be048f2c-6_1
SMILES:	CC(C)n1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN595
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.23

EDJ-MED-ee81482e-4_1



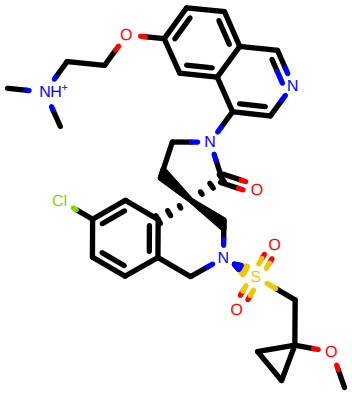
CID:	EDJ-MED-ee81482e-4_1
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN668
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.47

EDJ-MED-7d88f880-3_1



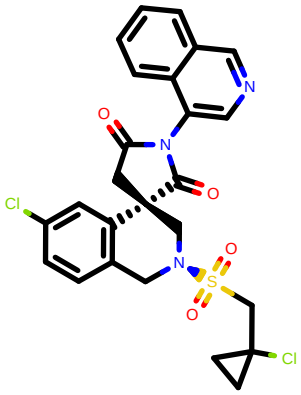
CID:	EDJ-MED-7d88f880-3_1
SMILES:	C[S@@](=N)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN639
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.48

MAT-POS-853c0ffa-10_1



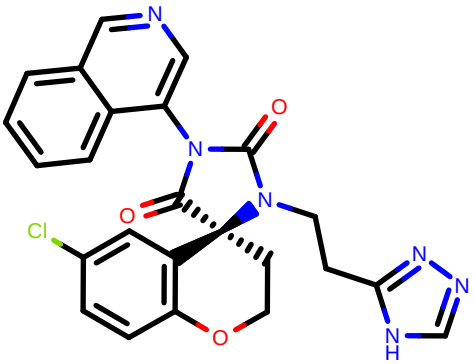
CID:	MAT-POS-853c0ffa-10_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN652
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.54

PET-UNK-94036022-5_1



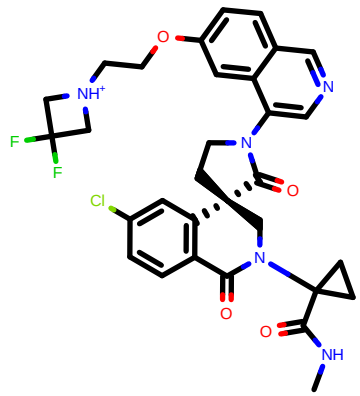
CID:	PET-UNK-94036022-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN557
DDG (kcal/mol):	-1.05
dDDG (kcal/mol):	0.25

VLA-UNK-f702bf1c-8_1



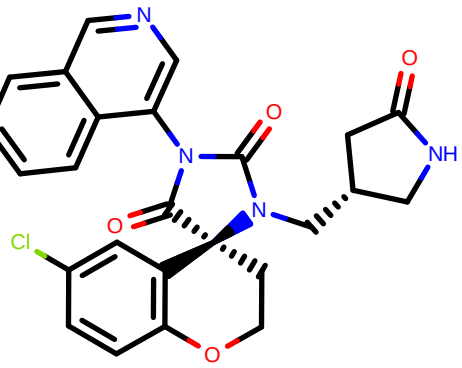
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncn6
RUN:	RUN490
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.18

EDJ-MED-dfa1d800-5_1



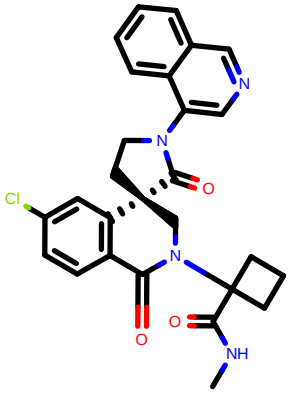
CID:	EDJ-MED-dfa1d800-5_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CC(C6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN653
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.27

VLA-UNK-f702bf1c-4_1



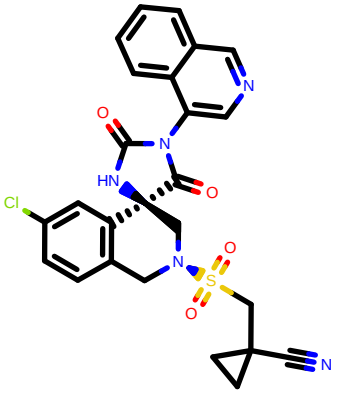
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CC(=O)NC6
RUN:	RUN471
DDG (kcal/mol):	-0.97
dDDG (kcal/mol):	0.20

EDJ-MED-98c0a822-3_1



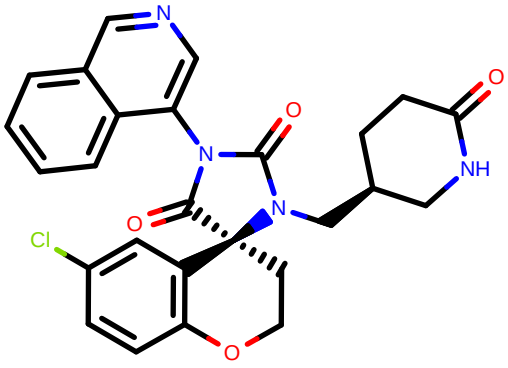
CID:	EDJ-MED-98c0a822-3_1
SMILES:	CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN526
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.20

MAT-POS-c2d406ed-1_1



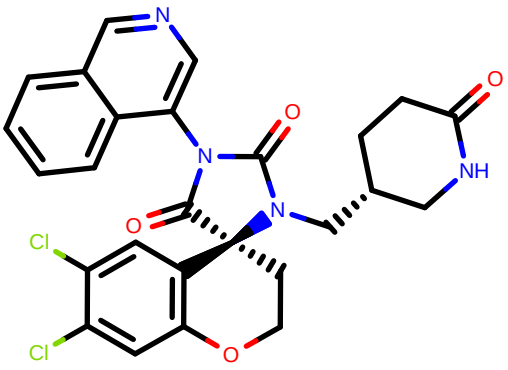
CID:	MAT-POS-c2d406ed-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN552
DDG (kcal/mol):	-0.95
dDDG (kcal/mol):	0.21

VLA-UNK-f702bf1c-5_2



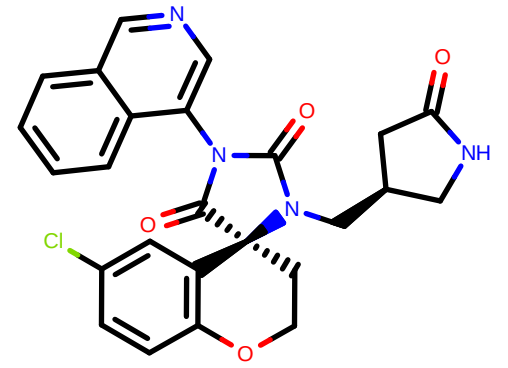
CID:	VLA-UNK-f702bf1c-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CCC(=O)NC6
RUN:	RUN508
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.17

JOH-MSK-b735e33c-1_1



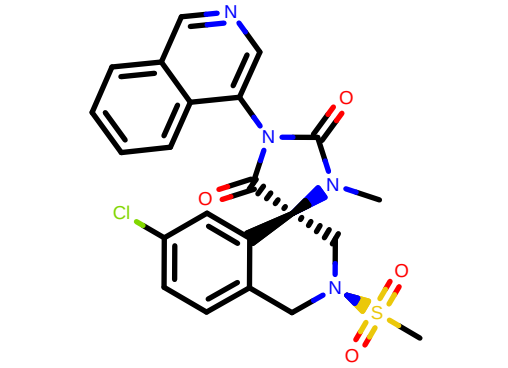
CID:	JOH-MSK-b735e33c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6
RUN:	RUN581
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.23

VLA-UNK-f702bf1c-4_2



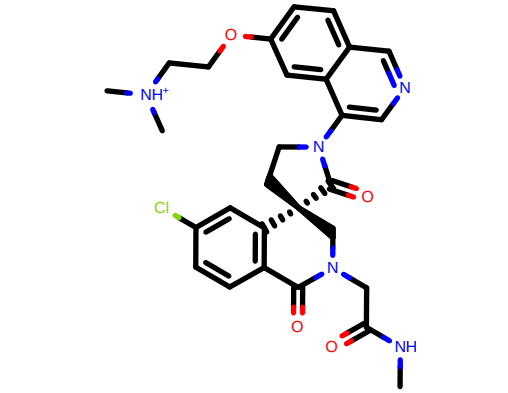
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NC6
RUN:	RUN483
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.23

MAT-POS-2e8b2191-8_1



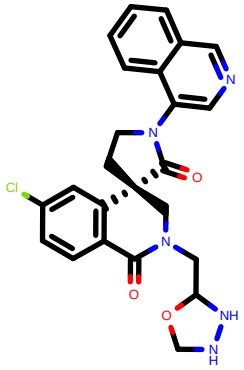
CID:	MAT-POS-2e8b2191-8_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN400
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.11

EDJ-MED-b6c6ee2b-5_1



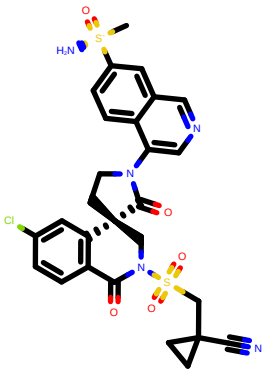
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN644
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.25

PET-UNK-aa57768f-1_1



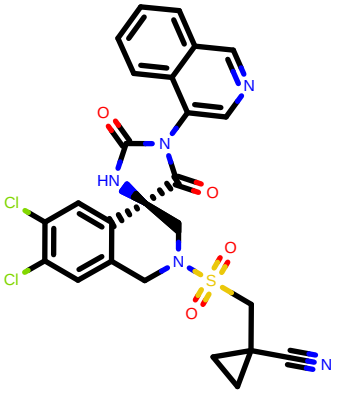
CID:	PET-UNK-aa57768f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN441
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.10

EDJ-MED-7d88f880-3_2



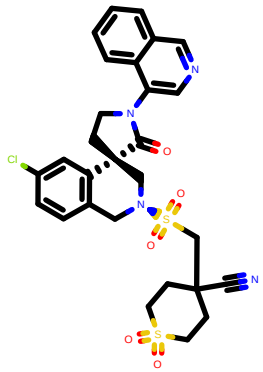
CID:	EDJ-MED-7d88f880-3_2
SMILES:	C[S@](=N)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN643
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.43

JOH-MSK-ccc6e4c0-1_1



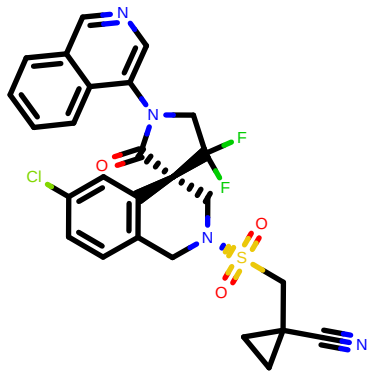
CID:	JOH-MSK-ccc6e4c0-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(c(c5)Cl)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN616
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-2_1



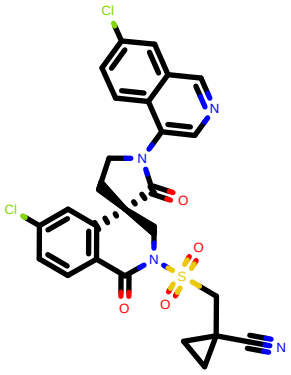
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN642
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.27

EDJ-MED-7e491f08-1_1



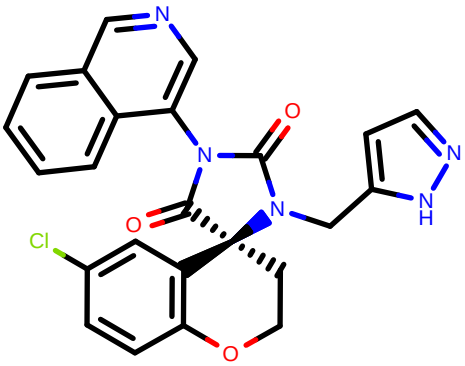
CID:	EDJ-MED-7e491f08-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN607
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.48

EDJ-MED-9f4ac58c-1_1



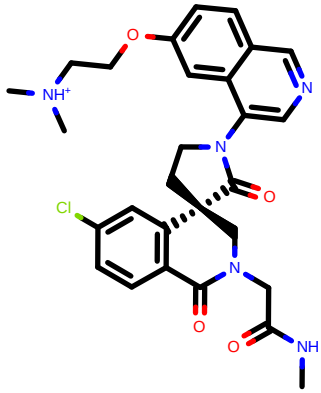
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	c1cc2c(cc1Cl)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN589
DDG (kcal/mol):	-0.74
dDDG (kcal/mol):	0.34

VLA-UNK-f702bf1c-2_1



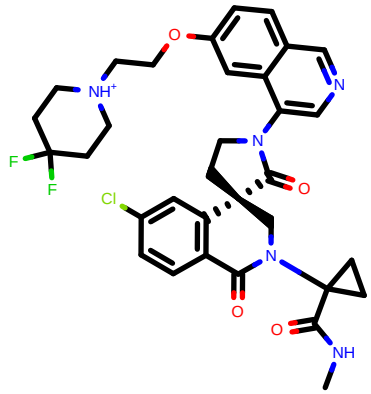
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6ccn[nH]6
RUN:	RUN422
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.13

MAT-POS-38eb6498-4_1



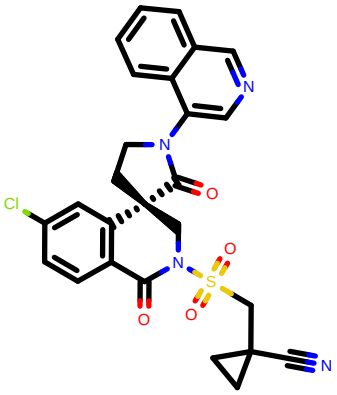
CID:	MAT-POS-38eb6498-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN638
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.24

EDJ-MED-dfa1d800-4_1



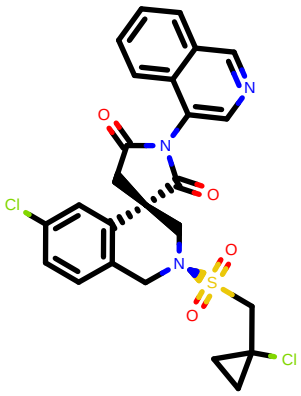
CID:	EDJ-MED-dfa1d800-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCC(CC6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN665
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.34

EDJ-MED-9f4ac58c-2_1



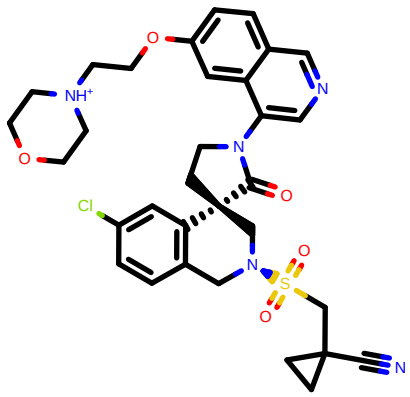
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN548
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.36

PET-UNK-94036022-12_1



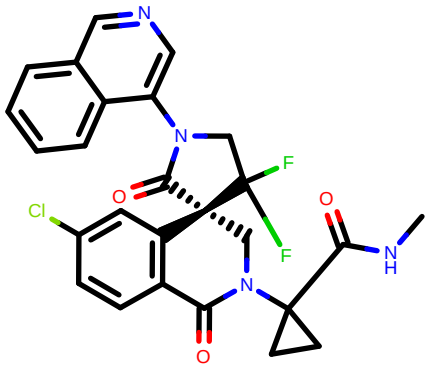
CID:	PET-UNK-94036022-12_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN542
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.35

EDJ-MED-468565e0-2_1



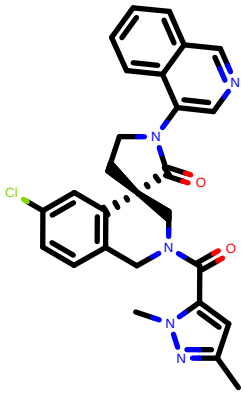
CID:	EDJ-MED-468565e0-2_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN659
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.48

EDJ-MED-7e491f08-2_1



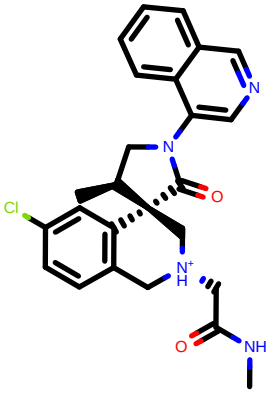
CID:	EDJ-MED-7e491f08-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(CC3(F)F)c5cncc6c5cccc6
RUN:	RUN567
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.12

EDJ-MED-cc48ee33-5_1



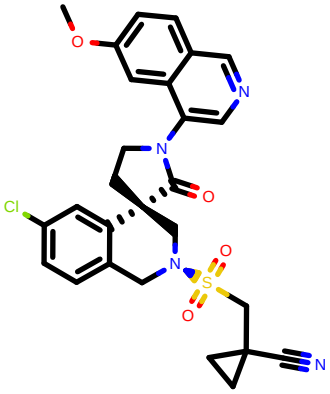
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	Cc1cc(n(n1)C)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN544
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-4_2



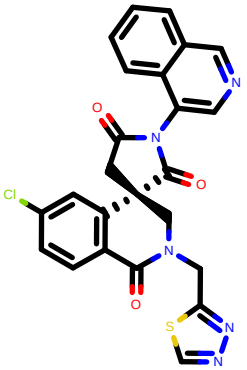
CID:	MAT-POS-50a80394-4_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN444
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.23

EDJ-MED-b6c6ee2b-3_1



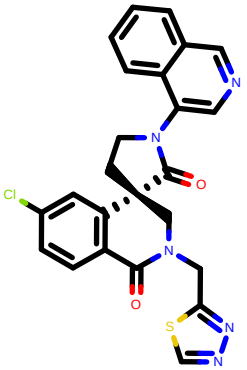
CID:	EDJ-MED-b6c6ee2b-3_1
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN613
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.33

PET-UNK-6af7266d-2_1



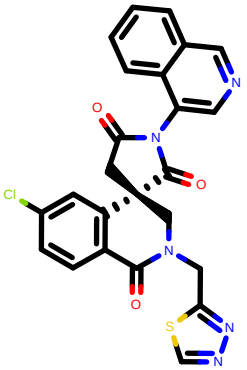
CID:	PET-UNK-6af7266d-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN500
DDG (kcal/mol):	-0.58
dDDG (kcal/mol):	0.09

PET-UNK-6af7266d-1_1



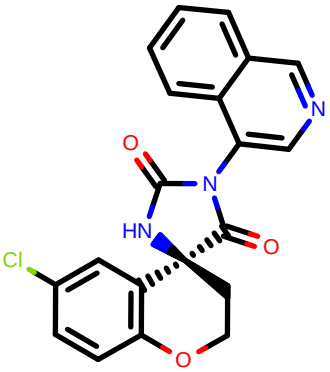
CID:	PET-UNK-6af7266d-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN465
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.12

PET-UNK-6af7266d-4_1



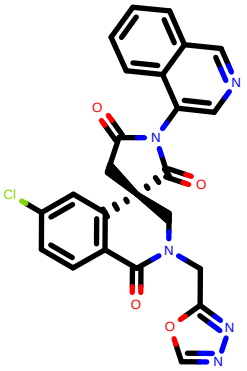
CID:	PET-UNK-6af7266d-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN505
DDG (kcal/mol):	-0.53
dDDG (kcal/mol):	0.08

VLA-UCB-29506327-1_1



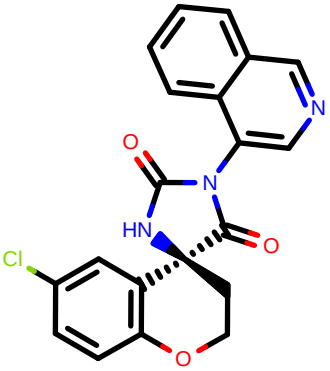
CID:	VLA-UCB-29506327-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN357
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.05

