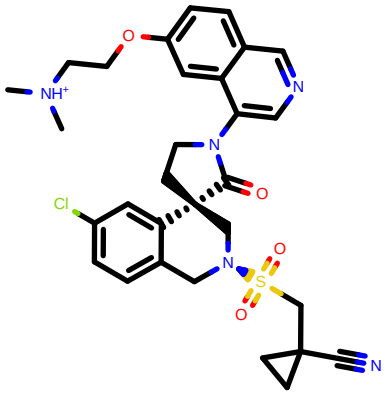
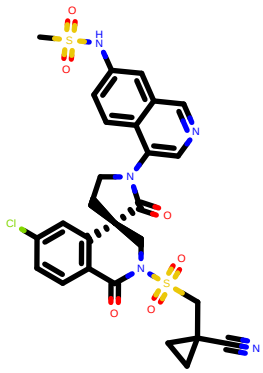
MAT-POS-38eb6498-1_2



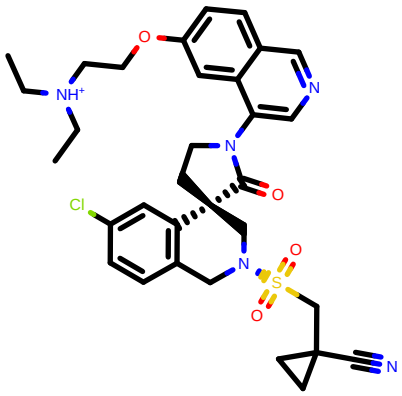
CID:	MAT-POS-38eb6498-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1905
DDG (kcal/mol):	-5.74
dDDG (kcal/mol):	0.57

EDJ-MED-9f4ac58c-3_1



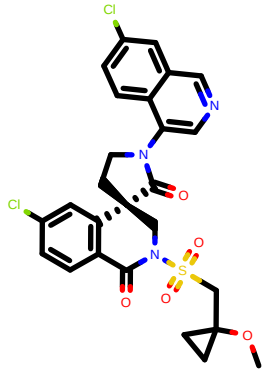
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1892
DDG (kcal/mol):	-4.68
dDDG (kcal/mol):	0.53

MAT-POS-40ad851a-3_2



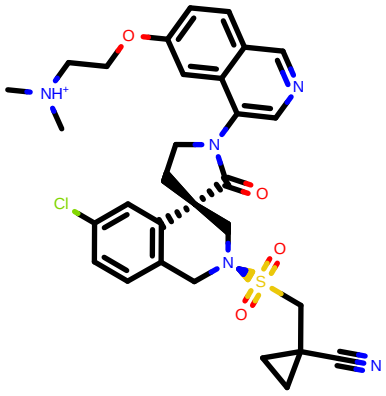
CID:	MAT-POS-40ad851a-3_2
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1927
DDG (kcal/mol):	-3.75
dDDG (kcal/mol):	0.57

EDJ-MED-9f4ac58c-5_1



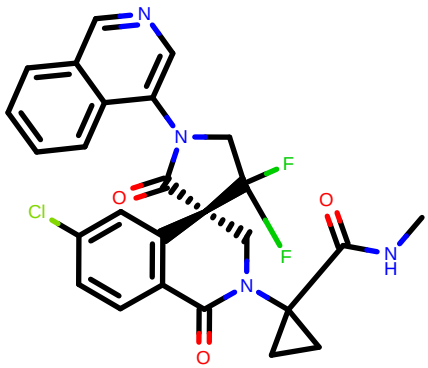
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl
RUN:	RUN1817
DDG (kcal/mol):	-3.43
dDDG (kcal/mol):	0.44

LUO-POS-8484f2d3-2_2



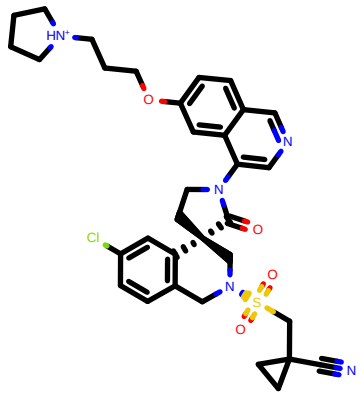
CID:	LUO-POS-8484f2d3-2_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1907
DDG (kcal/mol):	-3.06
dDDG (kcal/mol):	0.57

EDJ-MED-7e491f08-2_1



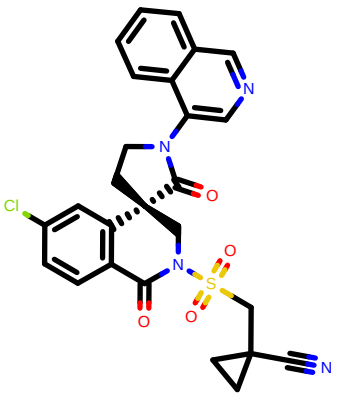
CID:	EDJ-MED-7e491f08-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(CC3(F)F)c5cncc6c5cccc6
RUN:	RUN1805
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.15

MAT-POS-40ad851a-5_2



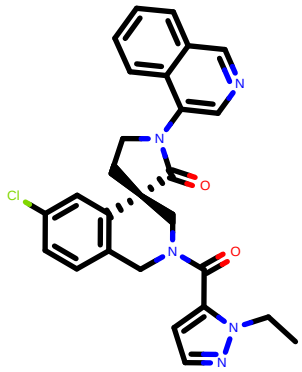
CID:	MAT-POS-40ad851a-5_2
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1934
DDG (kcal/mol):	-2.98
dDDG (kcal/mol):	0.68

EDJ-MED-9f4ac58c-2_1



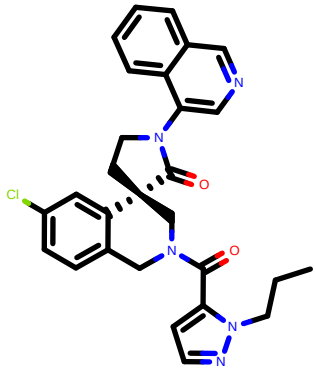
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1755
DDG (kcal/mol):	-2.85
dDDG (kcal/mol):	0.55

MAT-POS-be048f2c-5_1



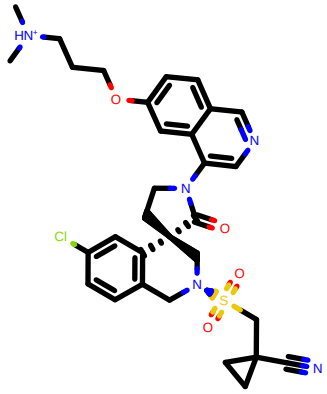
CID:	MAT-POS-be048f2c-5_1
SMILES:	CCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1739
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.15

MAT-POS-be048f2c-8_1



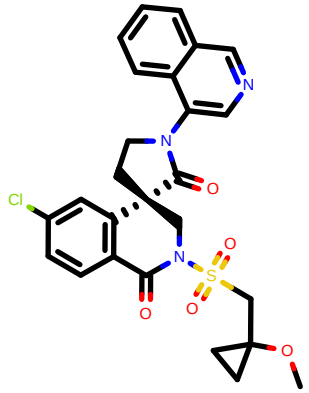
CID:	MAT-POS-be048f2c-8_1
SMILES:	CCCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1801
DDG (kcal/mol):	-2.76
dDDG (kcal/mol):	0.17

MAT-POS-40ad851a-4_1



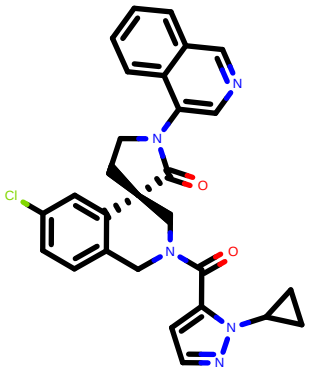
CID:	MAT-POS-40ad851a-4_1
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1915
DDG (kcal/mol):	-2.74
dDDG (kcal/mol):	0.64

EDJ-MED-9f4ac58c-6_1



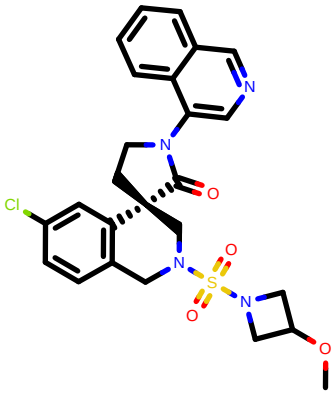
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1759
DDG (kcal/mol):	-2.72
dDDG (kcal/mol):	0.36

MAT-POS-be048f2c-7_1



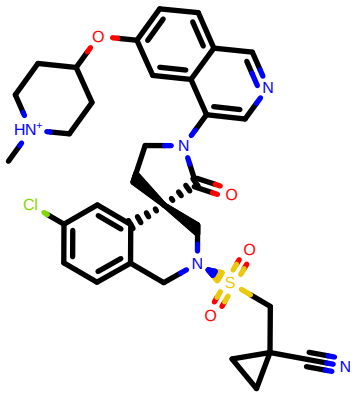
CID:	MAT-POS-be048f2c-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(Cc5c4cc(cc5)Cl)C(=O)c6ccnn6C7CC7
RUN:	RUN1787
DDG (kcal/mol):	-2.71
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-10_2



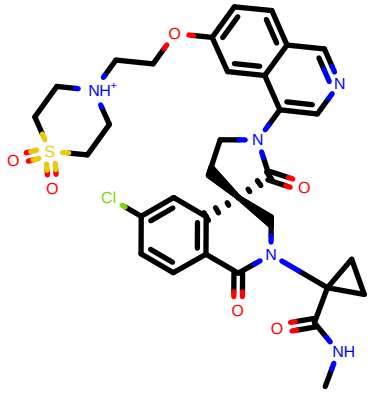
CID:	ALP-POS-ecbed2ba-10_2
SMILES:	COC1CN(C1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1714
DDG (kcal/mol):	-2.38
dDDG (kcal/mol):	0.72

LUO-POS-d1147590-1_2



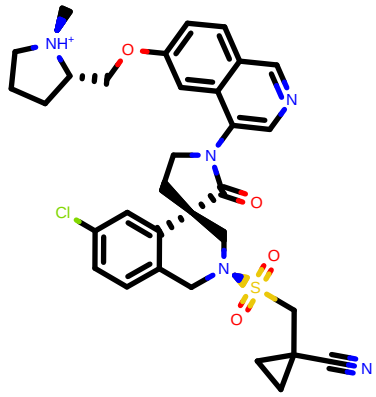
CID:	LUO-POS-d1147590-1_2
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1937
DDG (kcal/mol):	-2.37
dDDG (kcal/mol):	0.61

EDJ-MED-dfa1d800-3_1



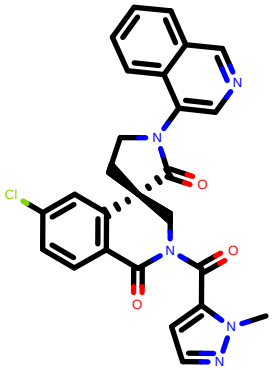
CID:	EDJ-MED-dfa1d800-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CCS(=O)(=O)CC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1946
DDG (kcal/mol):	-2.32
dDDG (kcal/mol):	0.34

MAT-POS-40ad851a-1_7



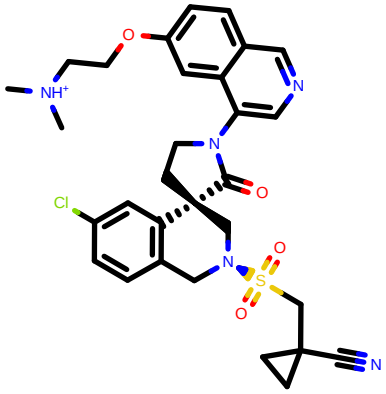
CID:	MAT-POS-40ad851a-1_7
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1938
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.61

EDJ-MED-cc48ee33-2_1



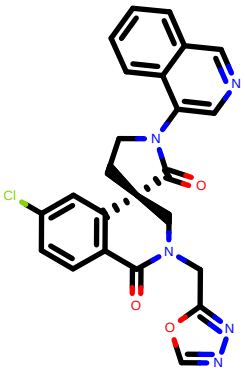
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	Cn1c(ccn1)C(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1730
DDG (kcal/mol):	-2.13
dDDG (kcal/mol):	0.18

LUO-POS-8484f2d3-1_2



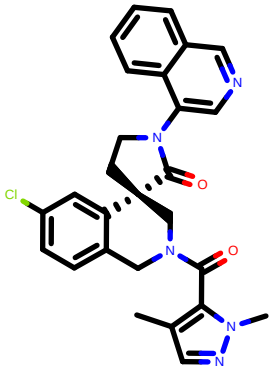
CID:	LUO-POS-8484f2d3-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1902
DDG (kcal/mol):	-2.09
dDDG (kcal/mol):	0.76

PET-UNK-aa57768f-1_1



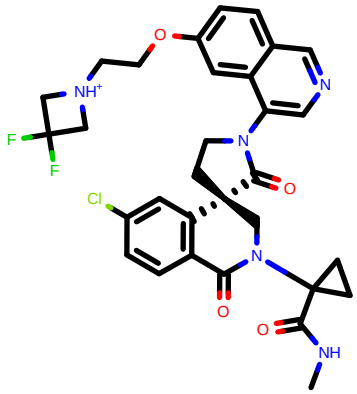
CID:	PET-UNK-aa57768f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN1605
DDG (kcal/mol):	-2.03
dDDG (kcal/mol):	0.15

EDJ-MED-cc48ee33-4_1



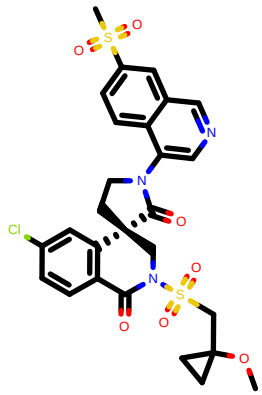
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	Cc1cnn(c1C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl)C
RUN:	RUN1731
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.17

EDJ-MED-dfa1d800-5_1



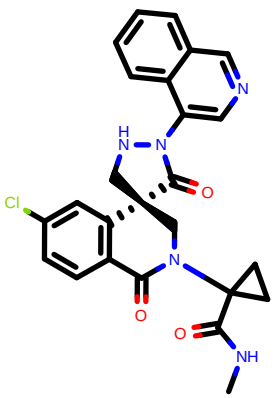
CID:	EDJ-MED-dfa1d800-5_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CC(C6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN1920
DDG (kcal/mol):	-1.93
dDDG (kcal/mol):	0.30

EDJ-MED-9f4ac58c-8_1



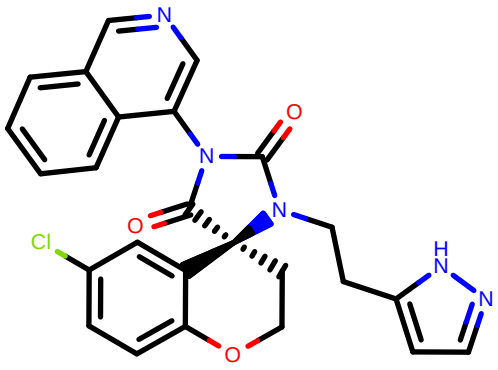
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1883
DDG (kcal/mol):	-1.91
dDDG (kcal/mol):	0.55

EDJ-MED-fed7ac0b-2_1



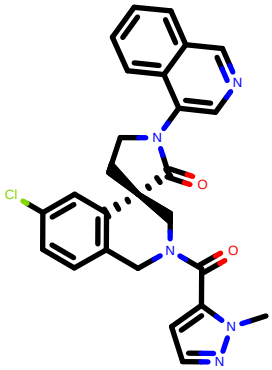
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CNN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1674
DDG (kcal/mol):	-1.83
dDDG (kcal/mol):	0.15

VLA-UNK-f702bf1c-1_1



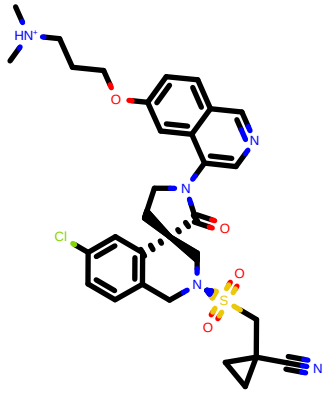
CID:	VLA-UNK-f702bf1c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6ccn[nH]6
RUN:	RUN1651
DDG (kcal/mol):	-1.82
dDDG (kcal/mol):	0.20

EDJ-MED-cc48ee33-3_1



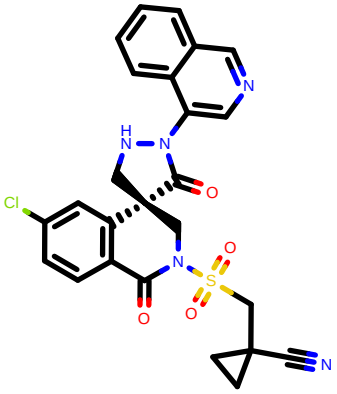
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1672
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.17

MAT-POS-40ad851a-4_2



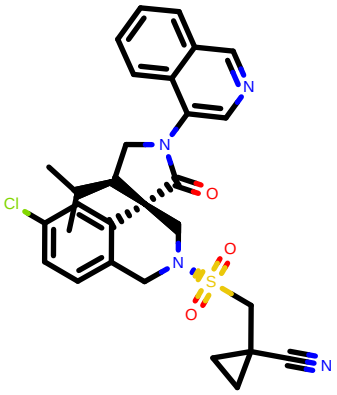
CID:	MAT-POS-40ad851a-4_2
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1914
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.57

EDJ-MED-fed7ac0b-3_1



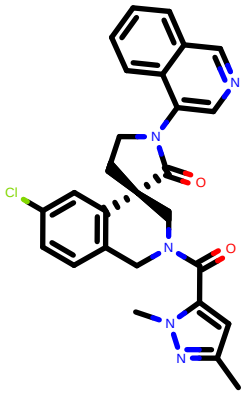
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CN3)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1784
DDG (kcal/mol):	-1.78
dDDG (kcal/mol):	0.46

MAT-POS-50a80394-3_2



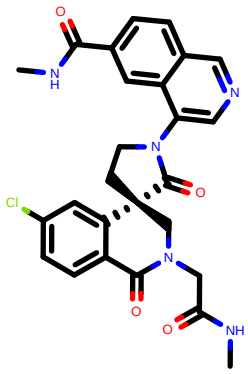
CID:	MAT-POS-50a80394-3_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1854
DDG (kcal/mol):	-1.77
dDDG (kcal/mol):	0.51

EDJ-MED-cc48ee33-5_1



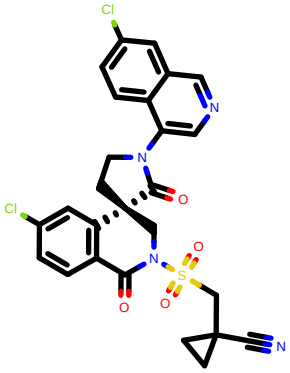
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	Cc1cc(n(n1)C)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1737
DDG (kcal/mol):	-1.76
dDDG (kcal/mol):	0.18

MAT-POS-38eb6498-6_1



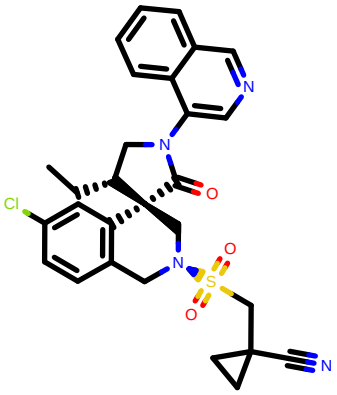
CID:	MAT-POS-38eb6498-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)C(=O)NC)c5cc(ccc5C1=O)Cl
RUN:	RUN1780
DDG (kcal/mol):	-1.64
dDDG (kcal/mol):	0.20

EDJ-MED-9f4ac58c-1_1



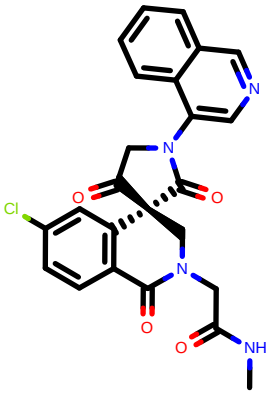
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	c1cc2c(cc1Cl)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1814
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.37

MAT-POS-50a80394-2_3



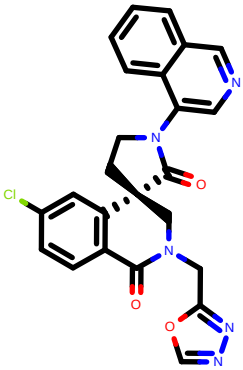
CID:	MAT-POS-50a80394-2_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN1827
DDG (kcal/mol):	-1.63
dDDG (kcal/mol):	0.76

EDJ-MED-a12e3a20-2_1



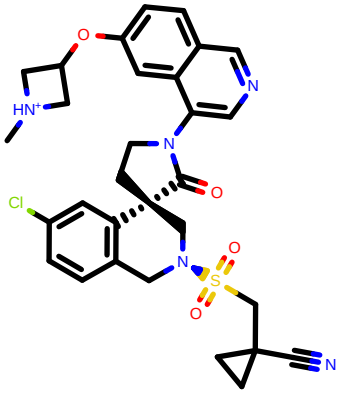
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=O)CN(C2=O)c4cncc5c4cccc5
RUN:	RUN1627
DDG (kcal/mol):	-1.61
dDDG (kcal/mol):	0.13

PET-UNK-aa57768f-7_1



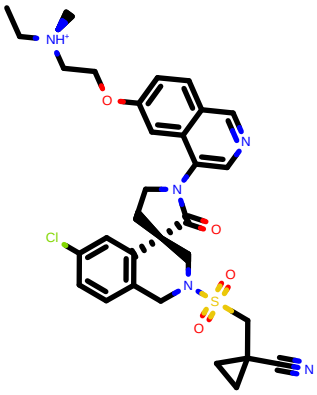
CID:	PET-UNK-aa57768f-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN1620
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.14

EDJ-MED-ee81482e-2_1



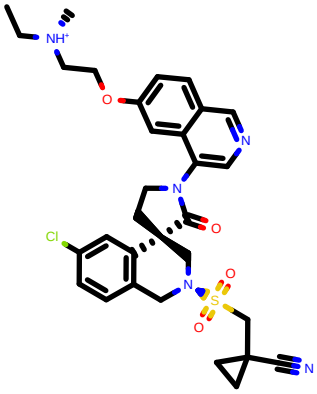
CID:	EDJ-MED-ee81482e-2_1
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1903
DDG (kcal/mol):	-1.57
dDDG (kcal/mol):	0.39

MAT-POS-40ad851a-2_3



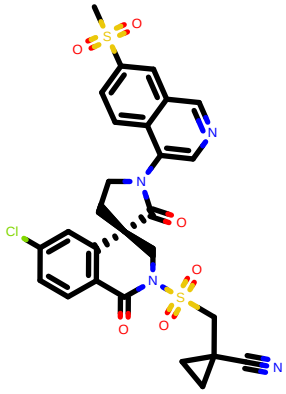
CID:	MAT-POS-40ad851a-2_3
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1911
DDG (kcal/mol):	-1.52
dDDG (kcal/mol):	0.57

MAT-POS-40ad851a-2_4



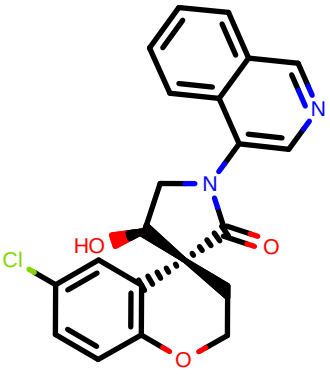
CID:	MAT-POS-40ad851a-2_4
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1910
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.74

EDJ-MED-9f4ac58c-4_1



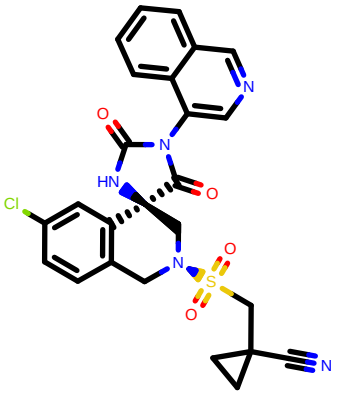
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1877
DDG (kcal/mol):	-1.41
dDDG (kcal/mol):	0.61

DAR-DIA-0f7b7cd9-9_1



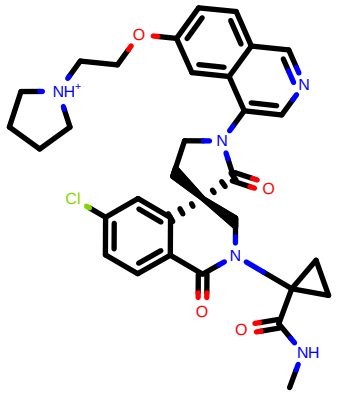
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1491
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.09

MAT-POS-c2d406ed-1_2



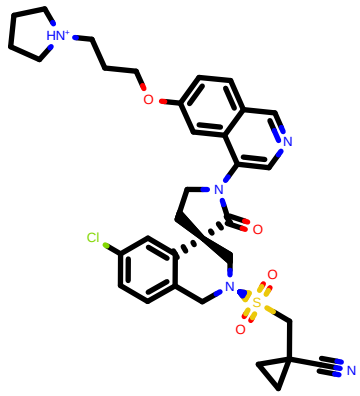
CID:	MAT-POS-c2d406ed-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN1771
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.41

EDJ-MED-dfa1d800-1_1



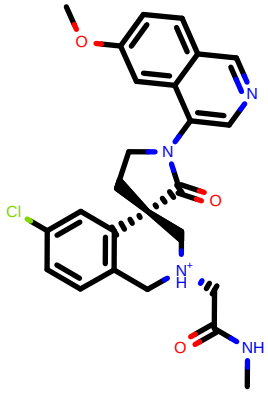
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1900
DDG (kcal/mol):	-1.30
dDDG (kcal/mol):	0.32

MAT-POS-40ad851a-5_1



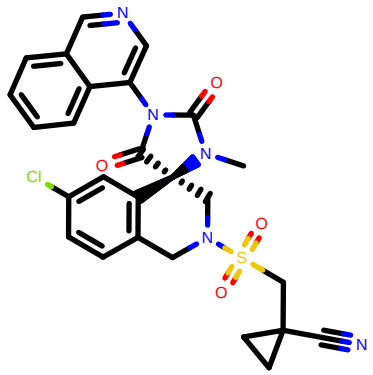
CID:	MAT-POS-40ad851a-5_1
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1943
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.83

EDJ-MED-b6c6ee2b-2_1



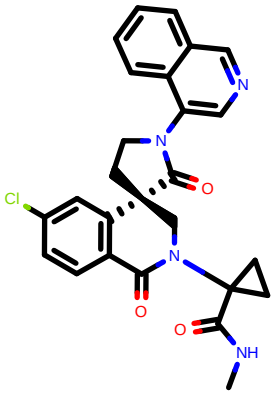
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN1639
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.30

MAT-POS-c2d406ed-2_2



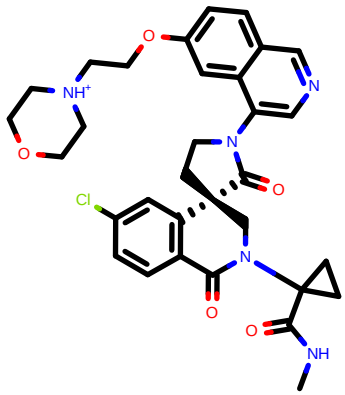
CID:	MAT-POS-c2d406ed-2_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1825
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.37

MAT-POS-576f7758-2_1



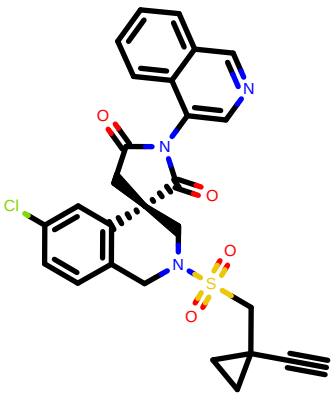
CID:	MAT-POS-576f7758-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1666
DDG (kcal/mol):	-1.26
dDDG (kcal/mol):	0.19

EDJ-MED-dfa1d800-2_1



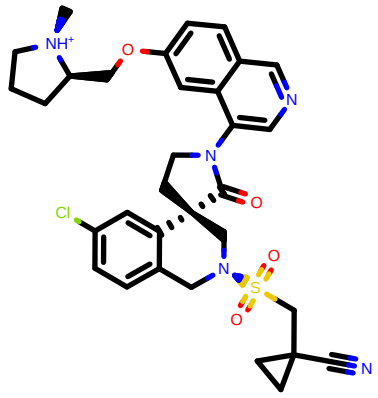
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCOCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1922
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.34

PET-UNK-94036022-4_2



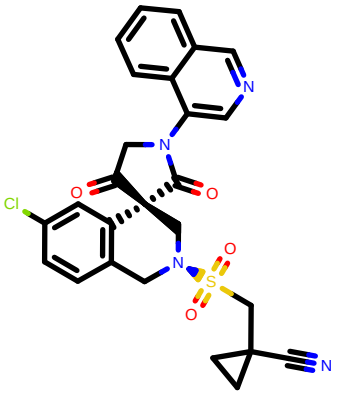
CID:	PET-UNK-94036022-4_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1810
DDG (kcal/mol):	-1.24
dDDG (kcal/mol):	0.35

MAT-POS-40ad851a-1_5



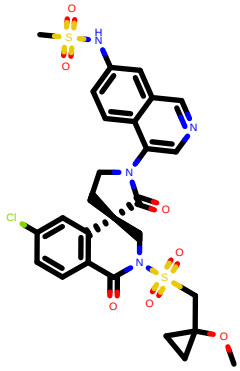
CID:	MAT-POS-40ad851a-1_5
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1924
DDG (kcal/mol):	-1.23
dDDG (kcal/mol):	0.74

EDJ-MED-a12e3a20-1_2



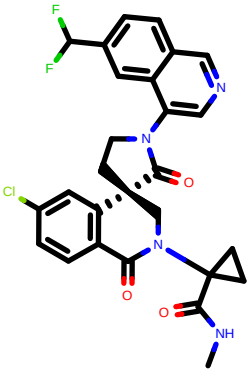
CID:	EDJ-MED-a12e3a20-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1793
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.57

EDJ-MED-9f4ac58c-7_1



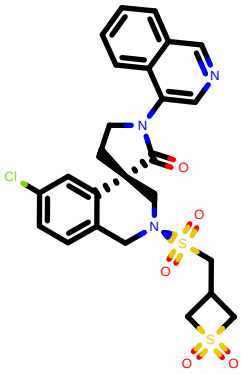
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1890
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.45

EDJ-MED-5cd3920d-4_1



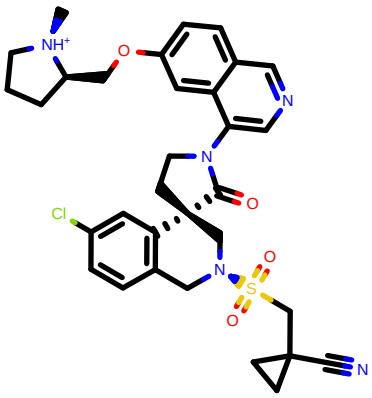
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)C(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1839
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-5_2



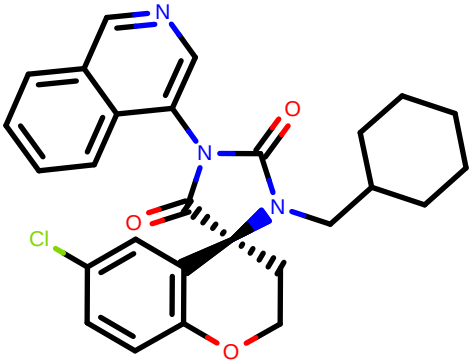
CID:	ALP-POS-ecbed2ba-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN1775
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.85

MAT-POS-40ad851a-1_1



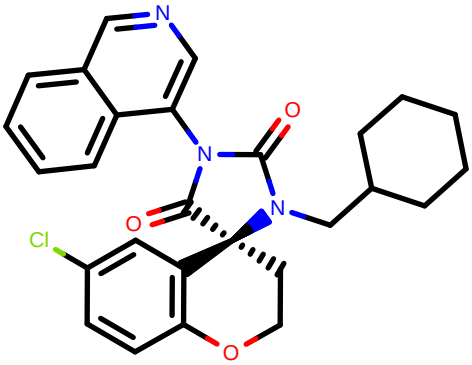
CID:	MAT-POS-40ad851a-1_1
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3ncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1925
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.56

VLA-UCB-34f3ed0c-14_1



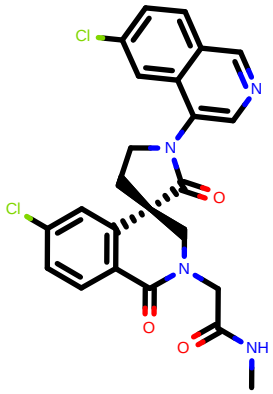
CID:	VLA-UCB-34f3ed0c-14_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN1635
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.20

VLA-UNK-f702bf1c-6_1



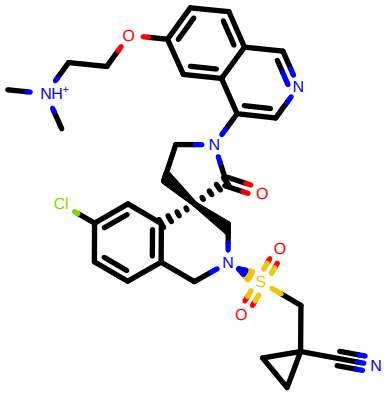
CID:	VLA-UNK-f702bf1c-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN1642
DDG (kcal/mol):	-1.11
dDDG (kcal/mol):	0.21

LUO-POS-8c3e556a-2_1



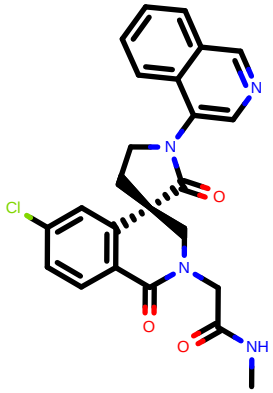
CID:	LUO-POS-8c3e556a-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1641
DDG (kcal/mol):	-1.10
dDDG (kcal/mol):	0.17

