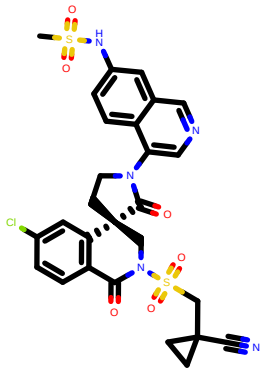
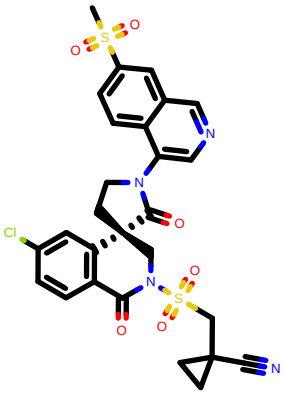
EDJ-MED-9f4ac58c-3_1



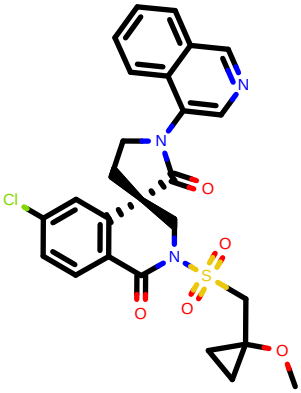
CID:	EDJ-MED-9f4ac58c-3_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1405
DDG (kcal/mol):	-4.44
dDDG (kcal/mol):	0.60

EDJ-MED-9f4ac58c-4_1



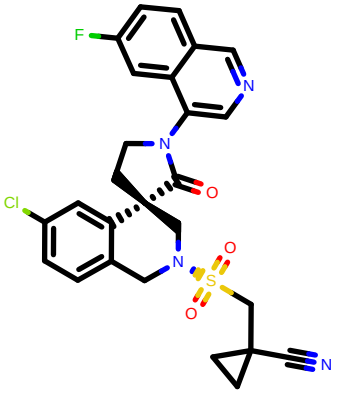
CID:	EDJ-MED-9f4ac58c-4_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1390
DDG (kcal/mol):	-3.62
dDDG (kcal/mol):	0.60

EDJ-MED-9f4ac58c-6_1



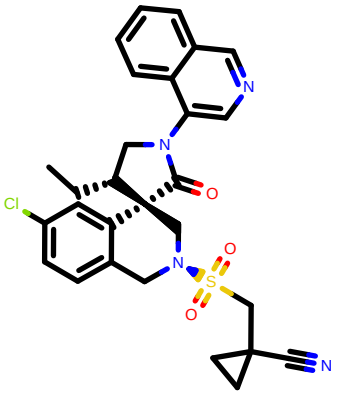
CID:	EDJ-MED-9f4ac58c-6_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1272
DDG (kcal/mol):	-3.35
dDDG (kcal/mol):	0.33

MAT-POS-853c0ffa-13_2



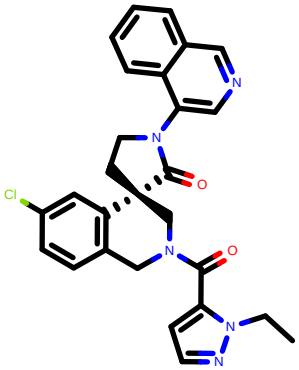
CID:	MAT-POS-853c0ffa-13_2
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1277
DDG (kcal/mol):	-2.94
dDDG (kcal/mol):	0.38

MAT-POS-50a80394-2_1



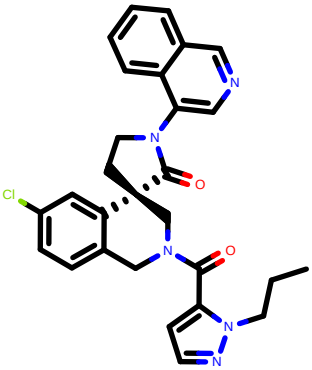
CID:	MAT-POS-50a80394-2_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN1337
DDG (kcal/mol):	-2.89
dDDG (kcal/mol):	0.45

MAT-POS-be048f2c-5_1



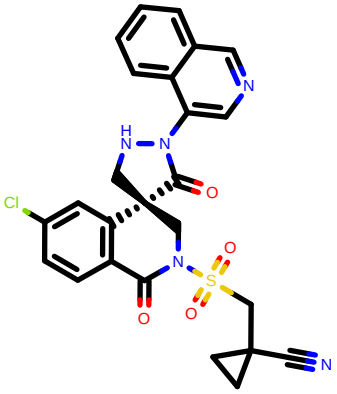
CID:	MAT-POS-be048f2c-5_1
SMILES:	CCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1252
DDG (kcal/mol):	-2.84
dDDG (kcal/mol):	0.13