PET-UNK-77d5678a-2_1



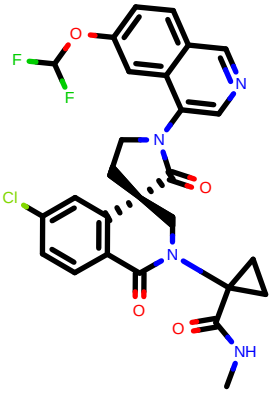
CID:	PET-UNK-77d5678a-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN497
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.08

VLA-UNK-cf7facf1-1_1



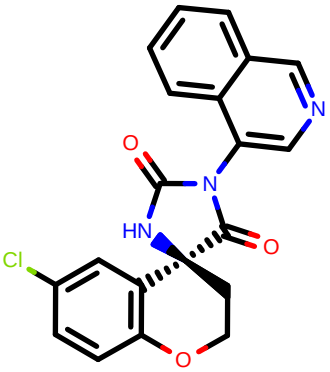
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN359
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.04

EDJ-MED-5cd3920d-3_1



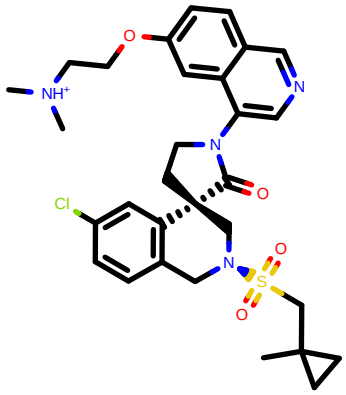
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN627
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.13

VLA-UCB-34f3ed0c-11_1



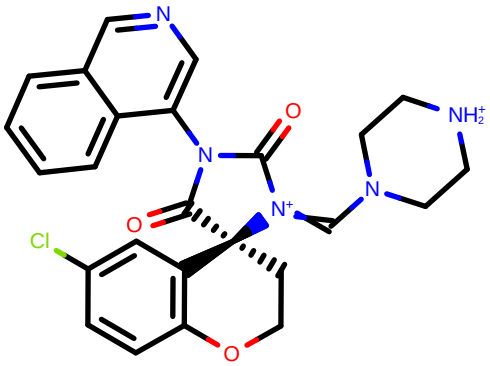
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN349
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.05

MAT-POS-853c0ffa-19_1



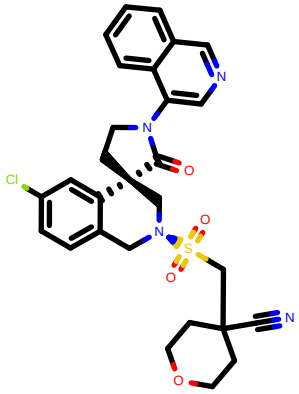
CID:	MAT-POS-853c0ffa-19_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN647
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.32

VLA-UCB-34f3ed0c-15_1



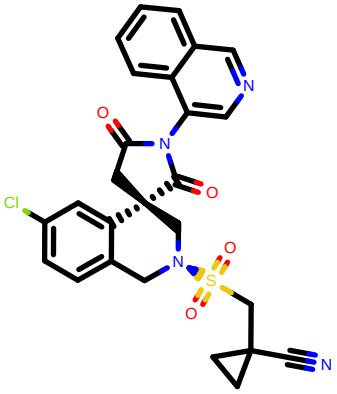
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+]CC6
RUN:	RUN467
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.32

ALP-POS-ecbed2ba-11_1



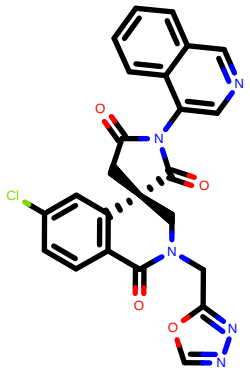
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN629
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.41

LUO-POS-868e8996-10_1



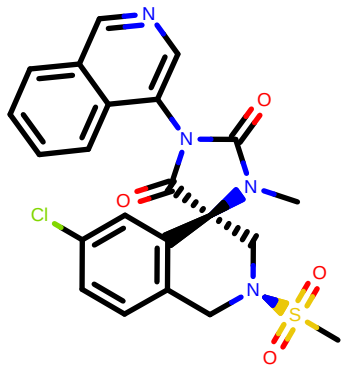
CID:	LUO-POS-868e8996-10_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN546
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.43

PET-UNK-77d5678a-5_1



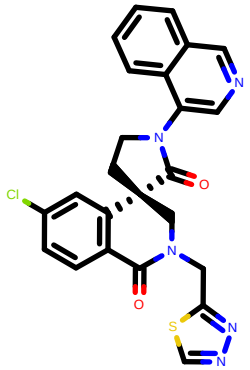
CID:	PET-UNK-77d5678a-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN494
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.09

EDJ-MED-7587a9ee-1_1



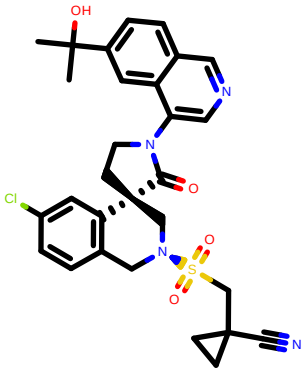
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN396
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.11

PET-UNK-6af7266d-3_1



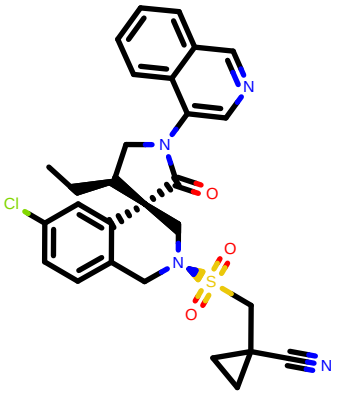
CID:	PET-UNK-6af7266d-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN466
DDG (kcal/mol):	-0.45
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-11_1



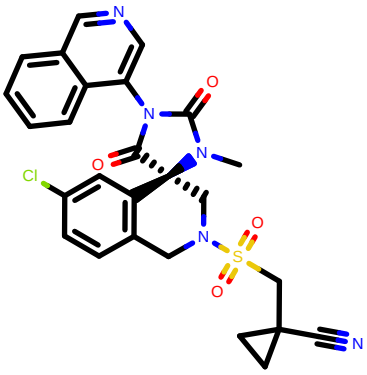
CID:	MAT-POS-853c0ffa-11_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN633
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.40

MAT-POS-50a80394-2_2



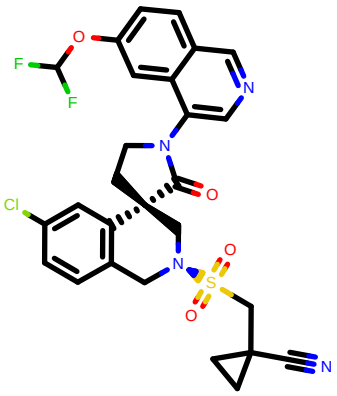
CID:	MAT-POS-50a80394-2_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN610
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.34

MAT-POS-c2d406ed-2_1



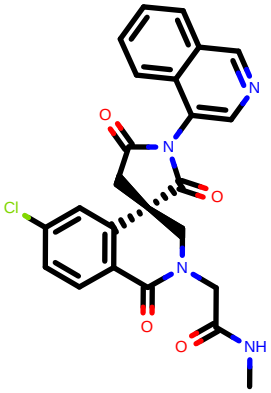
CID:	MAT-POS-c2d406ed-2_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN582
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.20

EDJ-MED-5cd3920d-1_1



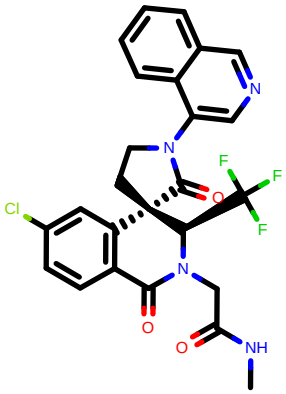
CID:	EDJ-MED-5cd3920d-1_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN649
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.27

MAT-POS-1bed62cf-2_1



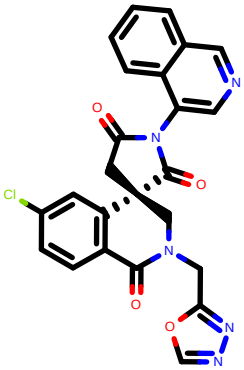
CID:	MAT-POS-1bed62cf-2_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN424
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.10

VLA-UNK-61877630-3_1



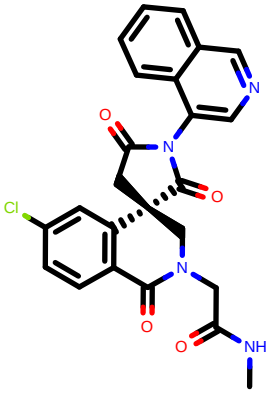
CID:	VLA-UNK-61877630-3_1
SMILES:	CNC(=O)CN1[C@@H]([C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)(F)F
RUN:	RUN587
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.13

12_-111-3e02a1cd-1_1



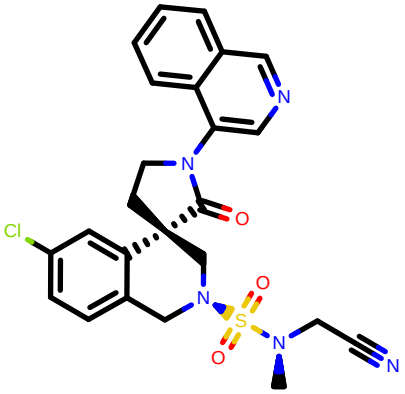
CID:	12_-111-3e02a1cd-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN502
DDG (kcal/mol):	-0.38
dDDG (kcal/mol):	0.09

LUO-POS-868e8996-8_1



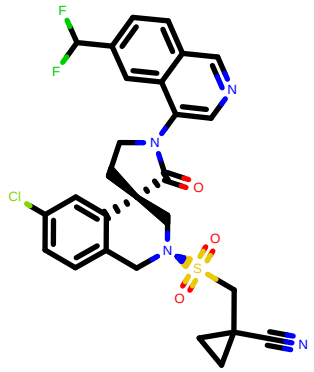
CID:	LUO-POS-868e8996-8_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN435
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-17_1



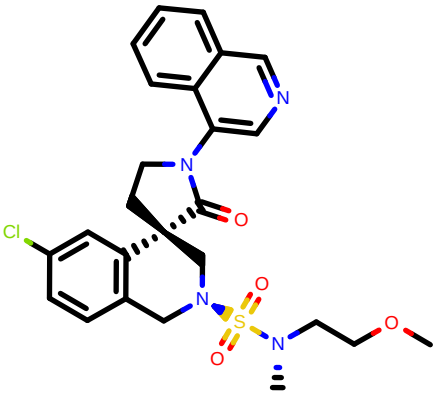
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	C[N@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN478
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.48

EDJ-MED-5cd3920d-2_1



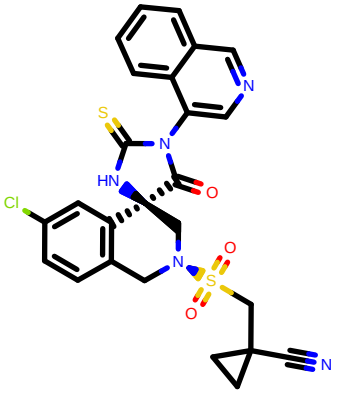
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN631
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-21_1



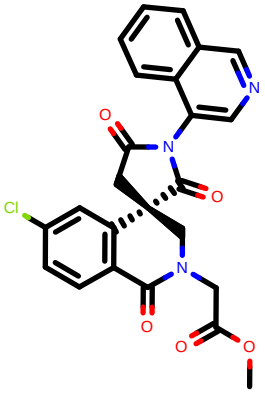
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	C[N@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN530
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.24

MAT-POS-c2d406ed-3_1



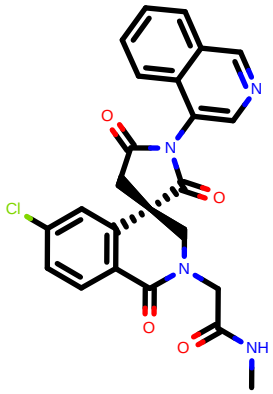
CID:	MAT-POS-c2d406ed-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN562
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.24

12_-111-3e02a1cd-2_1



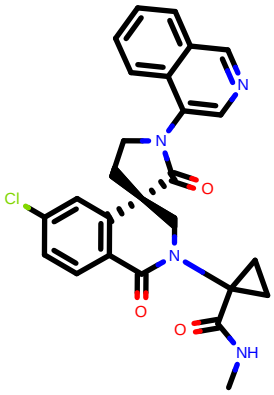
CID:	12_-111-3e02a1cd-2_1
SMILES:	COC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN454
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.08

LUO-POS-868e8996-7_1



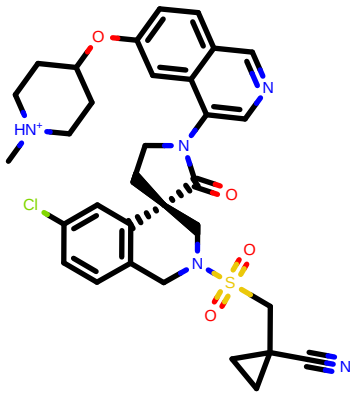
CID:	LUO-POS-868e8996-7_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN430
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.10

EDJ-MED-976a33d5-1_1



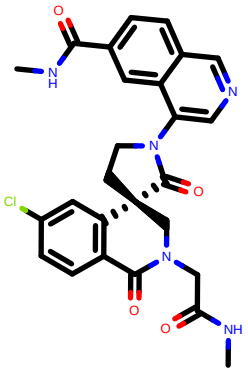
CID:	EDJ-MED-976a33d5-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN476
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.12

LUO-POS-d1147590-1_1



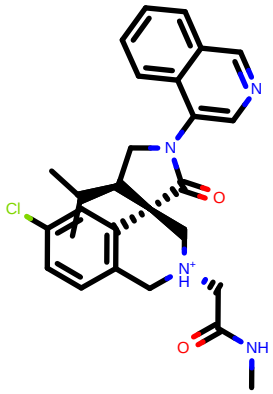
CID:	LUO-POS-d1147590-1_1
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN667
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.57

MAT-POS-38eb6498-6_1



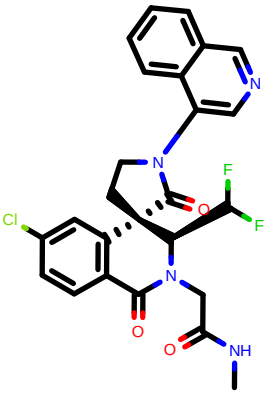
CID:	MAT-POS-38eb6498-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)C(=O)NC)c5cc(ccc5C1=O)Cl
RUN:	RUN553
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.14

MAT-POS-50a80394-6_2



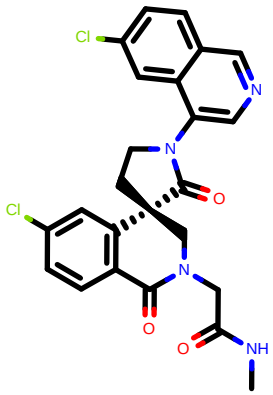
CID:	MAT-POS-50a80394-6_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN513
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.19

VLA-UNK-61877630-6_1



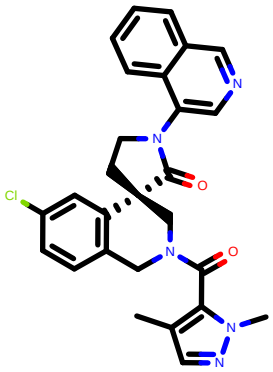
CID:	VLA-UNK-61877630-6_1
SMILES:	CNC(=O)CN1[C@@H]([C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)F
RUN:	RUN538
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.13

LUO-POS-8c3e556a-1_1



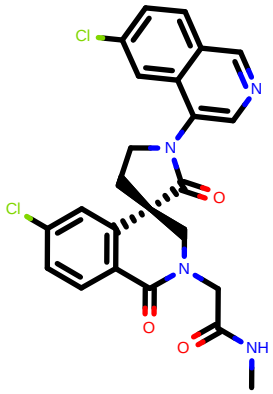
CID:	LUO-POS-8c3e556a-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN455
DDG (kcal/mol):	-0.28
dDDG (kcal/mol):	0.12

EDJ-MED-cc48ee33-4_1



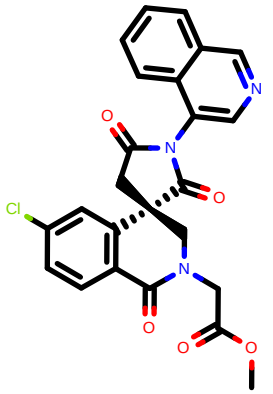
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	Cc1cnn(c1C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl)C
RUN:	RUN541
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.13

LUO-POS-8c3e556a-2_1



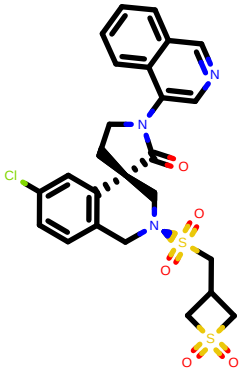
CID:	LUO-POS-8c3e556a-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN453
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.12

PET-UNK-77d5678a-6_1



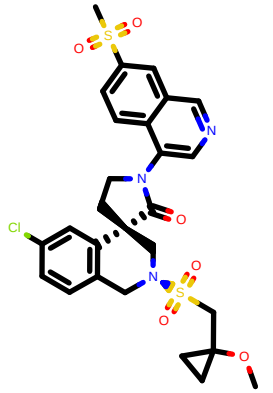
CID:	PET-UNK-77d5678a-6_1
SMILES:	COC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN457
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.09

ALP-POS-ecbed2ba-5_1



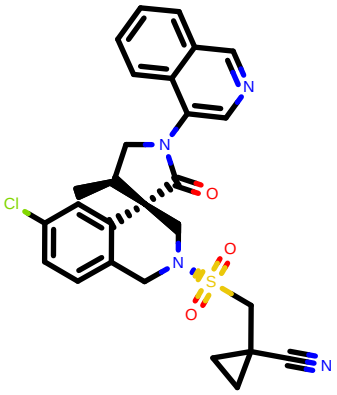
CID:	ALP-POS-ecbed2ba-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN565
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.66

MAT-POS-853c0ffa-16_1



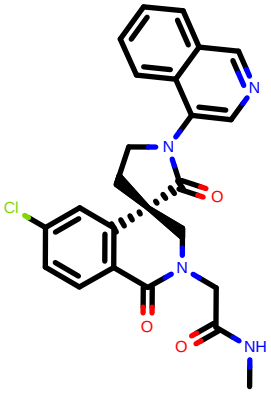
CID:	MAT-POS-853c0ffa-16_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN632
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-1_2



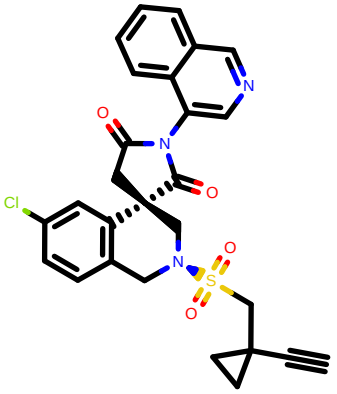
CID:	MAT-POS-50a80394-1_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN566
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.38

MIK-ENA-37e0b697-1_1



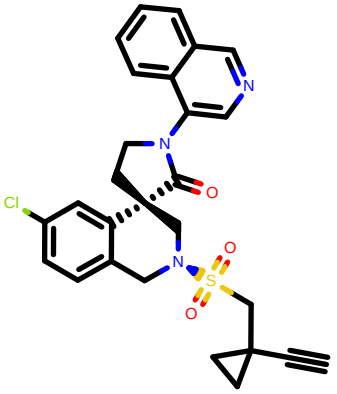
CID:	MIK-ENA-37e0b697-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN418
DDG (kcal/mol):	-0.22
dDDG (kcal/mol):	0.12

PET-UNK-94036022-4_1



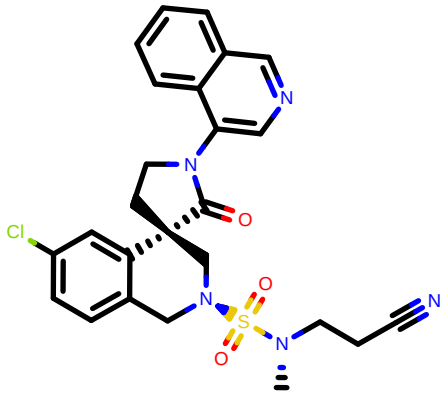
CID:	PET-UNK-94036022-4_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN576
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.27