MAT-POS-853c0ffa-9_2



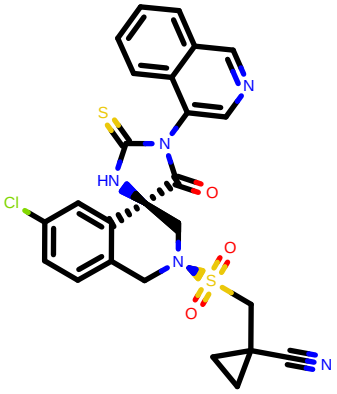
CID:	MAT-POS-853c0ffa-9_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1897
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.58

PET-UNK-14142a25-10_1



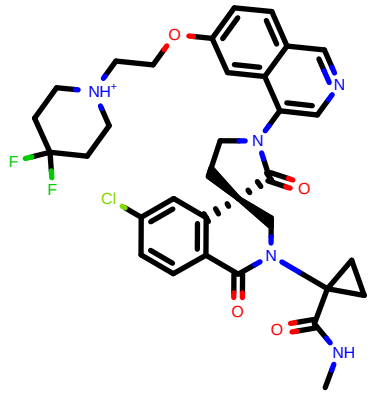
CID:	PET-UNK-14142a25-10_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1566
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.16

MAT-POS-c2d406ed-3_2



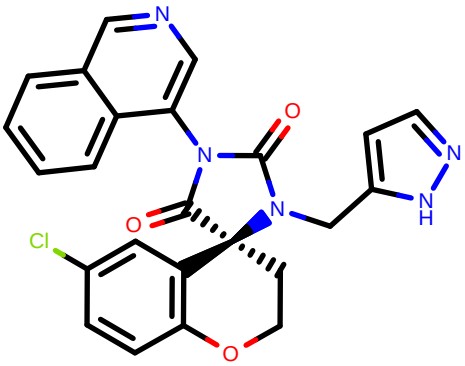
CID:	MAT-POS-c2d406ed-3_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN1786
DDG (kcal/mol):	-1.02
dDDG (kcal/mol):	0.35

EDJ-MED-dfa1d800-4_1



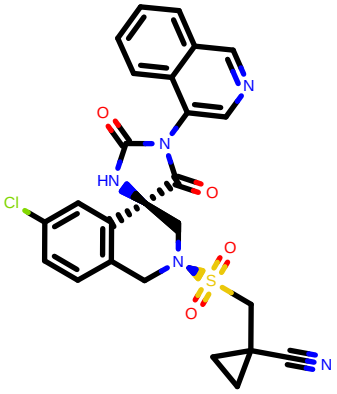
CID:	EDJ-MED-dfa1d800-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCC(CC6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN1944
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.48

VLA-UNK-f702bf1c-2_1



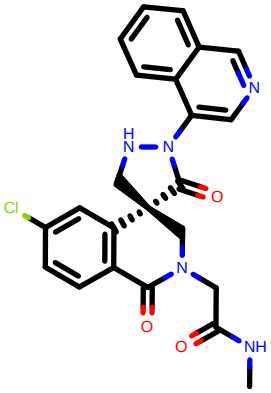
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6ccn[nH]6
RUN:	RUN1597
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.18

MAT-POS-c2d406ed-1_1



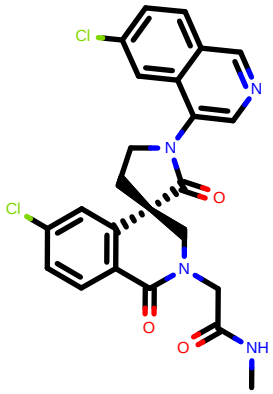
CID:	MAT-POS-c2d406ed-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN1781
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.25

EDJ-MED-fed7ac0b-1_1



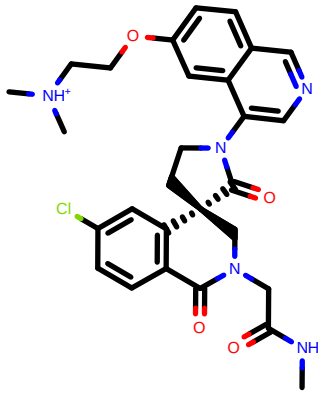
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	CNC(=O)CN1C[C@]2(CNN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1571
DDG (kcal/mol):	-1.00
dDDG (kcal/mol):	0.14

EDG-MED-b1ef7fe3-1_1



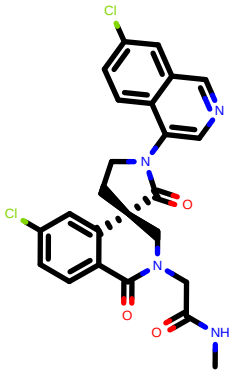
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1594
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.18

EDJ-MED-b6c6ee2b-5_1



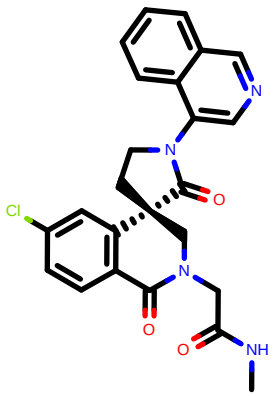
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN1886
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.28

EDG-MED-b1ef7fe3-4_1



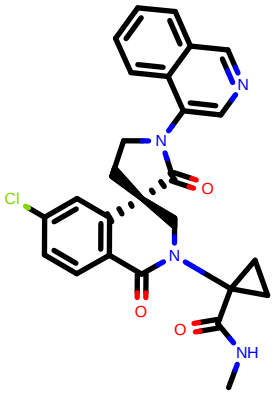
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1601
DDG (kcal/mol):	-0.99
dDDG (kcal/mol):	0.13

EDJ-MED-8bb691af-8_1



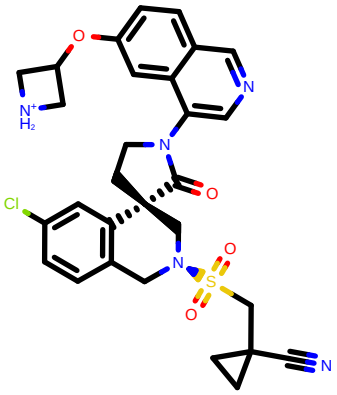
CID:	EDJ-MED-8bb691af-8_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1552
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.15

EDJ-MED-976a33d5-1_1



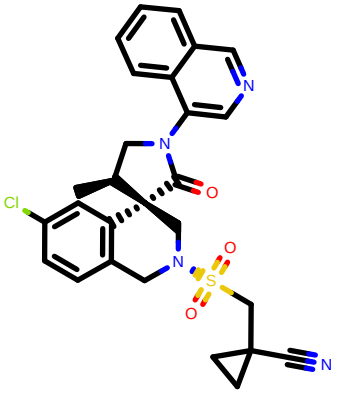
CID:	EDJ-MED-976a33d5-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1671
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.20

EDJ-MED-ee81482e-1_1



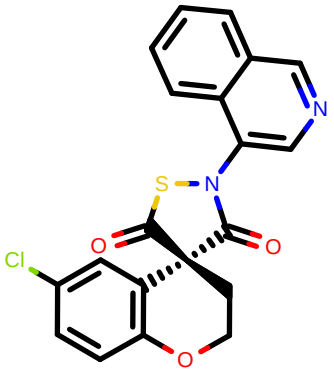
CID:	EDJ-MED-ee81482e-1_1
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1894
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.41

MAT-POS-50a80394-1_2



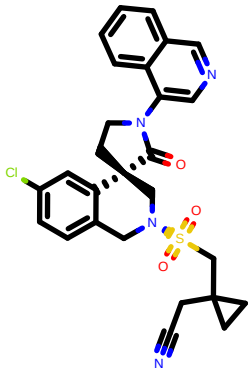
CID:	MAT-POS-50a80394-1_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1800
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.33

DAR-DIA-0f7b7cd9-8_1



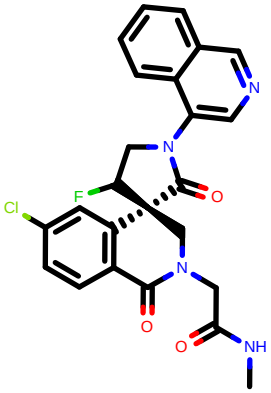
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C(=O)S3
RUN:	RUN1489
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-22_1



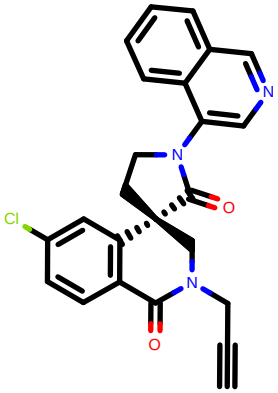
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)CC#N
RUN:	RUN1779
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.39

EDJ-MED-fd8ed875-5_1



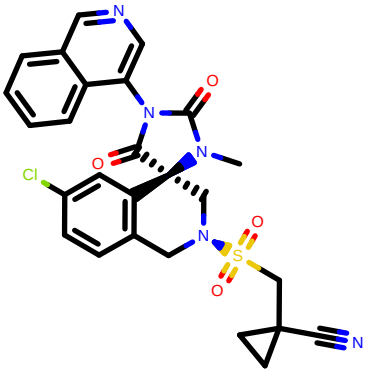
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cncc5c4cccc5)F
RUN:	RUN1631
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.13

PET-UNK-aa57768f-9_1



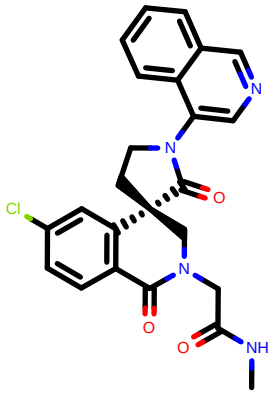
CID:	PET-UNK-aa57768f-9_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1519
DDG (kcal/mol):	-0.89
dDDG (kcal/mol):	0.17

MAT-POS-c2d406ed-2_1



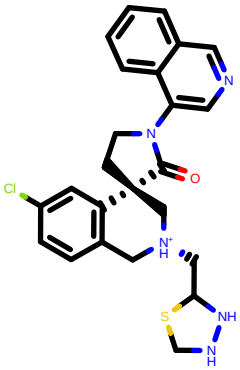
CID:	MAT-POS-c2d406ed-2_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN1823
DDG (kcal/mol):	-0.88
dDDG (kcal/mol):	0.31

LUO-POS-9931618f-1_1



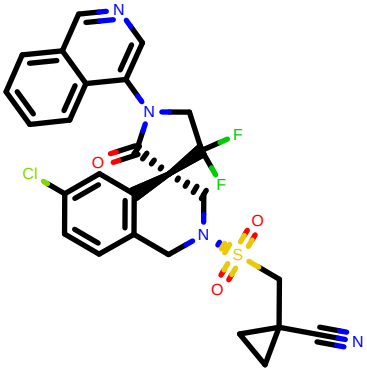
CID:	LUO-POS-9931618f-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1581
DDG (kcal/mol):	-0.85
dDDG (kcal/mol):	0.18

MAT-POS-96396902-1_1



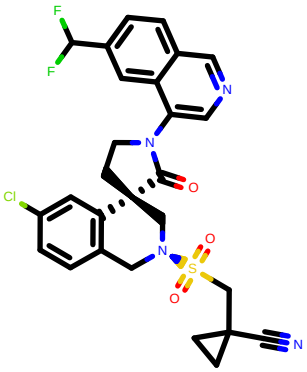
CID:	MAT-POS-96396902-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1587
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.24

EDJ-MED-7e491f08-1_1



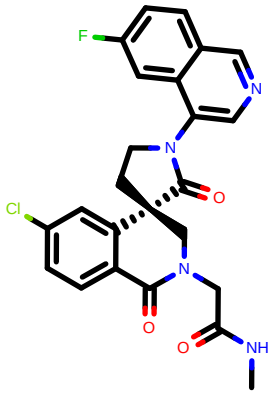
CID:	EDJ-MED-7e491f08-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN1834
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.74

EDJ-MED-5cd3920d-2_2



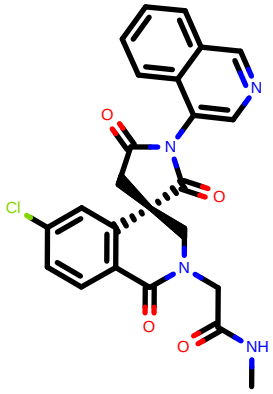
CID:	EDJ-MED-5cd3920d-2_2
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1860
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.58

EDG-MED-b1ef7fe3-2_1



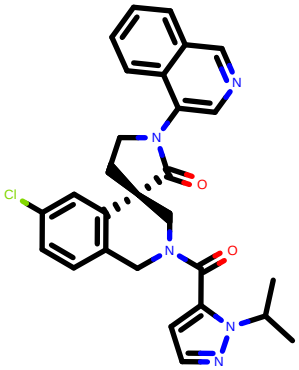
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1603
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.15

LUO-POS-868e8996-8_1



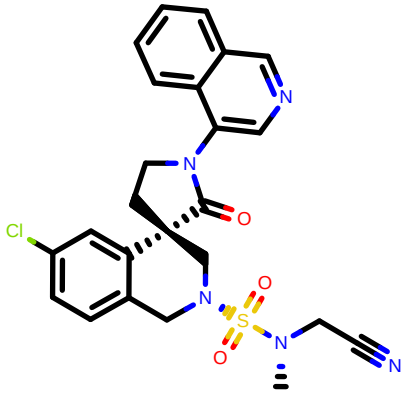
CID:	LUO-POS-868e8996-8_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1606
DDG (kcal/mol):	-0.80
dDDG (kcal/mol):	0.14

MAT-POS-be048f2c-6_1



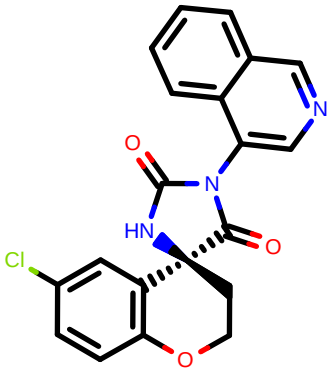
CID:	MAT-POS-be048f2c-6_1
SMILES:	CC(C)n1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1792
DDG (kcal/mol):	-0.76
dDDG (kcal/mol):	0.23

ALP-POS-ecbed2ba-17_4



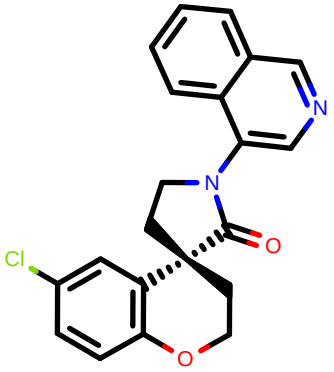
CID:	ALP-POS-ecbed2ba-17_4
SMILES:	C[N@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1663
DDG (kcal/mol):	-0.75
dDDG (kcal/mol):	0.55

VLA-UCB-34f3ed0c-11_1



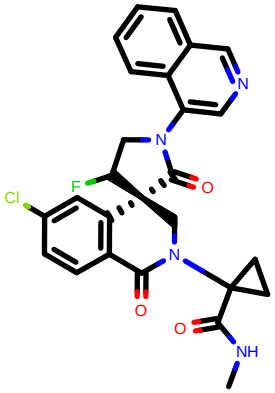
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1488
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.07

MAT-POS-983b399a-1_1



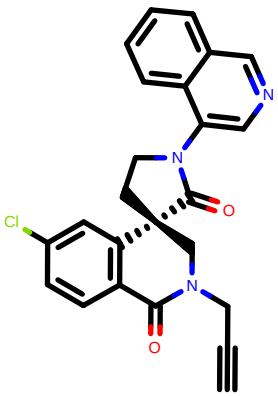
CID:	MAT-POS-983b399a-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1470
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.09

EDJ-MED-fd8ed875-6_1



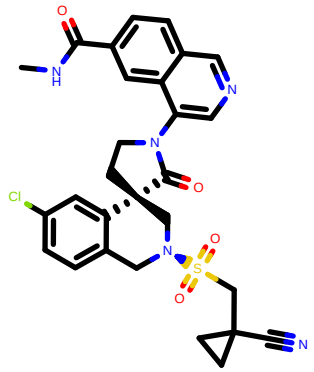
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	CNC(=O)C1(CC1)N2C[C@@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5cccc6)F
RUN:	RUN1747
DDG (kcal/mol):	-0.67
dDDG (kcal/mol):	0.17

PET-UNK-aa57768f-3_1



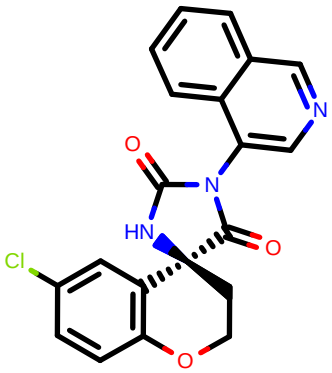
CID:	PET-UNK-aa57768f-3_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1515
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.29

MAT-POS-38eb6498-2_1



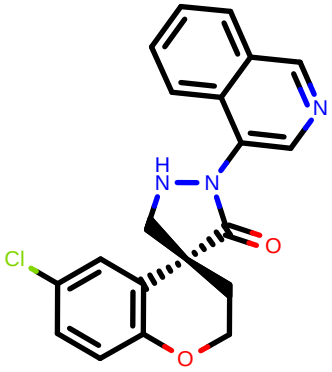
CID:	MAT-POS-38eb6498-2_1
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1871
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.41

VLA-UCB-29506327-1_1



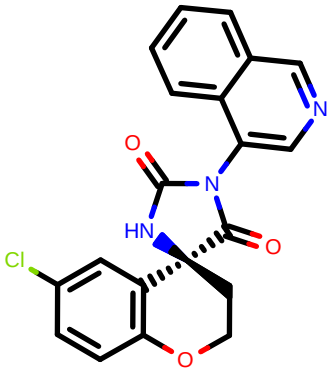
CID:	VLA-UCB-29506327-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1490
DDG (kcal/mol):	-0.65
dDDG (kcal/mol):	0.08

BEN-BAS-c2bc0d80-3_1



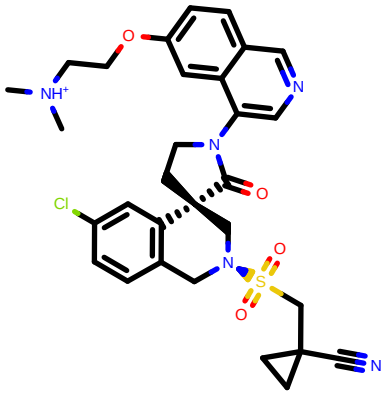
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3
RUN:	RUN1471
DDG (kcal/mol):	-0.64
dDDG (kcal/mol):	0.09

VLA-UNK-cf7facf1-1_1



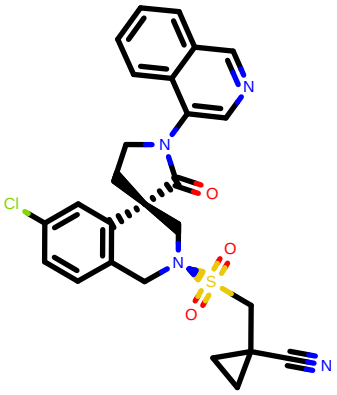
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1483
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.07

LUO-POS-8484f2d3-1_1



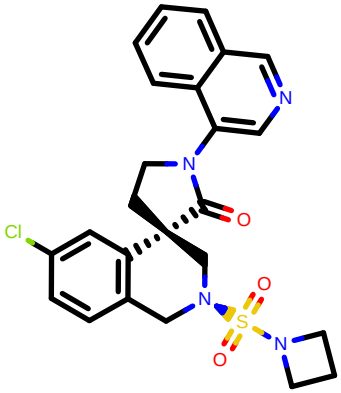
CID:	LUO-POS-8484f2d3-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1906
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.63

MIK-ENA-5d9157e9-1_2



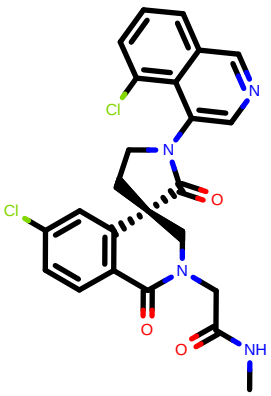
CID:	MIK-ENA-5d9157e9-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1720
DDG (kcal/mol):	-0.60
dDDG (kcal/mol):	0.56

ALP-POS-ecbed2ba-20_1



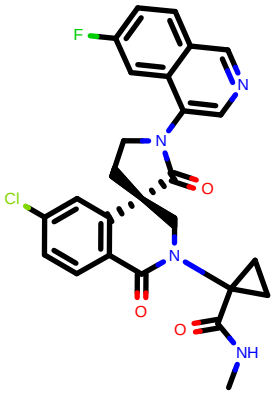
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN1619
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.60

MAT-POS-1d5ab790-3_1



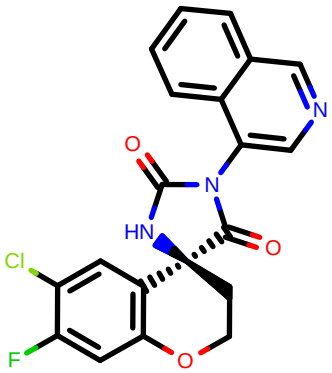
CID:	MAT-POS-1d5ab790-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1629
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.15

EDJ-MED-b6c6ee2b-7_1



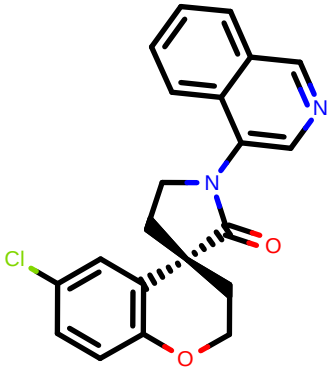
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1740
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.19

VLA-UNK-3a43cd95-1_1



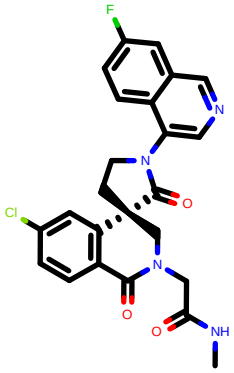
CID:	VLA-UNK-3a43cd95-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)F)Cl)NC3=O
RUN:	RUN1503
DDG (kcal/mol):	-0.57
dDDG (kcal/mol):	0.09

ALP-POS-477dc5b7-4_1



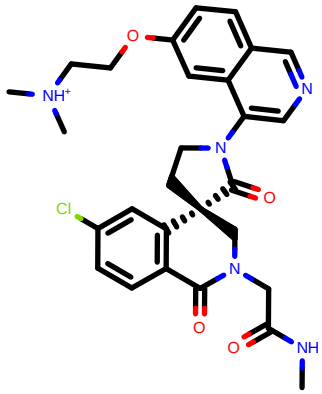
CID:	ALP-POS-477dc5b7-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1467
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.12

EDG-MED-b1ef7fe3-3_1



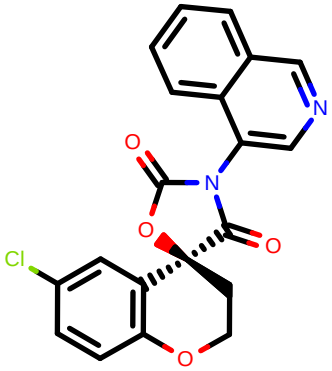
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1608
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.16

MAT-POS-38eb6498-4_1



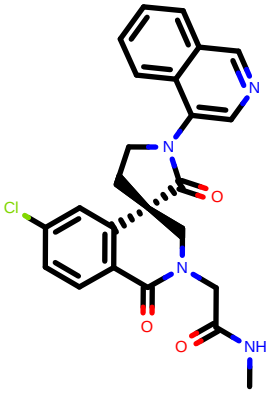
CID:	MAT-POS-38eb6498-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN1876
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.32

MAT-POS-90505e2b-1_1



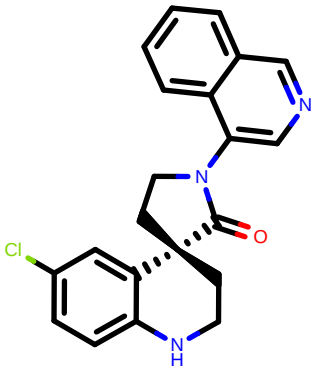
CID:	MAT-POS-90505e2b-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN1484
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.06

EDJ-MED-fd8ed875-3_1



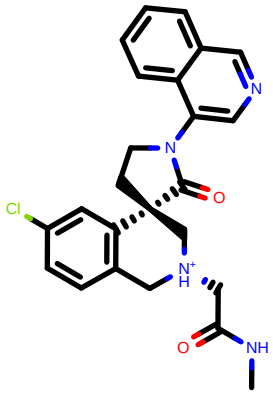
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	CNC(=O)CN1C[C@]2(C=CN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1576
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.12

DAR-DIA-6be260fc-5_1



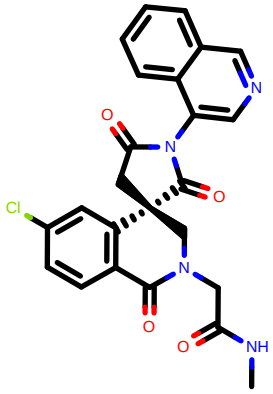
CID:	DAR-DIA-6be260fc-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl
RUN:	RUN1465
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.11

LUO-POS-868e8996-11_1



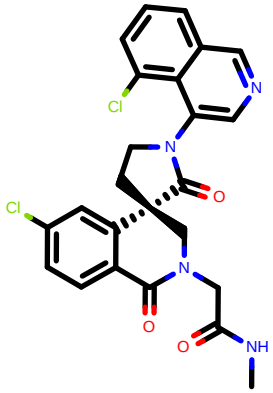
CID:	LUO-POS-868e8996-11_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1542
DDG (kcal/mol):	-0.51
dDDG (kcal/mol):	0.20

MAT-POS-1bed62cf-2_1



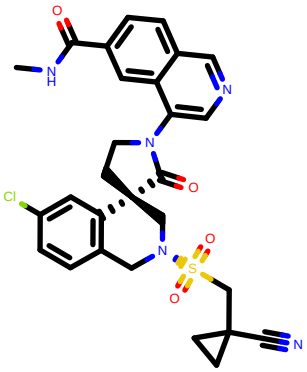
CID:	MAT-POS-1bed62cf-2_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1596
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.15

MAT-POS-853c0ffa-1_1



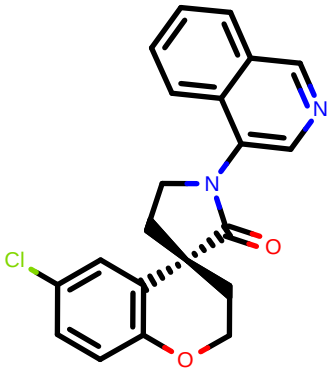
CID:	MAT-POS-853c0ffa-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1610
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.16

MAT-POS-38eb6498-2_2



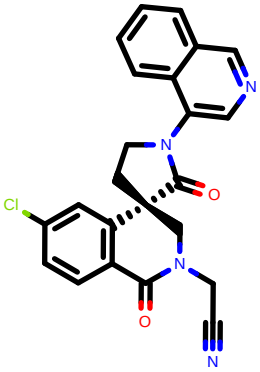
CID:	MAT-POS-38eb6498-2_2
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1872
DDG (kcal/mol):	-0.48
dDDG (kcal/mol):	0.47

EDJ-MED-159244ea-1_1



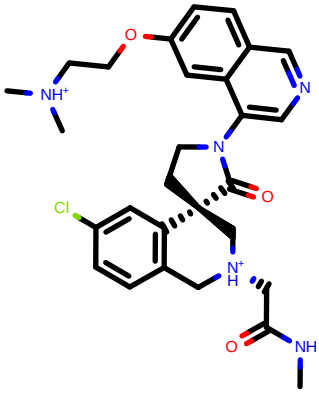
CID:	EDJ-MED-159244ea-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1469
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.10

PET-UNK-aa57768f-2_1



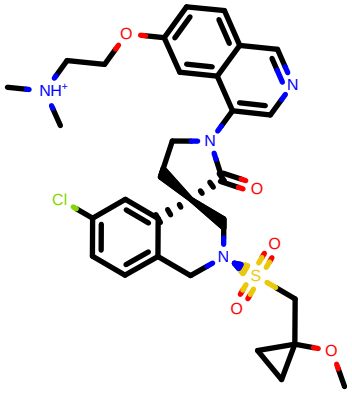
CID:	PET-UNK-aa57768f-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN1521
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.11

EDJ-MED-b6c6ee2b-1_1



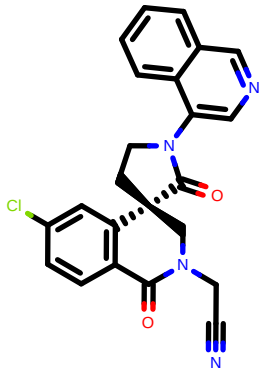
CID:	EDJ-MED-b6c6ee2b-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1844
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-10_1



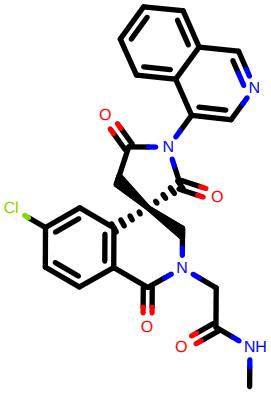
CID:	MAT-POS-853c0ffa-10_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN1895
DDG (kcal/mol):	-0.44
dDDG (kcal/mol):	0.43

PET-UNK-aa57768f-8_1



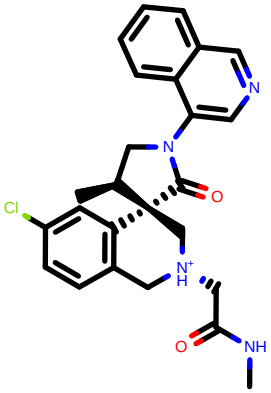
CID:	PET-UNK-aa57768f-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN1523
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.13

LUO-POS-868e8996-7_1



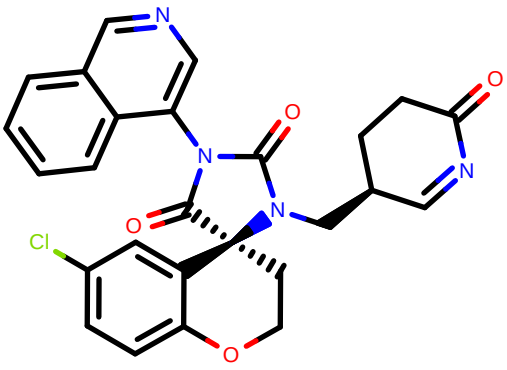
CID:	LUO-POS-868e8996-7_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1604
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.11

MAT-POS-50a80394-4_2



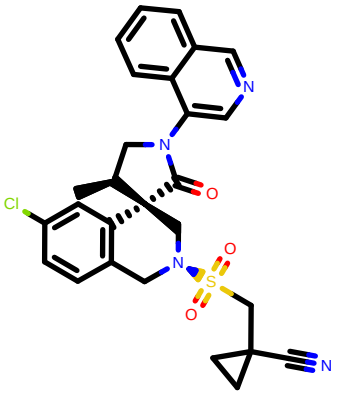
CID:	MAT-POS-50a80394-4_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1583
DDG (kcal/mol):	-0.42
dDDG (kcal/mol):	0.24

VLA-UNK-f702bf1c-5_2



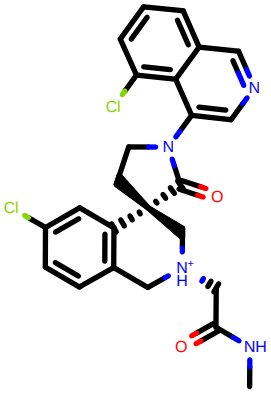
CID:	VLA-UNK-f702bf1c-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CCC(=O)NC6
RUN:	RUN1689
DDG (kcal/mol):	-0.37
dDDG (kcal/mol):	0.20

MAT-POS-50a80394-1_4



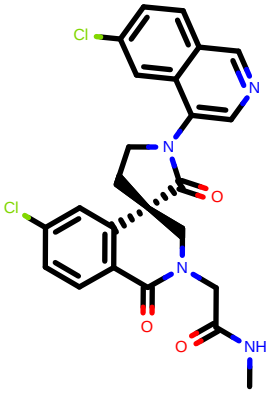
CID:	MAT-POS-50a80394-1_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1804
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.60

MAT-POS-b4d6b7fc-6_1



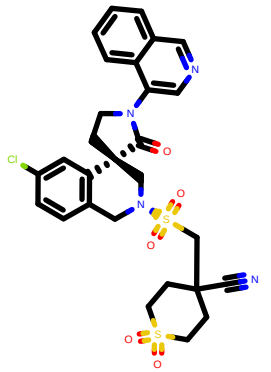
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1561
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.27

LUO-POS-8c3e556a-1_1



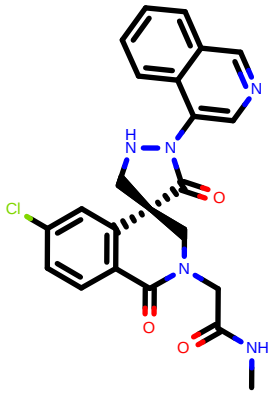
CID:	LUO-POS-8c3e556a-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1638
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.23

ALP-POS-ecbed2ba-2_2



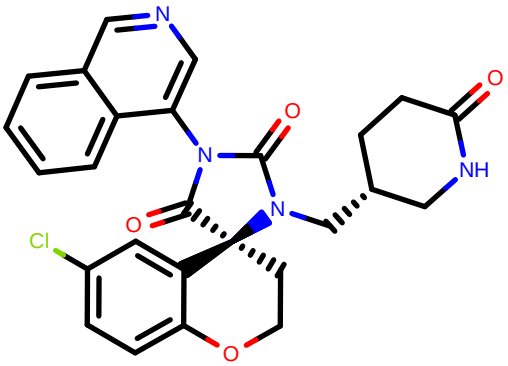
CID:	ALP-POS-ecbed2ba-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN1875
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.44

EDJ-MED-fed7ac0b-4_1



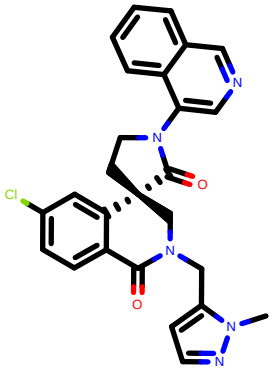
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	CNC(=O)CN1C[C@]2(C=NN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1567
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.17