PET-UNK-94036022-2_1



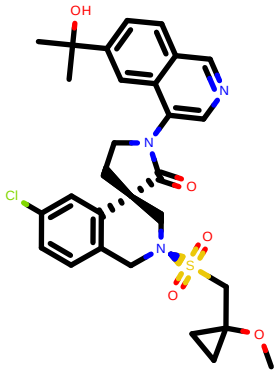
CID:	PET-UNK-94036022-2_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN550
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-16_1



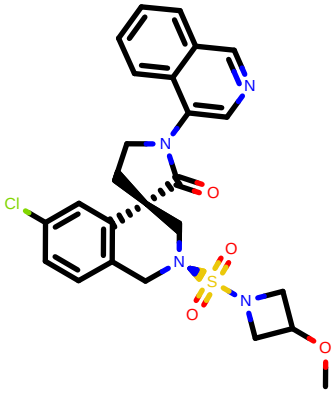
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN520
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.59

MAT-POS-853c0ffa-12_1



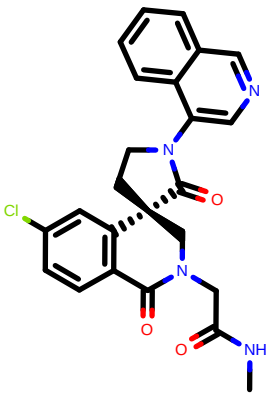
CID:	MAT-POS-853c0ffa-12_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN636
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.39

ALP-POS-ecbed2ba-10_1



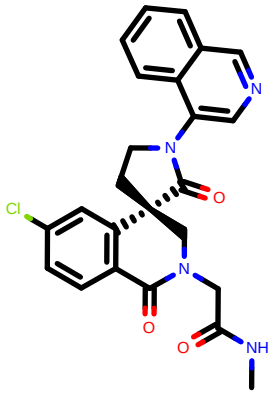
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	COC1CN(C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN522
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.33

LUO-POS-9931618f-1_1



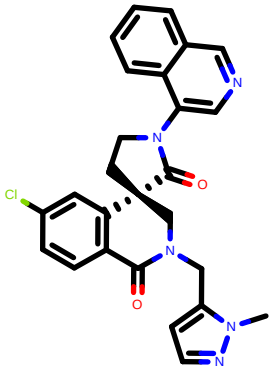
CID:	LUO-POS-9931618f-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN408
DDG (kcal/mol):	-0.17
dDDG (kcal/mol):	0.12

PET-UNK-14142a25-10_1



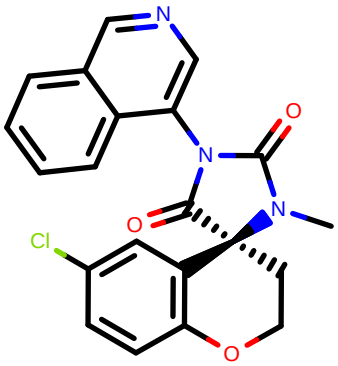
CID:	PET-UNK-14142a25-10_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN394
DDG (kcal/mol):	-0.16
dDDG (kcal/mol):	0.11

EDJ-MED-cc48ee33-7_1



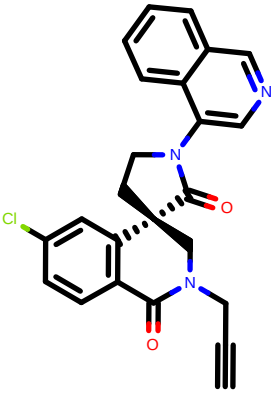
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN480
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.21

BEN-BAS-c2bc0d80-7_1



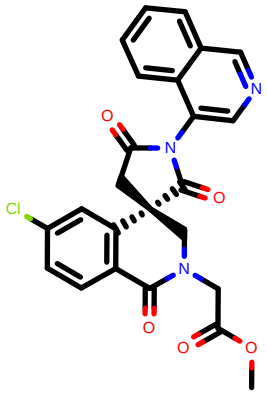
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN369
DDG (kcal/mol):	-0.11
dDDG (kcal/mol):	0.08

PET-UNK-aa57768f-3_1



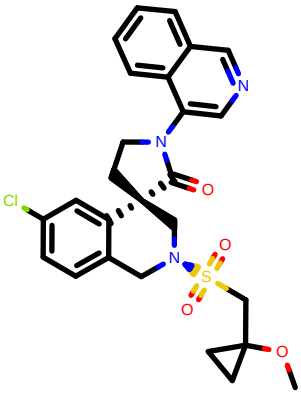
CID:	PET-UNK-aa57768f-3_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN377
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.09

PET-UNK-77d5678a-3_1



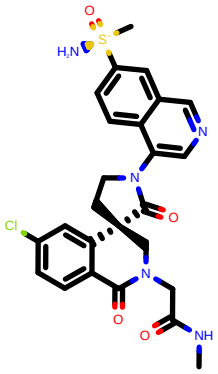
CID:	PET-UNK-77d5678a-3_1
SMILES:	COC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN464
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.08

ALP-POS-ecbed2ba-6_1



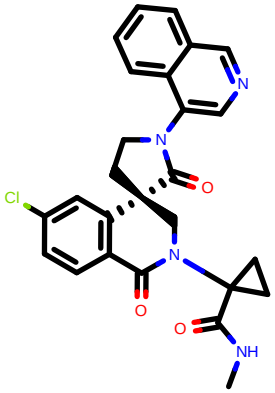
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN536
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.23

EDJ-MED-7d88f880-1_2



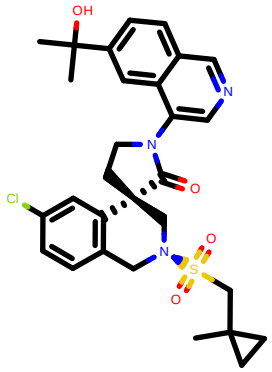
CID:	EDJ-MED-7d88f880-1_2
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)[S@](=N)(=O)C)c5cc(ccc5C1=O)Cl
RUN:	RUN564
DDG (kcal/mol):	-0.09
dDDG (kcal/mol):	0.14

MAT-POS-576f7758-2_1



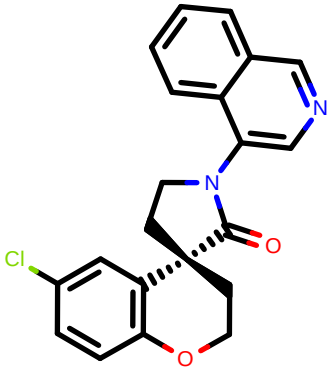
CID:	MAT-POS-576f7758-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN482
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-20_1



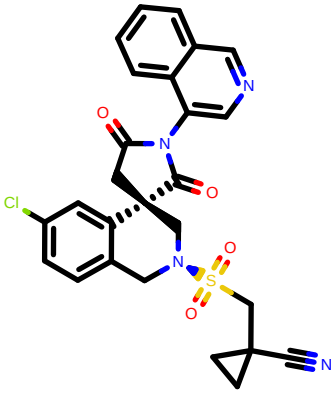
CID:	MAT-POS-853c0ffa-20_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN630
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.25

MAT-POS-983b399a-1_1



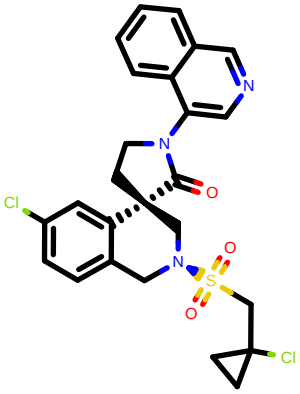
CID:	MAT-POS-983b399a-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN351
DDG (kcal/mol):	-0.07
dDDG (kcal/mol):	0.05

LUO-POS-868e8996-9_1



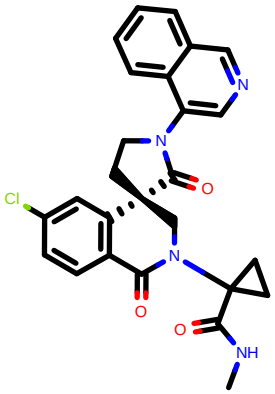
CID:	LUO-POS-868e8996-9_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN555
DDG (kcal/mol):	-0.06
dDDG (kcal/mol):	0.35

PET-UNK-94036022-10_1



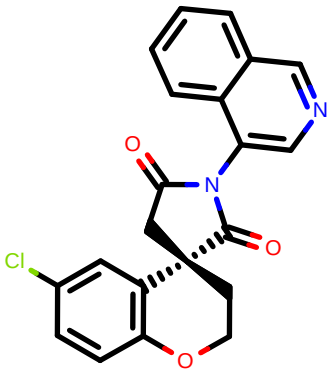
CID:	PET-UNK-94036022-10_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN506
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.22

MAT-POS-e48723dc-2_1



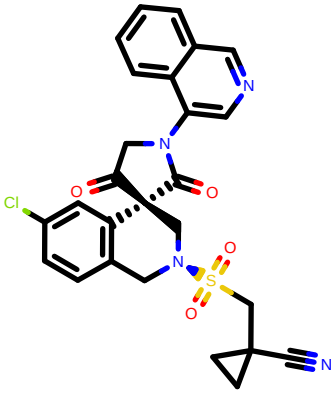
CID:	MAT-POS-e48723dc-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN495
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.12

VLA-UCB-50c39ae8-2_1



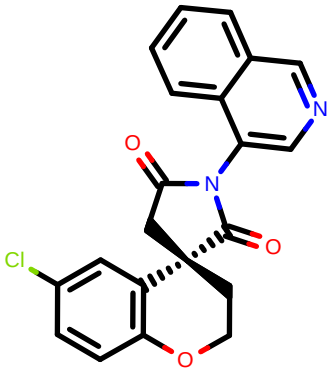
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN353
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.04

EDJ-MED-a12e3a20-1_1



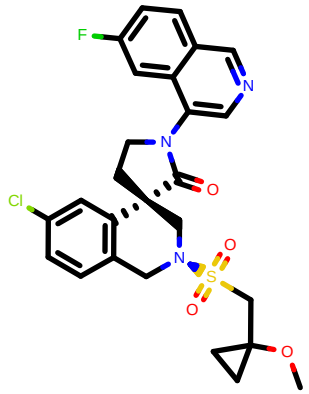
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN573
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.32

BEN-BAS-c2bc0d80-6_1



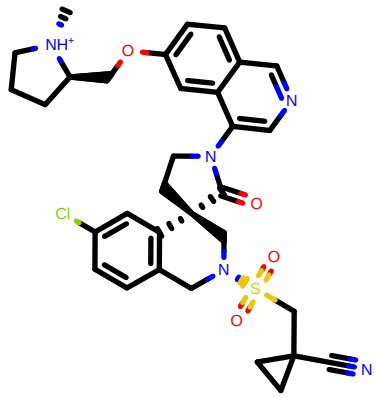
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN356
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.04

MAT-POS-853c0ffa-14_1



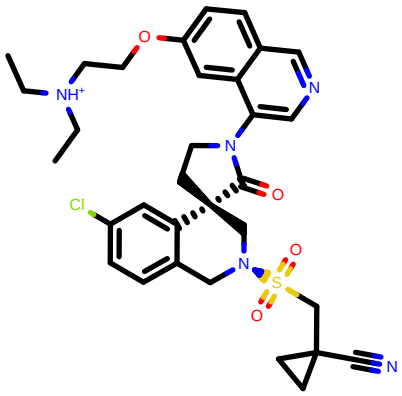
CID:	MAT-POS-853c0ffa-14_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN586
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.24

MAT-POS-40ad851a-1_1



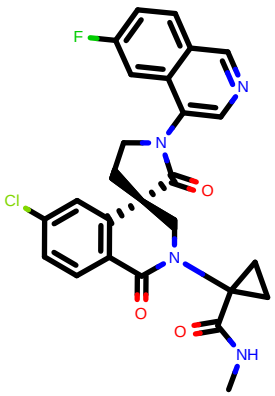
CID:	MAT-POS-40ad851a-1_1
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN663
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.69

MAT-POS-40ad851a-3_1



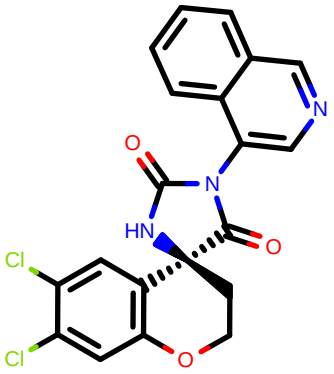
CID:	MAT-POS-40ad851a-3_1
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN671
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.81

EDJ-MED-b6c6ee2b-7_1



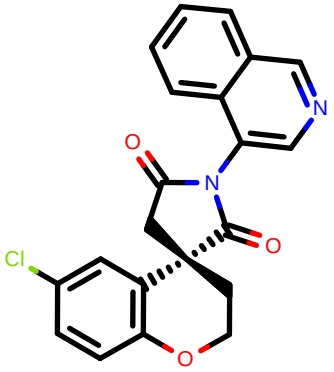
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl
RUN:	RUN531
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.12

VLA-UNK-56836b69-2_1



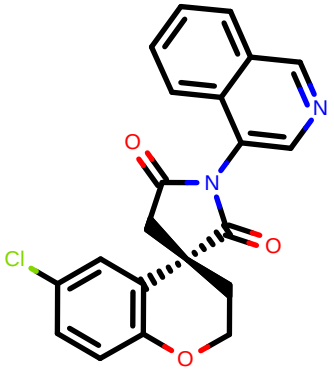
CID:	VLA-UNK-56836b69-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN368
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.11

VLA-UCB-05e51b3f-5_1



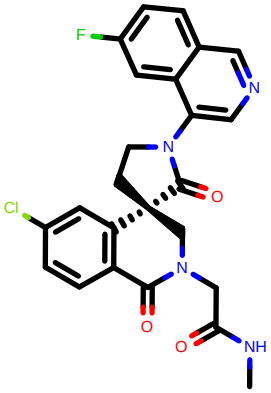
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN363
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.04

MAT-POS-94643566-1_1



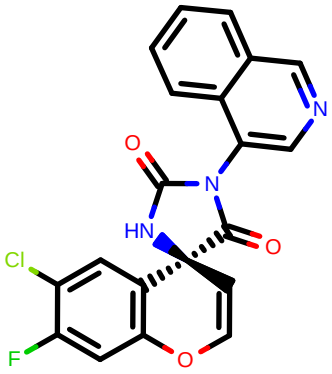
CID:	MAT-POS-94643566-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN361
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.03

EDJ-MED-b6c6ee2b-6_1



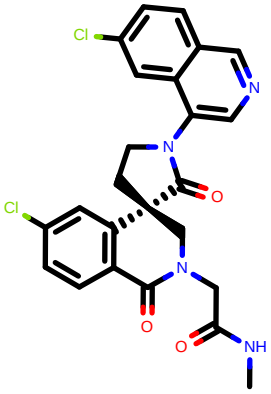
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN445
DDG (kcal/mol):	0.03
dDDG (kcal/mol):	0.11

VLA-UNK-3a43cd95-1_1



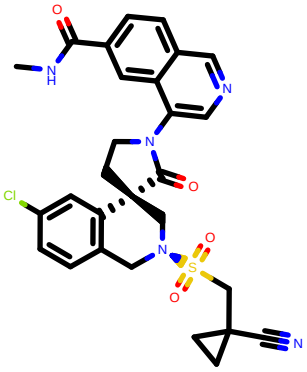
CID:	VLA-UNK-3a43cd95-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)F)Cl)NC3=O
RUN:	RUN366
DDG (kcal/mol):	0.04
dDDG (kcal/mol):	0.07

EDG-MED-b1ef7fe3-1_1



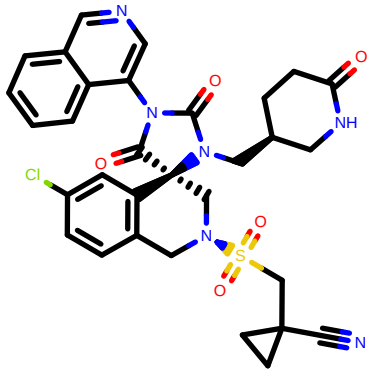
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN425
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.15

MAT-POS-38eb6498-2_1



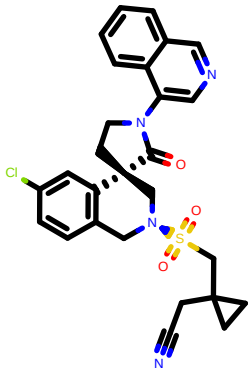
CID:	MAT-POS-38eb6498-2_1
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN626
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.25

JOH-MSK-949975c8-1_2



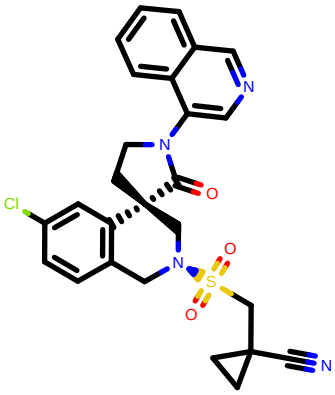
CID:	JOH-MSK-949975c8-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N(C3=O)C[C@H]7CCC(=O)NC7
RUN:	RUN670
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-22_1



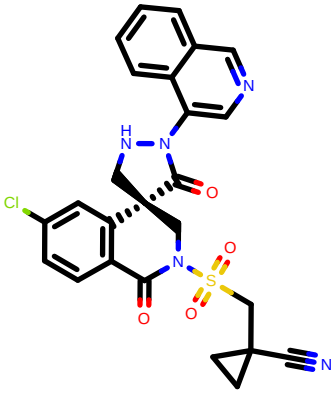
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN591
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.30

MIK-ENA-5d9157e9-2_1



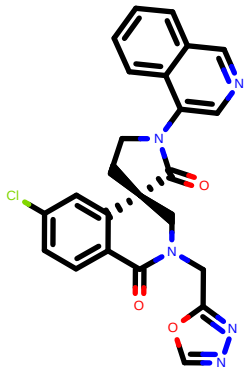
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN534
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.44

EDJ-MED-fed7ac0b-3_1



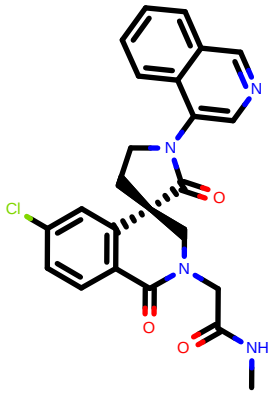
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CN3)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN560
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.29

PET-UNK-aa57768f-7_1



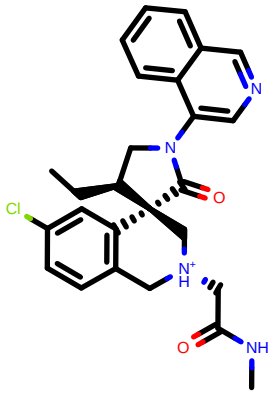
CID:	PET-UNK-aa57768f-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN450
DDG (kcal/mol):	0.06
dDDG (kcal/mol):	0.11

LUO-POS-9931618f-2_1



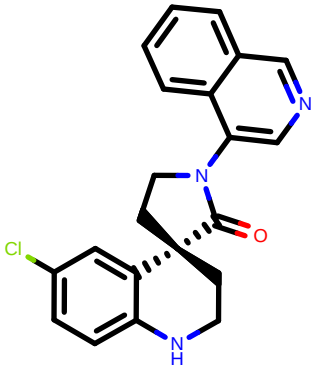
CID:	LUO-POS-9931618f-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN412
DDG (kcal/mol):	0.07
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-5_2



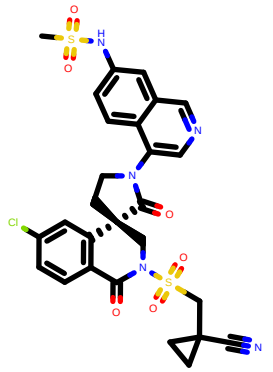
CID:	MAT-POS-50a80394-5_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN488
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.22

DAR-DIA-6be260fc-5_1



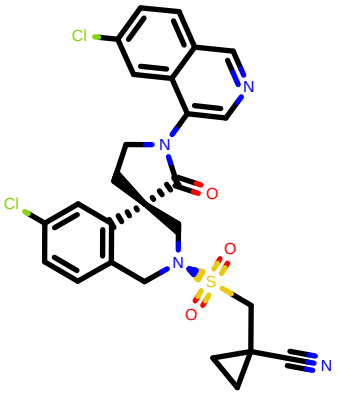
CID:	DAR-DIA-6be260fc-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl
RUN:	RUN352
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.07

EDJ-MED-9f4ac58c-3_1



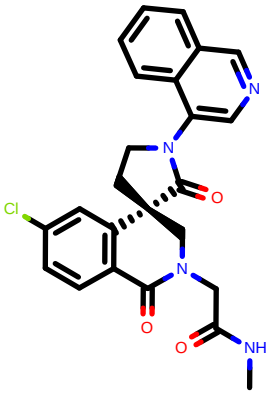
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN657
DDG (kcal/mol):	0.08
dDDG (kcal/mol):	0.56

EDJ-MED-b6c6ee2b-4_1



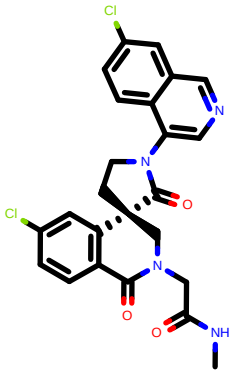
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN579
DDG (kcal/mol):	0.09
dDDG (kcal/mol):	0.37

PET-UNK-14142a25-1_1



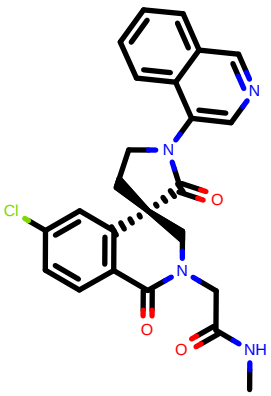
CID:	PET-UNK-14142a25-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN392
DDG (kcal/mol):	0.10
dDDG (kcal/mol):	0.11

EDG-MED-b1ef7fe3-4_1



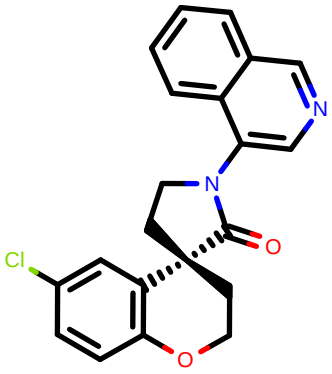
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN431
DDG (kcal/mol):	0.10
dDDG (kcal/mol):	0.11

MIK-ENA-794411b8-1_1



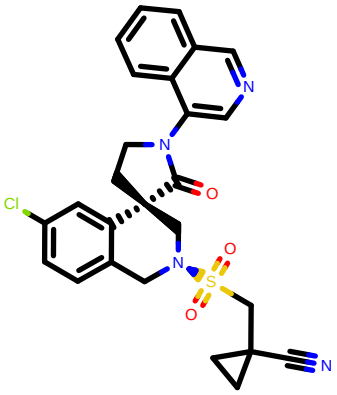
CID:	MIK-ENA-794411b8-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN421
DDG (kcal/mol):	0.10
dDDG (kcal/mol):	0.13

ALP-POS-477dc5b7-4_1



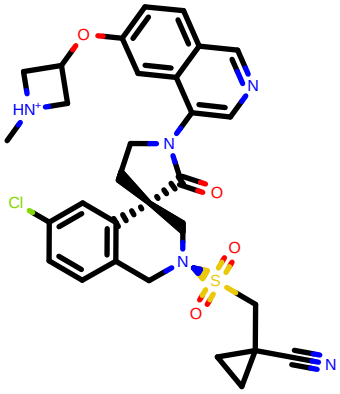
CID:	ALP-POS-477dc5b7-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN355
DDG (kcal/mol):	0.12
dDDG (kcal/mol):	0.06

ALP-POS-ecbed2ba-4_1



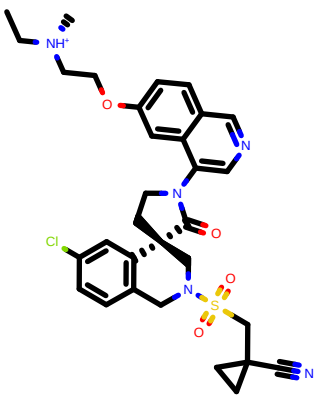
CID:	ALP-POS-ecbed2ba-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN529
DDG (kcal/mol):	0.12
dDDG (kcal/mol):	0.28

EDJ-MED-ee81482e-2_1



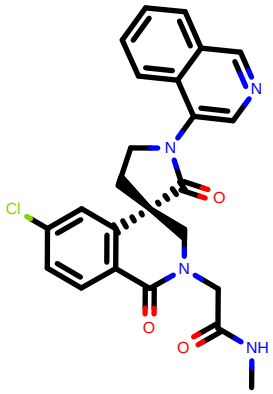
CID:	EDJ-MED-ee81482e-2_1
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN656
DDG (kcal/mol):	0.14
dDDG (kcal/mol):	0.50

MAT-POS-40ad851a-2_1



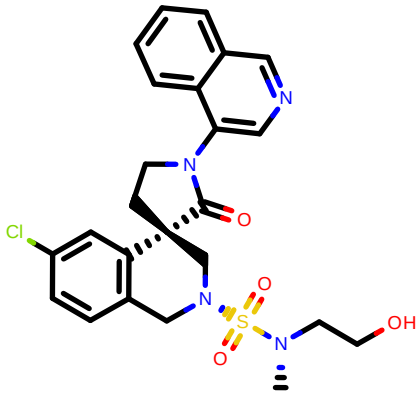
CID:	MAT-POS-40ad851a-2_1
SMILES:	CC[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN658
DDG (kcal/mol):	0.16
dDDG (kcal/mol):	0.65

EDJ-MED-8bb691af-8_1



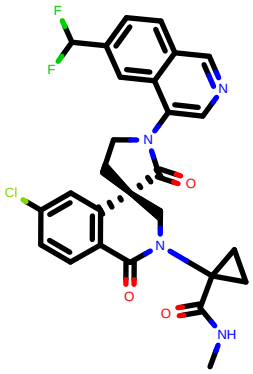
CID:	EDJ-MED-8bb691af-8_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN390
DDG (kcal/mol):	0.16
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-19_1



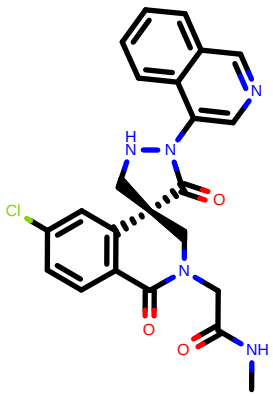
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	C[N@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN474
DDG (kcal/mol):	0.16
dDDG (kcal/mol):	0.27

EDJ-MED-5cd3920d-4_1



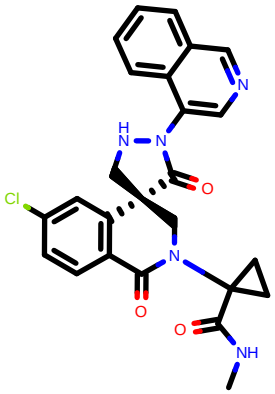
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)C(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN590
DDG (kcal/mol):	0.17
dDDG (kcal/mol):	0.14

EDJ-MED-fed7ac0b-4_1



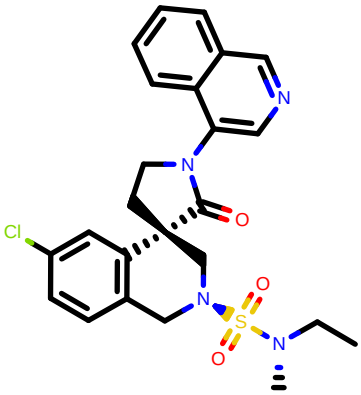
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	CNC(=O)CN1C[C@]2(C=NN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN401
DDG (kcal/mol):	0.19
dDDG (kcal/mol):	0.11

EDJ-MED-fed7ac0b-2_1



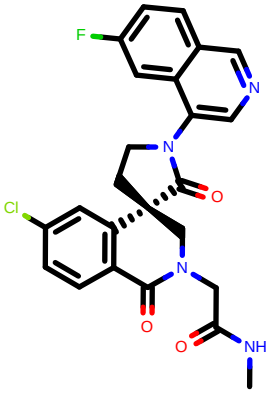
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CNN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN484
DDG (kcal/mol):	0.20
dDDG (kcal/mol):	0.13

ALP-POS-ecbed2ba-18_1



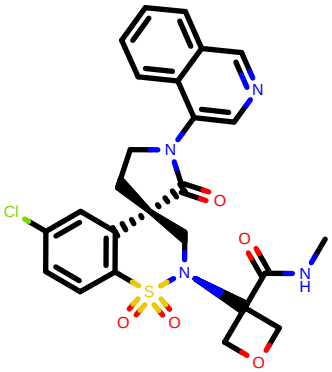
CID:	ALP-POS-ecbed2ba-18_1
SMILES:	CC[N@@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN446
DDG (kcal/mol):	0.22
dDDG (kcal/mol):	0.24

EDG-MED-b1ef7fe3-2_1



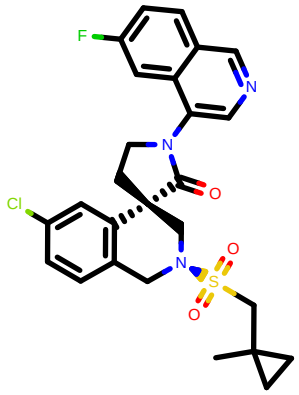
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN428
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.11

EDJ-MED-98c0a822-2_1



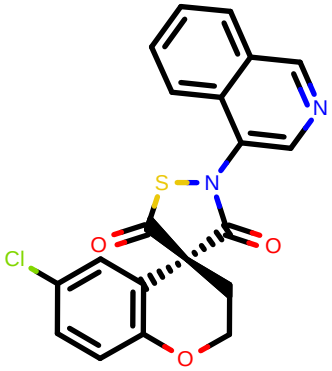
CID:	EDJ-MED-98c0a822-2_1
SMILES:	CNC(=O)C1(COC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN584
DDG (kcal/mol):	0.24
dDDG (kcal/mol):	0.25

MAT-POS-853c0ffa-21_1



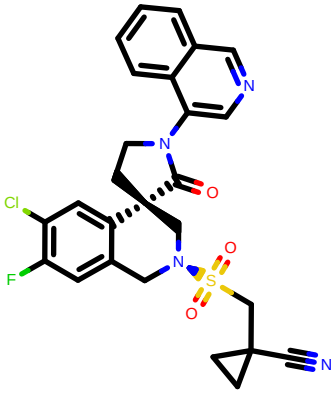
CID:	MAT-POS-853c0ffa-21_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN519
DDG (kcal/mol):	0.24
dDDG (kcal/mol):	0.23

DAR-DIA-0f7b7cd9-8_1



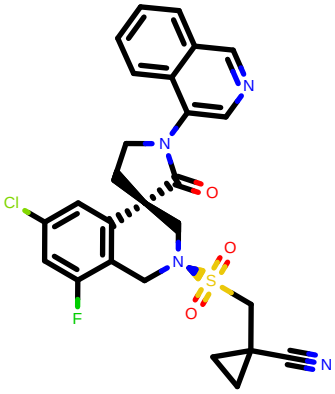
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C(=O)S3
RUN:	RUN376
DDG (kcal/mol):	0.25
dDDG (kcal/mol):	0.07

VLA-UNK-61877630-8_1



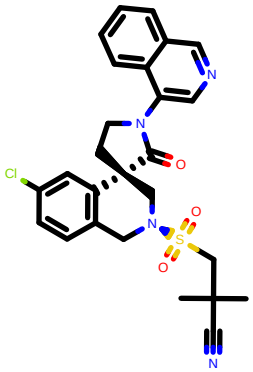
CID:	VLA-UNK-61877630-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(c(c5)F)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN605
DDG (kcal/mol):	0.28
dDDG (kcal/mol):	0.28

VLA-UNK-61877630-7_1



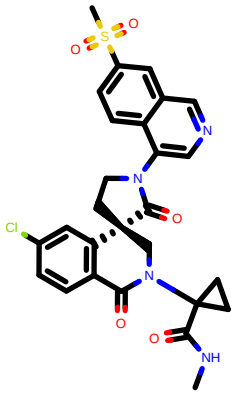
CID:	VLA-UNK-61877630-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5F)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN577
DDG (kcal/mol):	0.28
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-13_1



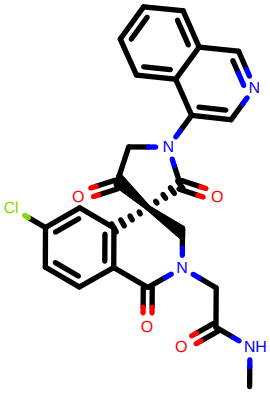
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN515
DDG (kcal/mol):	0.28
dDDG (kcal/mol):	0.34

EDJ-MED-976a33d5-2_1



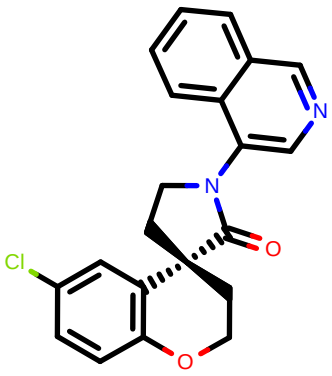
CID:	EDJ-MED-976a33d5-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN606
DDG (kcal/mol):	0.29
dDDG (kcal/mol):	0.16

EDJ-MED-a12e3a20-2_1



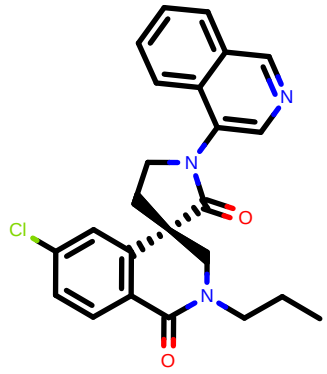
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=O)CN(C2=O)c4cncc5c4cccc5
RUN:	RUN462
DDG (kcal/mol):	0.30
dDDG (kcal/mol):	0.12

EDJ-MED-159244ea-1_1



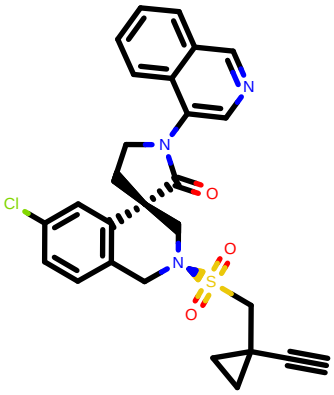
CID:	EDJ-MED-159244ea-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN342
DDG (kcal/mol):	0.32
dDDG (kcal/mol):	0.08

PET-UNK-aa57768f-9_1



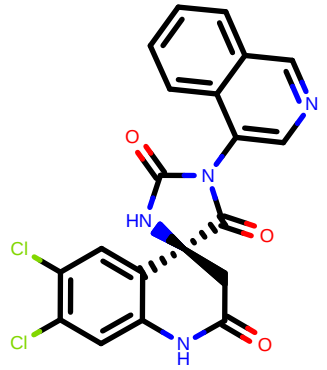
CID:	PET-UNK-aa57768f-9_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN372
DDG (kcal/mol):	0.32
dDDG (kcal/mol):	0.12

PET-UNK-94036022-9_1



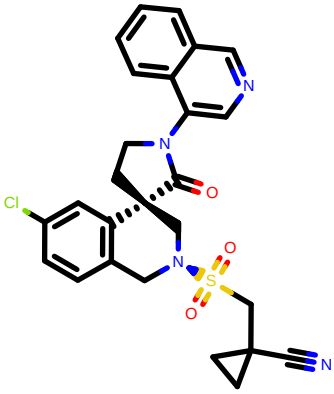
CID:	PET-UNK-94036022-9_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN551
DDG (kcal/mol):	0.33
dDDG (kcal/mol):	0.26

VLA-UNK-56836b69-5_1



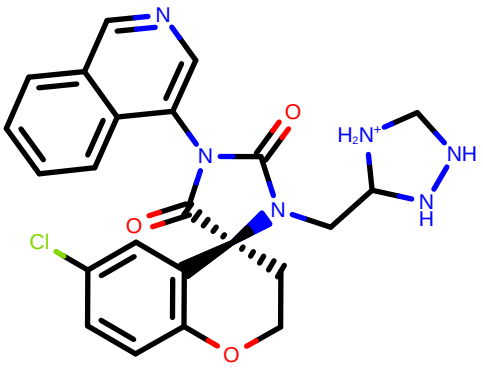
CID:	VLA-UNK-56836b69-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN387
DDG (kcal/mol):	0.36
dDDG (kcal/mol):	0.13

MIK-ENA-5d9157e9-1_1



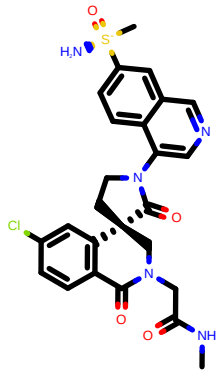
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN535
DDG (kcal/mol):	0.39
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-3_1



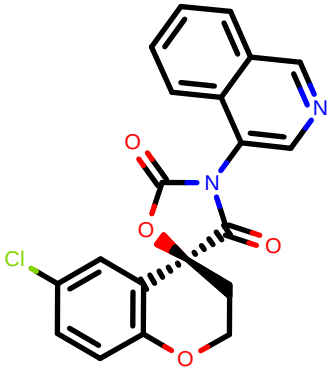
CID:	VLA-UNK-f702bf1c-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6[nH]ncn6
RUN:	RUN427
DDG (kcal/mol):	0.42
dDDG (kcal/mol):	0.15

EDJ-MED-7d88f880-1_1



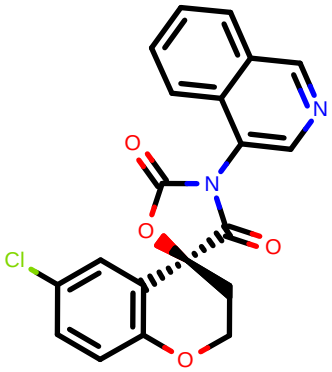
CID:	EDJ-MED-7d88f880-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)[S@@](=N)(=O)C)c5cc(ccc5C1=O)Cl
RUN:	RUN563
DDG (kcal/mol):	0.42
dDDG (kcal/mol):	0.17

MAT-POS-ec6d90b7-1_1



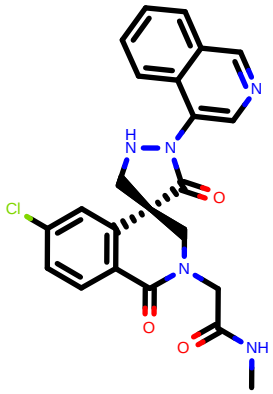
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN358
DDG (kcal/mol):	0.43
dDDG (kcal/mol):	0.04

MAT-POS-90505e2b-1_1



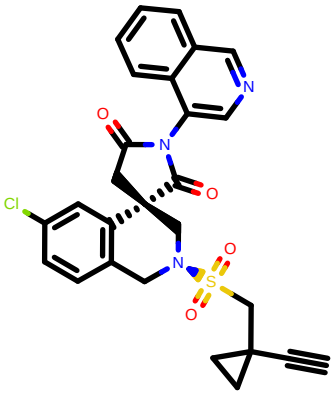
CID:	MAT-POS-90505e2b-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN350
DDG (kcal/mol):	0.44
dDDG (kcal/mol):	0.05

EDJ-MED-fed7ac0b-1_1



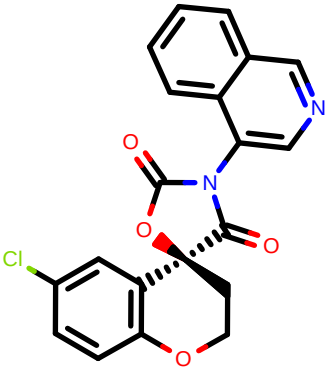
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	CNC(=O)CN1C[C@]2(CNN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN404
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.12