VLA-UNK-f702bf1c-5_1



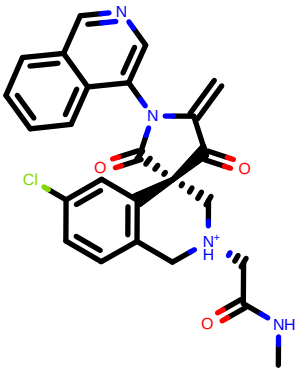
CID:	VLA-UNK-f702bf1c-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6
RUN:	RUN1688
DDG (kcal/mol):	-0.32
dDDG (kcal/mol):	0.23

EDJ-MED-cc48ee33-7_1



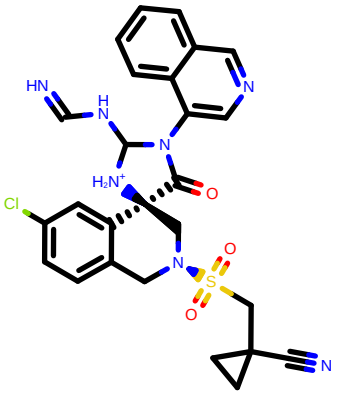
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1669
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.22

PET-UNK-94036022-7_1



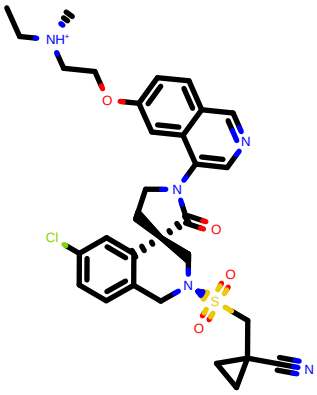
CID:	PET-UNK-94036022-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1643
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.36

LUO-POS-b5068a05-2_2



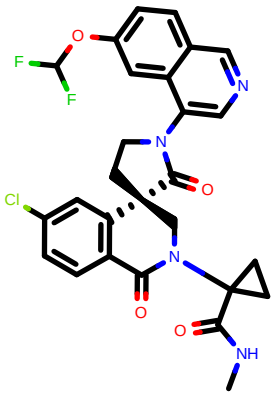
CID:	LUO-POS-b5068a05-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN1873
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.38

MAT-POS-40ad851a-2_2



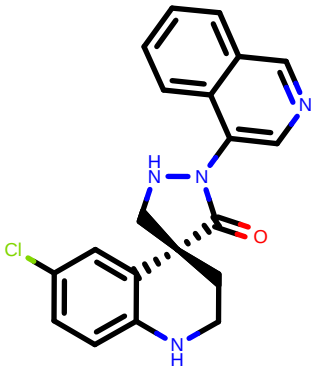
CID:	MAT-POS-40ad851a-2_2
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1912
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.70

EDJ-MED-5cd3920d-3_1



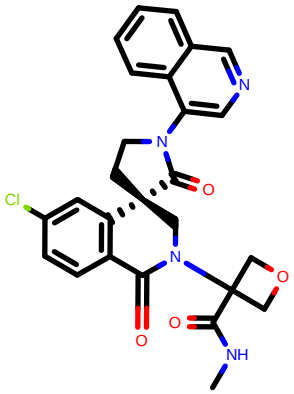
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1882
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.21

BRU-THA-55eab31a-1_1



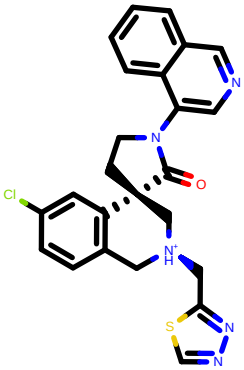
CID:	BRU-THA-55eab31a-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3
RUN:	RUN1480
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.12

EDJ-MED-98c0a822-4_1



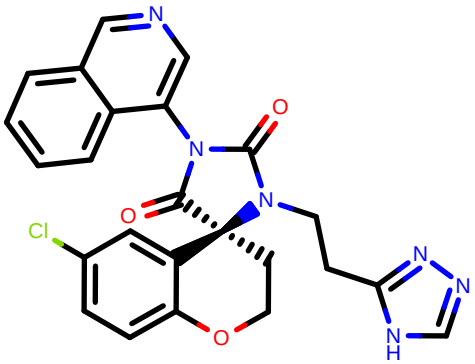
CID:	EDJ-MED-98c0a822-4_1
SMILES:	CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1734
DDG (kcal/mol):	-0.26
dDDG (kcal/mol):	0.20

PET-UNK-7e9559de-1_2



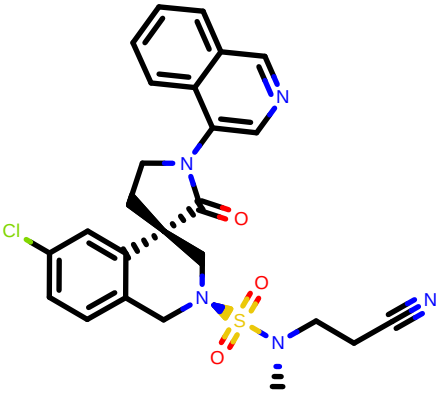
CID:	PET-UNK-7e9559de-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1578
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.22

VLA-UNK-f702bf1c-8_1



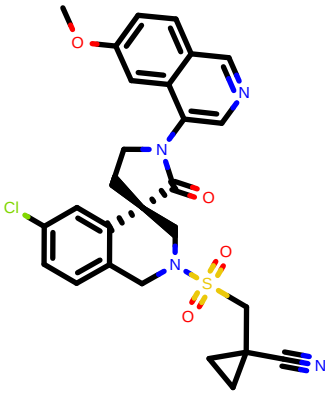
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncn6
RUN:	RUN1653
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-16_3



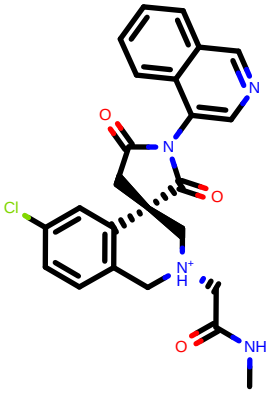
CID:	ALP-POS-ecbed2ba-16_3
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1718
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.59

EDJ-MED-b6c6ee2b-3_2



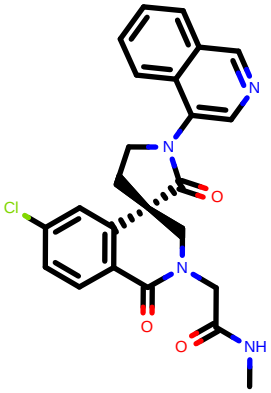
CID:	EDJ-MED-b6c6ee2b-3_2
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1838
DDG (kcal/mol):	-0.20
dDDG (kcal/mol):	0.56

MAT-POS-1bed62cf-3_1



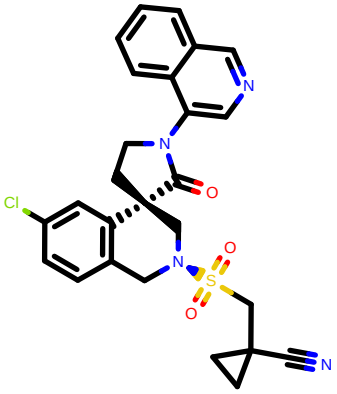
CID:	MAT-POS-1bed62cf-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1559
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.29

PET-UNK-14142a25-1_1



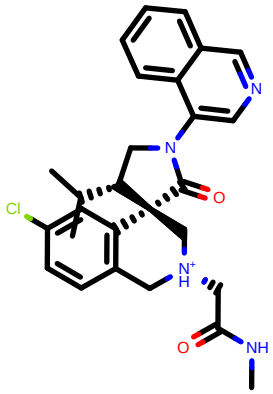
CID:	PET-UNK-14142a25-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1563
DDG (kcal/mol):	-0.14
dDDG (kcal/mol):	0.25

MIK-ENA-5d9157e9-1_1



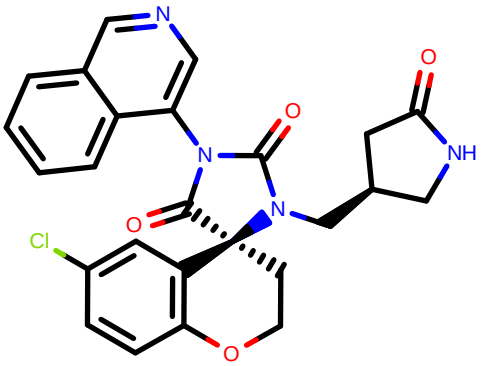
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1723
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.50

MAT-POS-50a80394-6_1



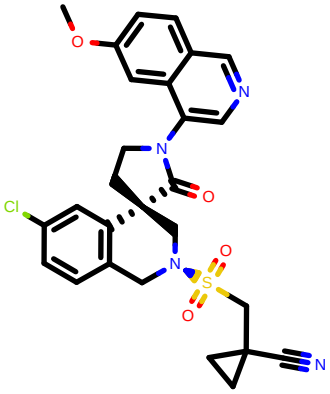
CID:	MAT-POS-50a80394-6_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1681
DDG (kcal/mol):	-0.13
dDDG (kcal/mol):	0.35

VLA-UNK-f702bf1c-4_2



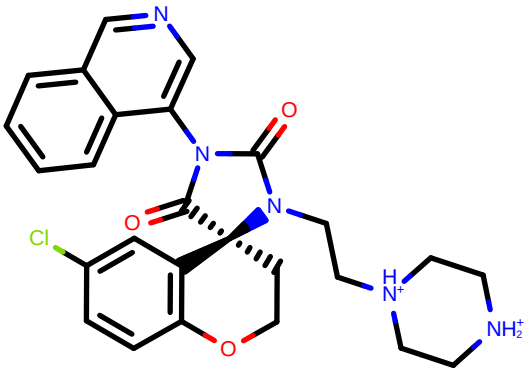
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NC6
RUN:	RUN1648
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.28

EDJ-MED-b6c6ee2b-3_1



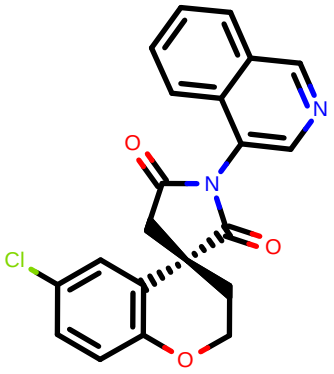
CID:	EDJ-MED-b6c6ee2b-3_1
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1833
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.44

VLA-UNK-f702bf1c-7_1



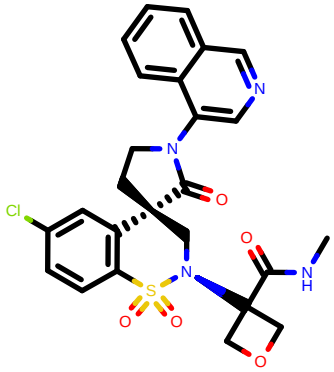
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCN6CC[NH2+]CC6
RUN:	RUN1691
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.25

MAT-POS-94643566-1_1



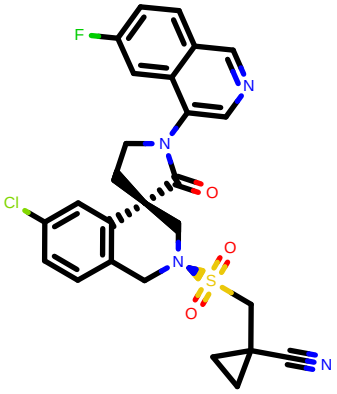
CID:	MAT-POS-94643566-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1482
DDG (kcal/mol):	-0.02
dDDG (kcal/mol):	0.02

EDJ-MED-98c0a822-2_2



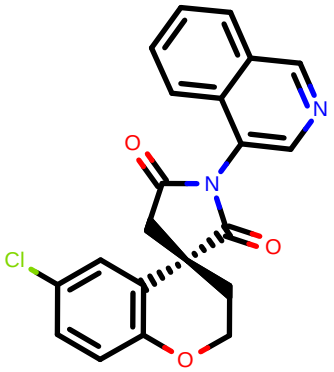
CID:	EDJ-MED-98c0a822-2_2
SMILES:	CNC(=O)C1(COC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1795
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.31

MAT-POS-853c0ffa-13_2



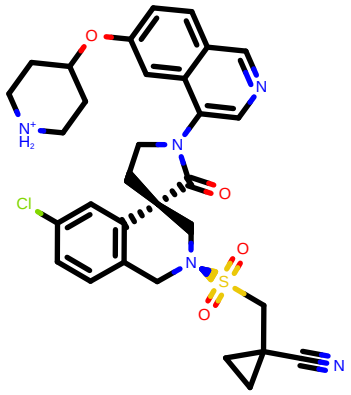
CID:	MAT-POS-853c0ffa-13_2
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1764
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.44

BEN-BAS-c2bc0d80-6_1



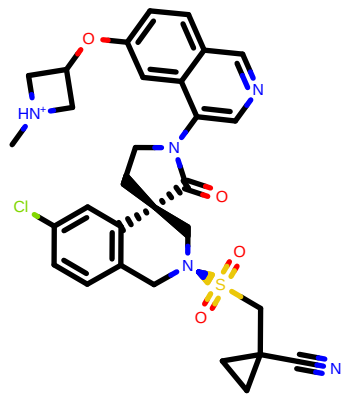
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1481
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.02

EDJ-MED-ee81482e-4_2



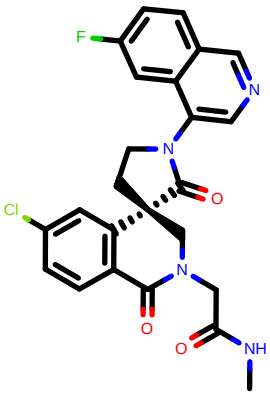
CID:	EDJ-MED-ee81482e-4_2
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1893
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.50

EDJ-MED-ee81482e-2_2



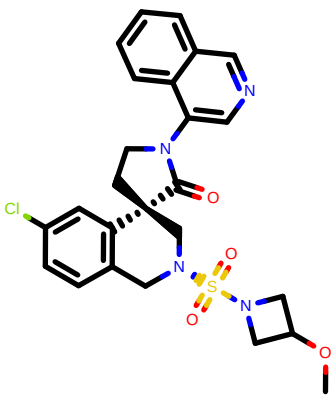
CID:	EDJ-MED-ee81482e-2_2
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1904
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.88

EDJ-MED-b6c6ee2b-6_1



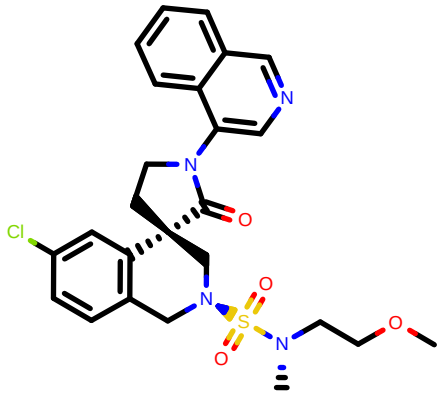
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1644
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-10_1



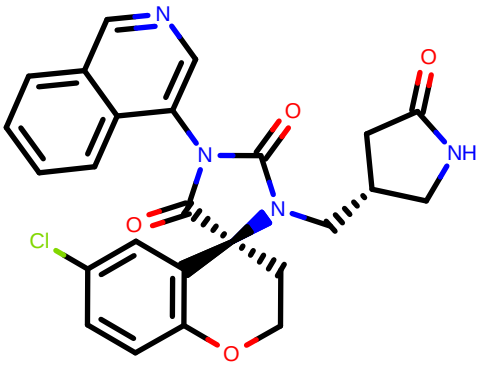
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	COC1CN(C1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1712
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.51

ALP-POS-ecbed2ba-21_1



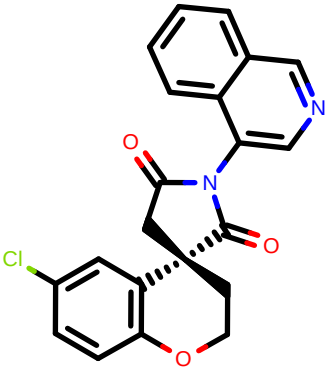
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	C[N@@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1722
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.45

VLA-UNK-f702bf1c-4_1



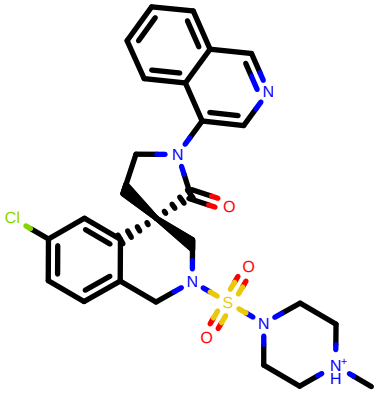
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CC(=O)NC6
RUN:	RUN1650
DDG (kcal/mol):	0.02
dDDG (kcal/mol):	0.23

VLA-UCB-50c39ae8-2_1



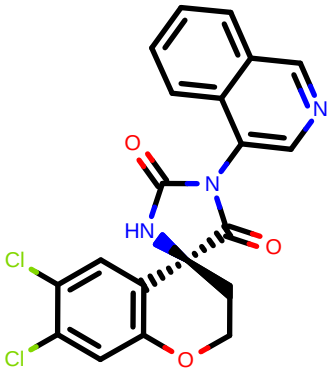
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1479
DDG (kcal/mol):	0.04
dDDG (kcal/mol):	0.04

LUO-POS-ed2cfb03-1_1



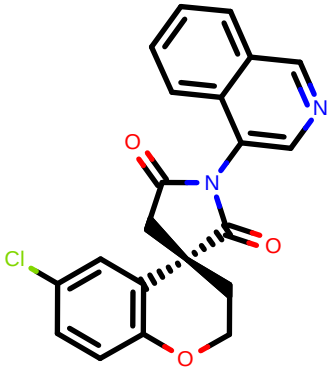
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1806
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.37

VLA-UNK-56836b69-2_1



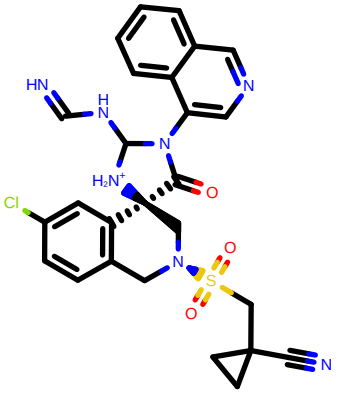
CID:	VLA-UNK-56836b69-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN1494
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.13

VLA-UCB-05e51b3f-5_1



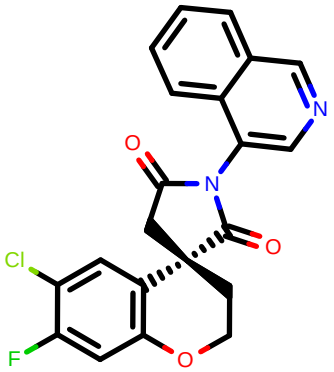
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1478
DDG (kcal/mol):	0.05
dDDG (kcal/mol):	0.04

LUO-POS-b5068a05-2_1



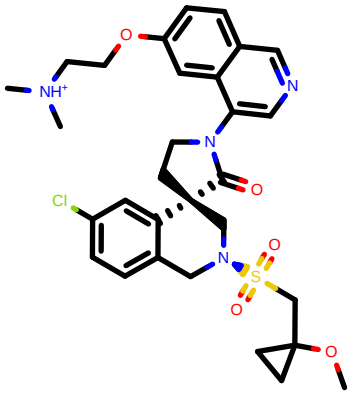
CID:	LUO-POS-b5068a05-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN1866
DDG (kcal/mol):	0.07
dDDG (kcal/mol):	0.27

VLA-UNK-3a43cd95-3_1



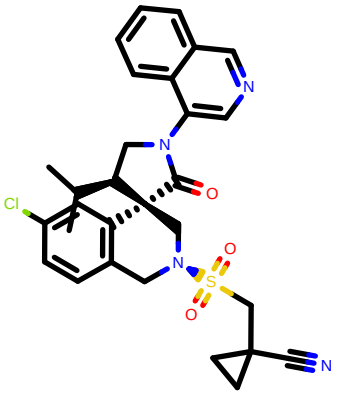
CID:	VLA-UNK-3a43cd95-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl
RUN:	RUN1499
DDG (kcal/mol):	0.10
dDDG (kcal/mol):	0.09

MAT-POS-853c0ffa-10_2



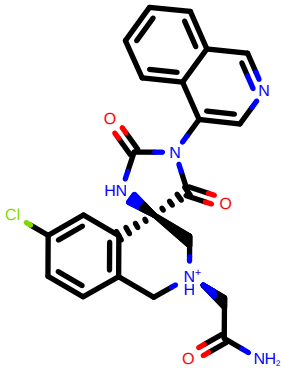
CID:	MAT-POS-853c0ffa-10_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN1899
DDG (kcal/mol):	0.14
dDDG (kcal/mol):	0.69

MAT-POS-50a80394-3_4



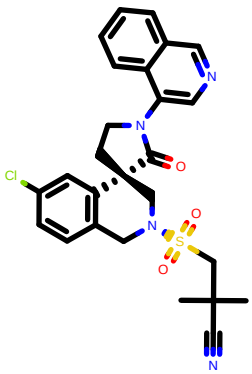
CID:	MAT-POS-50a80394-3_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1859
DDG (kcal/mol):	0.17
dDDG (kcal/mol):	0.46

VLA-MRT-a639d434-2_2



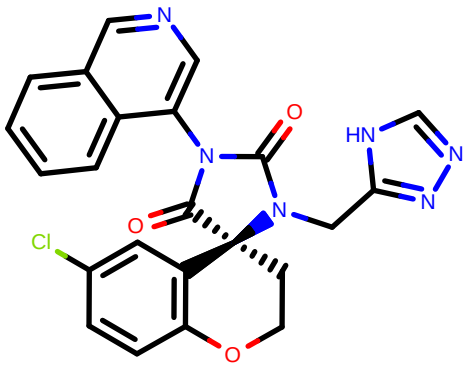
CID:	VLA-MRT-a639d434-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1528
DDG (kcal/mol):	0.18
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-13_2



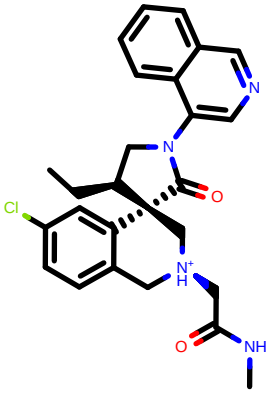
CID:	ALP-POS-ecbed2ba-13_2
SMILES:	CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN1707
DDG (kcal/mol):	0.21
dDDG (kcal/mol):	0.55

VLA-UNK-f702bf1c-3_1



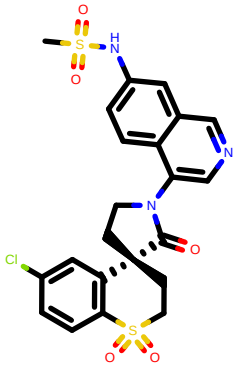
CID:	VLA-UNK-f702bf1c-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6[nH]ncn6
RUN:	RUN1598
DDG (kcal/mol):	0.21
dDDG (kcal/mol):	0.16

MAT-POS-50a80394-5_4



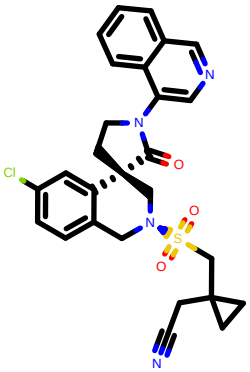
CID:	MAT-POS-50a80394-5_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1636
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.30

EDJ-MED-94fddcec-7_1



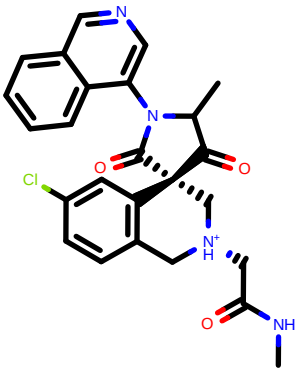
CID:	EDJ-MED-94fddcec-7_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1611
DDG (kcal/mol):	0.23
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-22_2



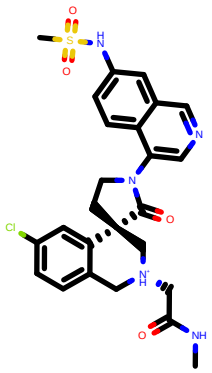
CID:	ALP-POS-ecbed2ba-22_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)CC#N
RUN:	RUN1772
DDG (kcal/mol):	0.24
dDDG (kcal/mol):	0.34

PET-UNK-94036022-14_1



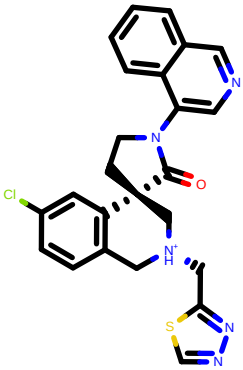
CID:	PET-UNK-94036022-14_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1645
DDG (kcal/mol):	0.24
dDDG (kcal/mol):	0.34

MAT-POS-b4d6b7fc-7_1



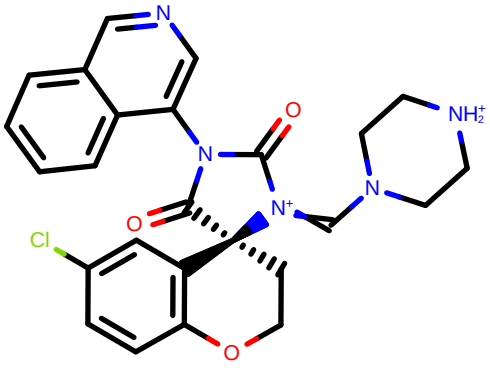
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN1753
DDG (kcal/mol):	0.25
dDDG (kcal/mol):	0.34

PET-UNK-7e9559de-1_1



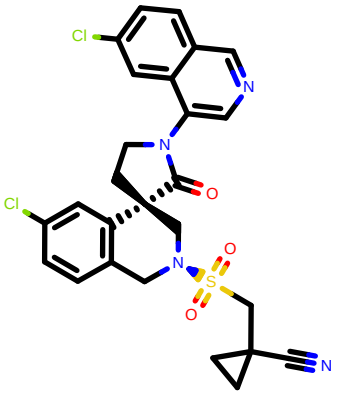
CID:	PET-UNK-7e9559de-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1574
DDG (kcal/mol):	0.26
dDDG (kcal/mol):	0.21

VLA-UCB-34f3ed0c-15_1



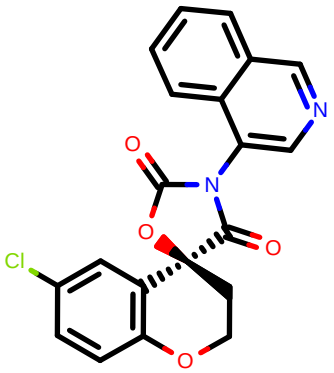
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+]CC6
RUN:	RUN1649
DDG (kcal/mol):	0.27
dDDG (kcal/mol):	0.42

EDJ-MED-b6c6ee2b-4_1



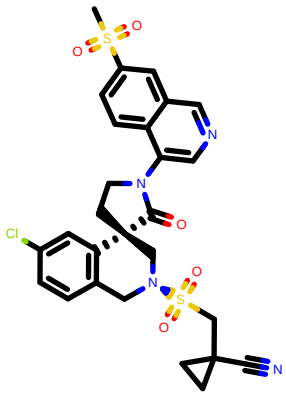
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1790
DDG (kcal/mol):	0.30
dDDG (kcal/mol):	0.48

MAT-POS-ec6d90b7-2_1



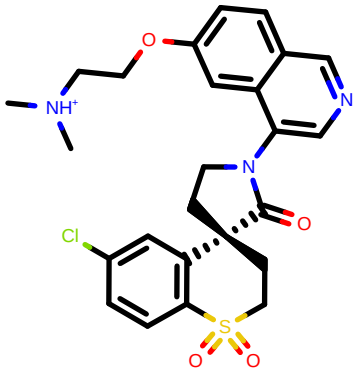
CID:	MAT-POS-ec6d90b7-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN1487
DDG (kcal/mol):	0.30
dDDG (kcal/mol):	0.07

MAT-POS-853c0ffa-15_1



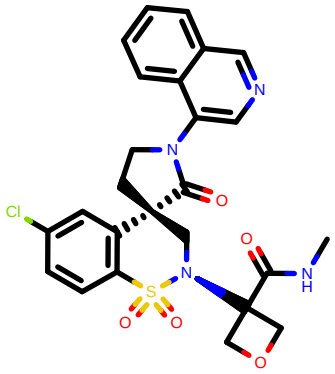
CID:	MAT-POS-853c0ffa-15_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1862
DDG (kcal/mol):	0.33
dDDG (kcal/mol):	0.53

EDJ-MED-d4864bdc-4_1



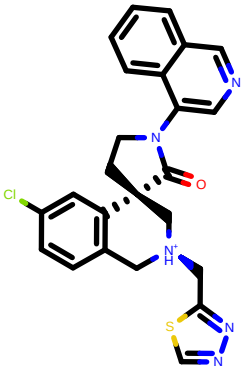
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1690
DDG (kcal/mol):	0.34
dDDG (kcal/mol):	0.27

EDJ-MED-98c0a822-2_1



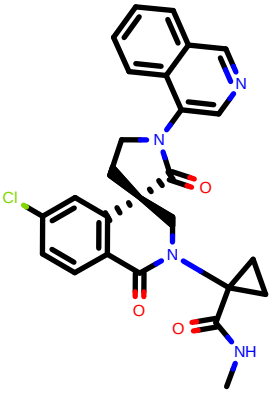
CID:	EDJ-MED-98c0a822-2_1
SMILES:	CNC(=O)C1(COC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1794
DDG (kcal/mol):	0.35
dDDG (kcal/mol):	0.28

PET-UNK-7e9559de-4_2



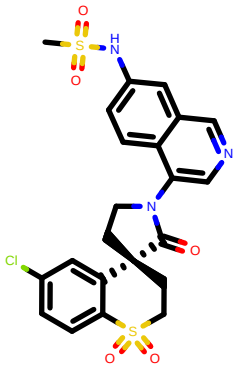
CID:	PET-UNK-7e9559de-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1577
DDG (kcal/mol):	0.35
dDDG (kcal/mol):	0.23

EDJ-MED-fd8ed875-4_1



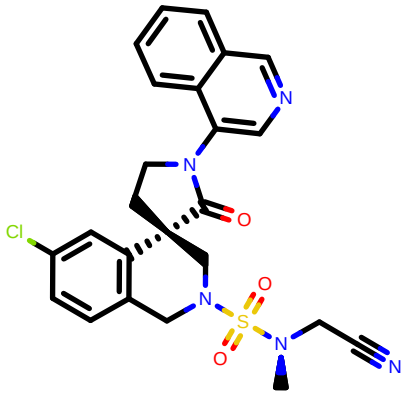
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(C=CN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1673
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.17

EDJ-MED-ede5c6cb-1_1



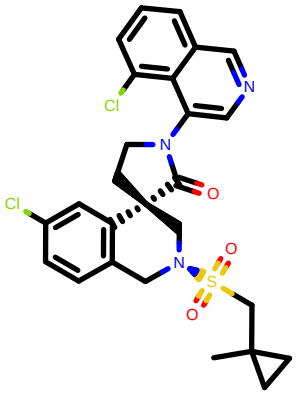
CID:	EDJ-MED-ede5c6cb-1_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1637
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-17_2



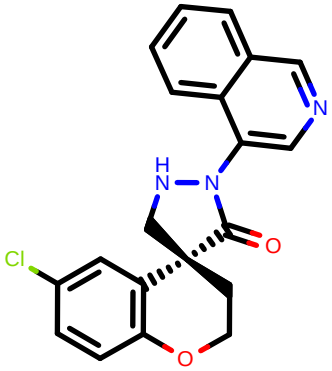
CID:	ALP-POS-ecbed2ba-17_2
SMILES:	C[N@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1659
DDG (kcal/mol):	0.43
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-17_2



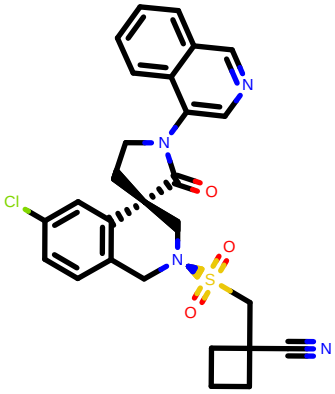
CID:	MAT-POS-853c0ffa-17_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1698
DDG (kcal/mol):	0.43
dDDG (kcal/mol):	0.43

BRU-THA-73c97d88-1_1



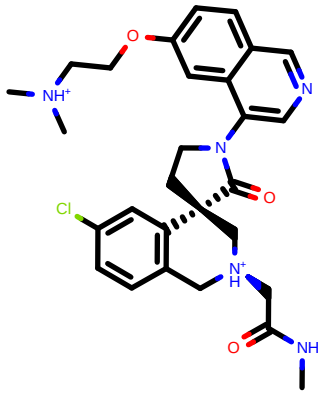
CID:	BRU-THA-73c97d88-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3
RUN:	RUN1474
DDG (kcal/mol):	0.44
dDDG (kcal/mol):	0.08

ALP-POS-ecbed2ba-8_1



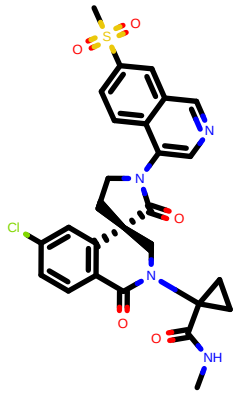
CID:	ALP-POS-ecbed2ba-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N
RUN:	RUN1773
DDG (kcal/mol):	0.44
dDDG (kcal/mol):	0.49

EDJ-MED-b6c6ee2b-1_2



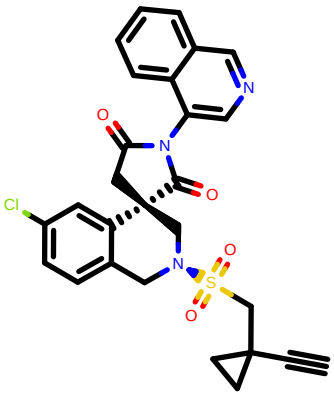
CID:	EDJ-MED-b6c6ee2b-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1856
DDG (kcal/mol):	0.45
dDDG (kcal/mol):	0.43