PET-UNK-94036022-11_1



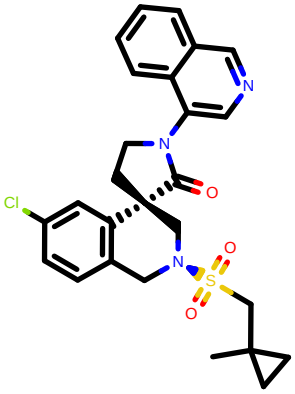
CID:	PET-UNK-94036022-11_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN559
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.27

MAT-POS-ec6d90b7-2_1



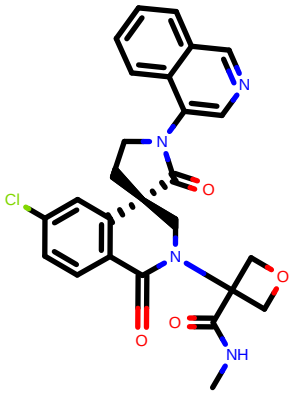
CID:	MAT-POS-ec6d90b7-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN370
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.04

ALP-POS-ecbed2ba-3_1



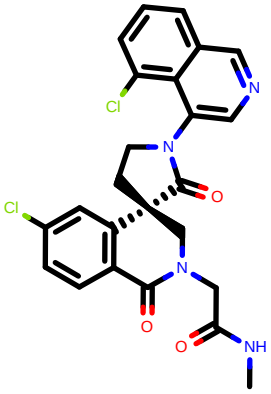
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN473
DDG (kcal/mol):	0.50
dDDG (kcal/mol):	0.23

EDJ-MED-98c0a822-4_1



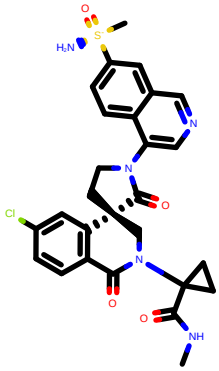
CID:	EDJ-MED-98c0a822-4_1
SMILES:	CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN528
DDG (kcal/mol):	0.50
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-1_1



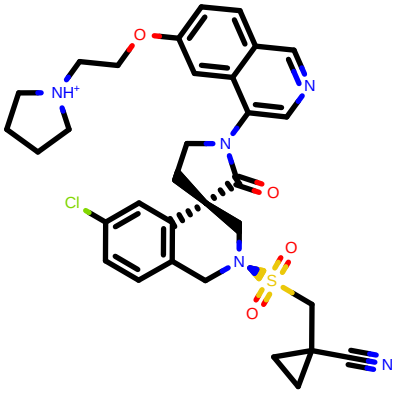
CID:	MAT-POS-853c0ffa-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN432
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.11

EDJ-MED-7d88f880-2_1



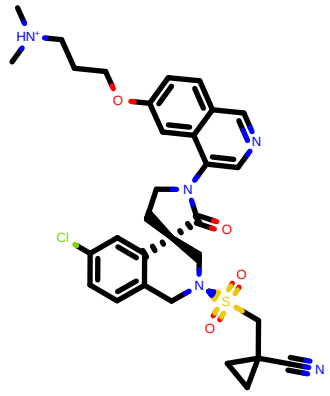
CID:	EDJ-MED-7d88f880-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)[S@@](=N)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN612
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.18

EDJ-MED-468565e0-1_1



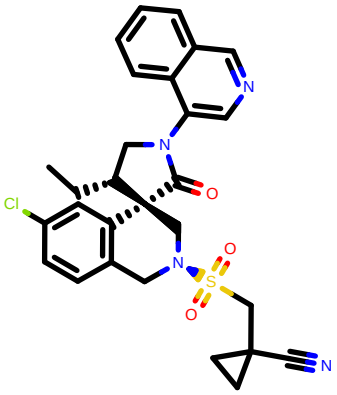
CID:	EDJ-MED-468565e0-1_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN666
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.55

MAT-POS-40ad851a-4_1



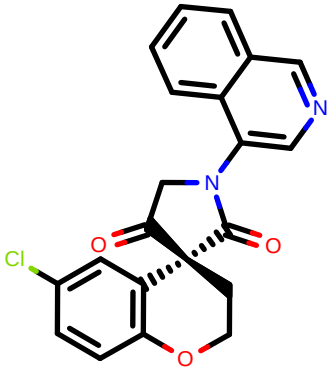
CID:	MAT-POS-40ad851a-4_1
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN654
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.51

MAT-POS-50a80394-2_1



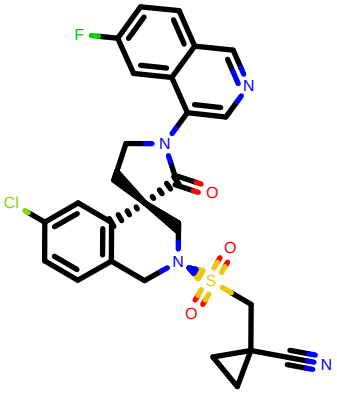
CID:	MAT-POS-50a80394-2_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN596
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.39

DAR-DIA-0f7b7cd9-9_1



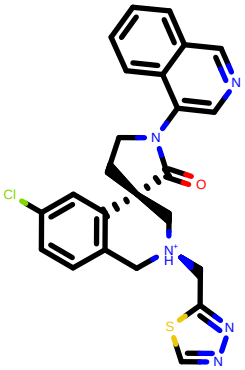
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN367
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.07

MAT-POS-853c0ffa-13_1



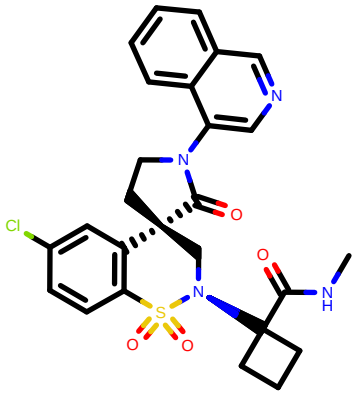
CID:	MAT-POS-853c0ffa-13_1
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN561
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.33

MAT-POS-96396902-1_1



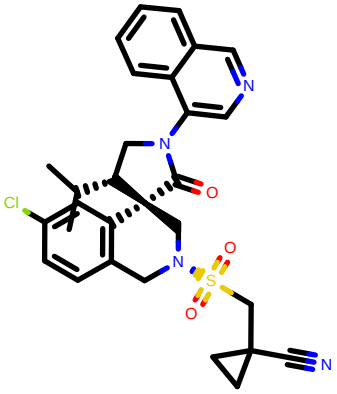
CID:	MAT-POS-96396902-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN442
DDG (kcal/mol):	0.55
dDDG (kcal/mol):	0.13

EDJ-MED-98c0a822-1_1



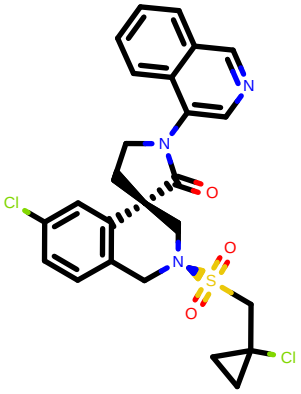
CID:	EDJ-MED-98c0a822-1_1
SMILES:	CNC(=O)C1(CCC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN588
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.62

MAT-POS-50a80394-3_1



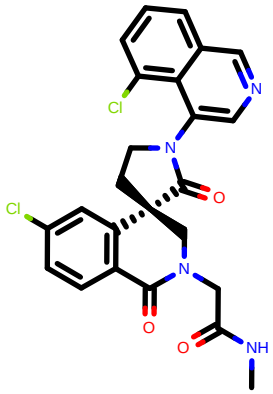
CID:	MAT-POS-50a80394-3_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN624
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.26

PET-UNK-94036022-3_1



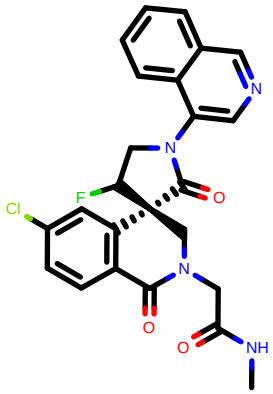
CID:	PET-UNK-94036022-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN512
DDG (kcal/mol):	0.63
dDDG (kcal/mol):	0.21

MAT-POS-1d5ab790-3_1



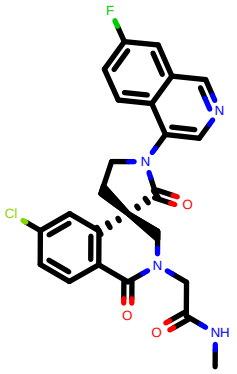
CID:	MAT-POS-1d5ab790-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN459
DDG (kcal/mol):	0.63
dDDG (kcal/mol):	0.11

EDJ-MED-fd8ed875-5_1



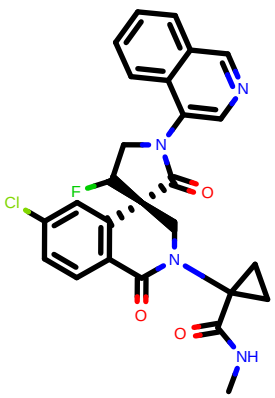
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cncc5c4cccc5)F
RUN:	RUN470
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.11

EDG-MED-b1ef7fe3-3_1



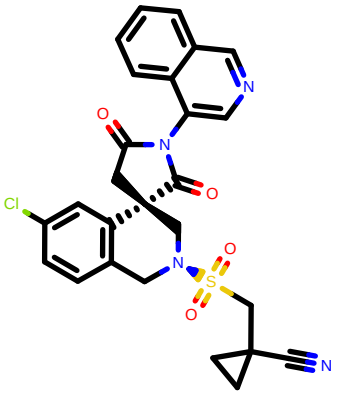
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN433
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.12

EDJ-MED-fd8ed875-6_1



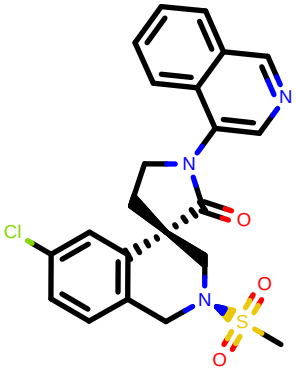
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	CNC(=O)C1(CC1)N2C[C@@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5cccc6)F
RUN:	RUN532
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.13

MAT-POS-1bed62cf-1_1



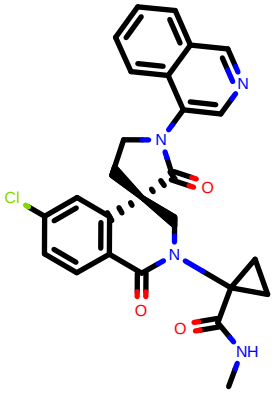
CID:	MAT-POS-1bed62cf-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN537
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.26

EDJ-MED-7587a9ee-3_1



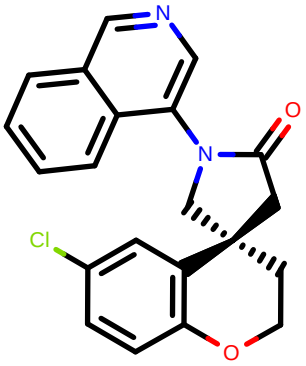
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN385
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.18

MAT-POS-e48723dc-1_1



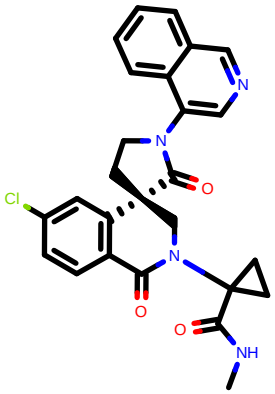
CID:	MAT-POS-e48723dc-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN493
DDG (kcal/mol):	0.66
dDDG (kcal/mol):	0.14

MAT-POS-983b399a-3_1



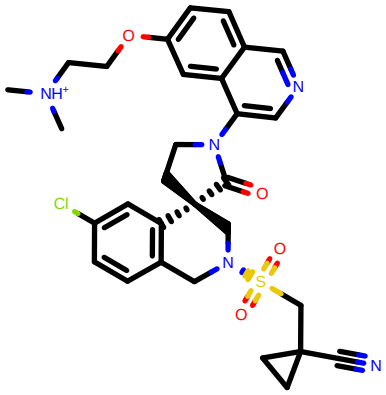
CID:	MAT-POS-983b399a-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN346
DDG (kcal/mol):	0.68
dDDG (kcal/mol):	0.07

EDJ-MED-fd8ed875-4_1



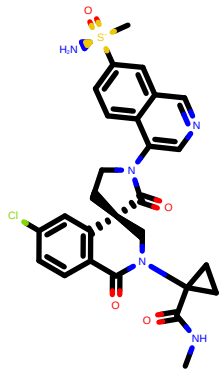
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(C=CN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN492
DDG (kcal/mol):	0.73
dDDG (kcal/mol):	0.11

MAT-POS-38eb6498-1_1



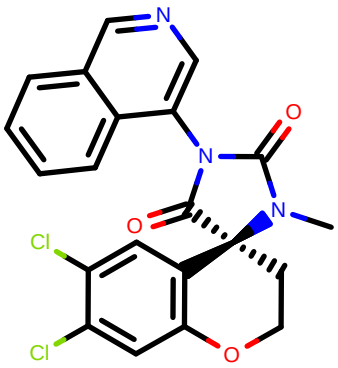
CID:	MAT-POS-38eb6498-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN650
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.46

EDJ-MED-7d88f880-2_2



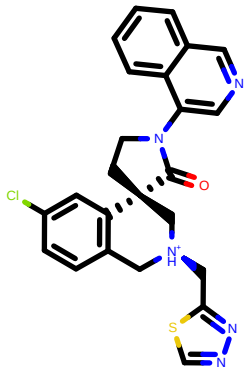
CID:	EDJ-MED-7d88f880-2_2
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)[S@](=N)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN611
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.17

VLA-UNK-56836b69-3_1



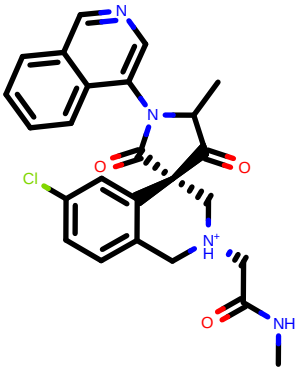
CID:	VLA-UNK-56836b69-3_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN364
DDG (kcal/mol):	0.79
dDDG (kcal/mol):	0.12

PET-UNK-7e9559de-4_1



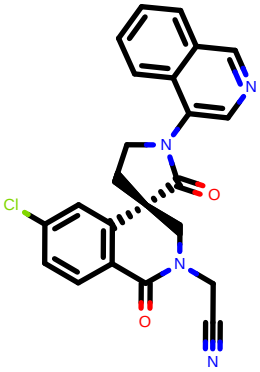
CID:	PET-UNK-7e9559de-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN449
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.14

PET-UNK-94036022-14_1



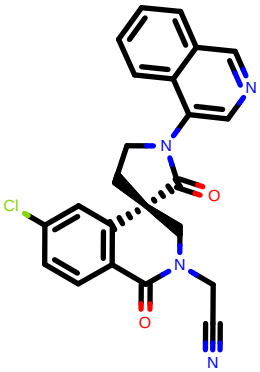
CID:	PET-UNK-94036022-14_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN489
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.32

PET-UNK-aa57768f-8_1



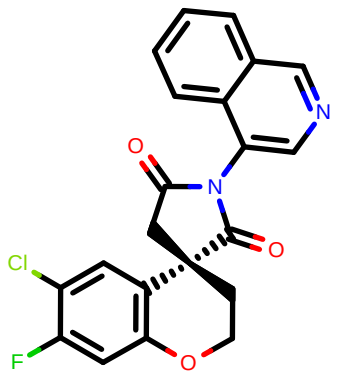
CID:	PET-UNK-aa57768f-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN381
DDG (kcal/mol):	0.84
dDDG (kcal/mol):	0.08

PET-UNK-aa57768f-2_1



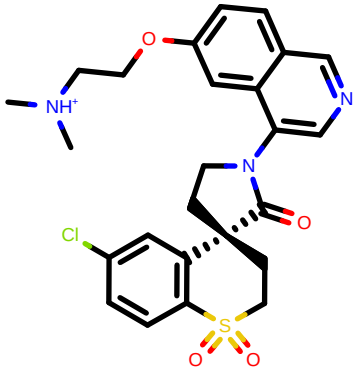
CID:	PET-UNK-aa57768f-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN380
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.09

VLA-UNK-3a43cd95-3_1



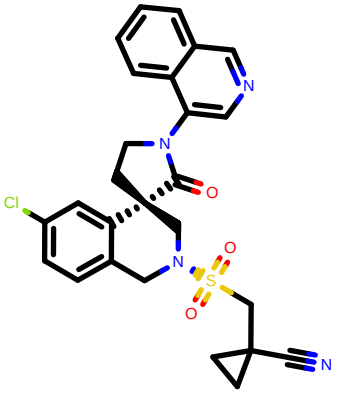
CID:	VLA-UNK-3a43cd95-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl
RUN:	RUN362
DDG (kcal/mol):	0.92
dDDG (kcal/mol):	0.08

EDJ-MED-d4864bdc-4_1



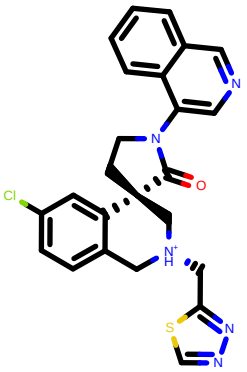
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN499
DDG (kcal/mol):	0.93
dDDG (kcal/mol):	0.26

EDJ-MED-8bb691af-6_1



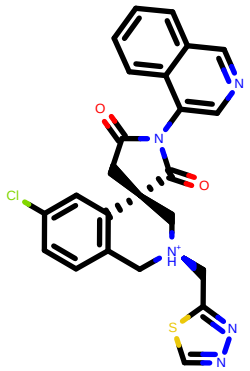
CID:	EDJ-MED-8bb691af-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN507
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.31

PET-UNK-7e9559de-1_1



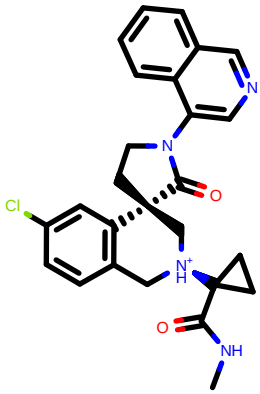
CID:	PET-UNK-7e9559de-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN415
DDG (kcal/mol):	1.00
dDDG (kcal/mol):	0.17

PET-UNK-77d5678a-1_1



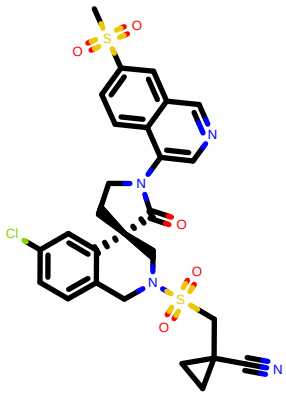
CID:	PET-UNK-77d5678a-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN485
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.14

MAT-POS-576f7758-1_1



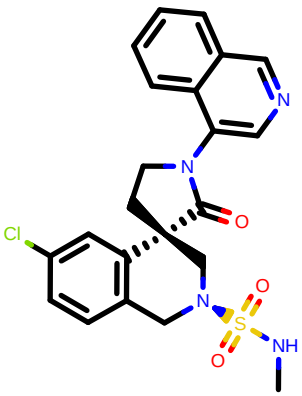
CID:	MAT-POS-576f7758-1_1
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN491
DDG (kcal/mol):	1.05
dDDG (kcal/mol):	0.14

MAT-POS-853c0ffa-15_1



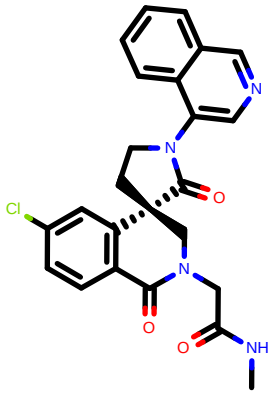
CID:	MAT-POS-853c0ffa-15_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN618
DDG (kcal/mol):	1.06
dDDG (kcal/mol):	0.33

LUO-POS-ed2cfb03-2_1



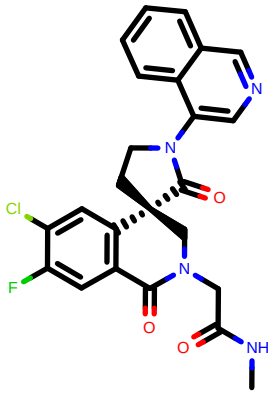
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN406
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.60