EDJ-MED-976a33d5-2_1



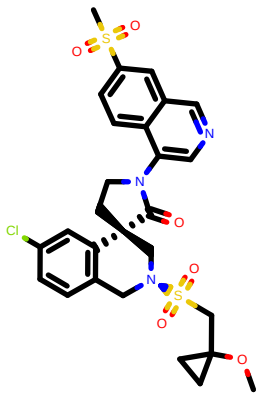
CID:	EDJ-MED-976a33d5-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1855
DDG (kcal/mol):	0.47
dDDG (kcal/mol):	0.19

PET-UNK-94036022-11_1



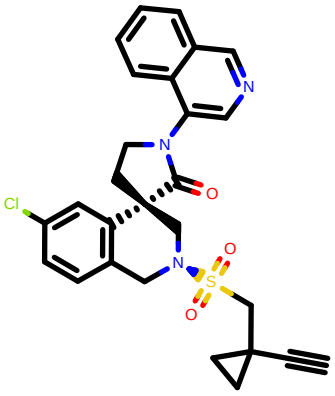
CID:	PET-UNK-94036022-11_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1812
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.35

MAT-POS-853c0ffa-16_1



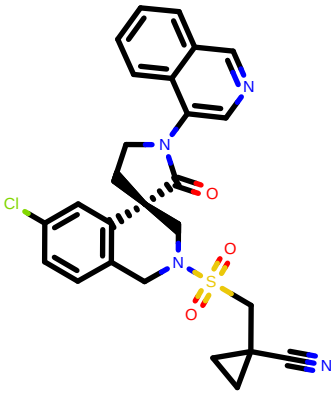
CID:	MAT-POS-853c0ffa-16_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1861
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.37

PET-UNK-94036022-2_1



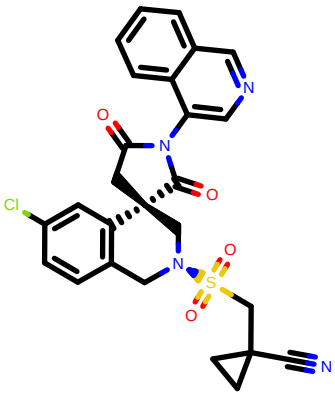
CID:	PET-UNK-94036022-2_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1745
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.39

MIK-ENA-5d9157e9-2_2



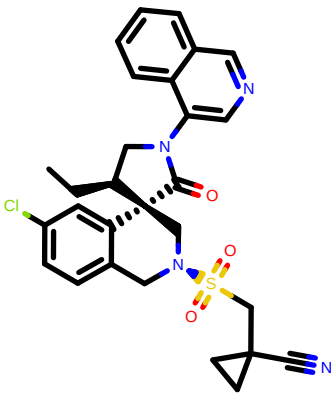
CID:	MIK-ENA-5d9157e9-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1727
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.43

LUO-POS-868e8996-10_1



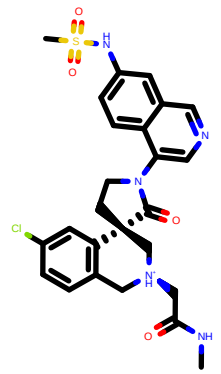
CID:	LUO-POS-868e8996-10_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1757
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.46

MAT-POS-50a80394-2_4



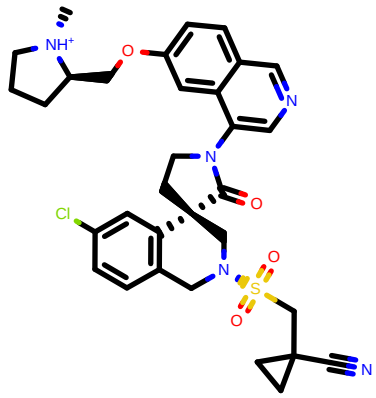
CID:	MAT-POS-50a80394-2_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1835
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.59

MAT-POS-b4d6b7fc-7_2



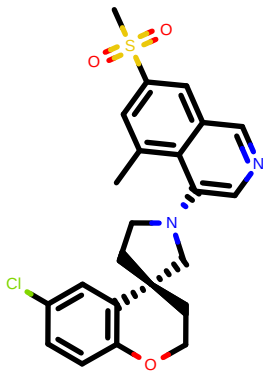
CID:	MAT-POS-b4d6b7fc-7_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN1783
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.37

MAT-POS-40ad851a-1_6



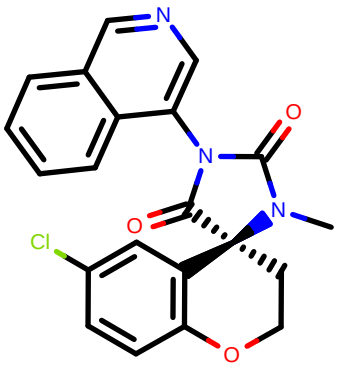
CID:	MAT-POS-40ad851a-1_6
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1932
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.76

EDJ-MED-d7486dd1-1_2



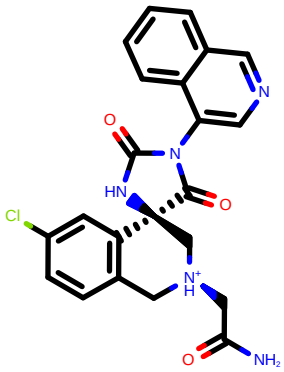
CID:	EDJ-MED-d7486dd1-1_2
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1517
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.17

BEN-BAS-c2bc0d80-7_1



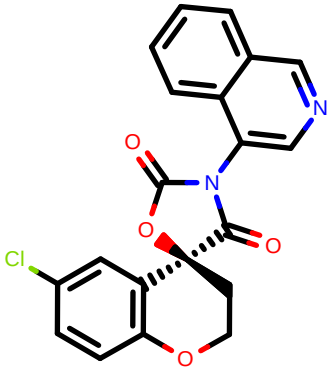
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN1495
DDG (kcal/mol):	0.55
dDDG (kcal/mol):	0.11

VLA-MRT-8c78ee15-4_2



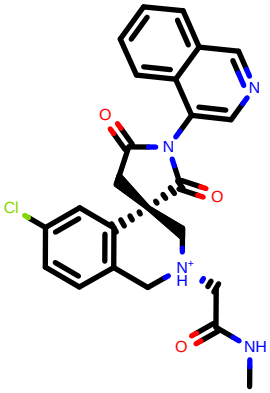
CID:	VLA-MRT-8c78ee15-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1525
DDG (kcal/mol):	0.56
dDDG (kcal/mol):	0.22

MAT-POS-ec6d90b7-1_1



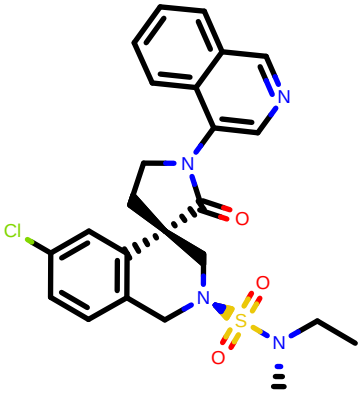
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN1485
DDG (kcal/mol):	0.58
dDDG (kcal/mol):	0.05

JOH-MSK-1f2dff76-1_1



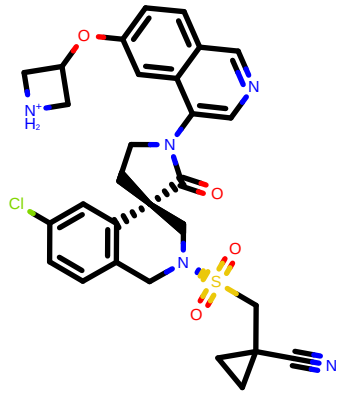
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1588
DDG (kcal/mol):	0.61
dDDG (kcal/mol):	0.28

ALP-POS-ecbed2ba-18_4



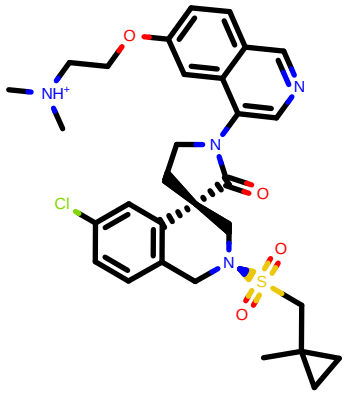
CID:	ALP-POS-ecbed2ba-18_4
SMILES:	CC[N@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1617
DDG (kcal/mol):	0.62
dDDG (kcal/mol):	0.56

EDJ-MED-ee81482e-1_2



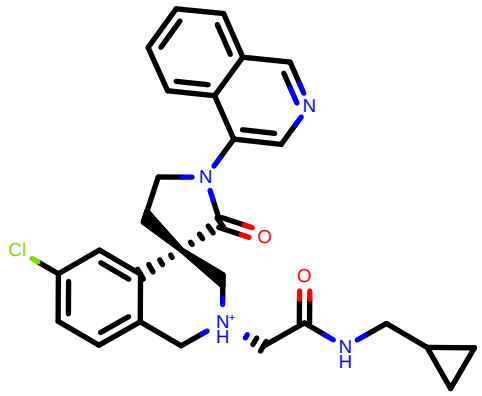
CID:	EDJ-MED-ee81482e-1_2
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1891
DDG (kcal/mol):	0.63
dDDG (kcal/mol):	0.51

MAT-POS-853c0ffa-19_2



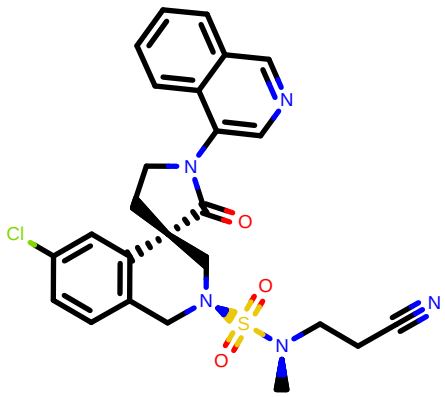
CID:	MAT-POS-853c0ffa-19_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN1887
DDG (kcal/mol):	0.63
dDDG (kcal/mol):	0.56

ALP-POS-ecbed2ba-12_1



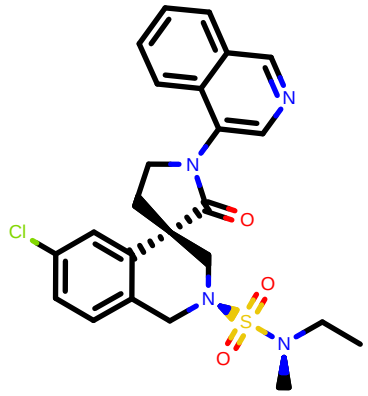
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN1665
DDG (kcal/mol):	0.64
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-16_2



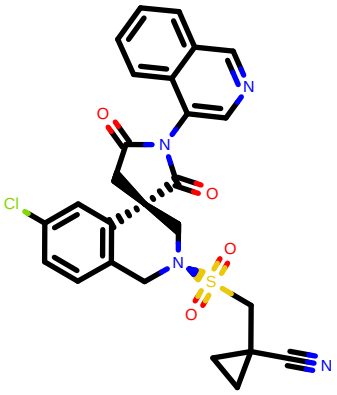
CID:	ALP-POS-ecbed2ba-16_2
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1710
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-18_3



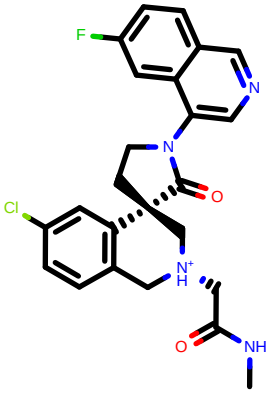
CID:	ALP-POS-ecbed2ba-18_3
SMILES:	CC[N@@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1615
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.56

MAT-POS-1bed62cf-1_2



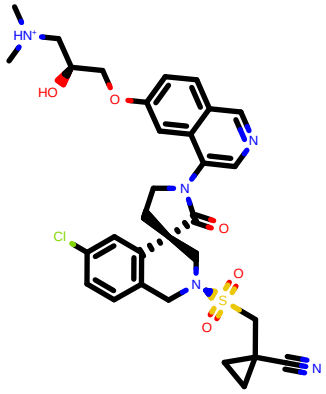
CID:	MAT-POS-1bed62cf-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1748
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.50

LUO-POS-b4dec3be-1_1



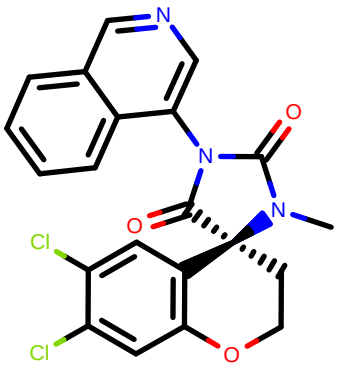
CID:	LUO-POS-b4dec3be-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1584
DDG (kcal/mol):	0.68
dDDG (kcal/mol):	0.27

EDJ-MED-ee81482e-3_3



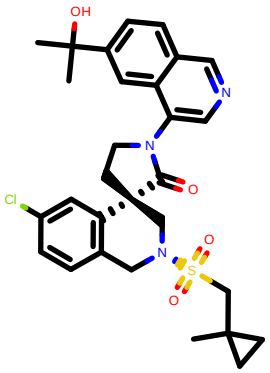
CID:	EDJ-MED-ee81482e-3_3
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1917
DDG (kcal/mol):	0.68
dDDG (kcal/mol):	1.04

VLA-UNK-56836b69-3_1



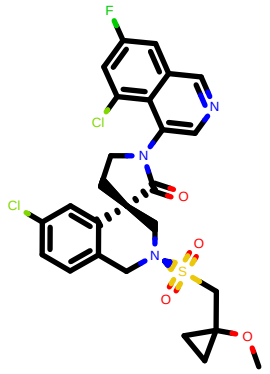
CID:	VLA-UNK-56836b69-3_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN1498
DDG (kcal/mol):	0.69
dDDG (kcal/mol):	0.14

MAT-POS-853c0ffa-20_1



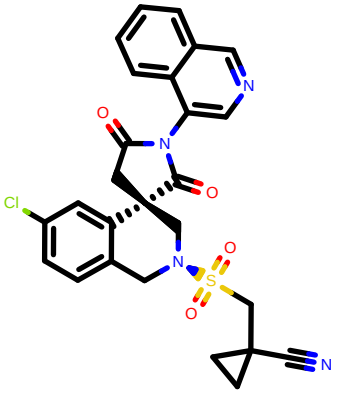
CID:	MAT-POS-853c0ffa-20_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN1852
DDG (kcal/mol):	0.69
dDDG (kcal/mol):	0.36

MAT-POS-853c0ffa-8_1



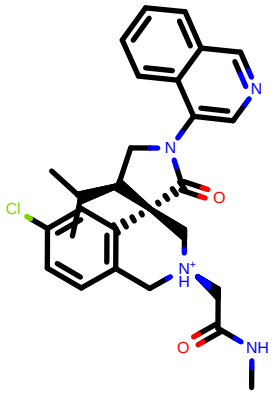
CID:	MAT-POS-853c0ffa-8_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1818
DDG (kcal/mol):	0.69
dDDG (kcal/mol):	0.28

LUO-POS-868e8996-9_1



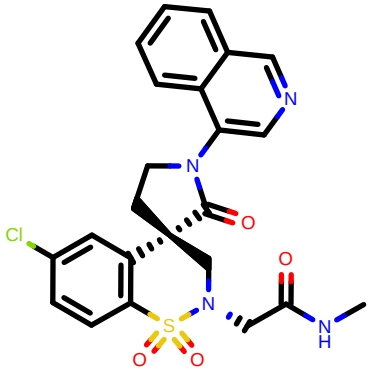
CID:	LUO-POS-868e8996-9_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1756
DDG (kcal/mol):	0.70
dDDG (kcal/mol):	0.36

MAT-POS-50a80394-6_4



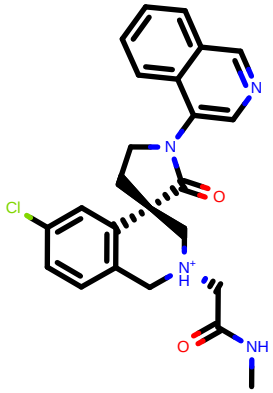
CID:	MAT-POS-50a80394-6_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1675
DDG (kcal/mol):	0.70
dDDG (kcal/mol):	0.27

ALP-POS-4483ae88-2_1



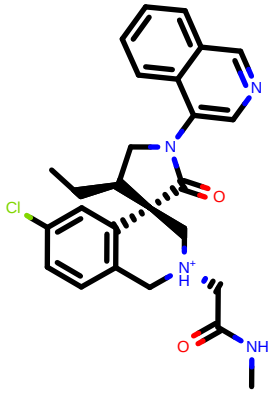
CID:	ALP-POS-4483ae88-2_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN1599
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.26

LUO-POS-868e8996-12_1



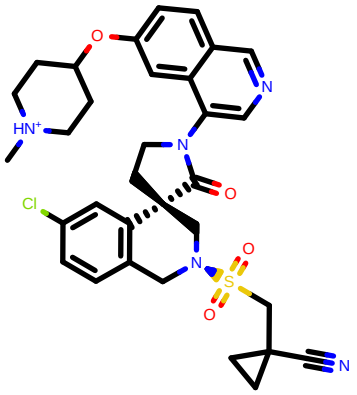
CID:	LUO-POS-868e8996-12_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1540
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.27

MAT-POS-50a80394-5_2



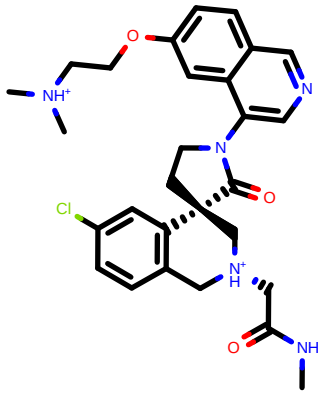
CID:	MAT-POS-50a80394-5_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1626
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.32

LUO-POS-d1147590-1_1



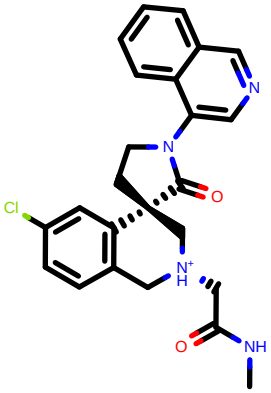
CID:	LUO-POS-d1147590-1_1
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1939
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.57

MAT-POS-38eb6498-3_1



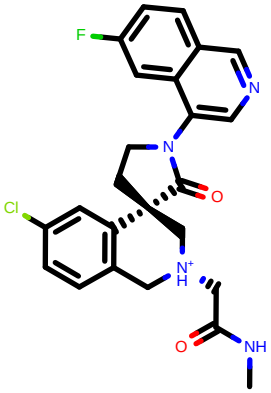
CID:	MAT-POS-38eb6498-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1840
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.51

MAT-POS-c7726e07-6_1



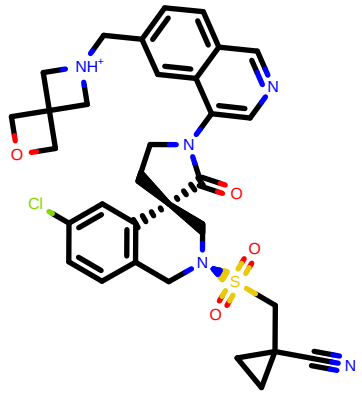
CID:	MAT-POS-c7726e07-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1539
DDG (kcal/mol):	0.73
dDDG (kcal/mol):	0.30

MAT-POS-b4d6b7fc-5_1



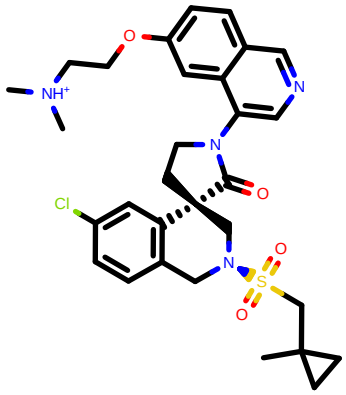
CID:	MAT-POS-b4d6b7fc-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1560
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.32

EDJ-MED-ee81482e-5_1



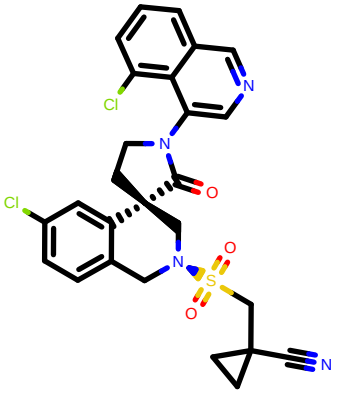
CID:	EDJ-MED-ee81482e-5_1
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@@](Cc7c6cc(cc7)Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN1919
DDG (kcal/mol):	0.77
dDDG (kcal/mol):	0.46

MAT-POS-853c0ffa-19_1



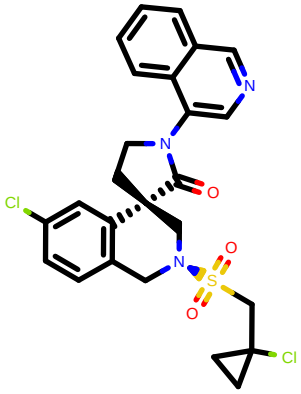
CID:	MAT-POS-853c0ffa-19_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN1888
DDG (kcal/mol):	0.78
dDDG (kcal/mol):	0.70

MAT-POS-853c0ffa-5_2



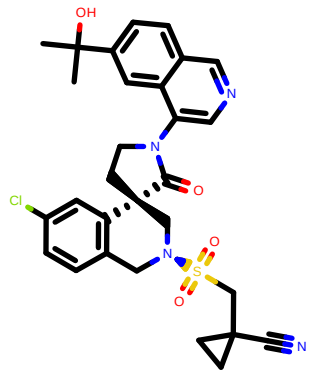
CID:	MAT-POS-853c0ffa-5_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1761
DDG (kcal/mol):	0.79
dDDG (kcal/mol):	0.57

PET-UNK-94036022-10_1



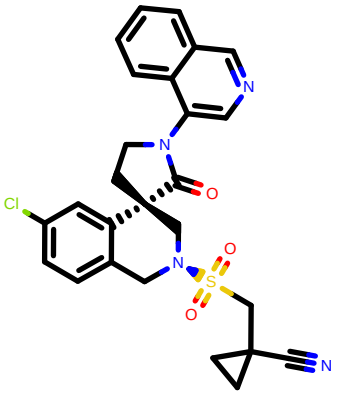
CID:	PET-UNK-94036022-10_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1686
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.33

MAT-POS-853c0ffa-11_1



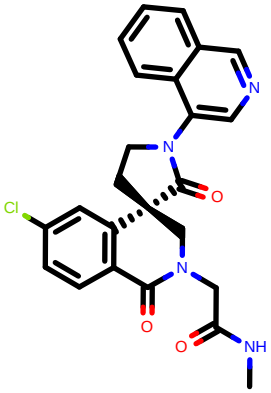
CID:	MAT-POS-853c0ffa-11_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1869
DDG (kcal/mol):	0.80
dDDG (kcal/mol):	0.44

EDJ-MED-8bb691af-6_1



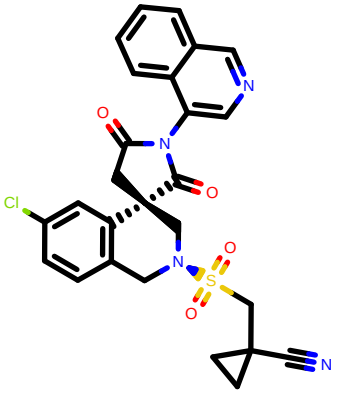
CID:	EDJ-MED-8bb691af-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1694
DDG (kcal/mol):	0.83
dDDG (kcal/mol):	0.52

LUO-POS-9931618f-2_1



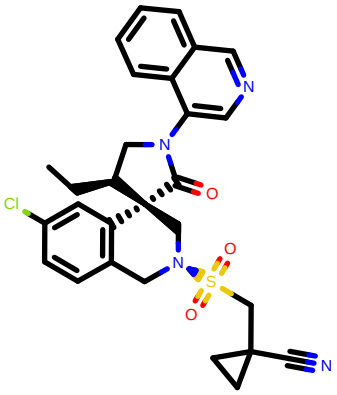
CID:	LUO-POS-9931618f-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1579
DDG (kcal/mol):	0.84
dDDG (kcal/mol):	0.23

LUO-POS-868e8996-9_2



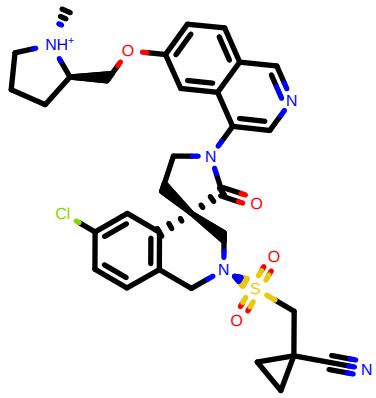
CID:	LUO-POS-868e8996-9_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1754
DDG (kcal/mol):	0.85
dDDG (kcal/mol):	0.53

MAT-POS-50a80394-2_2



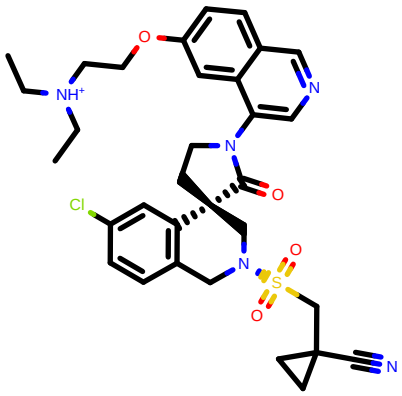
CID:	MAT-POS-50a80394-2_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1830
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.47

MAT-POS-40ad851a-1_2



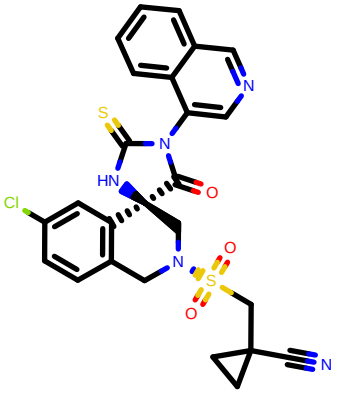
CID:	MAT-POS-40ad851a-1_2
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1941
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.48

MAT-POS-40ad851a-3_1



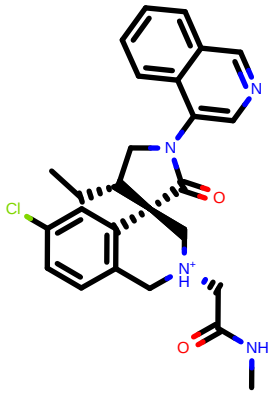
CID:	MAT-POS-40ad851a-3_1
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1929
DDG (kcal/mol):	0.87
dDDG (kcal/mol):	0.62

MAT-POS-c2d406ed-3_1



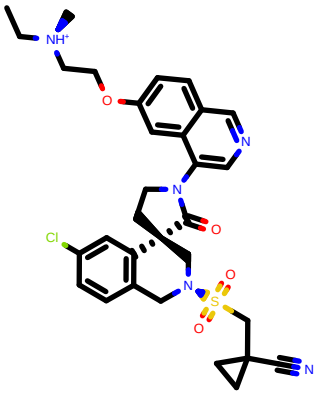
CID:	MAT-POS-c2d406ed-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN1785
DDG (kcal/mol):	0.89
dDDG (kcal/mol):	0.27

MAT-POS-50a80394-5_1



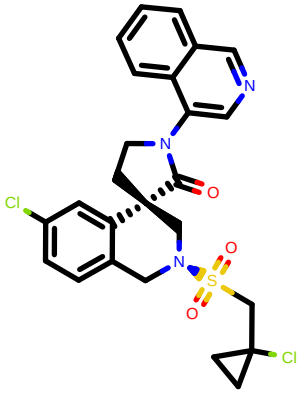
CID:	MAT-POS-50a80394-5_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1633
DDG (kcal/mol):	0.89
dDDG (kcal/mol):	0.22

MAT-POS-40ad851a-2_1



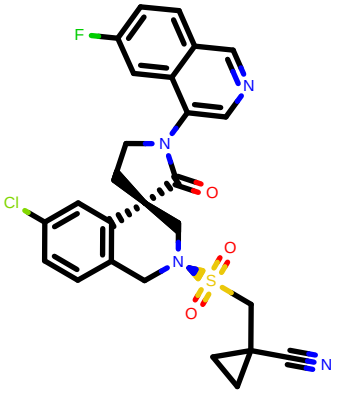
CID:	MAT-POS-40ad851a-2_1
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1909
DDG (kcal/mol):	0.89
dDDG (kcal/mol):	0.55

PET-UNK-94036022-3_1



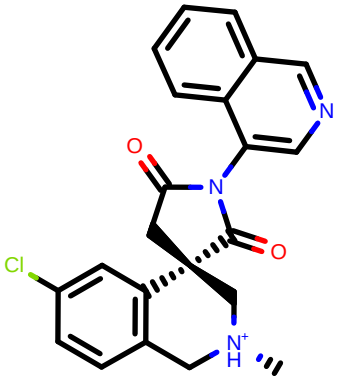
CID:	PET-UNK-94036022-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1687
DDG (kcal/mol):	0.90
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-13_1



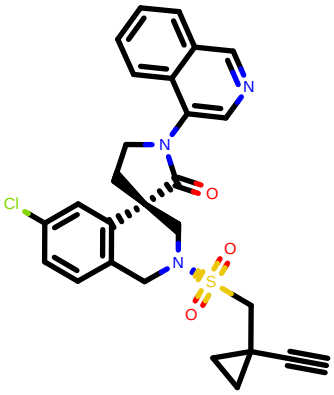
CID:	MAT-POS-853c0ffa-13_1
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1765
DDG (kcal/mol):	0.90
dDDG (kcal/mol):	0.43

JOH-MSK-51c67e7d-2_1



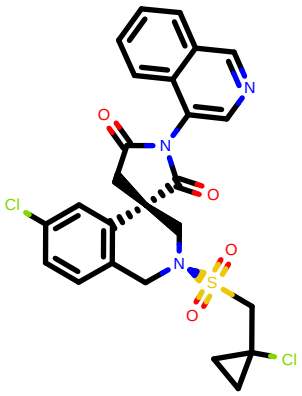
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1506
DDG (kcal/mol):	0.91
dDDG (kcal/mol):	0.16

PET-UNK-94036022-9_1



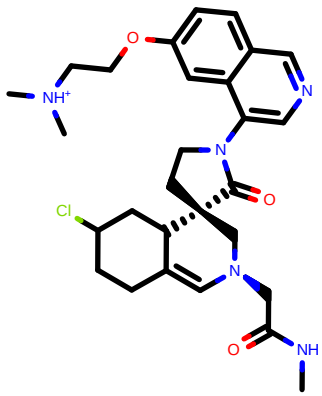
CID:	PET-UNK-94036022-9_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1735
DDG (kcal/mol):	0.91
dDDG (kcal/mol):	0.39

PET-UNK-94036022-12_1



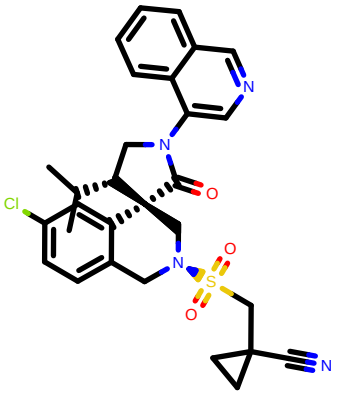
CID:	PET-UNK-94036022-12_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1749
DDG (kcal/mol):	0.93
dDDG (kcal/mol):	0.29

MAT-POS-38eb6498-3_2



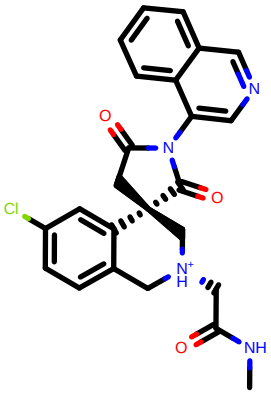
CID:	MAT-POS-38eb6498-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1851
DDG (kcal/mol):	0.94
dDDG (kcal/mol):	0.42

MAT-POS-50a80394-3_3



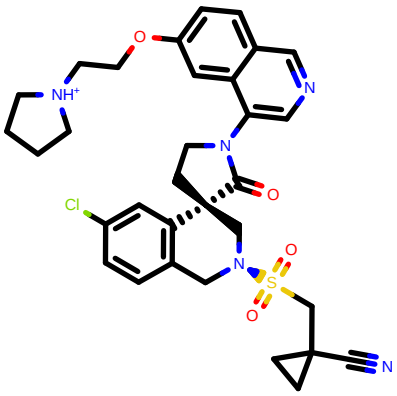
CID:	MAT-POS-50a80394-3_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1858
DDG (kcal/mol):	0.94
dDDG (kcal/mol):	0.80

JOH-MSK-1f2dff76-2_1



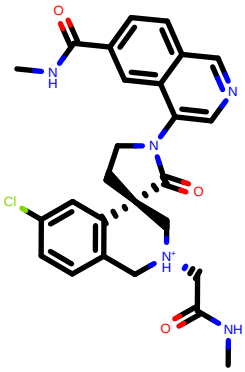
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1592
DDG (kcal/mol):	0.95
dDDG (kcal/mol):	0.28

EDJ-MED-468565e0-1_1



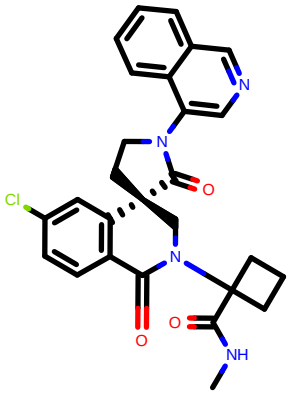
CID:	EDJ-MED-468565e0-1_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1933
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.49

MAT-POS-38eb6498-5_1



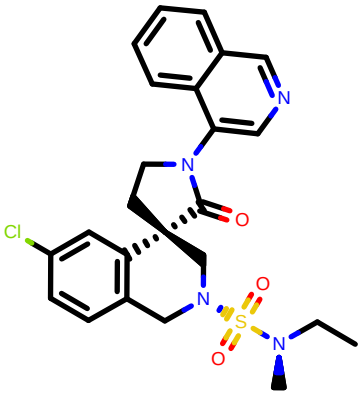
CID:	MAT-POS-38eb6498-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN1726
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.31

EDJ-MED-98c0a822-3_1



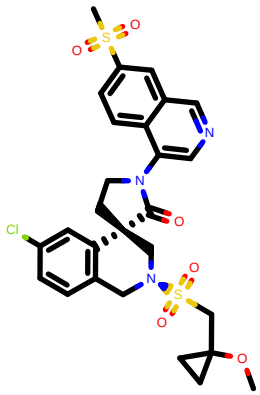
CID:	EDJ-MED-98c0a822-3_1
SMILES:	CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1733
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-18_1



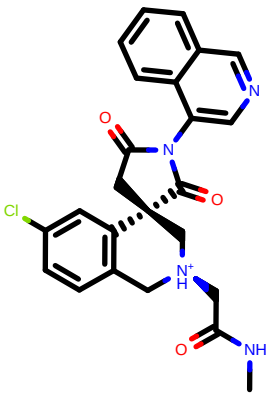
CID:	ALP-POS-ecbed2ba-18_1
SMILES:	CC[N@@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1612
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-16_2



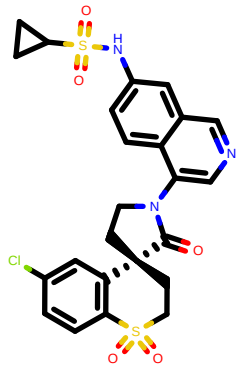
CID:	MAT-POS-853c0ffa-16_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1868
DDG (kcal/mol):	0.97
dDDG (kcal/mol):	0.78

JOH-MSK-1f2dff76-2_2



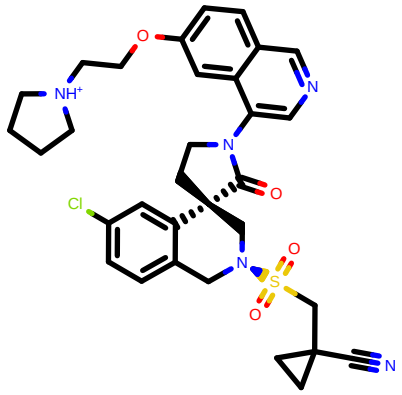
CID:	JOH-MSK-1f2dff76-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1595
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.28

EDJ-MED-ede5c6cb-2_1



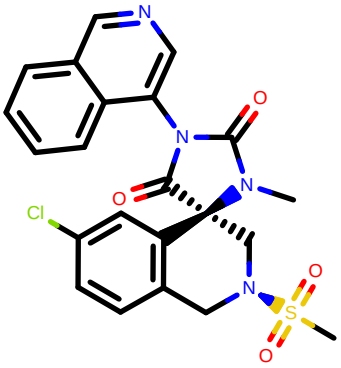
CID:	EDJ-MED-ede5c6cb-2_1
SMILES:	c1cc2c(cc1NS(=O)(=O)C3CC3)cncc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl
RUN:	RUN1750
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.27

EDJ-MED-468565e0-1_2



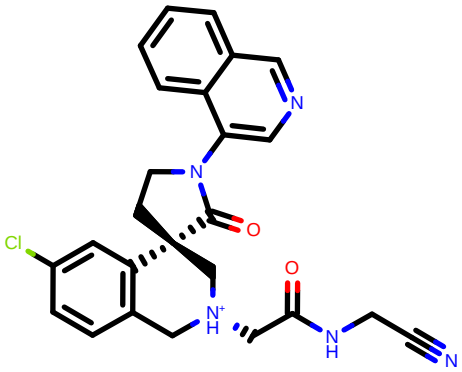
CID:	EDJ-MED-468565e0-1_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1940
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.63

EDJ-MED-7587a9ee-1_2



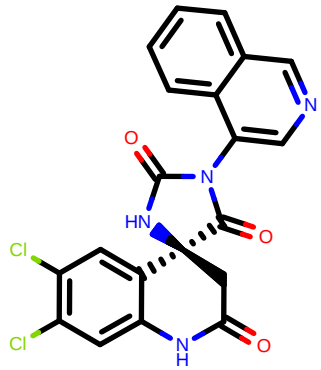
CID:	EDJ-MED-7587a9ee-1_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1547
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-14_1



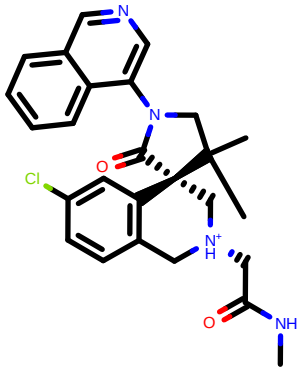
CID:	ALP-POS-ecbed2ba-14_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN1614
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.29

VLA-UNK-56836b69-5_1



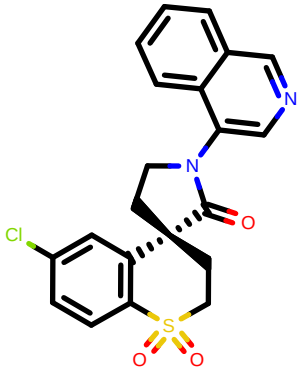
CID:	VLA-UNK-56836b69-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN1504
DDG (kcal/mol):	1.08
dDDG (kcal/mol):	0.14

MAT-POS-50a80394-7_1



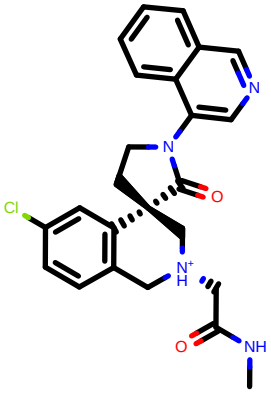
CID:	MAT-POS-50a80394-7_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN1630
DDG (kcal/mol):	1.09
dDDG (kcal/mol):	0.30

EDJ-MED-d4864bdc-3_1



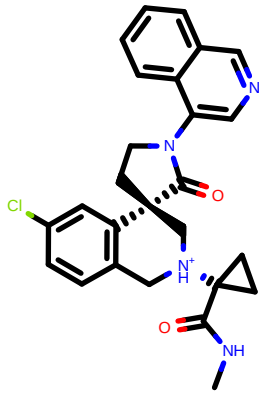
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1496
DDG (kcal/mol):	1.09
dDDG (kcal/mol):	0.25

EDJ-MED-8bb691af-4_1



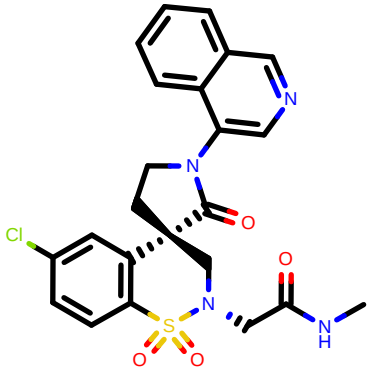
CID:	EDJ-MED-8bb691af-4_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1532
DDG (kcal/mol):	1.11
dDDG (kcal/mol):	0.29

ALP-POS-ecbed2ba-7_1



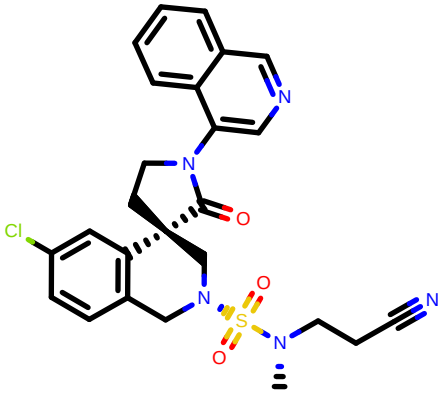
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1609
DDG (kcal/mol):	1.12
dDDG (kcal/mol):	0.29

ALP-POS-4483ae88-2_2



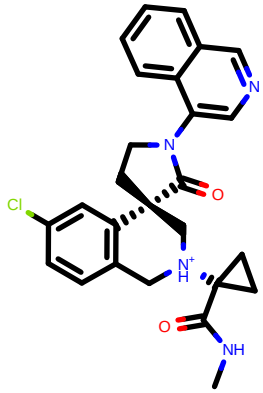
CID:	ALP-POS-4483ae88-2_2
SMILES:	CNC(=O)C[N@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN1607
DDG (kcal/mol):	1.12
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-16_4



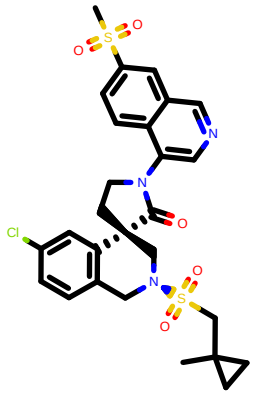
CID:	ALP-POS-ecbed2ba-16_4
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1719
DDG (kcal/mol):	1.15
dDDG (kcal/mol):	0.54

MAT-POS-576f7758-1_1



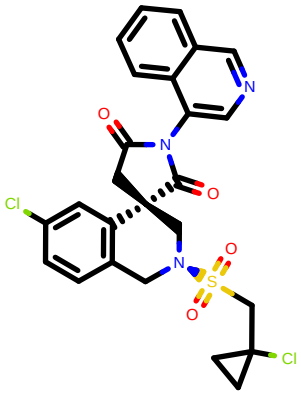
CID:	MAT-POS-576f7758-1_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1624
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.27

MAT-POS-853c0ffa-22_1



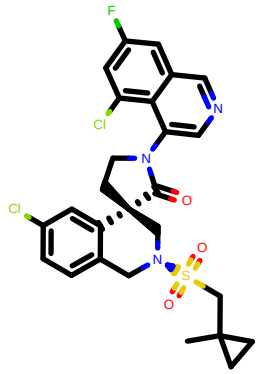
CID:	MAT-POS-853c0ffa-22_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1848
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.42

PET-UNK-94036022-5_1



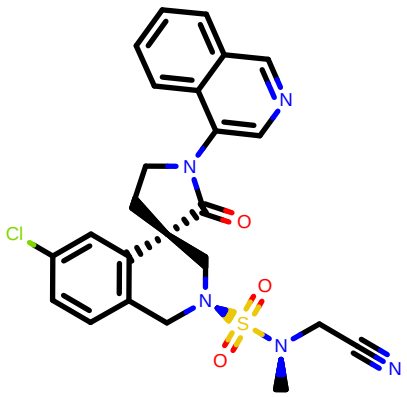
CID:	PET-UNK-94036022-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1741
DDG (kcal/mol):	1.17
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-18_2



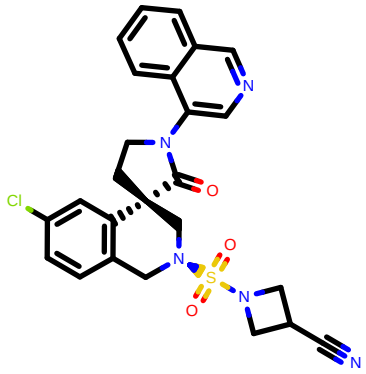
CID:	MAT-POS-853c0ffa-18_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1767
DDG (kcal/mol):	1.18
dDDG (kcal/mol):	0.40

ALP-POS-ecbed2ba-17_3



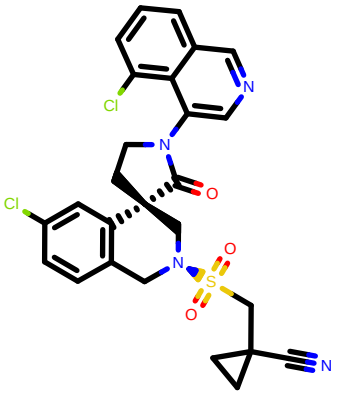
CID:	ALP-POS-ecbed2ba-17_3
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1668
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.45

ALP-POS-ecbed2ba-9_1



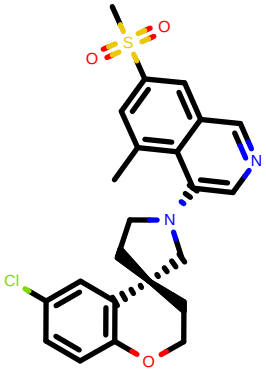
CID:	ALP-POS-ecbed2ba-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN1709
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.64

MAT-POS-1d5ab790-1_2



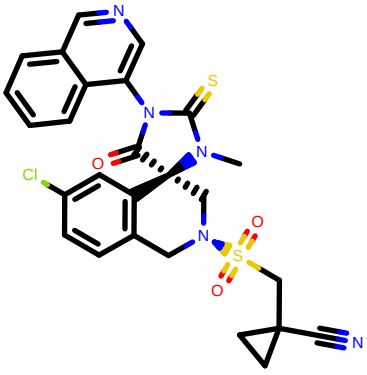
CID:	MAT-POS-1d5ab790-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1782
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.68

EDJ-MED-d7486dd1-1_1



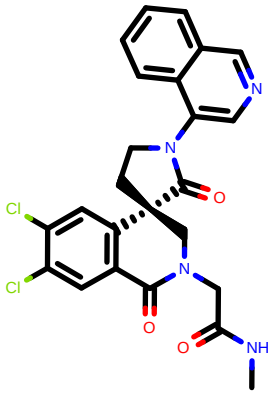
CID:	EDJ-MED-d7486dd1-1_1
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1514
DDG (kcal/mol):	1.23
dDDG (kcal/mol):	0.19

MAT-POS-c2d406ed-4_1



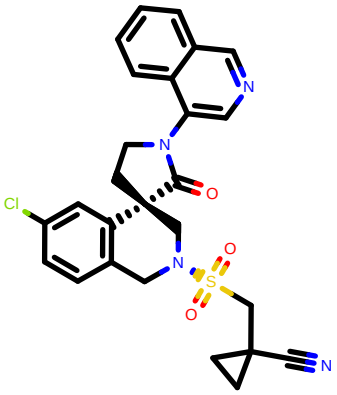
CID:	MAT-POS-c2d406ed-4_1
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1826
DDG (kcal/mol):	1.25
dDDG (kcal/mol):	0.35

ALP-POS-afe0272e-2_1



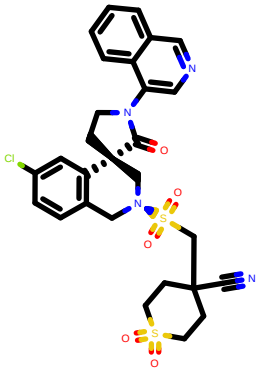
CID:	ALP-POS-afe0272e-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5C1=O)Cl)Cl
RUN:	RUN1625
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.22

EDJ-MED-8bb691af-6_2



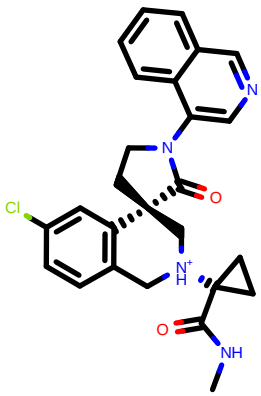
CID:	EDJ-MED-8bb691af-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1696
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.47

ALP-POS-ecbed2ba-2_1



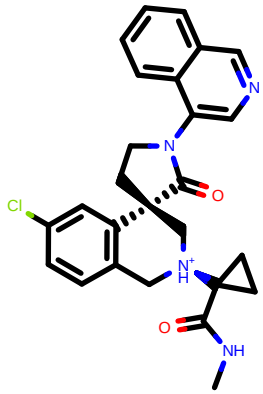
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN1880
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.56

MAT-POS-69786b79-1_1



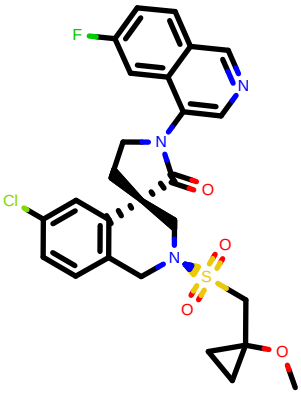
CID:	MAT-POS-69786b79-1_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1618
DDG (kcal/mol):	1.31
dDDG (kcal/mol):	0.26

MAT-POS-69786b79-1_2



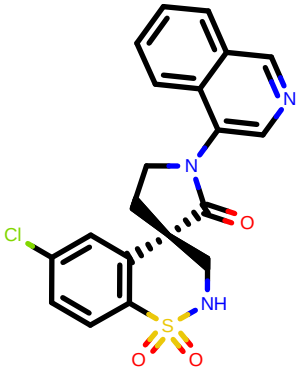
CID:	MAT-POS-69786b79-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1621
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-14_1



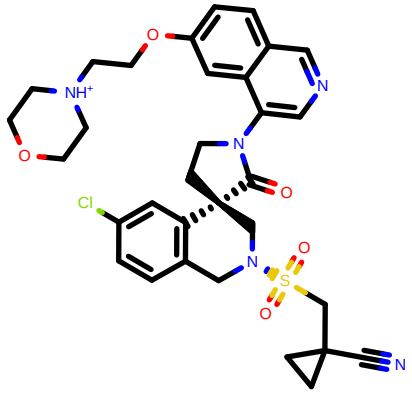
CID:	MAT-POS-853c0ffa-14_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1768
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.32

ALP-POS-4483ae88-1_1



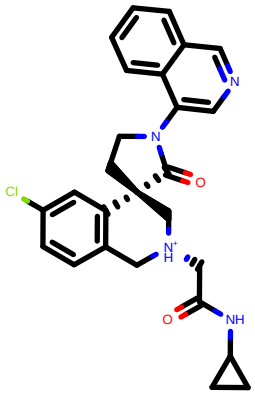
CID:	ALP-POS-4483ae88-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1512
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.17

EDJ-MED-468565e0-2_1



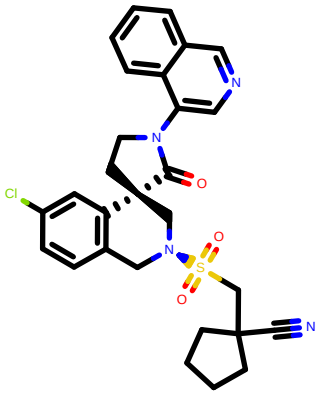
CID:	EDJ-MED-468565e0-2_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1931
DDG (kcal/mol):	1.35
dDDG (kcal/mol):	0.49

MAT-POS-69786b79-2_1



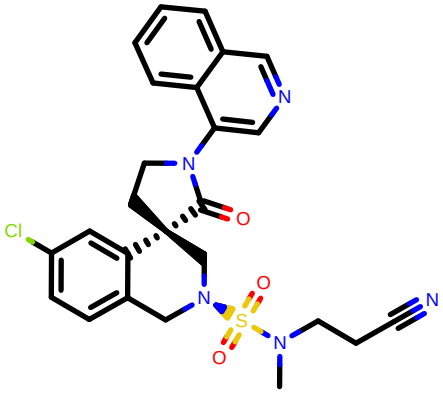
CID:	MAT-POS-69786b79-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN1622
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.38

ALP-POS-ecbed2ba-15_1



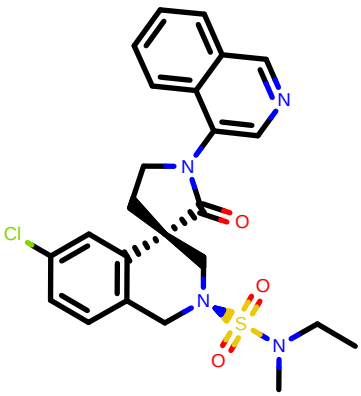
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN1819
DDG (kcal/mol):	1.37
dDDG (kcal/mol):	0.41

ALP-POS-ecbed2ba-16_1



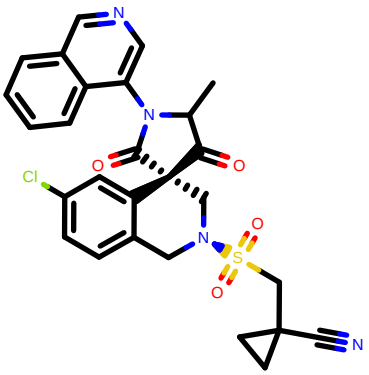
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1717
DDG (kcal/mol):	1.39
dDDG (kcal/mol):	0.49

ALP-POS-ecbed2ba-18_2



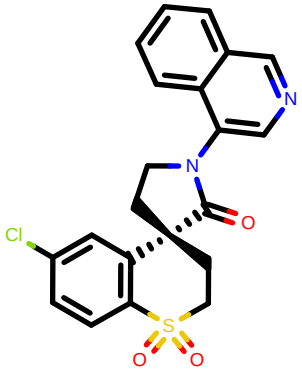
CID:	ALP-POS-ecbed2ba-18_2
SMILES:	CC[N@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1613
DDG (kcal/mol):	1.42
dDDG (kcal/mol):	0.37

PET-UNK-94036022-13_2



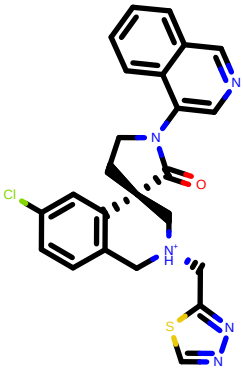
CID:	PET-UNK-94036022-13_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1847
DDG (kcal/mol):	1.45
dDDG (kcal/mol):	0.47

ALP-POS-41e2080f-1_1



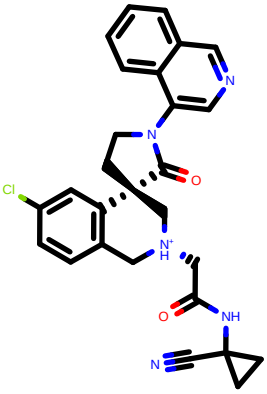
CID:	ALP-POS-41e2080f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1507
DDG (kcal/mol):	1.46
dDDG (kcal/mol):	0.19

PET-UNK-7e9559de-4_1



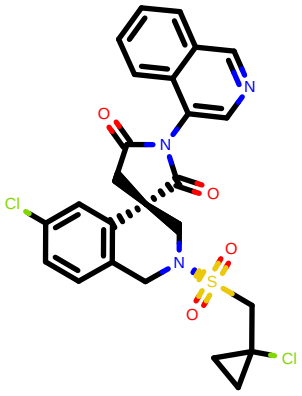
CID:	PET-UNK-7e9559de-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1575
DDG (kcal/mol):	1.46
dDDG (kcal/mol):	0.25

MAT-POS-69786b79-4_1



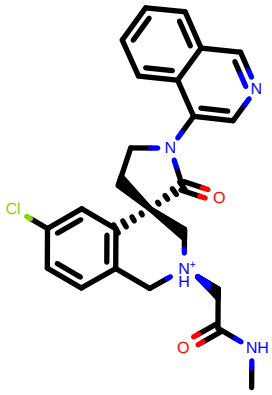
CID:	MAT-POS-69786b79-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN1729
DDG (kcal/mol):	1.46
dDDG (kcal/mol):	0.34

PET-UNK-94036022-5_2



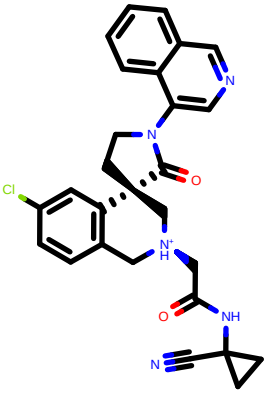
CID:	PET-UNK-94036022-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1743
DDG (kcal/mol):	1.50
dDDG (kcal/mol):	0.41

MAT-POS-c7726e07-6_2



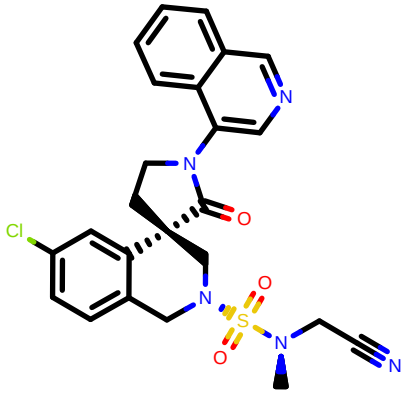
CID:	MAT-POS-c7726e07-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1543
DDG (kcal/mol):	1.50
dDDG (kcal/mol):	0.26

MAT-POS-69786b79-4_2



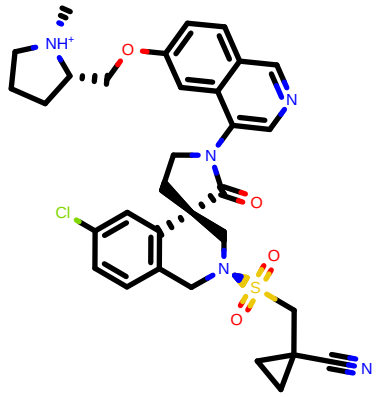
CID:	MAT-POS-69786b79-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN1736
DDG (kcal/mol):	1.53
dDDG (kcal/mol):	0.35

ALP-POS-ecbed2ba-17_1



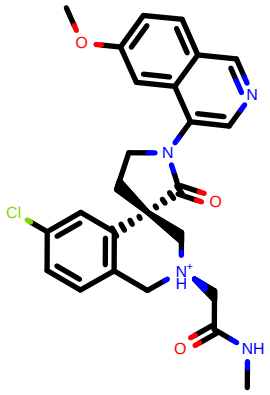
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1662
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.37

MAT-POS-40ad851a-1_8



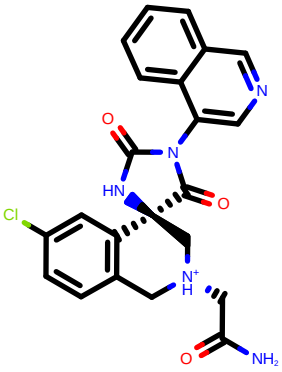
CID:	MAT-POS-40ad851a-1_8
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1930
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.66

EDJ-MED-b6c6ee2b-2_2



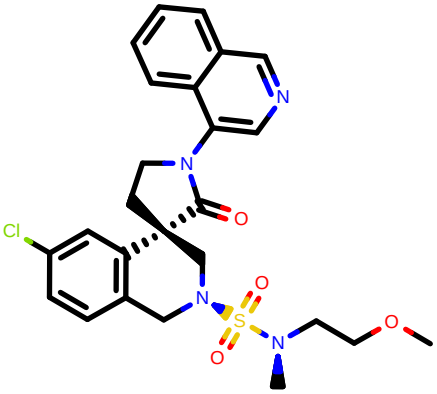
CID:	EDJ-MED-b6c6ee2b-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN1632
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.29

VLA-MRT-a639d434-2_1



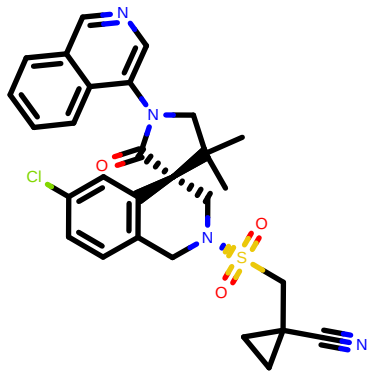
CID:	VLA-MRT-a639d434-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1526
DDG (kcal/mol):	1.57
dDDG (kcal/mol):	0.29

ALP-POS-ecbed2ba-21_2



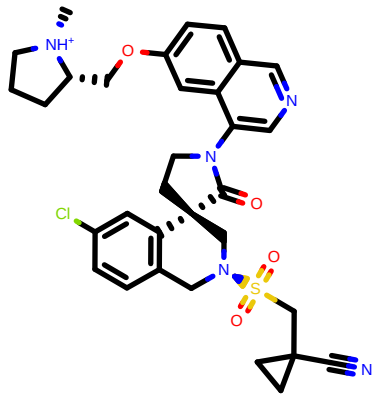
CID:	ALP-POS-ecbed2ba-21_2
SMILES:	C[N@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1724
DDG (kcal/mol):	1.58
dDDG (kcal/mol):	0.39

MAT-POS-50a80394-8_1



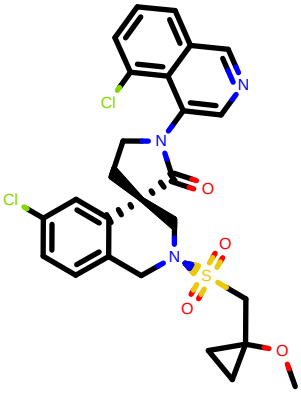
CID:	MAT-POS-50a80394-8_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN1832
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.80

MAT-POS-40ad851a-1_4



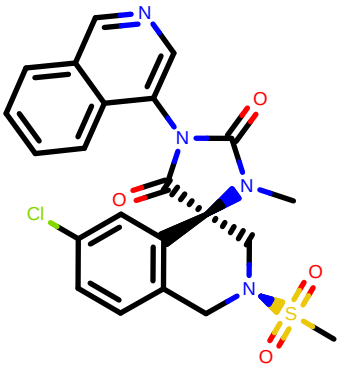
CID:	MAT-POS-40ad851a-1_4
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1926
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.58

MAT-POS-853c0ffa-7_1



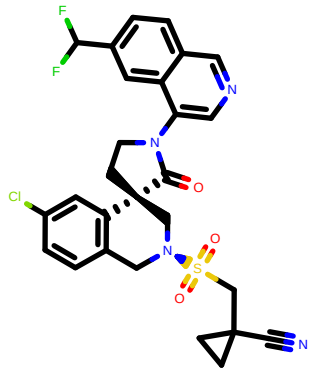
CID:	MAT-POS-853c0ffa-7_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1762
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.56

MAT-POS-2e8b2191-8_1



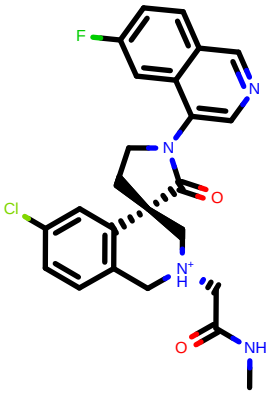
CID:	MAT-POS-2e8b2191-8_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1548
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.15

EDJ-MED-5cd3920d-2_1



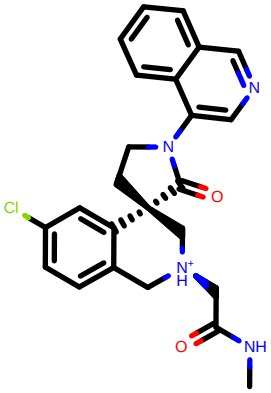
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1857
DDG (kcal/mol):	1.61
dDDG (kcal/mol):	0.45

LUO-POS-b4dec3be-2_1



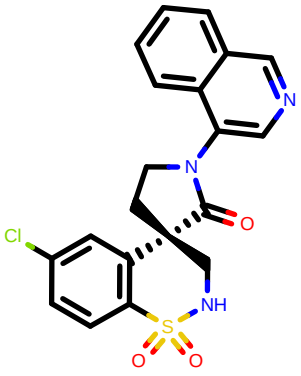
CID:	LUO-POS-b4dec3be-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1591
DDG (kcal/mol):	1.61
dDDG (kcal/mol):	0.29

LUO-POS-868e8996-11_2



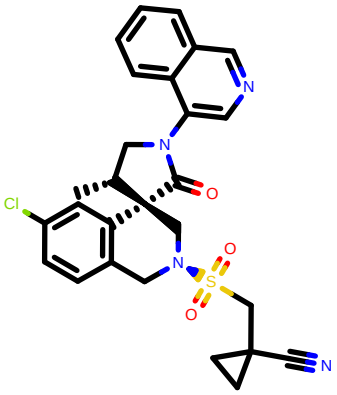
CID:	LUO-POS-868e8996-11_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1545
DDG (kcal/mol):	1.64
dDDG (kcal/mol):	0.26

EDJ-MED-f9b78f78-4_1



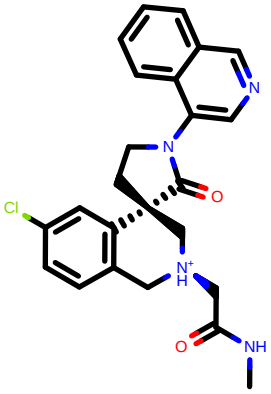
CID:	EDJ-MED-f9b78f78-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1513
DDG (kcal/mol):	1.65
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-1_1



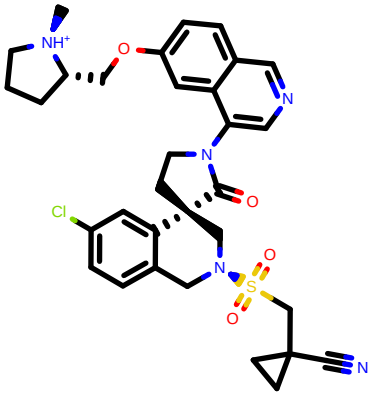
CID:	MAT-POS-50a80394-1_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1798
DDG (kcal/mol):	1.66
dDDG (kcal/mol):	0.46

LUO-POS-868e8996-12_2



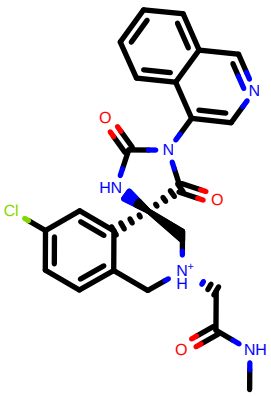
CID:	LUO-POS-868e8996-12_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1544
DDG (kcal/mol):	1.66
dDDG (kcal/mol):	0.25

MAT-POS-40ad851a-1_3



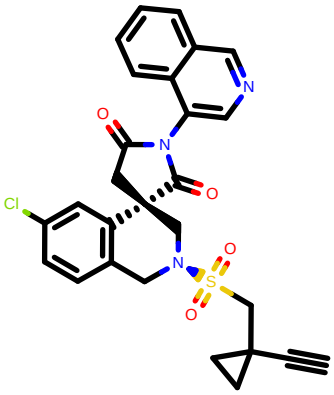
CID:	MAT-POS-40ad851a-1_3
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1923
DDG (kcal/mol):	1.68
dDDG (kcal/mol):	0.63

VLA-MRT-a639d434-1_1



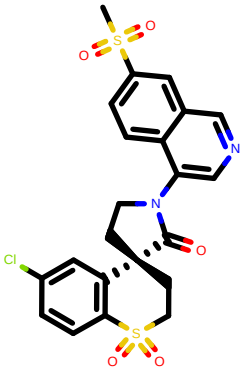
CID:	VLA-MRT-a639d434-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1549
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.26