EDJ-MED-fd8ed875-3_1



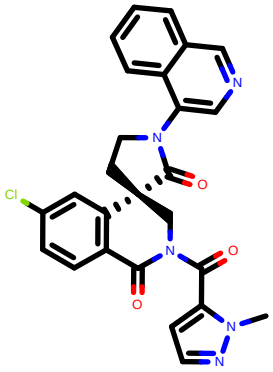
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	CNC(=O)CN1C[C@]2(C=CN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN413
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.11

VLA-UNK-61877630-5_1



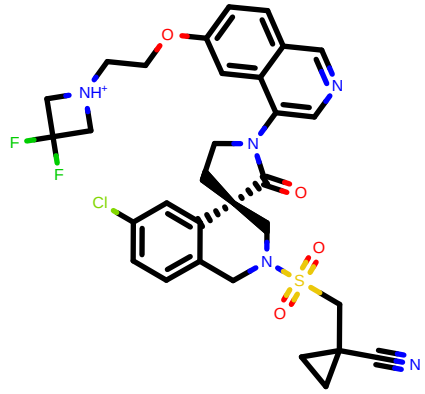
CID:	VLA-UNK-61877630-5_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5C1=O)F)Cl
RUN:	RUN461
DDG (kcal/mol):	1.11
dDDG (kcal/mol):	0.12

EDJ-MED-cc48ee33-2_1



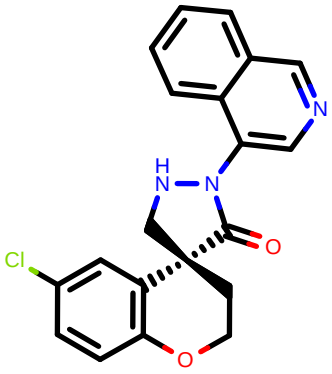
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	Cn1c(ccn1)C(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN554
DDG (kcal/mol):	1.13
dDDG (kcal/mol):	0.14

EDJ-MED-468565e0-5_1



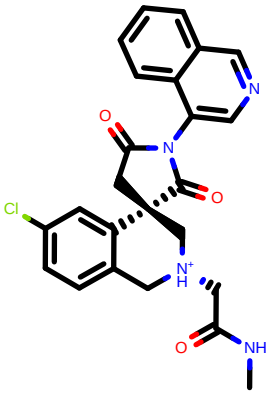
CID:	EDJ-MED-468565e0-5_1
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN669
DDG (kcal/mol):	1.15
dDDG (kcal/mol):	0.38

BRU-THA-73c97d88-1_1



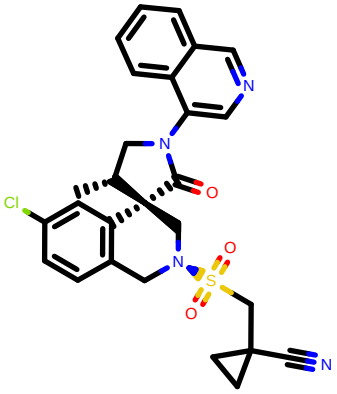
CID:	BRU-THA-73c97d88-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3
RUN:	RUN344
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.06

JOH-MSK-1f2dff76-1_1



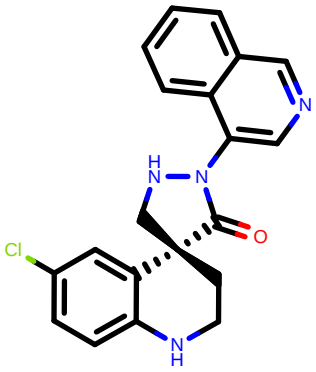
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN443
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-1_1



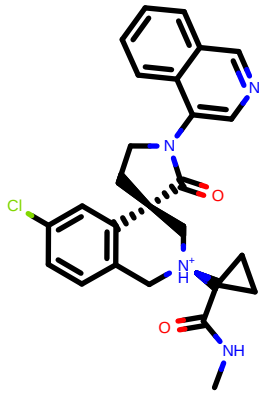
CID:	MAT-POS-50a80394-1_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN575
DDG (kcal/mol):	1.19
dDDG (kcal/mol):	0.29

BRU-THA-55eab31a-1_1



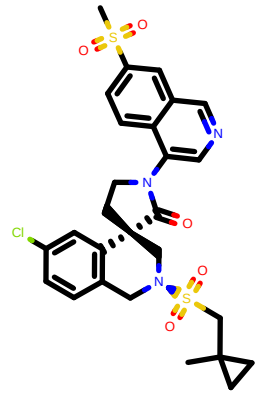
CID:	BRU-THA-55eab31a-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3
RUN:	RUN348
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.08

ALP-POS-ecbed2ba-7_1



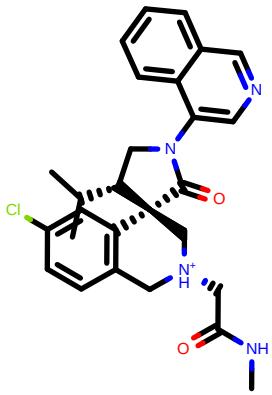
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN456
DDG (kcal/mol):	1.22
dDDG (kcal/mol):	0.15

MAT-POS-853c0ffa-22_1



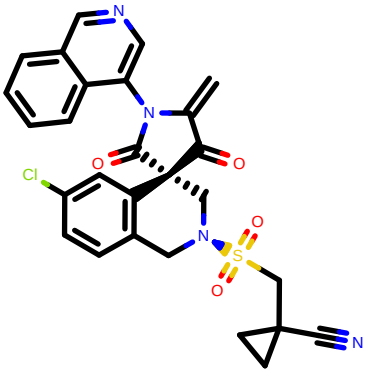
CID:	MAT-POS-853c0ffa-22_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN617
DDG (kcal/mol):	1.23
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-6_1



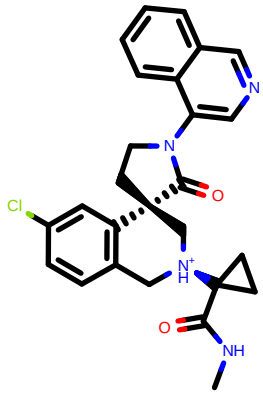
CID:	MAT-POS-50a80394-6_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN503
DDG (kcal/mol):	1.24
dDDG (kcal/mol):	0.20

PET-UNK-94036022-13_1



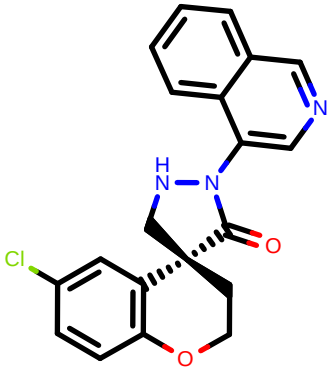
CID:	PET-UNK-94036022-13_1
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN614
DDG (kcal/mol):	1.28
dDDG (kcal/mol):	0.37

MAT-POS-69786b79-1_1



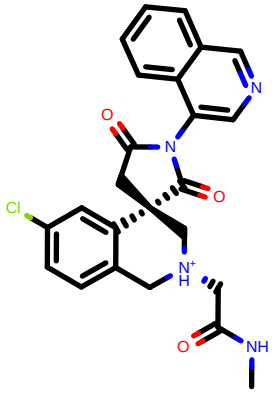
CID:	MAT-POS-69786b79-1_1
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN487
DDG (kcal/mol):	1.28
dDDG (kcal/mol):	0.18

BEN-BAS-c2bc0d80-3_1



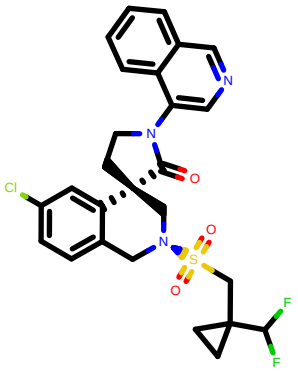
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3
RUN:	RUN354
DDG (kcal/mol):	1.28
dDDG (kcal/mol):	0.08

JOH-MSK-1f2dff76-2_1



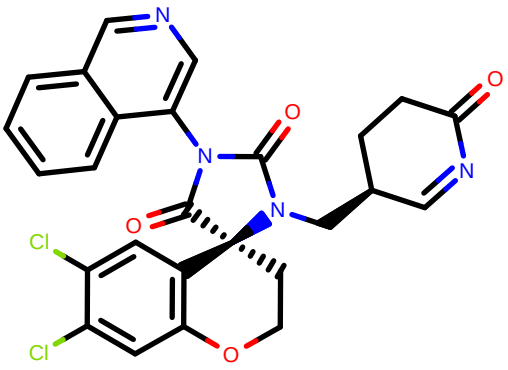
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN419
DDG (kcal/mol):	1.32
dDDG (kcal/mol):	0.25

EDJ-MED-5cd3920d-5_1



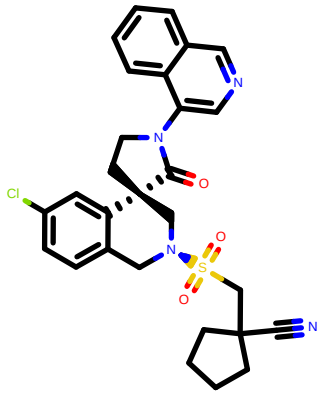
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN592
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.31

JOH-MSK-b735e33c-1_2



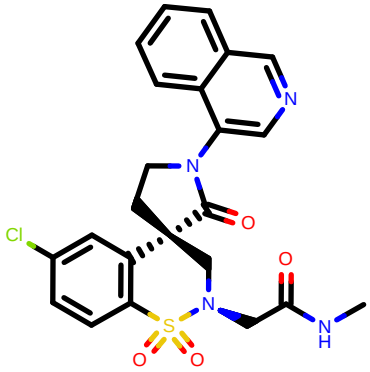
CID:	JOH-MSK-b735e33c-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)N(C3=O)C[C@H]6CCC(=O)NC6
RUN:	RUN580
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-15_1



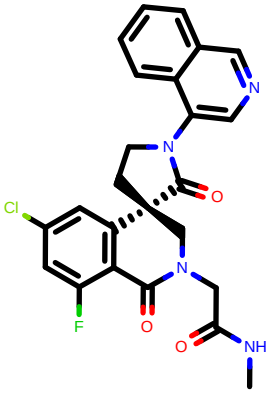
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN599
DDG (kcal/mol):	1.35
dDDG (kcal/mol):	0.44

ALP-POS-4483ae88-2_1



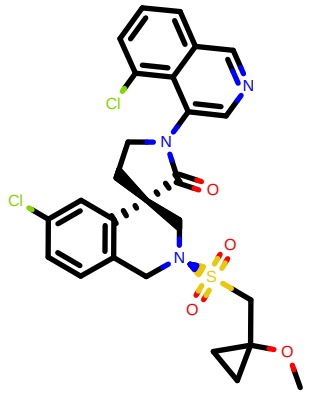
CID:	ALP-POS-4483ae88-2_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN434
DDG (kcal/mol):	1.44
dDDG (kcal/mol):	0.19

VLA-UNK-61877630-4_1



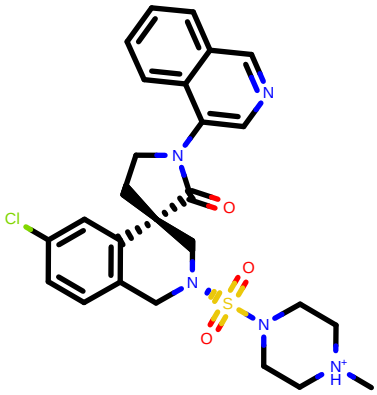
CID:	VLA-UNK-61877630-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(cc(c5C1=O)F)Cl
RUN:	RUN447
DDG (kcal/mol):	1.51
dDDG (kcal/mol):	0.13

MAT-POS-853c0ffa-7_1



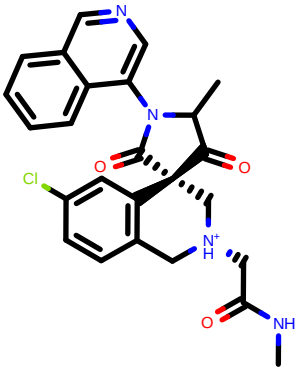
CID:	MAT-POS-853c0ffa-7_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN571
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.31

LUO-POS-ed2cfb03-1_1



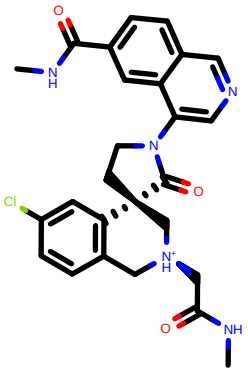
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN572
DDG (kcal/mol):	1.58
dDDG (kcal/mol):	0.59

PET-UNK-94036022-7_1



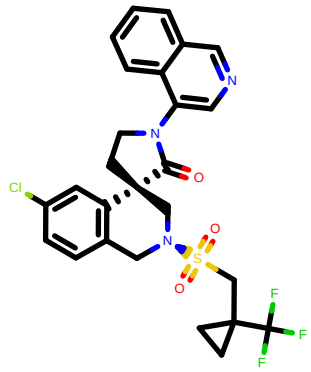
CID:	PET-UNK-94036022-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN463
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.29

MAT-POS-38eb6498-5_1



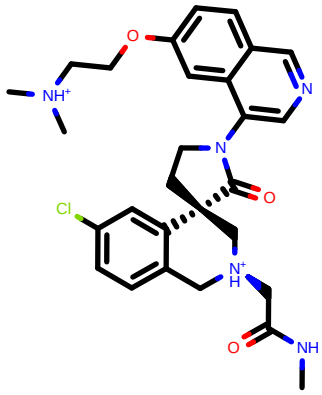
CID:	MAT-POS-38eb6498-5_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN527
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.19

VLA-UNK-61877630-10_1



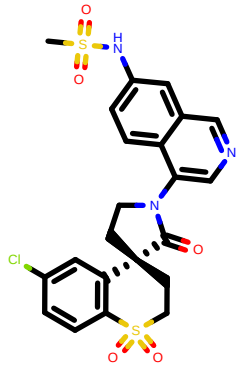
CID:	VLA-UNK-61877630-10_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN601
DDG (kcal/mol):	1.63
dDDG (kcal/mol):	0.33

EDJ-MED-b6c6ee2b-1_1



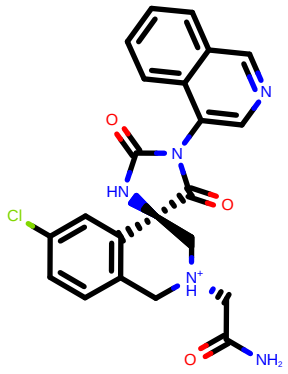
CID:	EDJ-MED-b6c6ee2b-1_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN625
DDG (kcal/mol):	1.64
dDDG (kcal/mol):	0.35

EDJ-MED-ede5c6cb-1_1



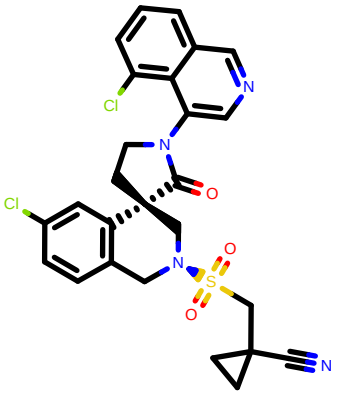
CID:	EDJ-MED-ede5c6cb-1_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN452
DDG (kcal/mol):	1.68
dDDG (kcal/mol):	0.16

VLA-MRT-a639d434-2_1



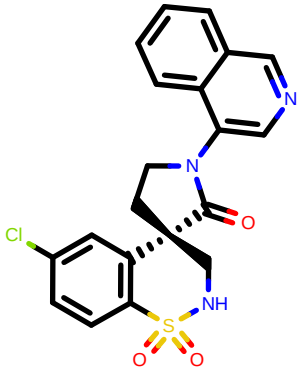
CID:	VLA-MRT-a639d434-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN420
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.22

MAT-POS-853c0ffa-5_1



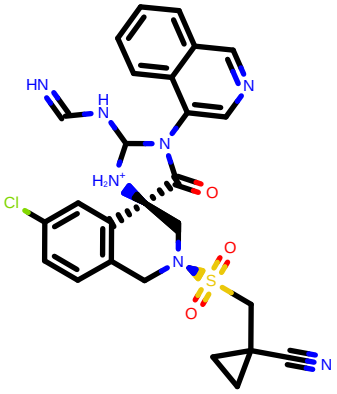
CID:	MAT-POS-853c0ffa-5_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN556
DDG (kcal/mol):	1.75
dDDG (kcal/mol):	0.36

EDJ-MED-f9b78f78-4_1



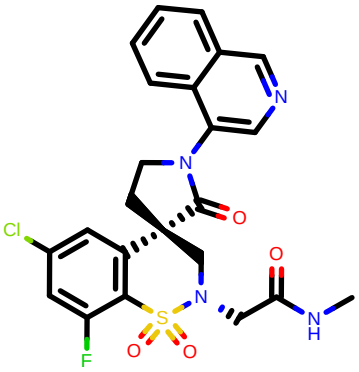
CID:	EDJ-MED-f9b78f78-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN382
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.12

LUO-POS-b5068a05-2_1



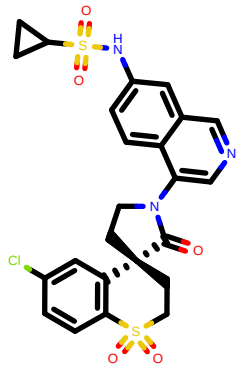
CID:	LUO-POS-b5068a05-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN622
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.30

VLA-UNK-f2612802-3_1



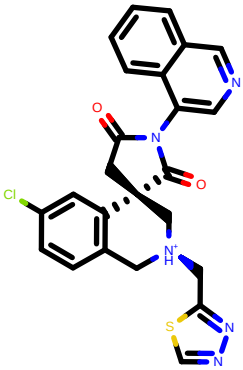
CID:	VLA-UNK-f2612802-3_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(cc(c5S1(=O)=O)F)Cl
RUN:	RUN501
DDG (kcal/mol):	1.77
dDDG (kcal/mol):	0.20

EDJ-MED-ede5c6cb-2_1



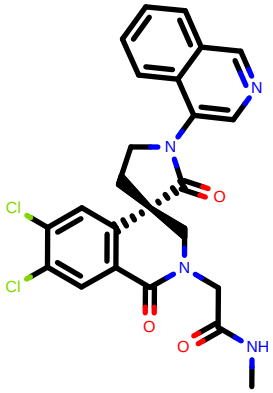
CID:	EDJ-MED-ede5c6cb-2_1
SMILES:	c1cc2c(cc1NS(=O)(=O)C3CC3)cncc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl
RUN:	RUN543
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.17

PET-UNK-77d5678a-4_1



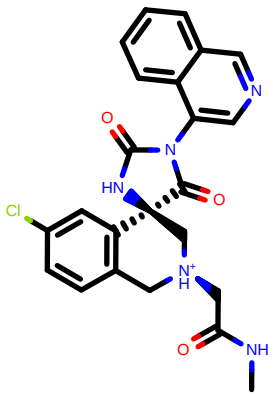
CID:	PET-UNK-77d5678a-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN479
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.17

ALP-POS-afe0272e-2_1



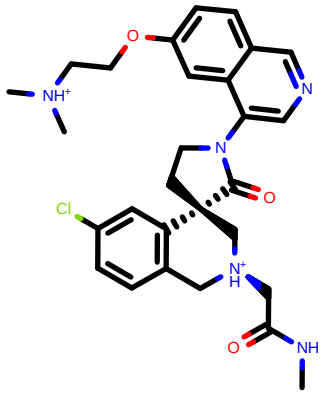
CID:	ALP-POS-afe0272e-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5C1=O)Cl)Cl
RUN:	RUN458
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.12

VLA-MRT-8c78ee15-3_1



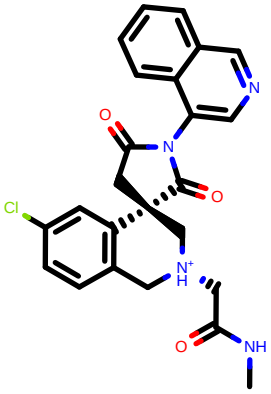
CID:	VLA-MRT-8c78ee15-3_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN410
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.18