PET-UNK-94036022-4_1



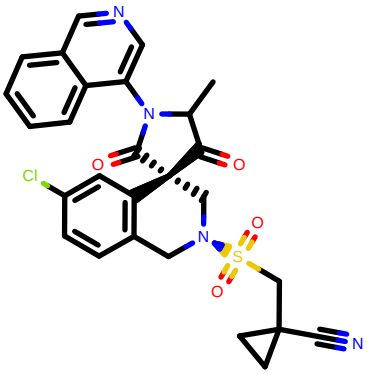
CID:	PET-UNK-94036022-4_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1797
DDG (kcal/mol):	1.71
dDDG (kcal/mol):	0.49

EDJ-MED-94fddcec-5_1



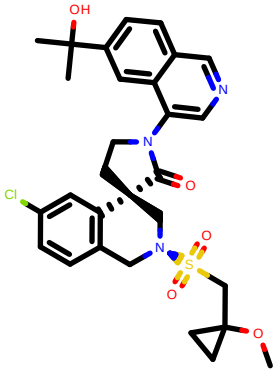
CID:	EDJ-MED-94fddcec-5_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1562
DDG (kcal/mol):	1.71
dDDG (kcal/mol):	0.23

PET-UNK-94036022-6_1



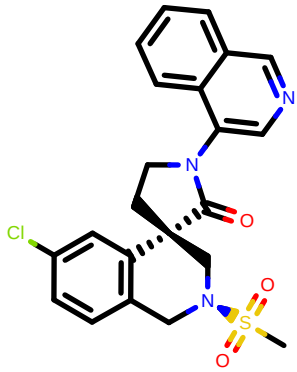
CID:	PET-UNK-94036022-6_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1841
DDG (kcal/mol):	1.72
dDDG (kcal/mol):	0.58

MAT-POS-853c0ffa-12_1



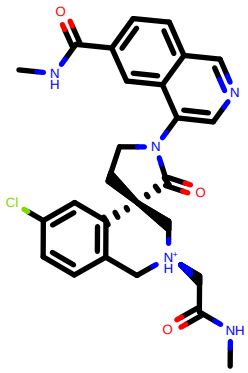
CID:	MAT-POS-853c0ffa-12_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN1870
DDG (kcal/mol):	1.72
dDDG (kcal/mol):	0.47

EDJ-MED-7587a9ee-3_1



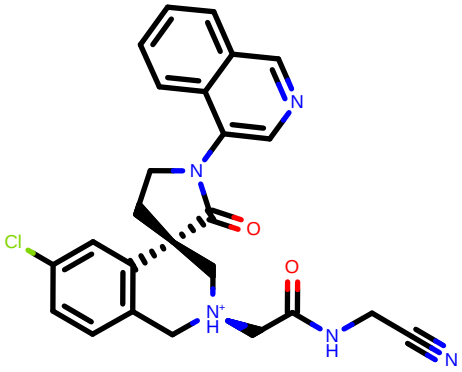
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1511
DDG (kcal/mol):	1.73
dDDG (kcal/mol):	0.23

MAT-POS-38eb6498-5_2



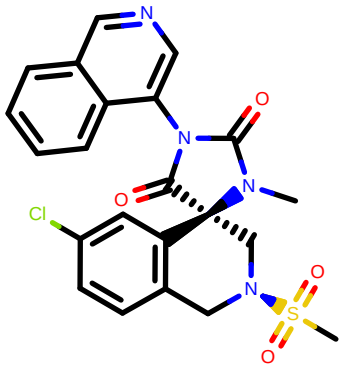
CID:	MAT-POS-38eb6498-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN1738
DDG (kcal/mol):	1.73
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-14_2



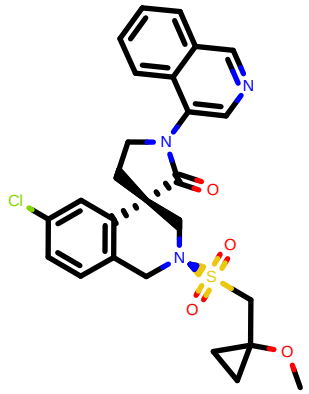
CID:	ALP-POS-ecbed2ba-14_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN1602
DDG (kcal/mol):	1.75
dDDG (kcal/mol):	0.26

EDJ-MED-7587a9ee-1_1



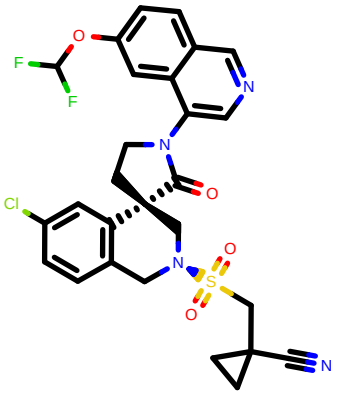
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1546
DDG (kcal/mol):	1.76
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-6_2



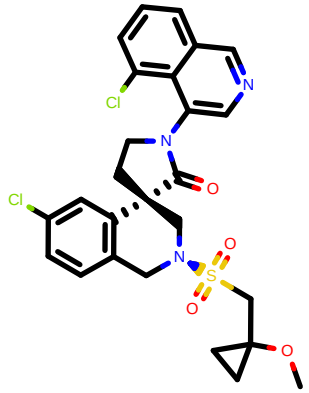
CID:	ALP-POS-ecbed2ba-6_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1697
DDG (kcal/mol):	1.78
dDDG (kcal/mol):	0.42

EDJ-MED-5cd3920d-1_2



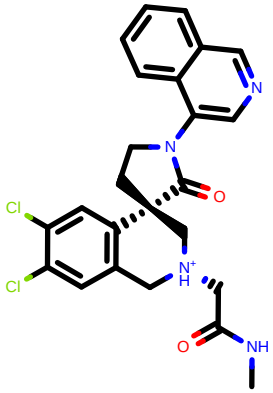
CID:	EDJ-MED-5cd3920d-1_2
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1889
DDG (kcal/mol):	1.78
dDDG (kcal/mol):	0.67

MAT-POS-853c0ffa-7_2



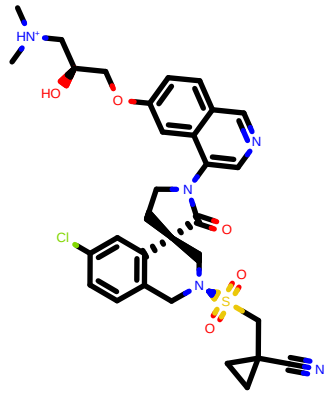
CID:	MAT-POS-853c0ffa-7_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1763
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.34

ALP-POS-afe0272e-1_1



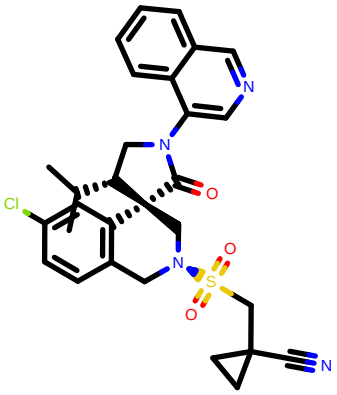
CID:	ALP-POS-afe0272e-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN1568
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.34

EDJ-MED-ee81482e-3_1



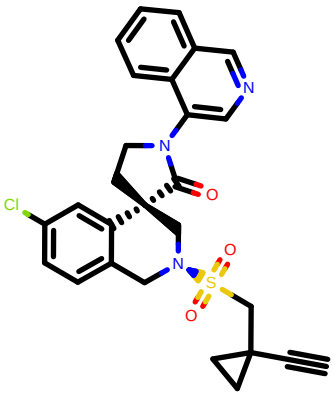
CID:	EDJ-MED-ee81482e-3_1
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1913
DDG (kcal/mol):	1.80
dDDG (kcal/mol):	0.77

MAT-POS-50a80394-3_1



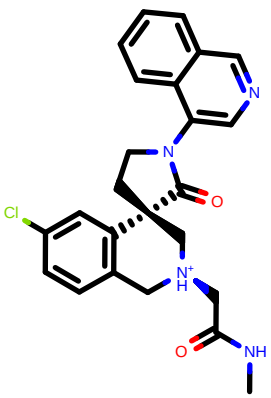
CID:	MAT-POS-50a80394-3_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1846
DDG (kcal/mol):	1.81
dDDG (kcal/mol):	0.73

PET-UNK-94036022-2_2



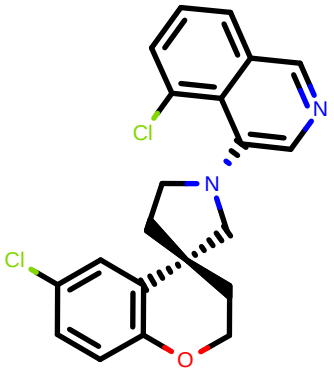
CID:	PET-UNK-94036022-2_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1744
DDG (kcal/mol):	1.81
dDDG (kcal/mol):	0.51

MAT-POS-c7726e07-5_2



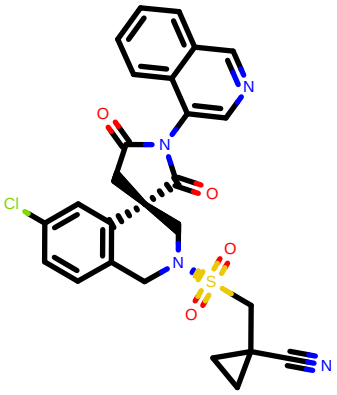
CID:	MAT-POS-c7726e07-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1535
DDG (kcal/mol):	1.82
dDDG (kcal/mol):	0.22

EDJ-MED-e78d5f1a-1_2



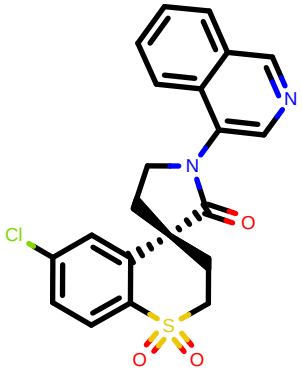
CID:	EDJ-MED-e78d5f1a-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1475
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.13

LUO-POS-868e8996-10_2



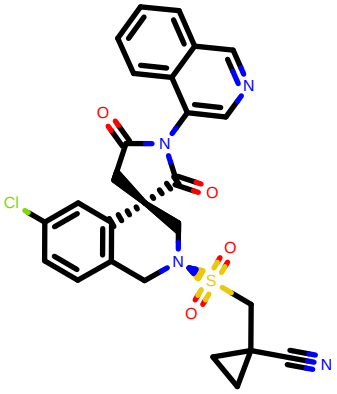
CID:	LUO-POS-868e8996-10_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1758
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.48

EDJ-MED-94fddcec-4_1



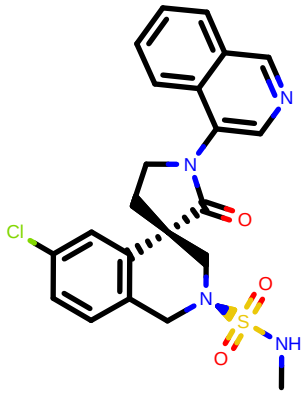
CID:	EDJ-MED-94fddcec-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1502
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.21

MAT-POS-1bed62cf-1_1



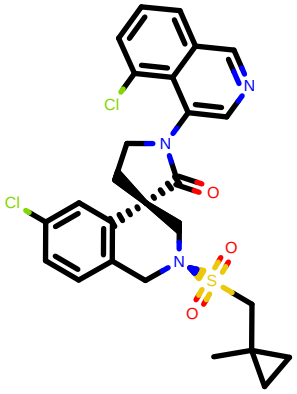
CID:	MAT-POS-1bed62cf-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1752
DDG (kcal/mol):	1.83
dDDG (kcal/mol):	0.37

LUO-POS-ed2cfb03-2_1



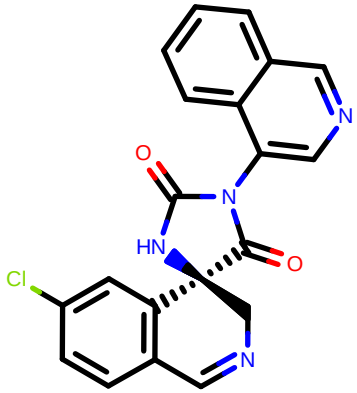
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	CNS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1557
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.27

MAT-POS-853c0ffa-17_1



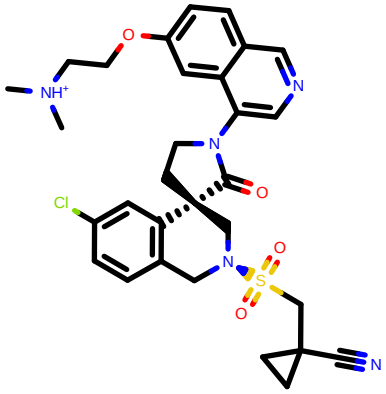
CID:	MAT-POS-853c0ffa-17_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1693
DDG (kcal/mol):	1.85
dDDG (kcal/mol):	0.43

VLA-MRT-8c78ee15-2_1



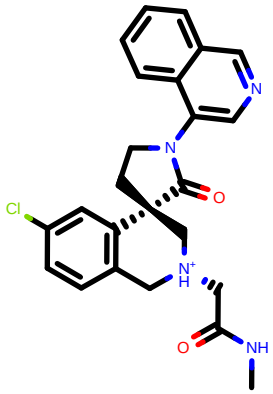
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1497
DDG (kcal/mol):	1.86
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-9_1



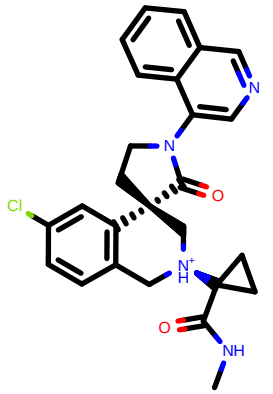
CID:	MAT-POS-853c0ffa-9_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1896
DDG (kcal/mol):	1.86
dDDG (kcal/mol):	0.51

MAT-POS-c7726e07-5_1



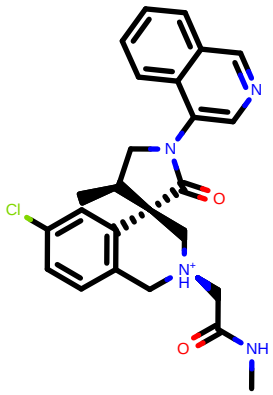
CID:	MAT-POS-c7726e07-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1538
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.27

MAT-POS-576f7758-1_2



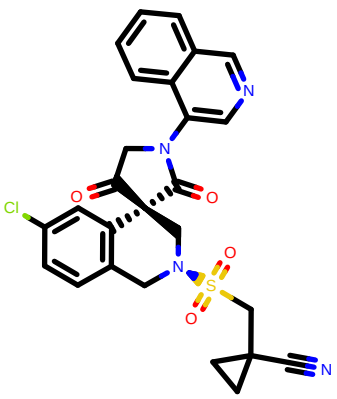
CID:	MAT-POS-576f7758-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1628
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.25

MAT-POS-50a80394-4_4



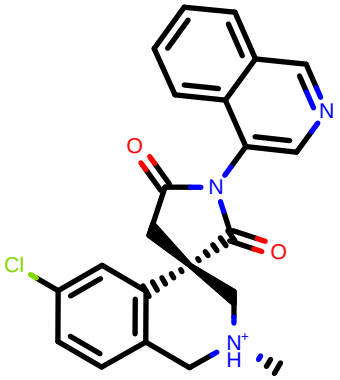
CID:	MAT-POS-50a80394-4_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1585
DDG (kcal/mol):	1.87
dDDG (kcal/mol):	0.25

EDJ-MED-a12e3a20-1_1



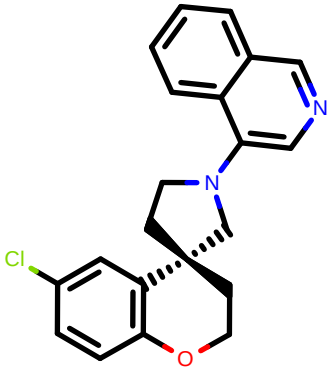
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1788
DDG (kcal/mol):	1.88
dDDG (kcal/mol):	0.41

JOH-MSK-51c67e7d-1_1



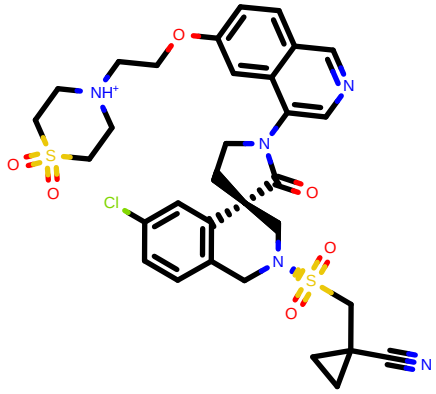
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1505
DDG (kcal/mol):	1.89
dDDG (kcal/mol):	0.18

EDJ-MED-159244ea-2_1



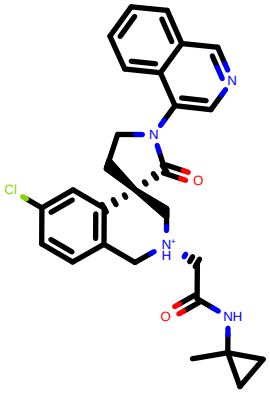
CID:	EDJ-MED-159244ea-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1464
DDG (kcal/mol):	1.91
dDDG (kcal/mol):	0.12

EDJ-MED-468565e0-3_2



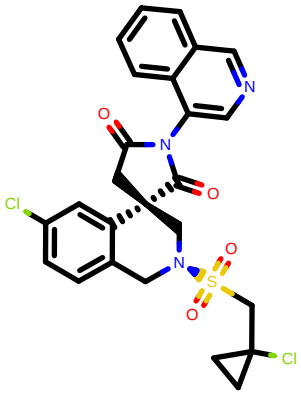
CID:	EDJ-MED-468565e0-3_2
SMILES:	c1cc2cncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1945
DDG (kcal/mol):	1.92
dDDG (kcal/mol):	0.60

MAT-POS-69786b79-3_1



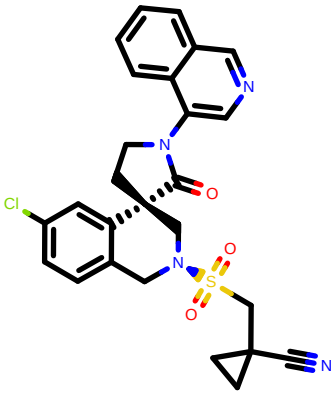
CID:	MAT-POS-69786b79-3_1
SMILES:	CC1(CC1)NC(=O)C[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1667
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.38

PET-UNK-94036022-12_2



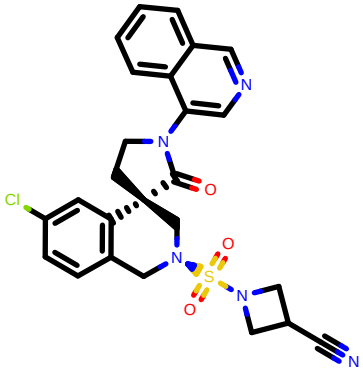
CID:	PET-UNK-94036022-12_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1751
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.38

MIK-ENA-5d9157e9-2_1



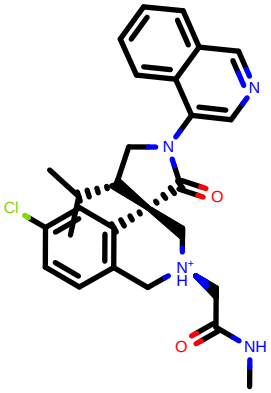
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1725
DDG (kcal/mol):	1.93
dDDG (kcal/mol):	0.45

ALP-POS-ecbed2ba-9_2



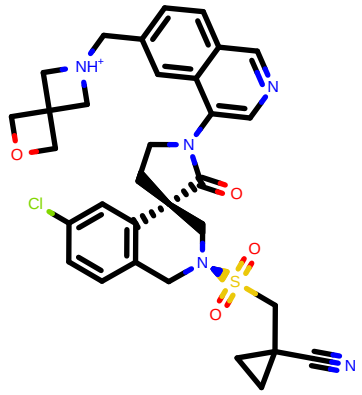
CID:	ALP-POS-ecbed2ba-9_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN1700
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.73

MAT-POS-50a80394-6_3



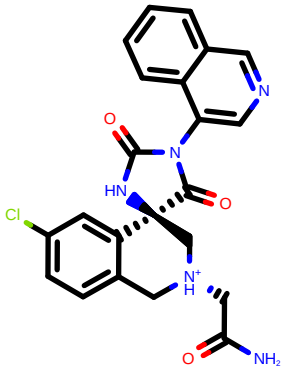
CID:	MAT-POS-50a80394-6_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1684
DDG (kcal/mol):	1.98
dDDG (kcal/mol):	0.31

EDJ-MED-ee81482e-5_2



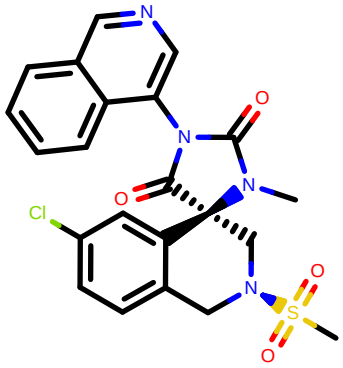
CID:	EDJ-MED-ee81482e-5_2
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@](Cc7c6cc(cc7)Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN1921
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.49

VLA-MRT-8c78ee15-4_1



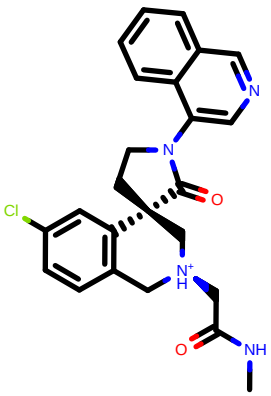
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1524
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.29

MAT-POS-2e8b2191-8_2



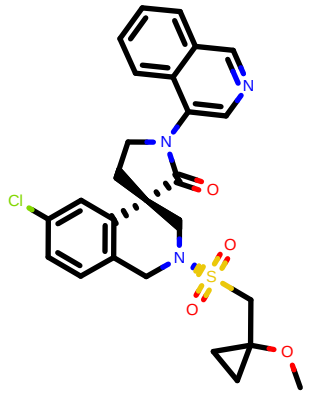
CID:	MAT-POS-2e8b2191-8_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1556
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.16

EDJ-MED-8bb691af-4_2



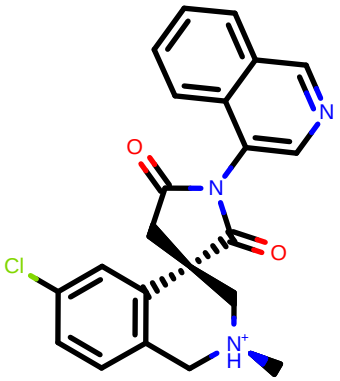
CID:	EDJ-MED-8bb691af-4_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1530
DDG (kcal/mol):	2.00
dDDG (kcal/mol):	0.28

ALP-POS-ecbed2ba-6_1



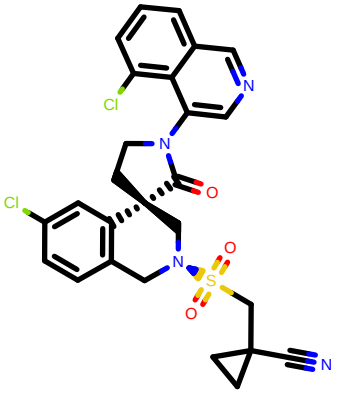
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1704
DDG (kcal/mol):	2.01
dDDG (kcal/mol):	0.38

JOH-MSK-51c67e7d-2_2



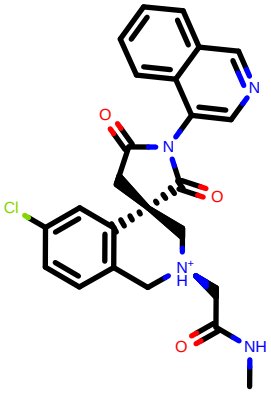
CID:	JOH-MSK-51c67e7d-2_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1509
DDG (kcal/mol):	2.04
dDDG (kcal/mol):	0.15

MAT-POS-1d5ab790-1_1



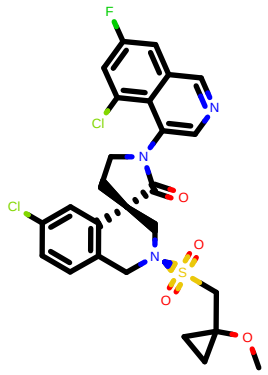
CID:	MAT-POS-1d5ab790-1_1
SMILES:	c1cc2ncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1777
DDG (kcal/mol):	2.04
dDDG (kcal/mol):	0.59

JOH-MSK-1f2dff76-1_2



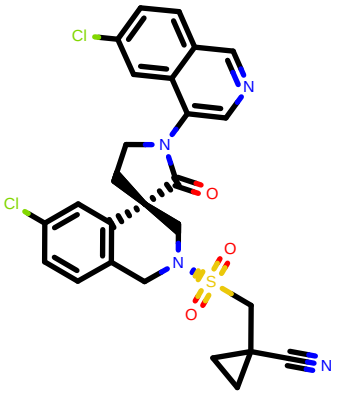
CID:	JOH-MSK-1f2dff76-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1593
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-8_2



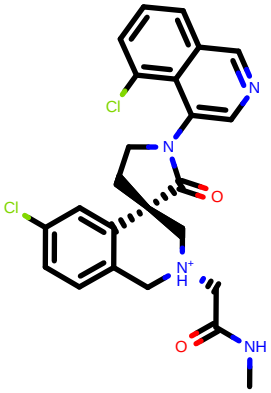
CID:	MAT-POS-853c0ffa-8_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1822
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.37

EDJ-MED-b6c6ee2b-4_2



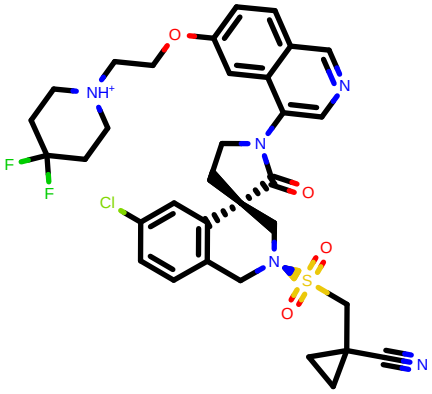
CID:	EDJ-MED-b6c6ee2b-4_2
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1796
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.47

MAT-POS-1d5ab790-2_1



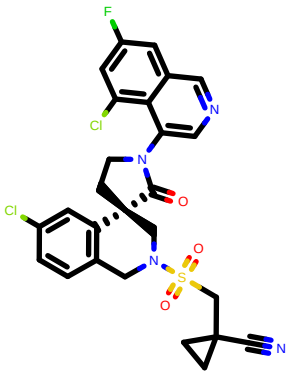
CID:	MAT-POS-1d5ab790-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1569
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.34

EDJ-MED-468565e0-4_1



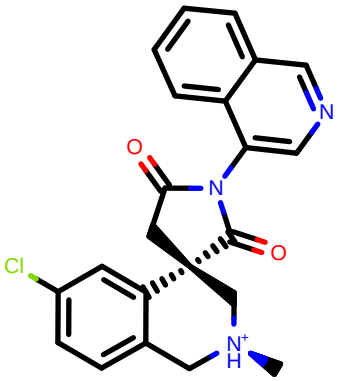
CID:	EDJ-MED-468565e0-4_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCC(CC3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1947
DDG (kcal/mol):	2.06
dDDG (kcal/mol):	0.76

MAT-POS-853c0ffa-6_2



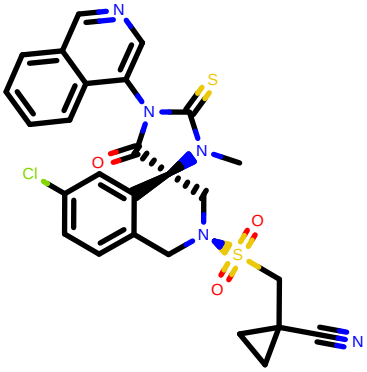
CID:	MAT-POS-853c0ffa-6_2
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1815
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.54

JOH-MSK-51c67e7d-1_2



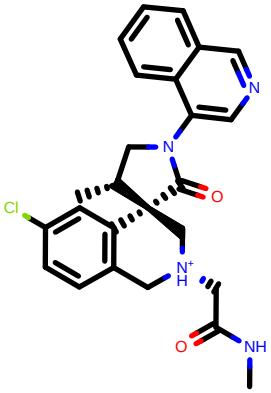
CID:	JOH-MSK-51c67e7d-1_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1508
DDG (kcal/mol):	2.08
dDDG (kcal/mol):	0.15

MAT-POS-c2d406ed-4_2



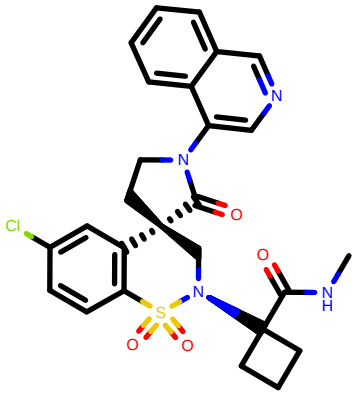
CID:	MAT-POS-c2d406ed-4_2
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1829
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.33

MAT-POS-50a80394-4_1



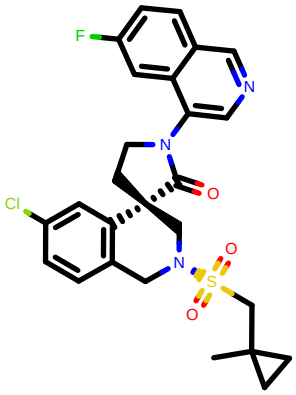
CID:	MAT-POS-50a80394-4_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1582
DDG (kcal/mol):	2.11
dDDG (kcal/mol):	0.26

EDJ-MED-98c0a822-1_2



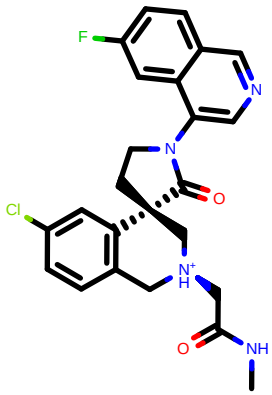
CID:	EDJ-MED-98c0a822-1_2
SMILES:	CNC(=O)C1(CCC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1791
DDG (kcal/mol):	2.13
dDDG (kcal/mol):	0.43

MAT-POS-853c0ffa-21_1



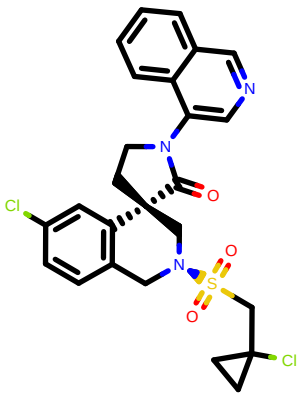
CID:	MAT-POS-853c0ffa-21_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1699
DDG (kcal/mol):	2.14
dDDG (kcal/mol):	0.33

MAT-POS-b4d6b7fc-5_2



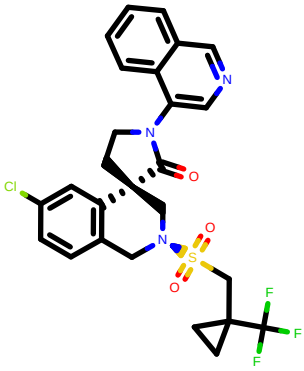
CID:	MAT-POS-b4d6b7fc-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1564
DDG (kcal/mol):	2.14
dDDG (kcal/mol):	0.28

PET-UNK-94036022-10_2



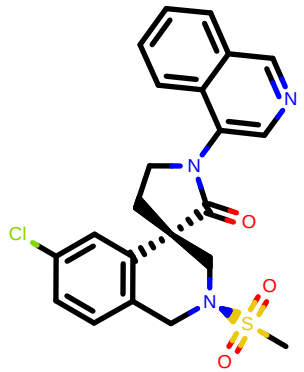
CID:	PET-UNK-94036022-10_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1677
DDG (kcal/mol):	2.15
dDDG (kcal/mol):	0.40

EDJ-MED-5cd3920d-6_2



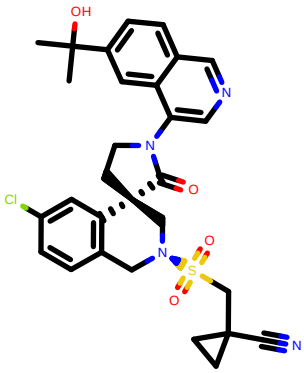
CID:	EDJ-MED-5cd3920d-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN1831
DDG (kcal/mol):	2.15
dDDG (kcal/mol):	0.66

EDJ-MED-7587a9ee-3_2



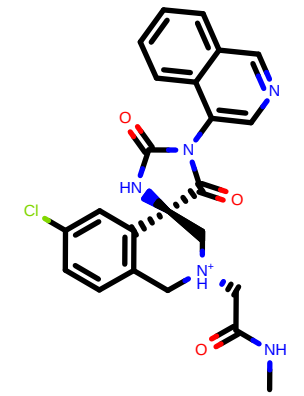
CID:	EDJ-MED-7587a9ee-3_2
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1510
DDG (kcal/mol):	2.16
dDDG (kcal/mol):	0.27

MAT-POS-853c0ffa-11_2



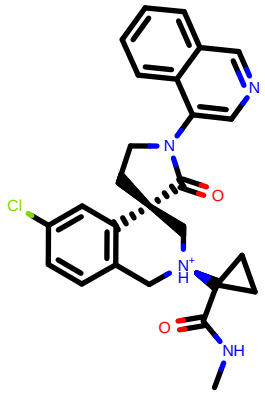
CID:	MAT-POS-853c0ffa-11_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1874
DDG (kcal/mol):	2.17
dDDG (kcal/mol):	0.63

VLA-MRT-8c78ee15-3_1



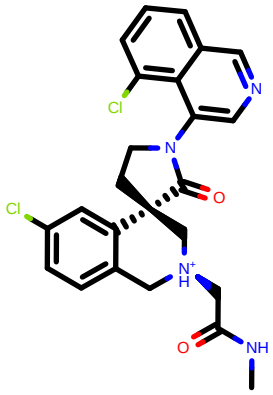
CID:	VLA-MRT-8c78ee15-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1551
DDG (kcal/mol):	2.17
dDDG (kcal/mol):	0.30