MAT-POS-38eb6498-3_1



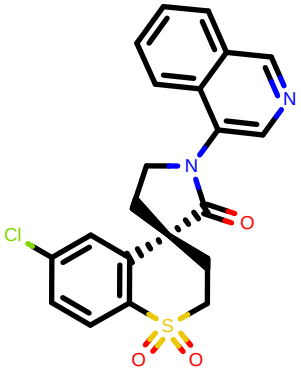
CID:	MAT-POS-38eb6498-3_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN609
DDG (kcal/mol):	1.89
dDDG (kcal/mol):	0.38

MAT-POS-1bed62cf-3_1



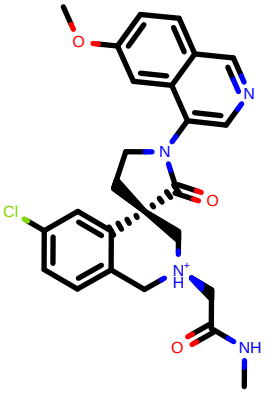
CID:	MAT-POS-1bed62cf-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN409
DDG (kcal/mol):	1.91
dDDG (kcal/mol):	0.24

ALP-POS-41e2080f-1_1



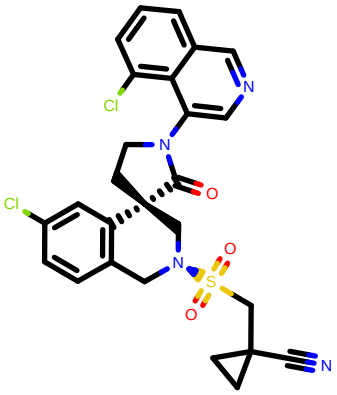
CID:	ALP-POS-41e2080f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN365
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.11

EDJ-MED-b6c6ee2b-2_1



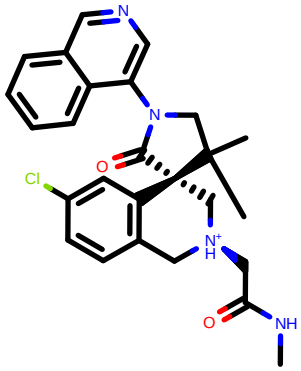
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN472
DDG (kcal/mol):	1.94
dDDG (kcal/mol):	0.21

MAT-POS-1d5ab790-1_1



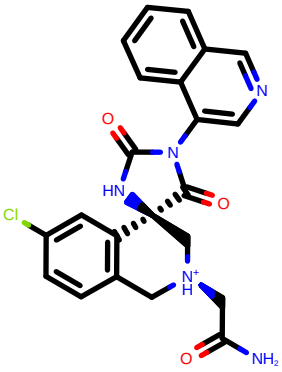
CID:	MAT-POS-1d5ab790-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN569
DDG (kcal/mol):	1.94
dDDG (kcal/mol):	0.40

MAT-POS-50a80394-7_1



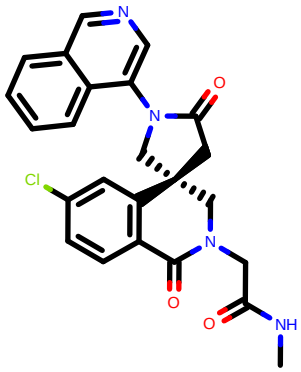
CID:	MAT-POS-50a80394-7_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN511
DDG (kcal/mol):	1.95
dDDG (kcal/mol):	0.19

VLA-MRT-8c78ee15-4_1



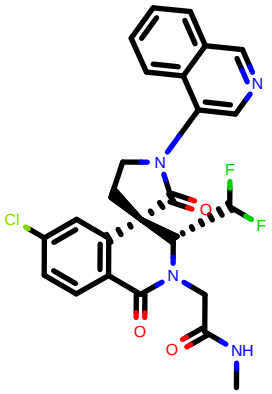
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN397
DDG (kcal/mol):	1.97
dDDG (kcal/mol):	0.18

EDJ-MED-8bb691af-9_1



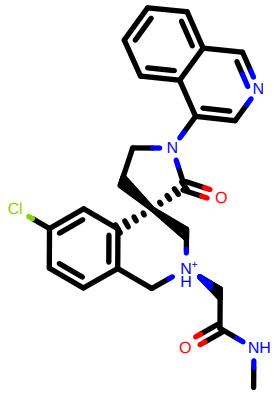
CID:	EDJ-MED-8bb691af-9_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN399
DDG (kcal/mol):	1.98
dDDG (kcal/mol):	0.15

VLA-UNK-61877630-6_2



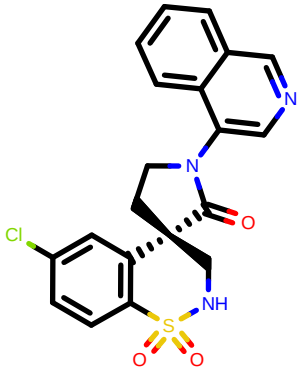
CID:	VLA-UNK-61877630-6_2
SMILES:	CNC(=O)CN1[C@H]([C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)F
RUN:	RUN540
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.17

MAT-POS-c7726e07-5_1



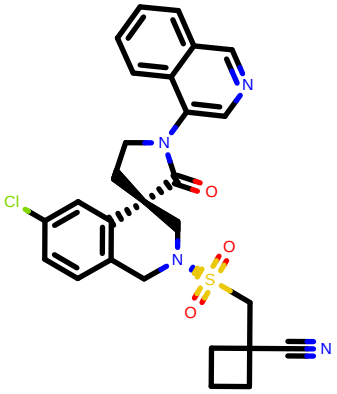
CID:	MAT-POS-c7726e07-5_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN407
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.19

ALP-POS-4483ae88-1_1



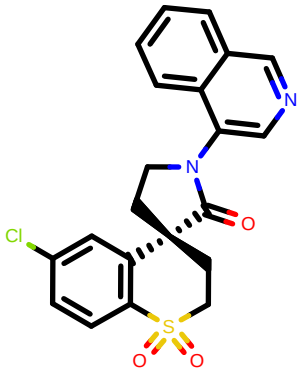
CID:	ALP-POS-4483ae88-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN373
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-8_1



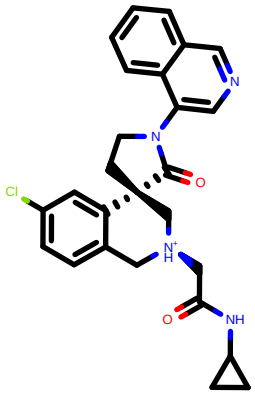
CID:	ALP-POS-ecbed2ba-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N
RUN:	RUN558
DDG (kcal/mol):	2.02
dDDG (kcal/mol):	0.51

EDJ-MED-d4864bdc-3_1



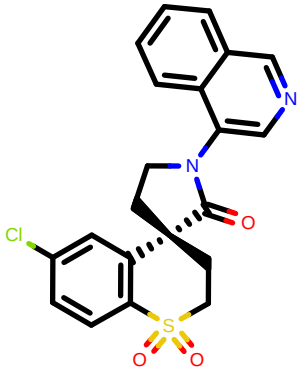
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN371
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.13

MAT-POS-69786b79-2_1



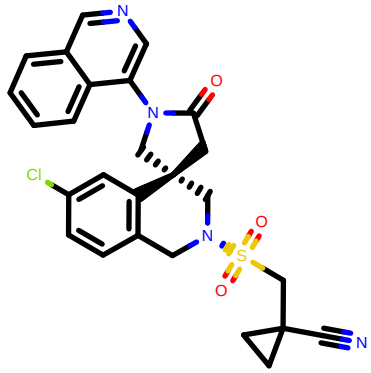
CID:	MAT-POS-69786b79-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN468
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.21

EDJ-MED-94fddcec-4_1



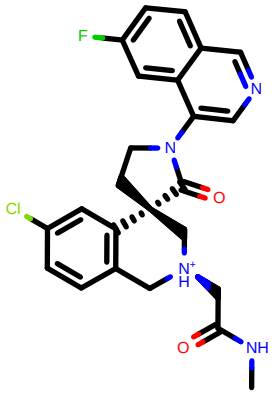
CID:	EDJ-MED-94fddcec-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN383
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.14

EDJ-MED-8bb691af-5_1



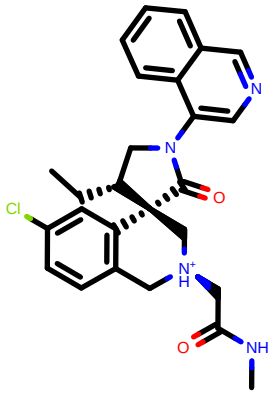
CID:	EDJ-MED-8bb691af-5_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN510
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.40

LUO-POS-b4dec3be-1_1



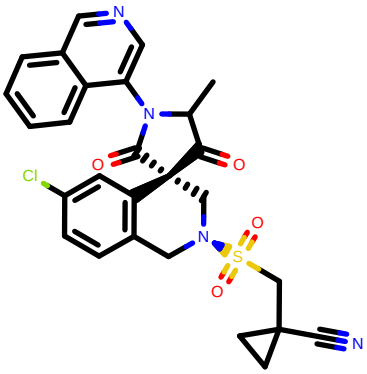
CID:	LUO-POS-b4dec3be-1_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN437
DDG (kcal/mol):	2.12
dDDG (kcal/mol):	0.18

MAT-POS-50a80394-5_1



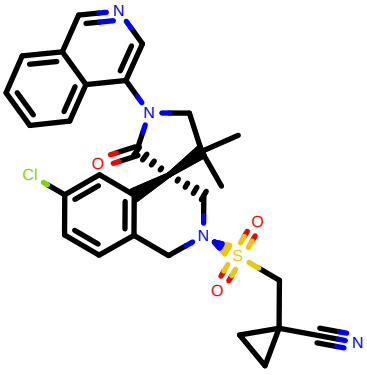
CID:	MAT-POS-50a80394-5_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN475
DDG (kcal/mol):	2.16
dDDG (kcal/mol):	0.21

PET-UNK-94036022-6_1



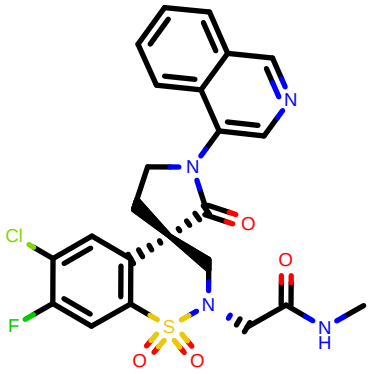
CID:	PET-UNK-94036022-6_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN615
DDG (kcal/mol):	2.17
dDDG (kcal/mol):	0.40

MAT-POS-50a80394-8_1



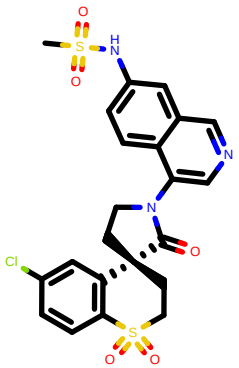
CID:	MAT-POS-50a80394-8_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN603
DDG (kcal/mol):	2.18
dDDG (kcal/mol):	0.45

VLA-UNK-f2612802-2_1



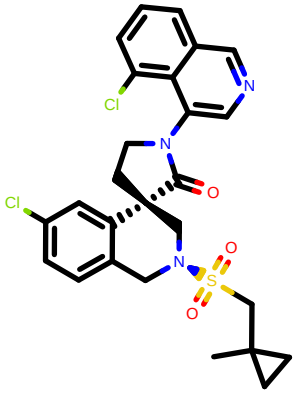
CID:	VLA-UNK-f2612802-2_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5S1(=O)=O)F)Cl
RUN:	RUN514
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.20

EDJ-MED-94fddcec-7_1



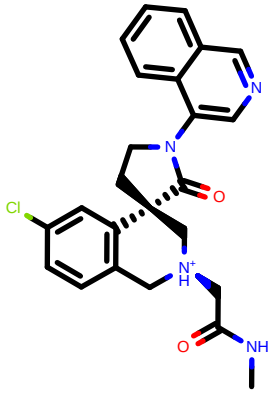
CID:	EDJ-MED-94fddcec-7_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN438
DDG (kcal/mol):	2.21
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-17_1



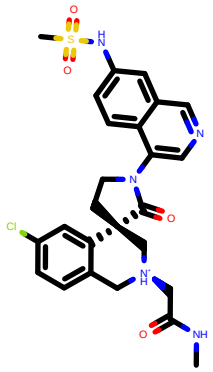
CID:	MAT-POS-853c0ffa-17_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN516
DDG (kcal/mol):	2.26
dDDG (kcal/mol):	0.26

LUO-POS-868e8996-11_1



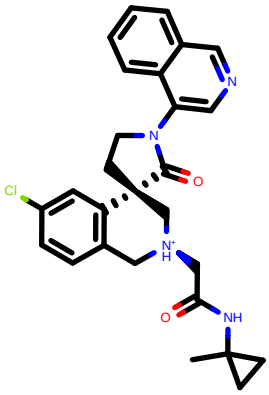
CID:	LUO-POS-868e8996-11_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN411
DDG (kcal/mol):	2.28
dDDG (kcal/mol):	0.17

MAT-POS-b4d6b7fc-7_1



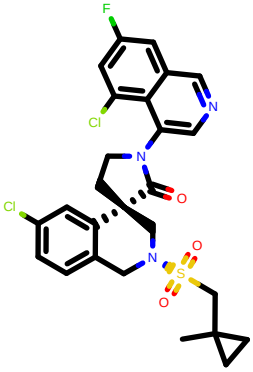
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN568
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.21

MAT-POS-69786b79-3_1



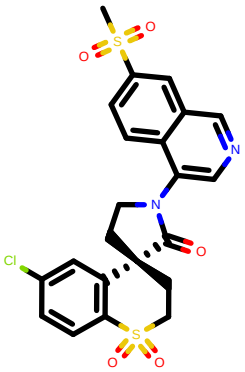
CID:	MAT-POS-69786b79-3_1
SMILES:	CC1(CC1)NC(=O)C[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN523
DDG (kcal/mol):	2.36
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-18_1



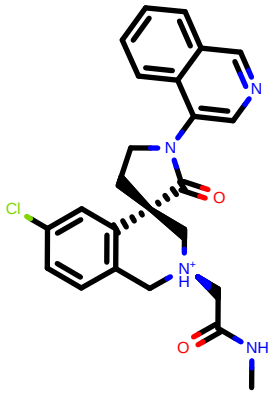
CID:	MAT-POS-853c0ffa-18_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN549
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.25

EDJ-MED-94fddcec-5_1



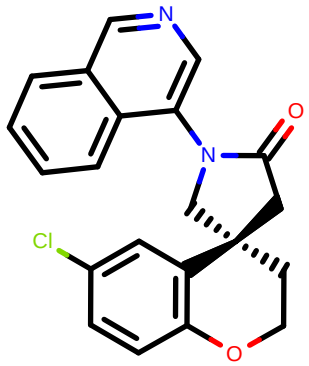
CID:	EDJ-MED-94fddcec-5_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN402
DDG (kcal/mol):	2.39
dDDG (kcal/mol):	0.13

EDJ-MED-8bb691af-4_1



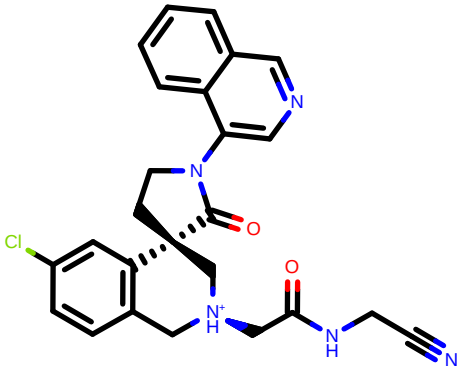
CID:	EDJ-MED-8bb691af-4_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN405
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.19

EDJ-MED-159244ea-3_1



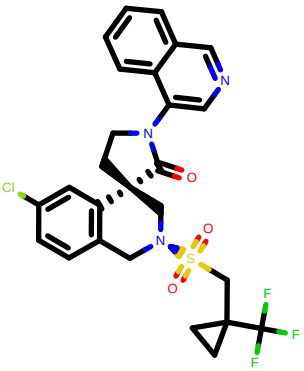
CID:	EDJ-MED-159244ea-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN341
DDG (kcal/mol):	2.43
dDDG (kcal/mol):	0.11

ALP-POS-ecbed2ba-14_1



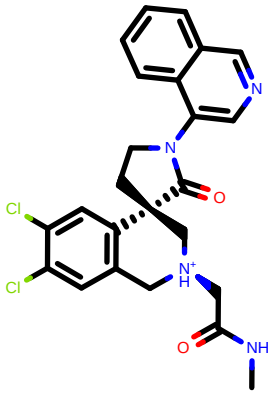
CID:	ALP-POS-ecbed2ba-14_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN436
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.20

EDJ-MED-5cd3920d-6_1



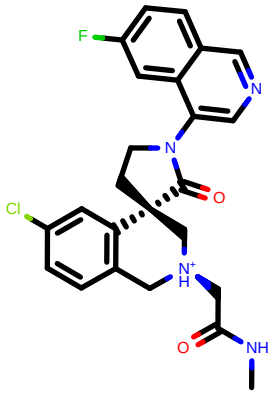
CID:	EDJ-MED-5cd3920d-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN604
DDG (kcal/mol):	2.46
dDDG (kcal/mol):	0.38

ALP-POS-afe0272e-1_1



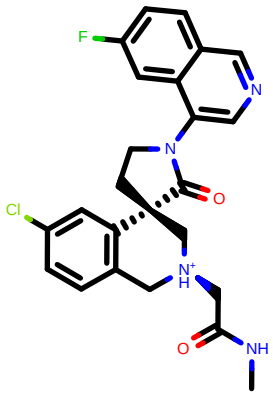
CID:	ALP-POS-afe0272e-1_1
SMILES:	CNC(=O)C[N@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN439
DDG (kcal/mol):	2.46
dDDG (kcal/mol):	0.24

LUO-POS-b4dec3be-2_1



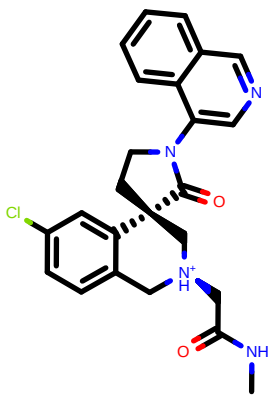
CID:	LUO-POS-b4dec3be-2_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN451
DDG (kcal/mol):	2.51
dDDG (kcal/mol):	0.19

MAT-POS-b4d6b7fc-5_1



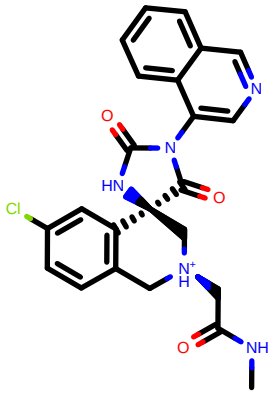
CID:	MAT-POS-b4d6b7fc-5_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN414
DDG (kcal/mol):	2.57
dDDG (kcal/mol):	0.19

LUO-POS-868e8996-12_1



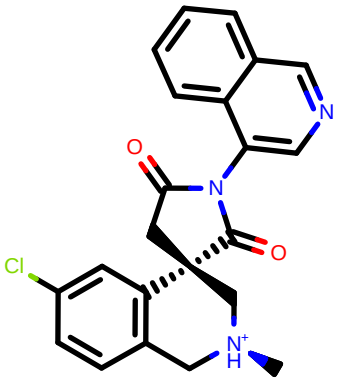
CID:	LUO-POS-868e8996-12_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN417
DDG (kcal/mol):	2.57
dDDG (kcal/mol):	0.21

VLA-MRT-a639d434-1_1



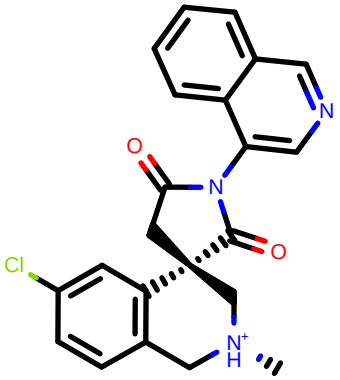
CID:	VLA-MRT-a639d434-1_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN393
DDG (kcal/mol):	2.62
dDDG (kcal/mol):	0.18

JOH-MSK-51c67e7d-1_1



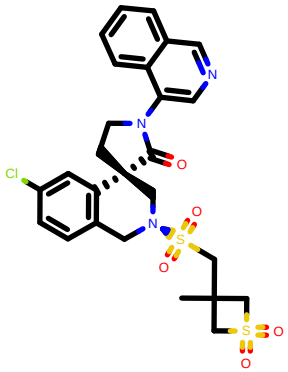
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN386
DDG (kcal/mol):	2.65
dDDG (kcal/mol):	0.09

JOH-MSK-51c67e7d-2_1



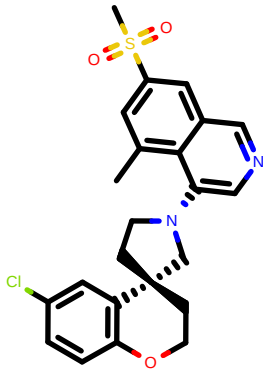
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN389
DDG (kcal/mol):	2.68
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-1_1



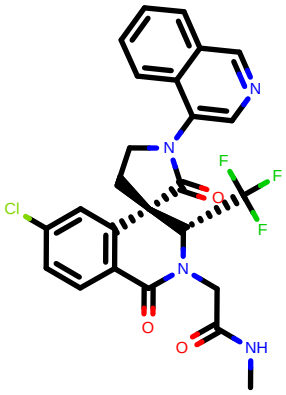
CID:	ALP-POS-ecbed2ba-1_1
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN585
DDG (kcal/mol):	2.69
dDDG (kcal/mol):	0.55

EDJ-MED-d7486dd1-1_1



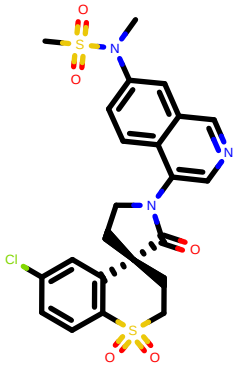
CID:	EDJ-MED-d7486dd1-1_1
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN378
DDG (kcal/mol):	2.69
dDDG (kcal/mol):	0.16

VLA-UNK-61877630-3_2



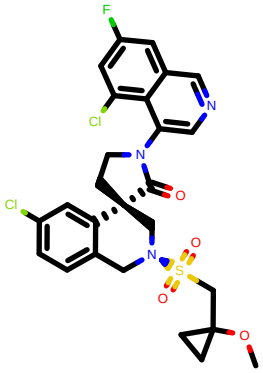
CID:	VLA-UNK-61877630-3_2
SMILES:	CNC(=O)CN1[C@H]([C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl)C(F)(F)F
RUN:	RUN574
DDG (kcal/mol):	2.69
dDDG (kcal/mol):	0.17

EDJ-MED-94fddcec-6_1



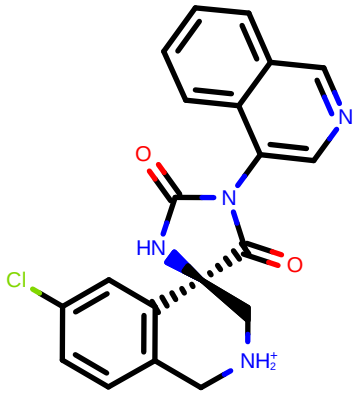
CID:	EDJ-MED-94fddcec-6_1
SMILES:	C[N@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN481
DDG (kcal/mol):	2.70
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-8_1



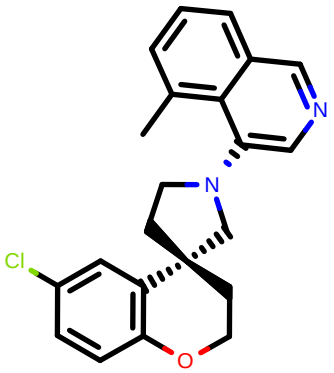
CID:	MAT-POS-853c0ffa-8_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN598
DDG (kcal/mol):	2.73
dDDG (kcal/mol):	0.27

VLA-MRT-a639d434-3_1



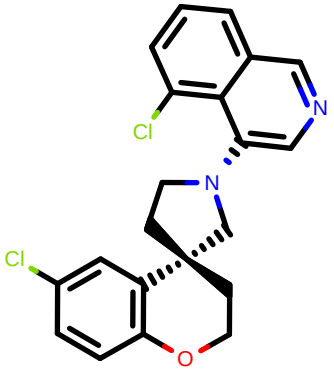
CID:	VLA-MRT-a639d434-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN384
DDG (kcal/mol):	2.76
dDDG (kcal/mol):	0.18

EDJ-MED-a6bab6fb-1_1



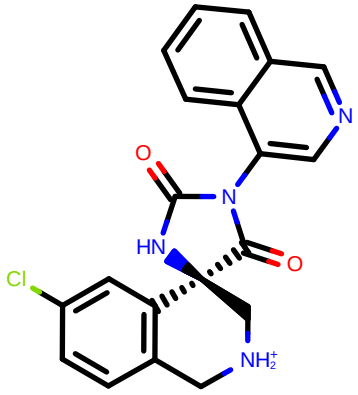
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN345
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.10

EDJ-MED-e78d5f1a-1_1



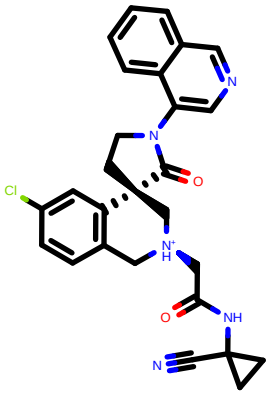
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN347
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.10

VLA-MRT-8c78ee15-1_1



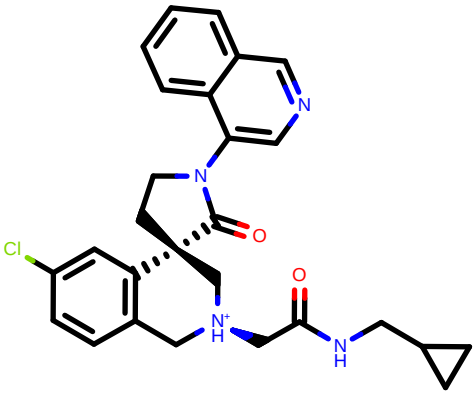
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN388
DDG (kcal/mol):	2.87
dDDG (kcal/mol):	0.16

MAT-POS-69786b79-4_1



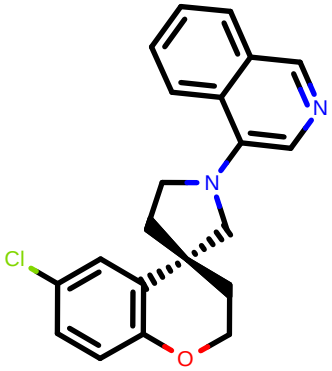
CID:	MAT-POS-69786b79-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN521
DDG (kcal/mol):	2.87
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-12_1



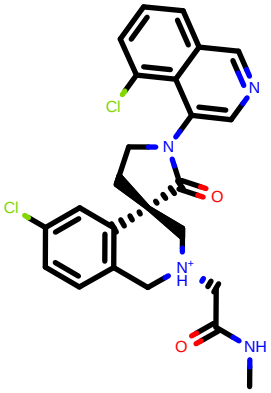
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN517
DDG (kcal/mol):	2.90
dDDG (kcal/mol):	0.22

EDJ-MED-159244ea-2_1



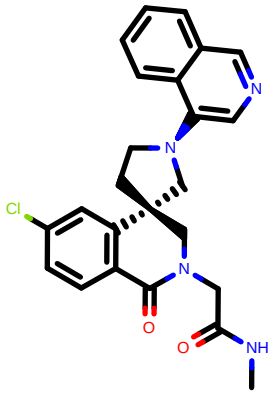
CID:	EDJ-MED-159244ea-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN343
DDG (kcal/mol):	2.91
dDDG (kcal/mol):	0.11

MAT-POS-1d5ab790-2_1



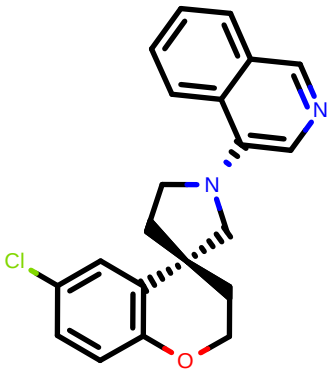
CID:	MAT-POS-1d5ab790-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN426
DDG (kcal/mol):	2.92
dDDG (kcal/mol):	0.24

EDJ-MED-8bb691af-7_1



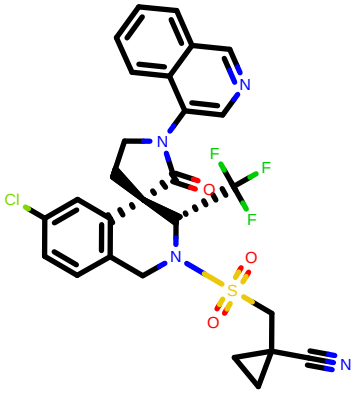
CID:	EDJ-MED-8bb691af-7_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN391
DDG (kcal/mol):	2.93
dDDG (kcal/mol):	0.14

MAT-POS-983b399a-2_1



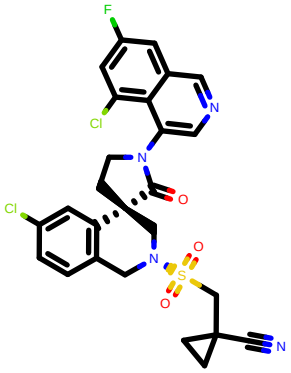
CID:	MAT-POS-983b399a-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN340
DDG (kcal/mol):	3.03
dDDG (kcal/mol):	0.11

VLA-UNK-61877630-9_2



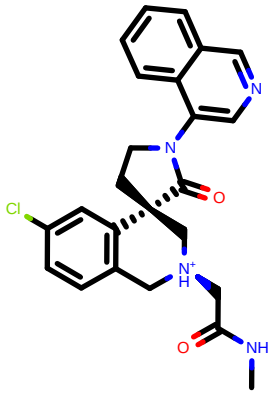
CID:	VLA-UNK-61877630-9_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@]4(C3=O)c5cc(ccc5C[N@@]([C@H]4C(F)(F)F)S(=O)(=O)CC6(CC6)C#N)Cl
RUN:	RUN620
DDG (kcal/mol):	3.11
dDDG (kcal/mol):	0.31

MAT-POS-853c0ffa-6_1



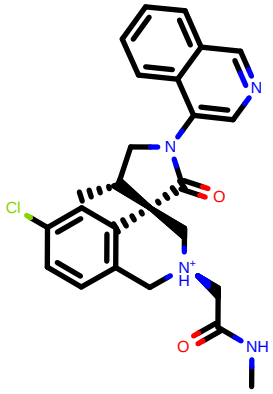
CID:	MAT-POS-853c0ffa-6_1
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN600
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.28

MAT-POS-c7726e07-6_1



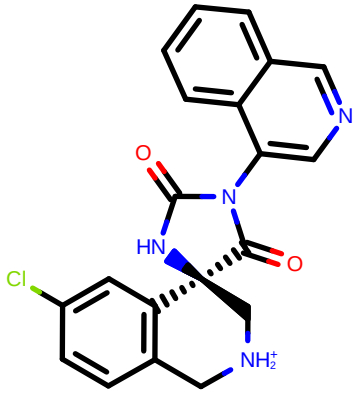
CID:	MAT-POS-c7726e07-6_1
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN429
DDG (kcal/mol):	3.29
dDDG (kcal/mol):	0.21

MAT-POS-50a80394-4_1



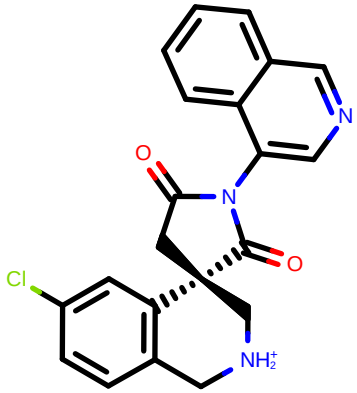
CID:	MAT-POS-50a80394-4_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN440
DDG (kcal/mol):	3.31
dDDG (kcal/mol):	0.19

VLA-MRT-8c78ee15-2_1



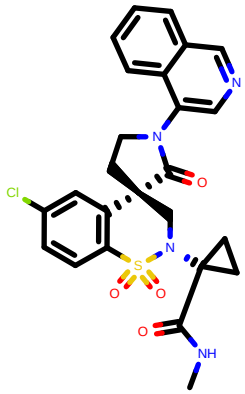
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN379
DDG (kcal/mol):	3.34
dDDG (kcal/mol):	0.18

JOH-MSK-1f2dff76-3_1



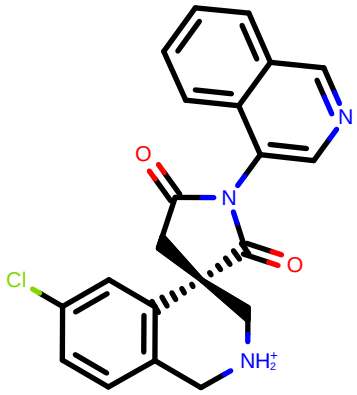
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN374
DDG (kcal/mol):	3.51
dDDG (kcal/mol):	0.15

EDJ-MED-976a33d5-3_1



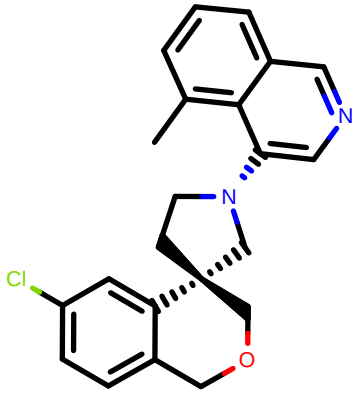
CID:	EDJ-MED-976a33d5-3_1
SMILES:	CNC(=O)C1(CC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN524
DDG (kcal/mol):	3.53
dDDG (kcal/mol):	0.49

JOH-MSK-1f2dff76-4_1



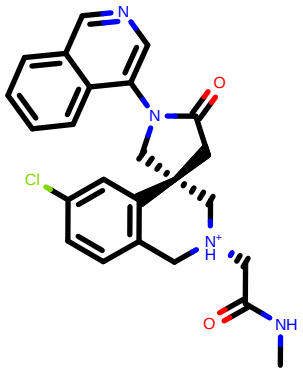
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN375
DDG (kcal/mol):	3.69
dDDG (kcal/mol):	0.15

EDJ-MED-f3cfbbb5-1_1



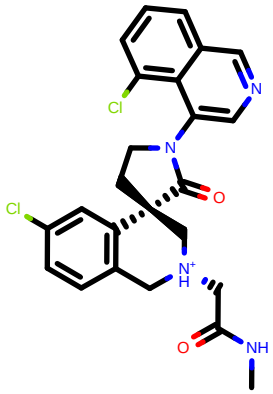
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN360
DDG (kcal/mol):	3.77
dDDG (kcal/mol):	0.10

EDJ-MED-8bb691af-3_1



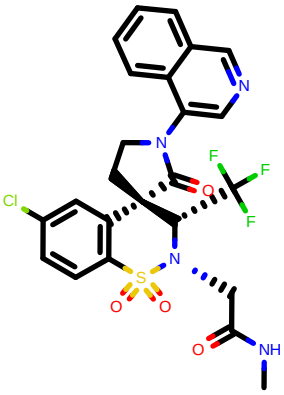
CID:	EDJ-MED-8bb691af-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN395
DDG (kcal/mol):	3.96
dDDG (kcal/mol):	0.23

MAT-POS-b4d6b7fc-6_1



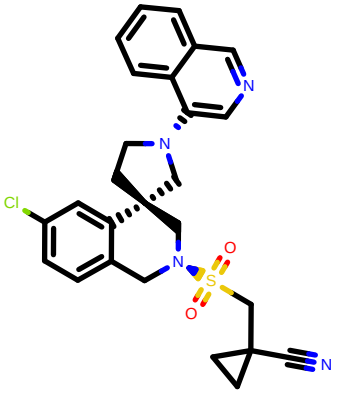
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN416
DDG (kcal/mol):	4.13
dDDG (kcal/mol):	0.25

VLA-UNK-f2612802-1_2



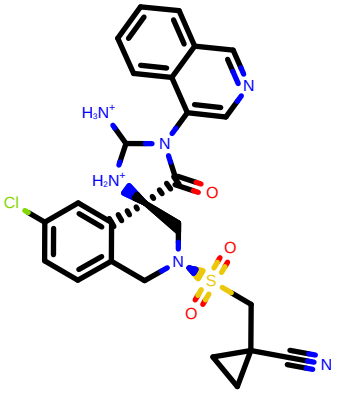
CID:	VLA-UNK-f2612802-1_2
SMILES:	CNC(=O)C[N@]1[C@H]([C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl)C(F)(F)F
RUN:	RUN602
DDG (kcal/mol):	4.54
dDDG (kcal/mol):	0.33

EDJ-MED-8bb691af-2_1



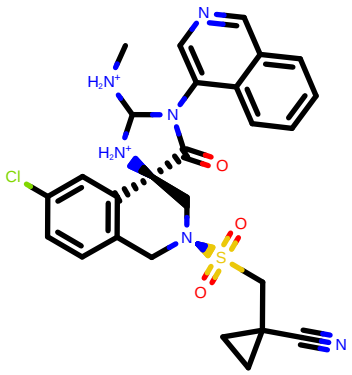
CID:	EDJ-MED-8bb691af-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN486
DDG (kcal/mol):	4.90
dDDG (kcal/mol):	0.31

LUO-POS-eaf50f21-1_1



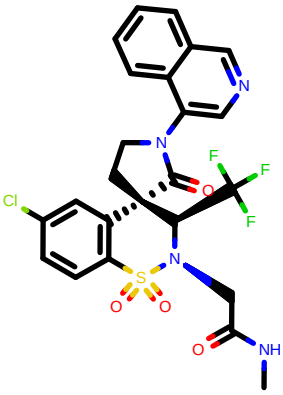
CID:	LUO-POS-eaf50f21-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)[NH+]=C3N
RUN:	RUN597
DDG (kcal/mol):	5.00
dDDG (kcal/mol):	0.27

LUO-POS-eaf50f21-2_1



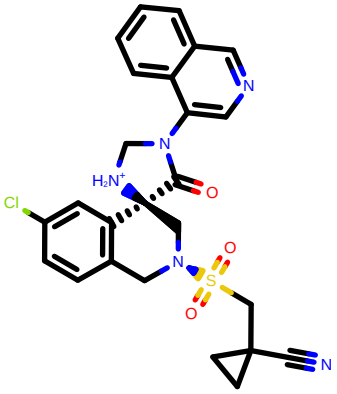
CID:	LUO-POS-eaf50f21-2_1
SMILES:	C/[NH+]=C/1\N[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN621
DDG (kcal/mol):	5.09
dDDG (kcal/mol):	0.29

VLA-UNK-f2612802-1_1



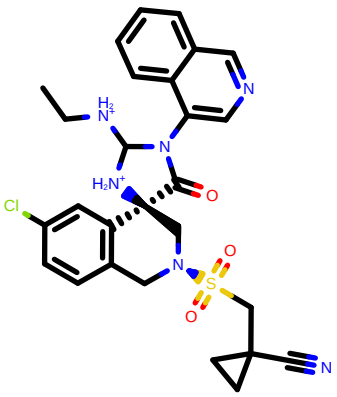
CID:	VLA-UNK-f2612802-1_1
SMILES:	CNC(=O)C[N@]1[C@@H][C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl)C(F)(F)F
RUN:	RUN608
DDG (kcal/mol):	5.11
dDDG (kcal/mol):	0.23

EDG-MED-00af8776-1_1



CID:	EDG-MED-00af8776-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN533
DDG (kcal/mol):	5.40
dDDG (kcal/mol):	0.30

LUO-POS-eaf50f21-5_1



CID:	LUO-POS-eaf50f21-5_1
SMILES:	CC/[NH+]=C/1\N[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN635
DDG (kcal/mol):	5.53
dDDG (kcal/mol):	0.33