ALP-POS-ecbed2ba-7_2



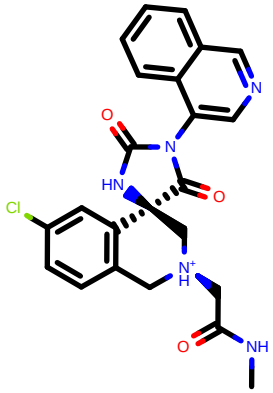
CID:	ALP-POS-ecbed2ba-7_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1600
DDG (kcal/mol):	2.17
dDDG (kcal/mol):	0.24

MAT-POS-1d5ab790-2_2



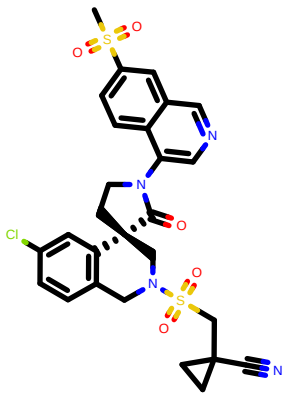
CID:	MAT-POS-1d5ab790-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1573
DDG (kcal/mol):	2.18
dDDG (kcal/mol):	0.26

VLA-MRT-a639d434-1_2



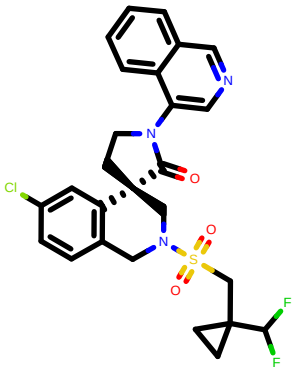
CID:	VLA-MRT-a639d434-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1558
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-15_2



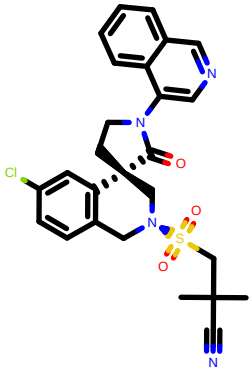
CID:	MAT-POS-853c0ffa-15_2
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1864
DDG (kcal/mol):	2.21
dDDG (kcal/mol):	0.60

EDJ-MED-5cd3920d-5_1



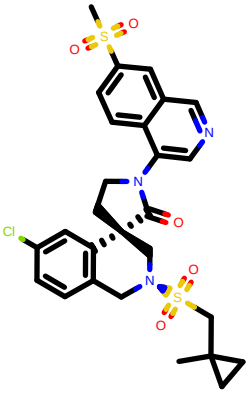
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN1803
DDG (kcal/mol):	2.25
dDDG (kcal/mol):	0.47

ALP-POS-ecbed2ba-13_1



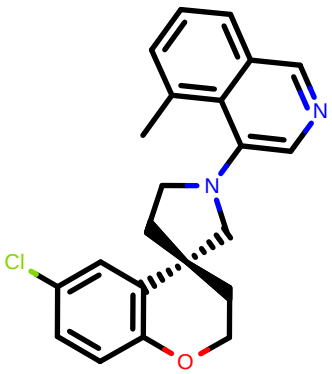
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	CC(C)(CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN1715
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.48

MAT-POS-853c0ffa-22_2



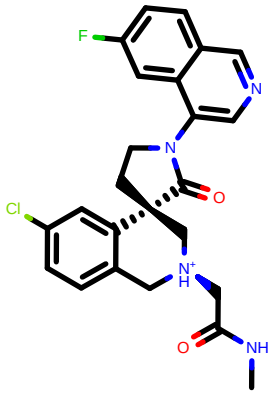
CID:	MAT-POS-853c0ffa-22_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1850
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.67

EDJ-MED-a6bab6fb-1_2



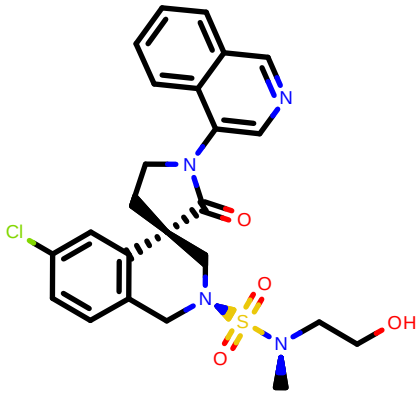
CID:	EDJ-MED-a6bab6fb-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1466
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.15

LUO-POS-b4dec3be-2_2



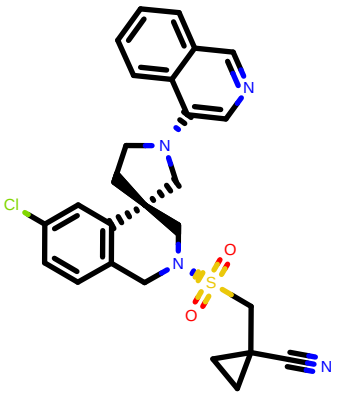
CID:	LUO-POS-b4dec3be-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1589
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-19_1



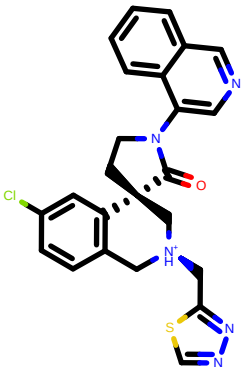
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	C[N@@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1670
DDG (kcal/mol):	2.34
dDDG (kcal/mol):	0.41

EDJ-MED-8bb691af-2_2



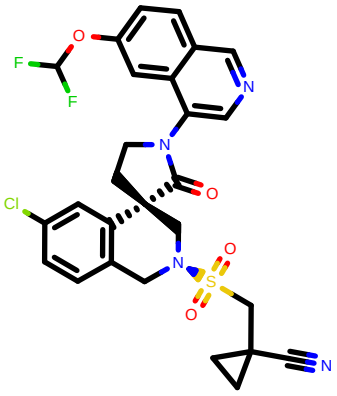
CID:	EDJ-MED-8bb691af-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1655
DDG (kcal/mol):	2.36
dDDG (kcal/mol):	0.45

MAT-POS-96396902-1_2



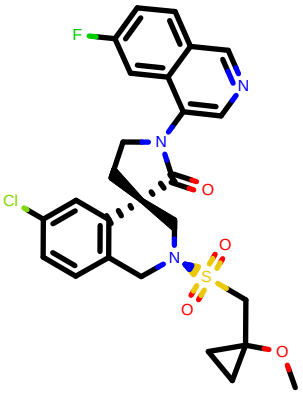
CID:	MAT-POS-96396902-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1586
DDG (kcal/mol):	2.36
dDDG (kcal/mol):	0.28

EDJ-MED-5cd3920d-1_1



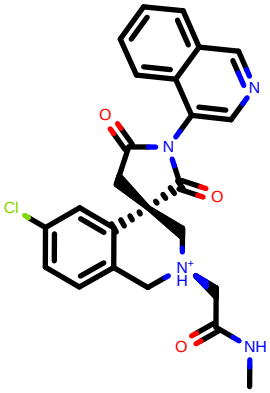
CID:	EDJ-MED-5cd3920d-1_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1884
DDG (kcal/mol):	2.39
dDDG (kcal/mol):	0.49

MAT-POS-853c0ffa-14_2



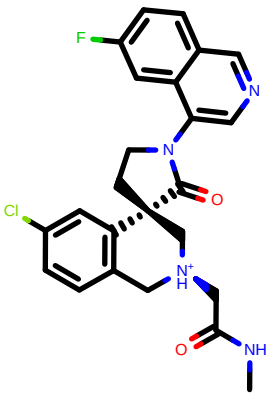
CID:	MAT-POS-853c0ffa-14_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1770
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.35

MAT-POS-1bed62cf-3_2



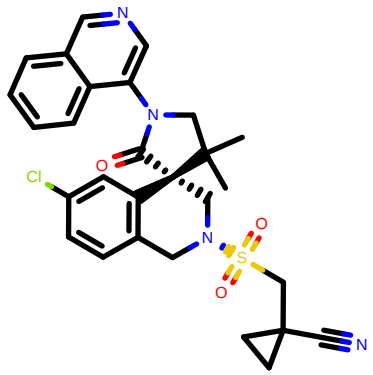
CID:	MAT-POS-1bed62cf-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1555
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.23

LUO-POS-b4dec3be-1_2



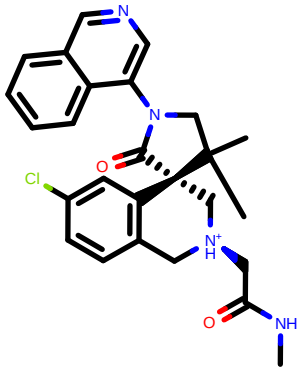
CID:	LUO-POS-b4dec3be-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1590
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-8_2



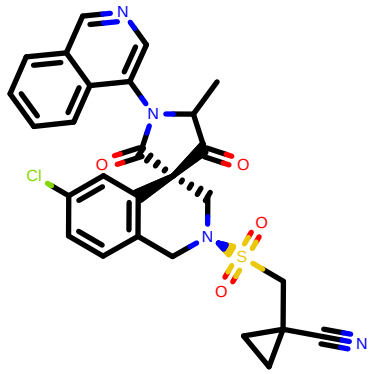
CID:	MAT-POS-50a80394-8_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN1828
DDG (kcal/mol):	2.40
dDDG (kcal/mol):	0.86

MAT-POS-50a80394-7_2



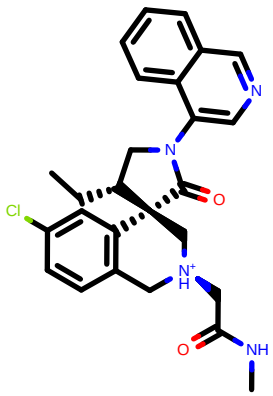
CID:	MAT-POS-50a80394-7_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN1640
DDG (kcal/mol):	2.44
dDDG (kcal/mol):	0.26

PET-UNK-94036022-6_2



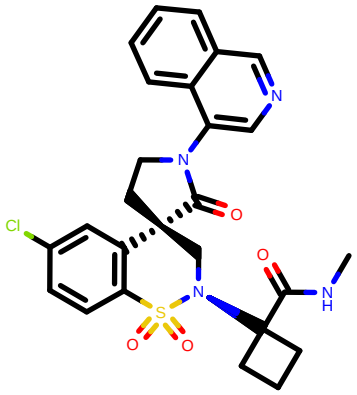
CID:	PET-UNK-94036022-6_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1843
DDG (kcal/mol):	2.44
dDDG (kcal/mol):	0.62

MAT-POS-50a80394-5_3



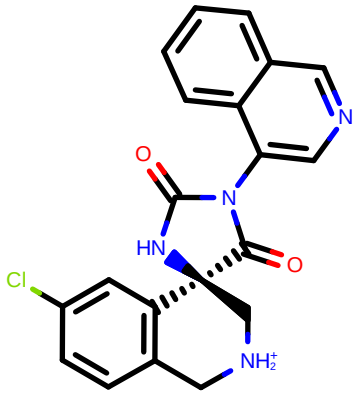
CID:	MAT-POS-50a80394-5_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1634
DDG (kcal/mol):	2.46
dDDG (kcal/mol):	0.33

EDJ-MED-98c0a822-1_1



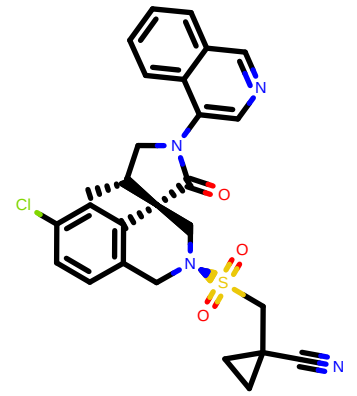
CID:	EDJ-MED-98c0a822-1_1
SMILES:	CNC(=O)C1(CCC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1789
DDG (kcal/mol):	2.47
dDDG (kcal/mol):	0.53

VLA-MRT-a639d434-3_1



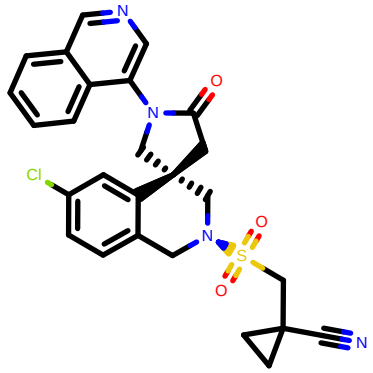
CID:	VLA-MRT-a639d434-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1500
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.22

MAT-POS-50a80394-1_3



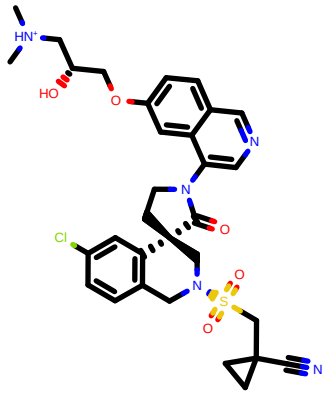
CID:	MAT-POS-50a80394-1_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1799
DDG (kcal/mol):	2.48
dDDG (kcal/mol):	0.34

EDJ-MED-8bb691af-5_2



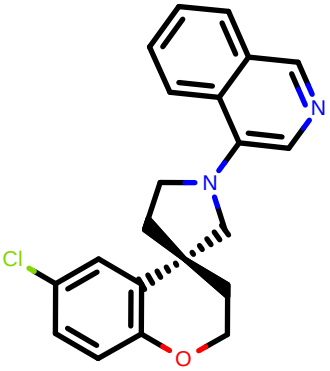
CID:	EDJ-MED-8bb691af-5_2
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1695
DDG (kcal/mol):	2.50
dDDG (kcal/mol):	0.50

EDJ-MED-ee81482e-3_4



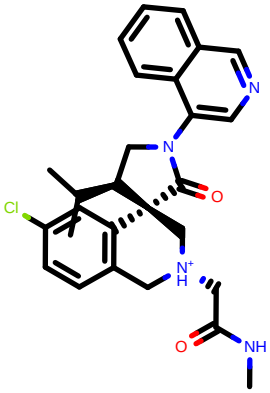
CID:	EDJ-MED-ee81482e-3_4
SMILES:	C[NH+](C)C[C@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1918
DDG (kcal/mol):	2.51
dDDG (kcal/mol):	0.76

MAT-POS-983b399a-2_2



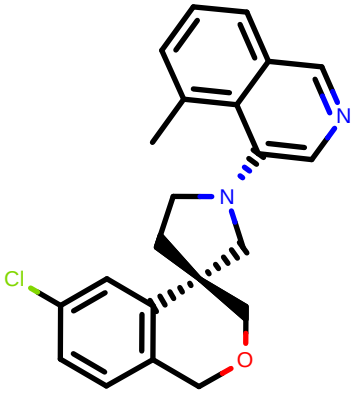
CID:	MAT-POS-983b399a-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1461
DDG (kcal/mol):	2.52
dDDG (kcal/mol):	0.14

MAT-POS-50a80394-6_2



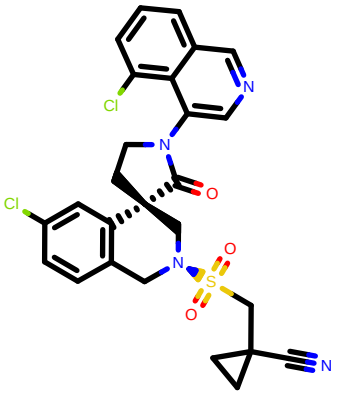
CID:	MAT-POS-50a80394-6_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1683
DDG (kcal/mol):	2.54
dDDG (kcal/mol):	0.32

EDJ-MED-f3cfbbb5-1_2



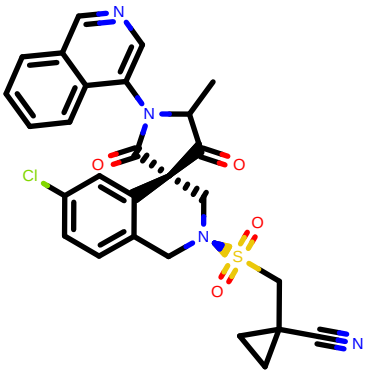
CID:	EDJ-MED-f3cfbbb5-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN1473
DDG (kcal/mol):	2.56
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-5_1



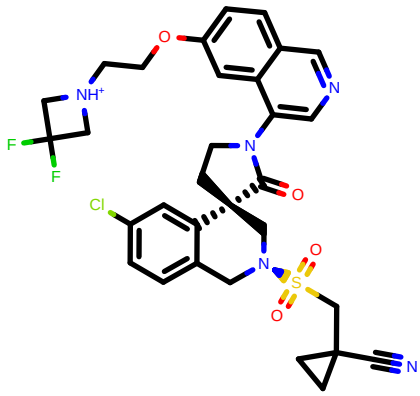
CID:	MAT-POS-853c0ffa-5_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1760
DDG (kcal/mol):	2.56
dDDG (kcal/mol):	0.63

PET-UNK-94036022-13_1



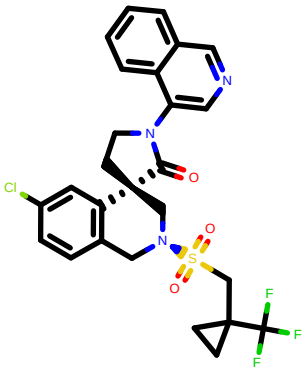
CID:	PET-UNK-94036022-13_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1845
DDG (kcal/mol):	2.60
dDDG (kcal/mol):	0.59

EDJ-MED-468565e0-5_1



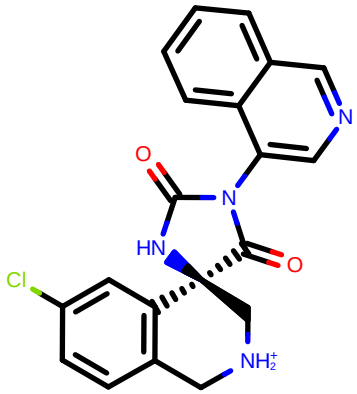
CID:	EDJ-MED-468565e0-5_1
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1936
DDG (kcal/mol):	2.62
dDDG (kcal/mol):	0.78

EDJ-MED-5cd3920d-6_1



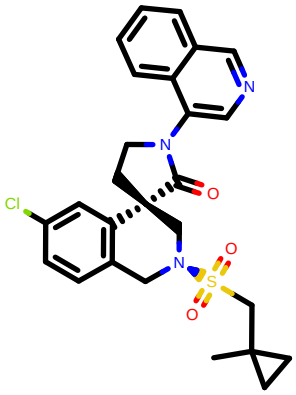
CID:	EDJ-MED-5cd3920d-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN1836
DDG (kcal/mol):	2.63
dDDG (kcal/mol):	0.45

VLA-MRT-8c78ee15-1_1



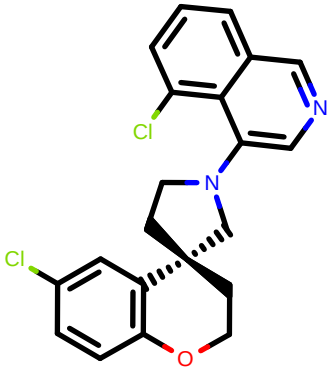
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1492
DDG (kcal/mol):	2.65
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-3_2



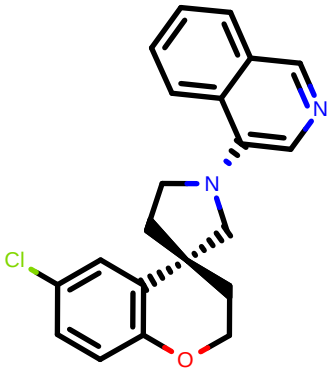
CID:	ALP-POS-ecbed2ba-3_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1661
DDG (kcal/mol):	2.72
dDDG (kcal/mol):	0.37

EDJ-MED-e78d5f1a-1_1



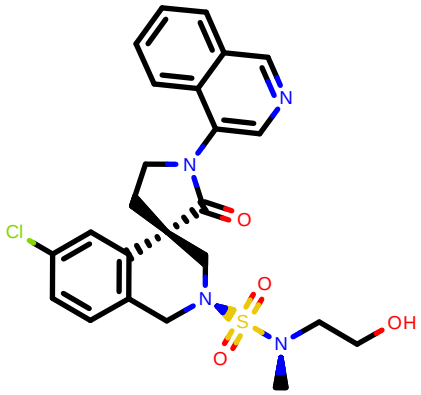
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1476
DDG (kcal/mol):	2.75
dDDG (kcal/mol):	0.14

EDJ-MED-159244ea-2_2



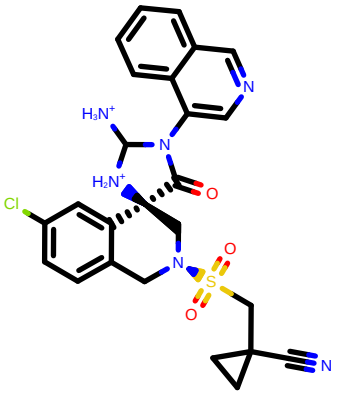
CID:	EDJ-MED-159244ea-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1463
DDG (kcal/mol):	2.77
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-19_3



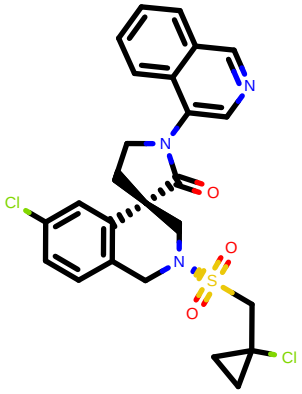
CID:	ALP-POS-ecbed2ba-19_3
SMILES:	C[N@@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1682
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	1.03

LUO-POS-eaf50f21-1_1



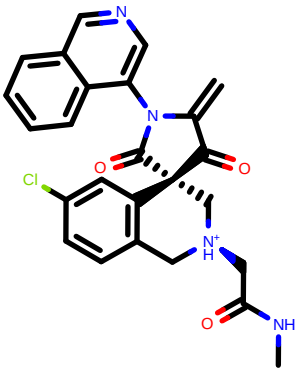
CID:	LUO-POS-eaf50f21-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)[NH+]=C3N
RUN:	RUN1809
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.42

PET-UNK-94036022-3_2



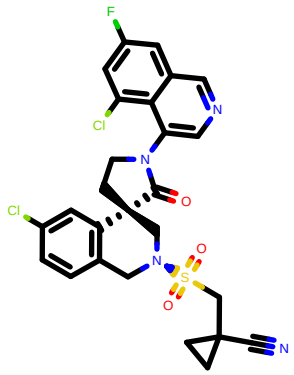
CID:	PET-UNK-94036022-3_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1685
DDG (kcal/mol):	2.78
dDDG (kcal/mol):	0.31

PET-UNK-94036022-7_2



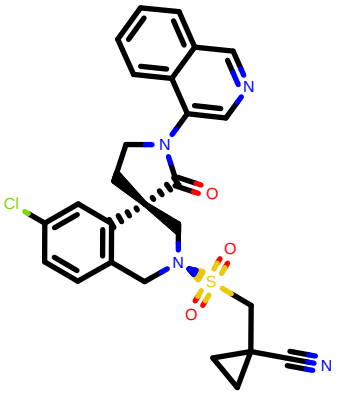
CID:	PET-UNK-94036022-7_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1646
DDG (kcal/mol):	2.83
dDDG (kcal/mol):	0.27

MAT-POS-853c0ffa-6_1



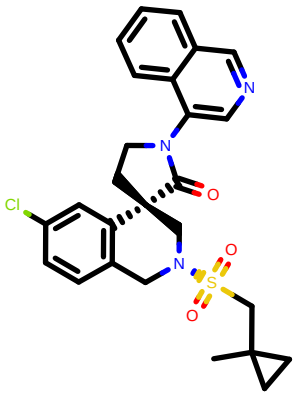
CID:	MAT-POS-853c0ffa-6_1
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1811
DDG (kcal/mol):	2.84
dDDG (kcal/mol):	0.54

ALP-POS-ecbed2ba-4_1



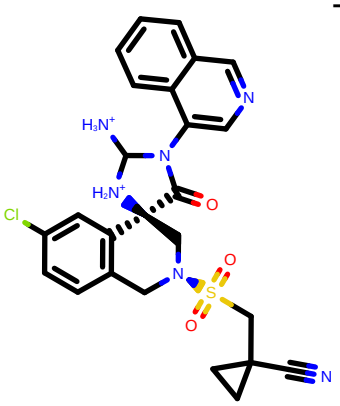
CID:	ALP-POS-ecbed2ba-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1702
DDG (kcal/mol):	2.85
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-3_1



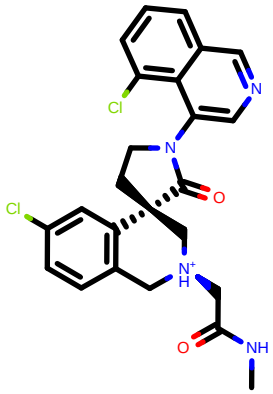
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1660
DDG (kcal/mol):	2.86
dDDG (kcal/mol):	0.28

LUO-POS-eaf50f21-1_2



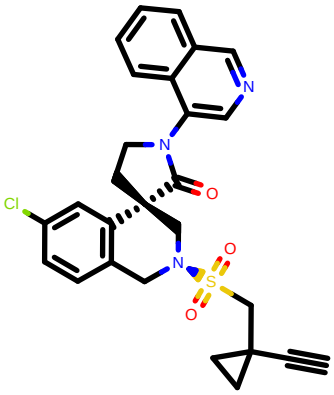
CID:	LUO-POS-eaf50f21-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)[NH+]=C3N
RUN:	RUN1813
DDG (kcal/mol):	2.87
dDDG (kcal/mol):	0.51

MAT-POS-b4d6b7fc-6_2



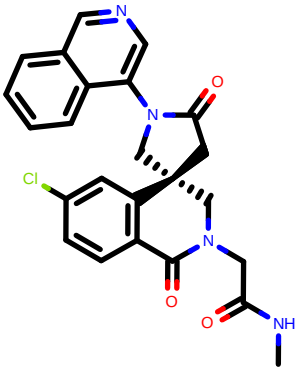
CID:	MAT-POS-b4d6b7fc-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1565
DDG (kcal/mol):	2.89
dDDG (kcal/mol):	0.34

PET-UNK-94036022-9_2



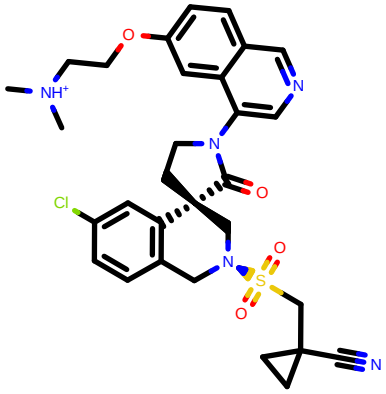
CID:	PET-UNK-94036022-9_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1746
DDG (kcal/mol):	2.90
dDDG (kcal/mol):	0.48

EDJ-MED-8bb691af-9_1



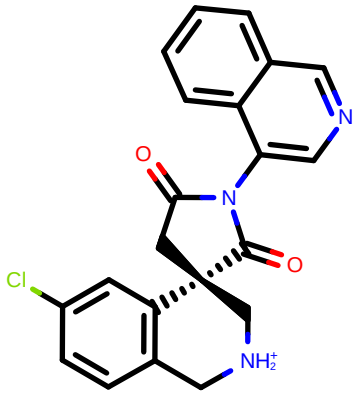
CID:	EDJ-MED-8bb691af-9_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1553
DDG (kcal/mol):	2.91
dDDG (kcal/mol):	0.17

LUO-POS-8484f2d3-2_1



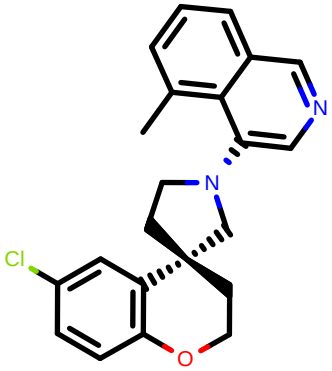
CID:	LUO-POS-8484f2d3-2_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1898
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.69

JOH-MSK-1f2dff76-4_1



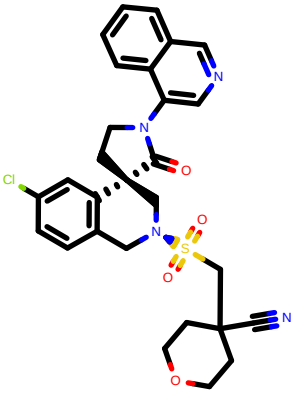
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN1493
DDG (kcal/mol):	2.96
dDDG (kcal/mol):	0.18

EDJ-MED-a6bab6fb-1_1



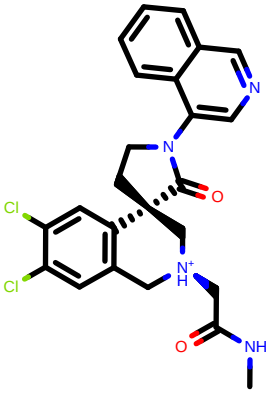
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1477
DDG (kcal/mol):	3.00
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-11_1



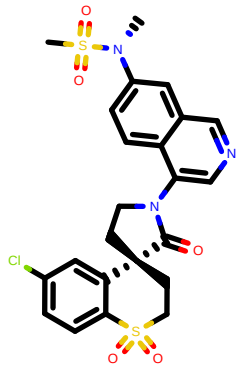
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN1842
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.51

ALP-POS-afe0272e-1_2



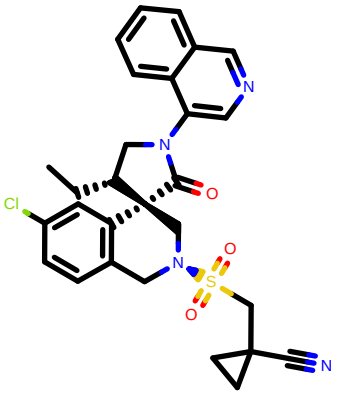
CID:	ALP-POS-afe0272e-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN1572
DDG (kcal/mol):	3.01
dDDG (kcal/mol):	0.43

EDJ-MED-94fddcec-6_2



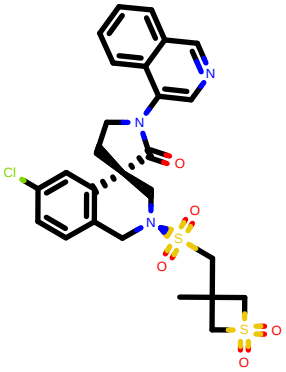
CID:	EDJ-MED-94fddcec-6_2
SMILES:	C[N@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1656
DDG (kcal/mol):	3.02
dDDG (kcal/mol):	0.27

MAT-POS-50a80394-2_1



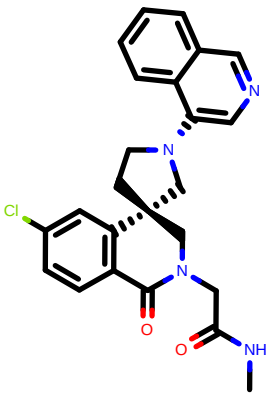
CID:	MAT-POS-50a80394-2_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1824
DDG (kcal/mol):	3.04
dDDG (kcal/mol):	0.30

ALP-POS-ecbed2ba-1_2



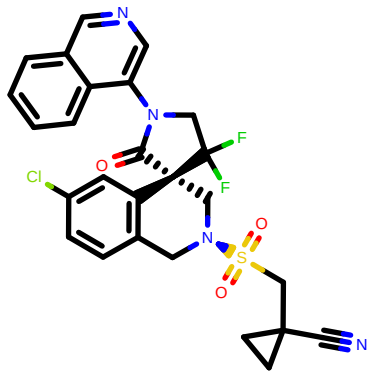
CID:	ALP-POS-ecbed2ba-1_2
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1821
DDG (kcal/mol):	3.07
dDDG (kcal/mol):	0.60

EDJ-MED-8bb691af-7_2



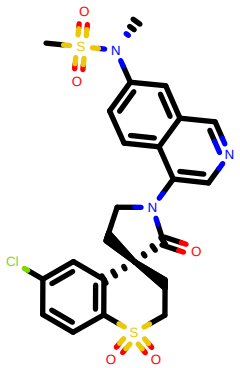
CID:	EDJ-MED-8bb691af-7_2
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1531
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.24

EDJ-MED-7e491f08-1_2



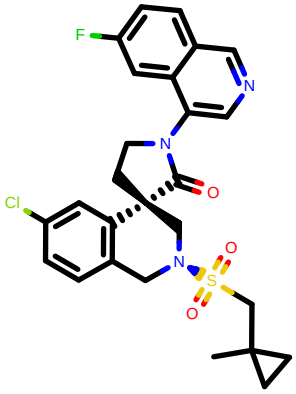
CID:	EDJ-MED-7e491f08-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN1837
DDG (kcal/mol):	3.09
dDDG (kcal/mol):	0.76

EDJ-MED-94fddcec-6_1



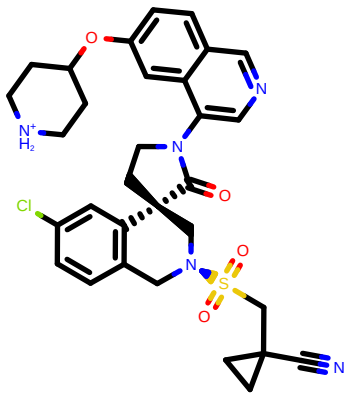
CID:	EDJ-MED-94fddcec-6_1
SMILES:	C[N@@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1658
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-21_2



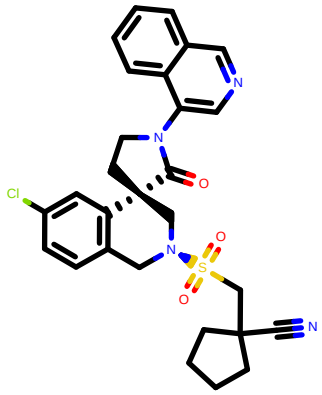
CID:	MAT-POS-853c0ffa-21_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1703
DDG (kcal/mol):	3.15
dDDG (kcal/mol):	0.42

EDJ-MED-ee81482e-4_1



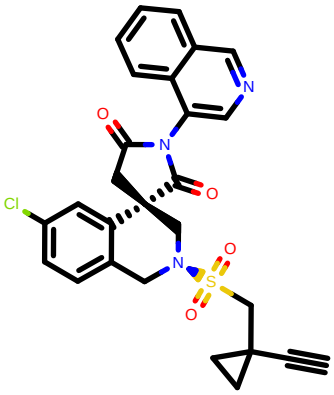
CID:	EDJ-MED-ee81482e-4_1
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1908
DDG (kcal/mol):	3.15
dDDG (kcal/mol):	0.61

ALP-POS-ecbed2ba-15_2



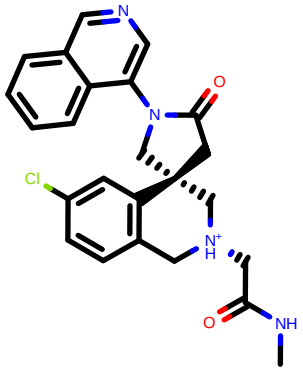
CID:	ALP-POS-ecbed2ba-15_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN1820
DDG (kcal/mol):	3.18
dDDG (kcal/mol):	0.54

PET-UNK-94036022-11_2



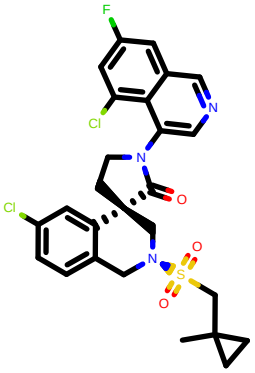
CID:	PET-UNK-94036022-11_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1802
DDG (kcal/mol):	3.18
dDDG (kcal/mol):	0.39

EDJ-MED-8bb691af-3_1



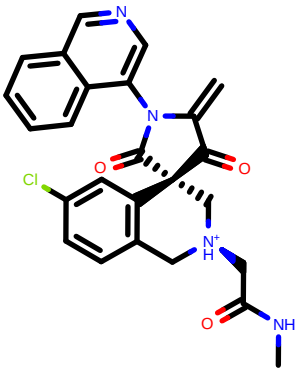
CID:	EDJ-MED-8bb691af-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1527
DDG (kcal/mol):	3.19
dDDG (kcal/mol):	0.31

MAT-POS-853c0ffa-18_1



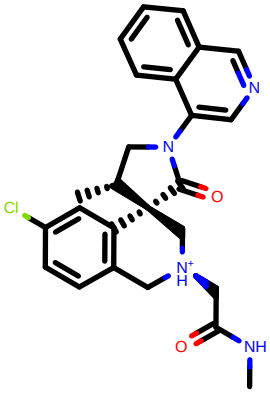
CID:	MAT-POS-853c0ffa-18_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1774
DDG (kcal/mol):	3.21
dDDG (kcal/mol):	0.39

PET-UNK-94036022-14_2



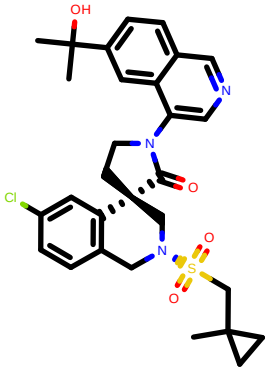
CID:	PET-UNK-94036022-14_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1647
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.29

MAT-POS-50a80394-4_3



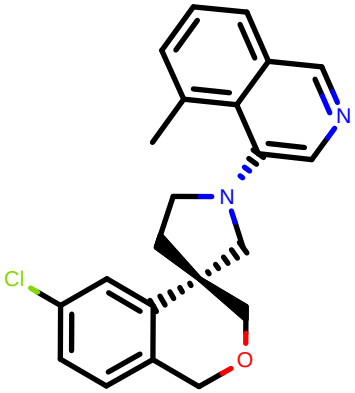
CID:	MAT-POS-50a80394-4_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1580
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.38

MAT-POS-853c0ffa-20_2



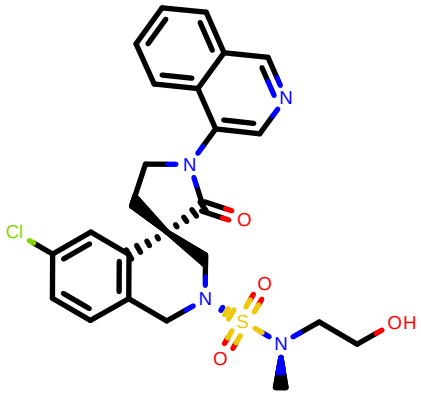
CID:	MAT-POS-853c0ffa-20_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN1853
DDG (kcal/mol):	3.27
dDDG (kcal/mol):	0.31

EDJ-MED-f3cfbbb5-1_1



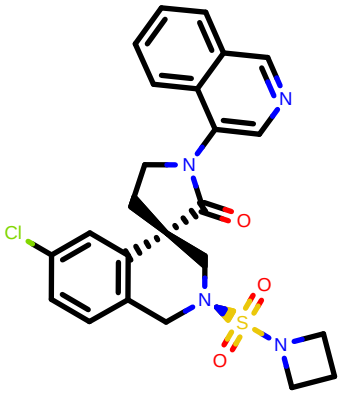
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN1472
DDG (kcal/mol):	3.28
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-19_2



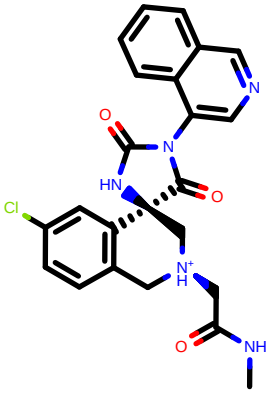
CID:	ALP-POS-ecbed2ba-19_2
SMILES:	C[N@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1676
DDG (kcal/mol):	3.29
dDDG (kcal/mol):	0.42

ALP-POS-ecbed2ba-20_2



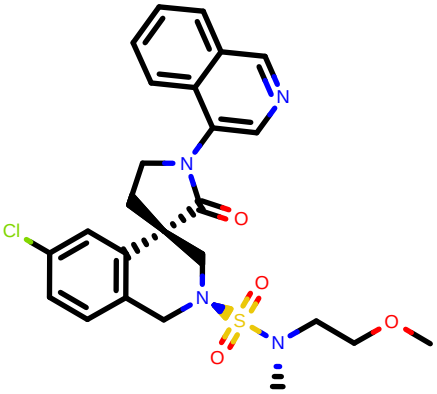
CID:	ALP-POS-ecbed2ba-20_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN1616
DDG (kcal/mol):	3.31
dDDG (kcal/mol):	0.86

VLA-MRT-8c78ee15-3_2



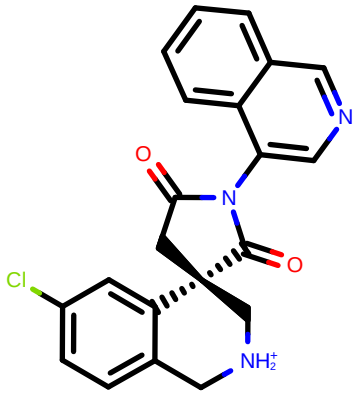
CID:	VLA-MRT-8c78ee15-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1554
DDG (kcal/mol):	3.33
dDDG (kcal/mol):	0.31

ALP-POS-ecbed2ba-21_3



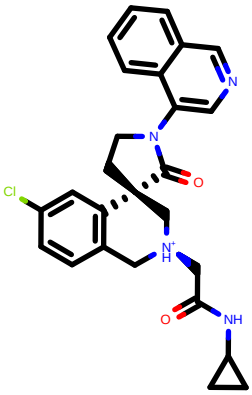
CID:	ALP-POS-ecbed2ba-21_3
SMILES:	C[N@@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1721
DDG (kcal/mol):	3.37
dDDG (kcal/mol):	0.77

JOH-MSK-1f2dff76-3_1



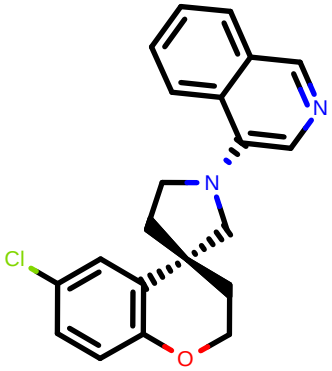
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN1501
DDG (kcal/mol):	3.40
dDDG (kcal/mol):	0.18

MAT-POS-69786b79-2_2



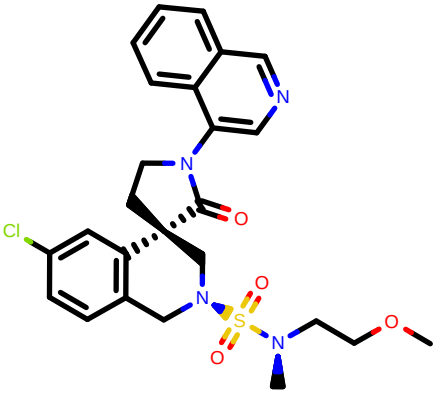
CID:	MAT-POS-69786b79-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN1623
DDG (kcal/mol):	3.40
dDDG (kcal/mol):	0.30

MAT-POS-983b399a-2_1



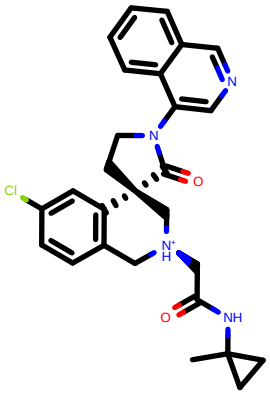
CID:	MAT-POS-983b399a-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN1462
DDG (kcal/mol):	3.45
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-21_4



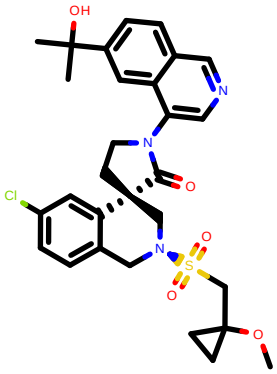
CID:	ALP-POS-ecbed2ba-21_4
SMILES:	C[N@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1728
DDG (kcal/mol):	3.51
dDDG (kcal/mol):	0.81

MAT-POS-69786b79-3_2



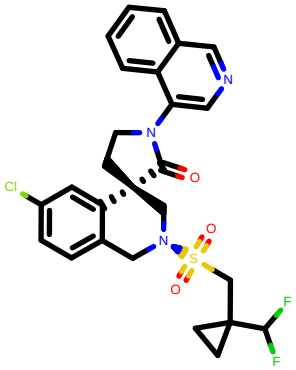
CID:	MAT-POS-69786b79-3_2
SMILES:	CC1(CC1)NC(=O)C[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1678
DDG (kcal/mol):	3.53
dDDG (kcal/mol):	0.38

MAT-POS-853c0ffa-12_2



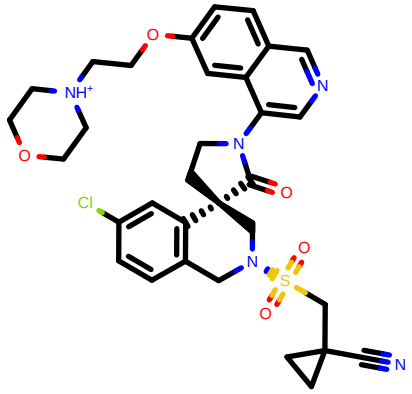
CID:	MAT-POS-853c0ffa-12_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN1865
DDG (kcal/mol):	3.55
dDDG (kcal/mol):	0.55

EDJ-MED-5cd3920d-5_2



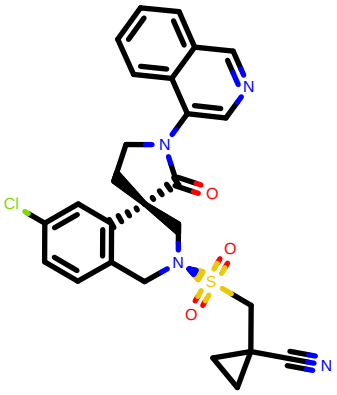
CID:	EDJ-MED-5cd3920d-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN1807
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.50

EDJ-MED-468565e0-2_2



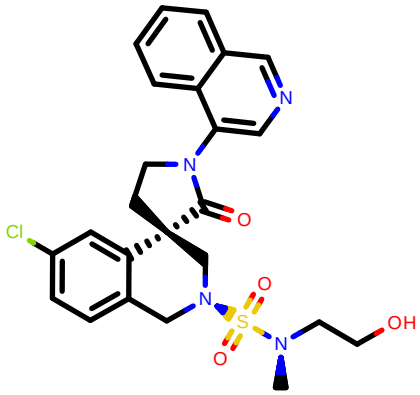
CID:	EDJ-MED-468565e0-2_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1942
DDG (kcal/mol):	3.56
dDDG (kcal/mol):	0.56

ALP-POS-ecbed2ba-4_2



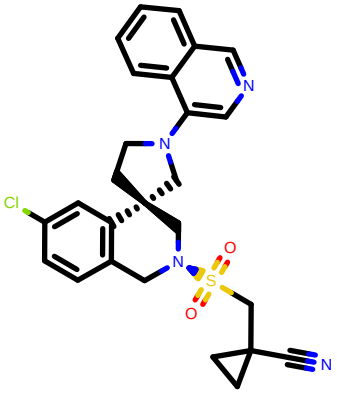
CID:	ALP-POS-ecbed2ba-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1701
DDG (kcal/mol):	3.57
dDDG (kcal/mol):	0.61

ALP-POS-ecbed2ba-19_4



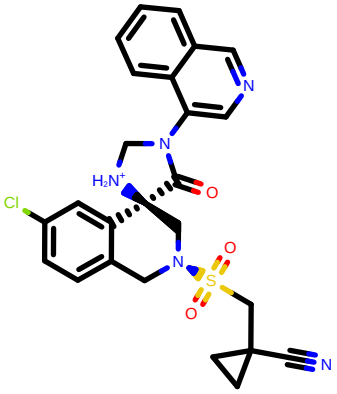
CID:	ALP-POS-ecbed2ba-19_4
SMILES:	C[N@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1680
DDG (kcal/mol):	3.67
dDDG (kcal/mol):	0.57

EDJ-MED-8bb691af-2_1



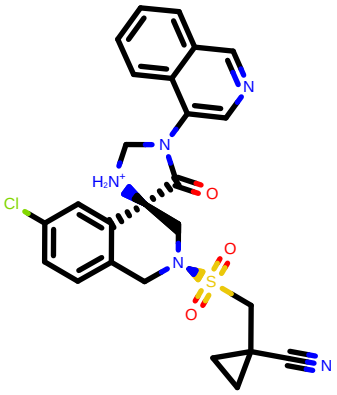
CID:	EDJ-MED-8bb691af-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1652
DDG (kcal/mol):	3.68
dDDG (kcal/mol):	0.42

EDG-MED-0c930815-1_1



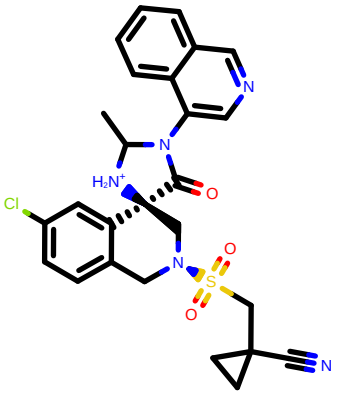
CID:	EDG-MED-0c930815-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1706
DDG (kcal/mol):	3.82
dDDG (kcal/mol):	0.45

EDG-MED-00af8776-1_1



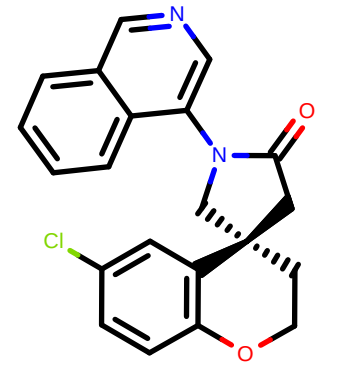
CID:	EDG-MED-00af8776-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1708
DDG (kcal/mol):	3.83
dDDG (kcal/mol):	0.39

EDG-MED-b6bce001-2_2



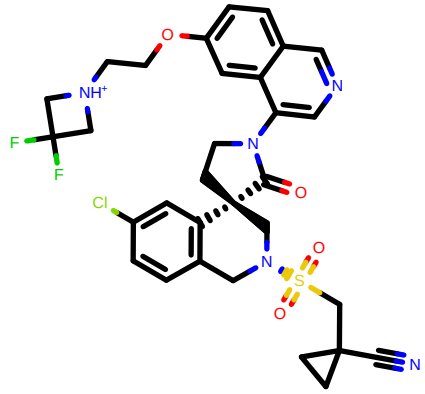
CID:	EDG-MED-b6bce001-2_2
SMILES:	CC1=[NH+][C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1778
DDG (kcal/mol):	3.84
dDDG (kcal/mol):	0.46

EDJ-MED-159244ea-3_1



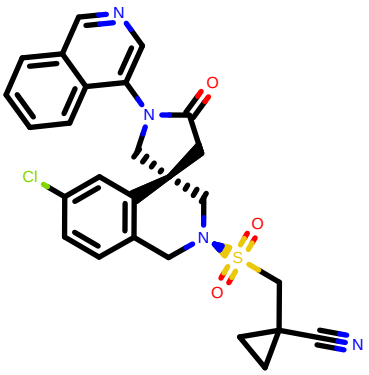
CID:	EDJ-MED-159244ea-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN1468
DDG (kcal/mol):	3.84
dDDG (kcal/mol):	0.12

EDJ-MED-468565e0-5_2



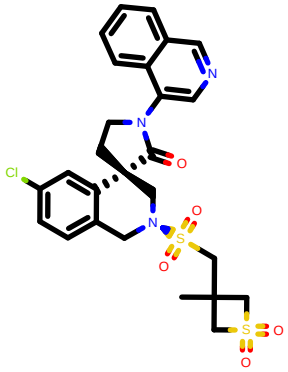
CID:	EDJ-MED-468565e0-5_2
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1928
DDG (kcal/mol):	3.85
dDDG (kcal/mol):	0.53

EDJ-MED-8bb691af-5_1



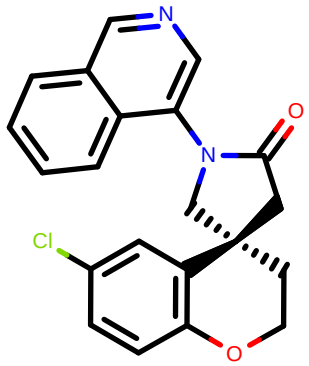
CID:	EDJ-MED-8bb691af-5_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1692
DDG (kcal/mol):	3.85
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-1_1



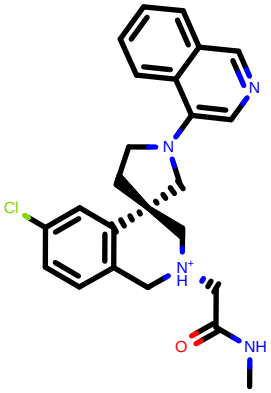
CID:	ALP-POS-ecbed2ba-1_1
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1816
DDG (kcal/mol):	3.88
dDDG (kcal/mol):	0.58

MAT-POS-983b399a-3_1



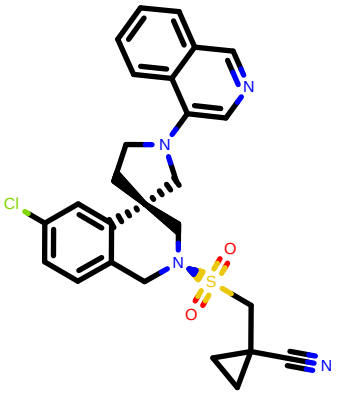
CID:	MAT-POS-983b399a-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN1486
DDG (kcal/mol):	3.89
dDDG (kcal/mol):	0.13

EDJ-MED-8bb691af-1_3



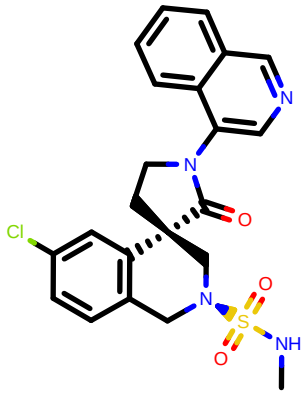
CID:	EDJ-MED-8bb691af-1_3
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1520
DDG (kcal/mol):	3.94
dDDG (kcal/mol):	0.28

EDJ-MED-8bb691af-2_4



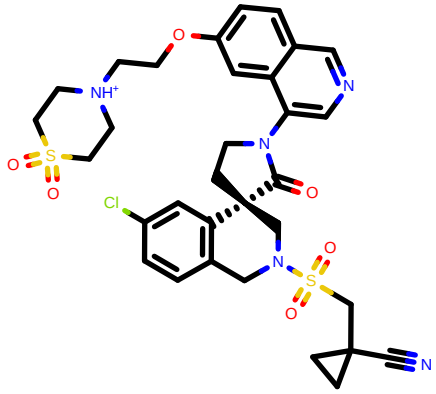
CID:	EDJ-MED-8bb691af-2_4
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1657
DDG (kcal/mol):	3.99
dDDG (kcal/mol):	0.49

LUO-POS-ed2cfb03-2_2



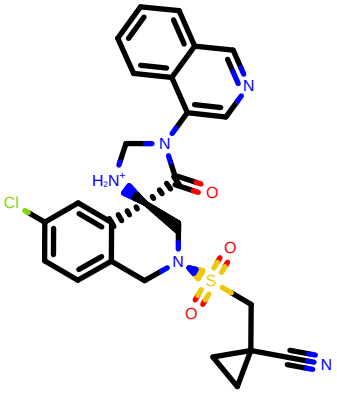
CID:	LUO-POS-ed2cfb03-2_2
SMILES:	CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1550
DDG (kcal/mol):	4.08
dDDG (kcal/mol):	0.61

EDJ-MED-468565e0-3_1



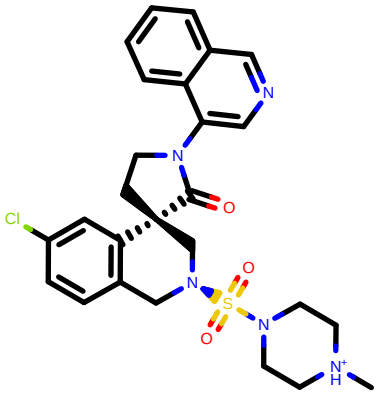
CID:	EDJ-MED-468565e0-3_1
SMILES:	c1cc2ncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1935
DDG (kcal/mol):	4.11
dDDG (kcal/mol):	0.40

EDG-MED-b6bce001-1_2



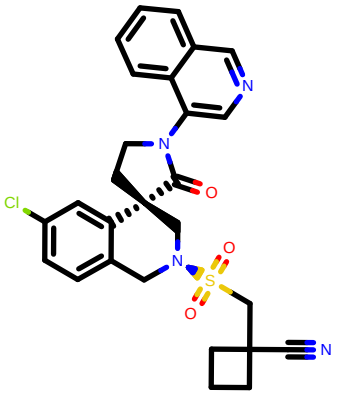
CID:	EDG-MED-b6bce001-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1713
DDG (kcal/mol):	4.13
dDDG (kcal/mol):	0.73

LUO-POS-ed2cfb03-1_2



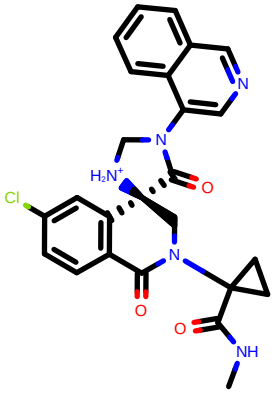
CID:	LUO-POS-ed2cfb03-1_2
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1808
DDG (kcal/mol):	4.20
dDDG (kcal/mol):	0.83

ALP-POS-ecbed2ba-8_2



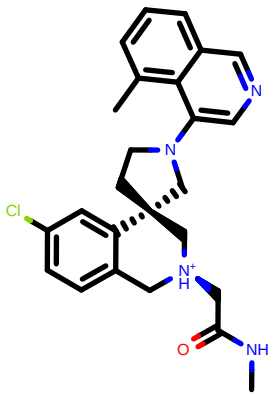
CID:	ALP-POS-ecbed2ba-8_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N
RUN:	RUN1766
DDG (kcal/mol):	4.20
dDDG (kcal/mol):	0.60

EDJ-MED-fd8ed875-2_1



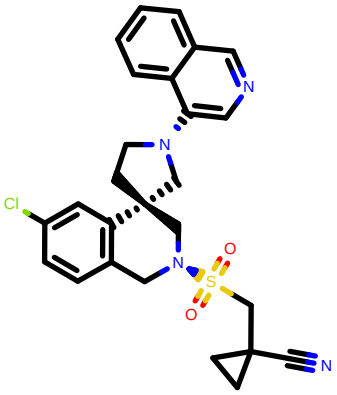
CID:	EDJ-MED-fd8ed875-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(C=[NH+]3)c5cncc6c5cccc6
RUN:	RUN1679
DDG (kcal/mol):	4.31
dDDG (kcal/mol):	0.19

EDJ-MED-3656d29d-1_3



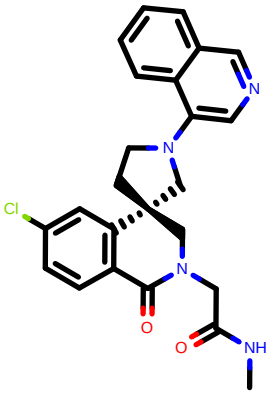
CID:	EDJ-MED-3656d29d-1_3
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1541
DDG (kcal/mol):	4.33
dDDG (kcal/mol):	0.27

EDJ-MED-8bb691af-2_3



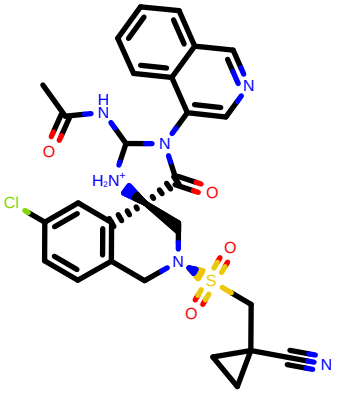
CID:	EDJ-MED-8bb691af-2_3
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1654
DDG (kcal/mol):	4.36
dDDG (kcal/mol):	0.33

EDJ-MED-8bb691af-7_1



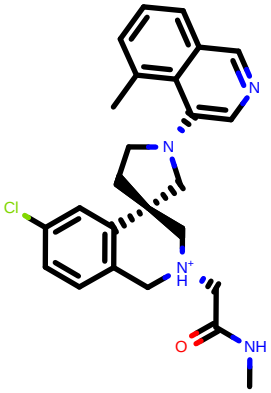
CID:	EDJ-MED-8bb691af-7_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1534
DDG (kcal/mol):	4.36
dDDG (kcal/mol):	0.21

LUO-POS-eaf50f21-3_1



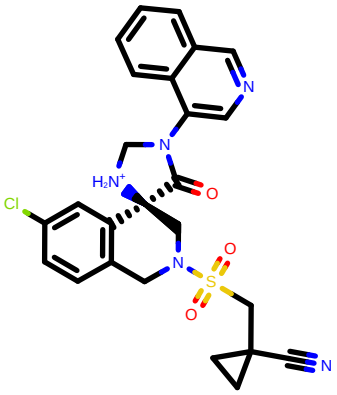
CID:	LUO-POS-eaf50f21-3_1
SMILES:	CC(=O)NC1=[NH+][C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5ncc6c5cccc6
RUN:	RUN1879
DDG (kcal/mol):	4.50
dDDG (kcal/mol):	0.74

EDJ-MED-3656d29d-1_2



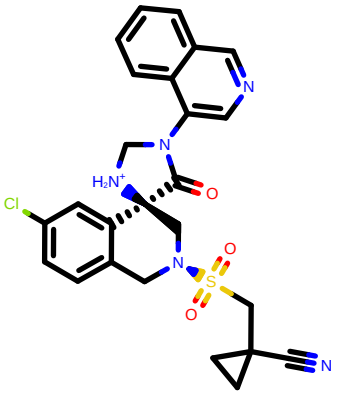
CID:	EDJ-MED-3656d29d-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1533
DDG (kcal/mol):	4.53
dDDG (kcal/mol):	0.27

EDG-MED-b6bce001-1_1



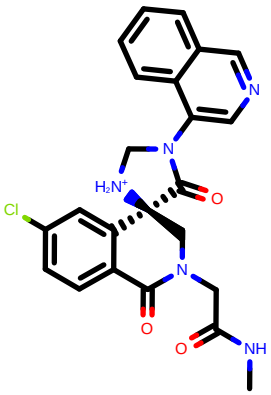
CID:	EDG-MED-b6bce001-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1716
DDG (kcal/mol):	4.67
dDDG (kcal/mol):	0.41

EDG-MED-0c930815-1_2



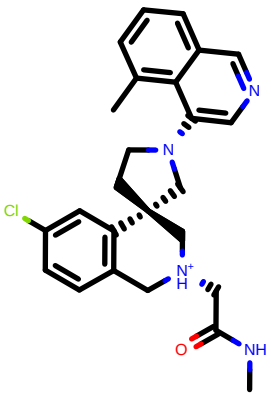
CID:	EDG-MED-0c930815-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1705
DDG (kcal/mol):	4.70
dDDG (kcal/mol):	0.47

EDJ-MED-fd8ed875-1_1



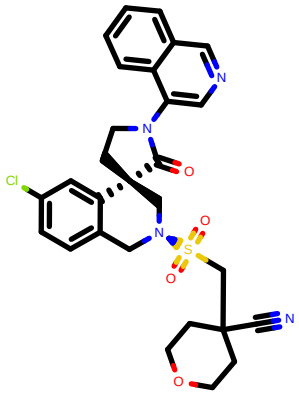
CID:	EDJ-MED-fd8ed875-1_1
SMILES:	CNC(=O)CN1C[C@]2(c3cc(ccc3C1=O)Cl)C(=O)N(C=[NH+]2)c4cncc5c4cccc5
RUN:	RUN1570
DDG (kcal/mol):	4.73
dDDG (kcal/mol):	0.18

EDJ-MED-3656d29d-1_1



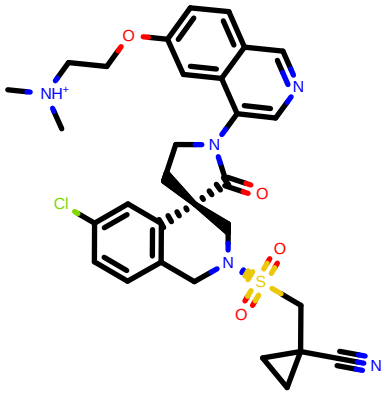
CID:	EDJ-MED-3656d29d-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1536
DDG (kcal/mol):	4.84
dDDG (kcal/mol):	0.43

ALP-POS-ecbed2ba-11_2



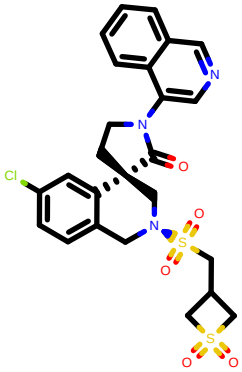
CID:	ALP-POS-ecbed2ba-11_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN1849
DDG (kcal/mol):	4.90
dDDG (kcal/mol):	0.49

MAT-POS-38eb6498-1_1



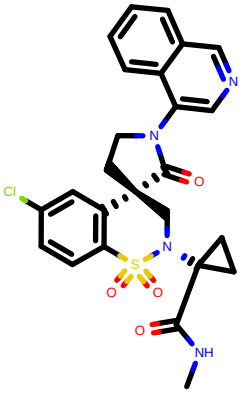
CID:	MAT-POS-38eb6498-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1901
DDG (kcal/mol):	4.94
dDDG (kcal/mol):	0.57

ALP-POS-ecbed2ba-5_1



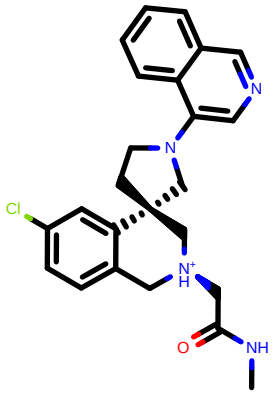
CID:	ALP-POS-ecbed2ba-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN1769
DDG (kcal/mol):	5.02
dDDG (kcal/mol):	0.56

EDJ-MED-976a33d5-3_1



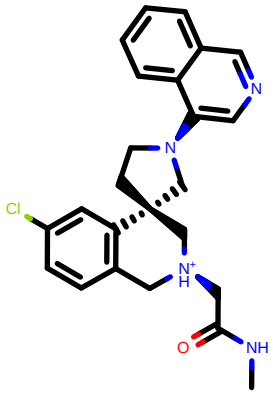
CID:	EDJ-MED-976a33d5-3_1
SMILES:	CNC(=O)C1(CC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1732
DDG (kcal/mol):	5.10
dDDG (kcal/mol):	0.62

EDJ-MED-8bb691af-1_2



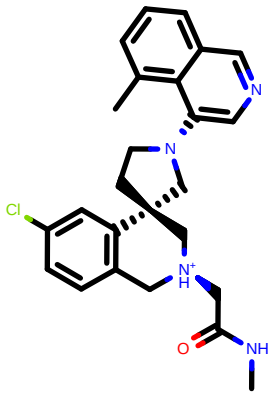
CID:	EDJ-MED-8bb691af-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1518
DDG (kcal/mol):	5.11
dDDG (kcal/mol):	0.24

EDJ-MED-8bb691af-1_4



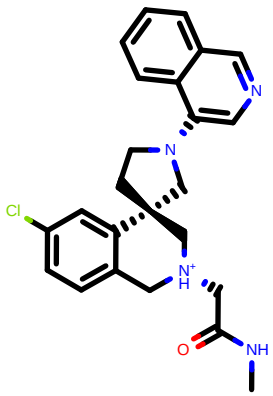
CID:	EDJ-MED-8bb691af-1_4
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1522
DDG (kcal/mol):	5.13
dDDG (kcal/mol):	0.27

EDJ-MED-3656d29d-1_4



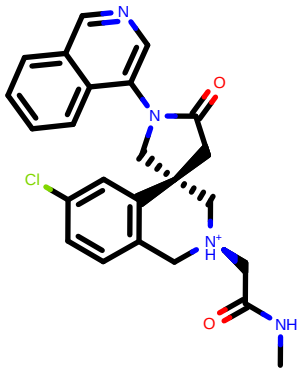
CID:	EDJ-MED-3656d29d-1_4
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1537
DDG (kcal/mol):	5.15
dDDG (kcal/mol):	0.30

EDJ-MED-8bb691af-1_1



CID:	EDJ-MED-8bb691af-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1516
DDG (kcal/mol):	5.16
dDDG (kcal/mol):	0.26

EDJ-MED-8bb691af-3_2



CID:	EDJ-MED-8bb691af-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1529
DDG (kcal/mol):	5.44
dDDG (kcal/mol):	0.38