MAT-POS-be048f2c-8_1



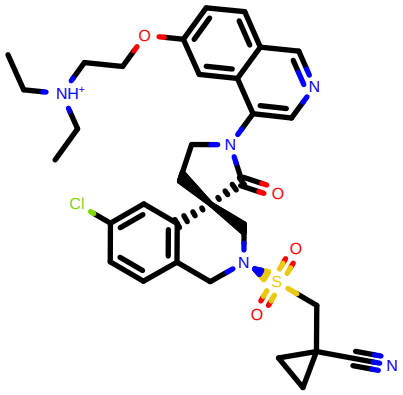
CID:	MAT-POS-be048f2c-8_1
SMILES:	CCCn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1314
DDG (kcal/mol):	-2.77
dDDG (kcal/mol):	0.15

EDJ-MED-fed7ac0b-3_1



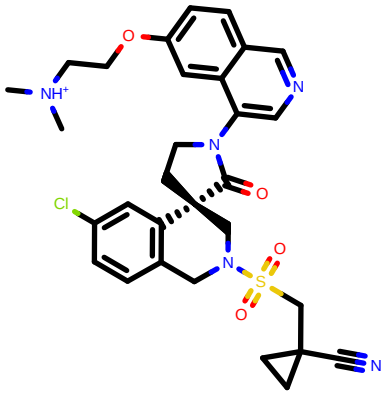
CID:	EDJ-MED-fed7ac0b-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@]4(CN3)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1297
DDG (kcal/mol):	-2.75
dDDG (kcal/mol):	0.39

MAT-POS-40ad851a-3_2



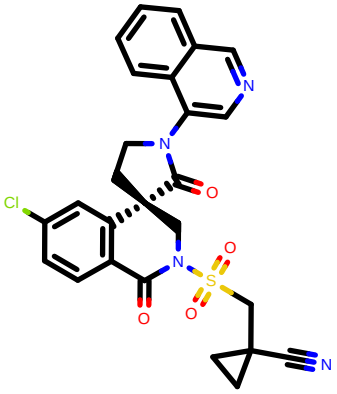
CID:	MAT-POS-40ad851a-3_2
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1440
DDG (kcal/mol):	-2.73
dDDG (kcal/mol):	0.79

LUO-POS-8484f2d3-2_2



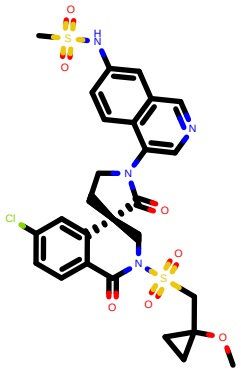
CID:	LUO-POS-8484f2d3-2_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1420
DDG (kcal/mol):	-2.55
dDDG (kcal/mol):	0.67

EDJ-MED-9f4ac58c-2_1



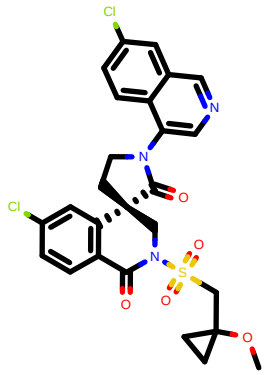
CID:	EDJ-MED-9f4ac58c-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1268
DDG (kcal/mol):	-2.35
dDDG (kcal/mol):	0.48

EDJ-MED-9f4ac58c-7_1



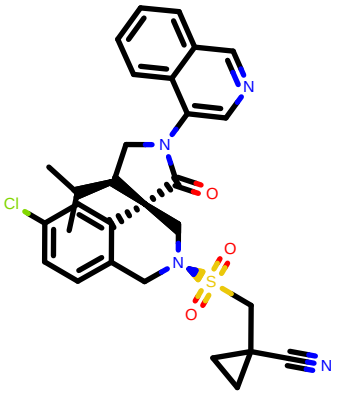
CID:	EDJ-MED-9f4ac58c-7_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1403
DDG (kcal/mol):	-2.27
dDDG (kcal/mol):	0.45

EDJ-MED-9f4ac58c-5_1



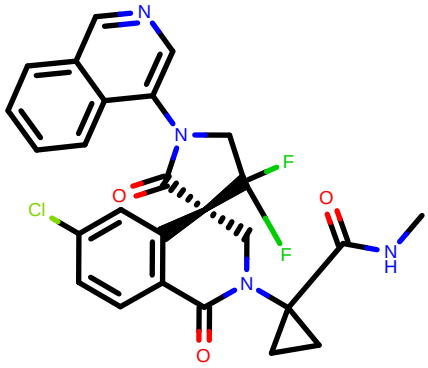
CID:	EDJ-MED-9f4ac58c-5_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)Cl)c6cc(ccc6C2=O)Cl
RUN:	RUN1330
DDG (kcal/mol):	-2.24
dDDG (kcal/mol):	0.39

MAT-POS-50a80394-3_4



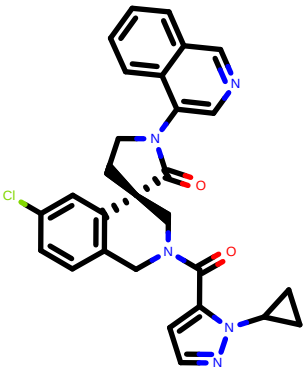
CID:	MAT-POS-50a80394-3_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1372
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.67

EDJ-MED-7e491f08-2_1



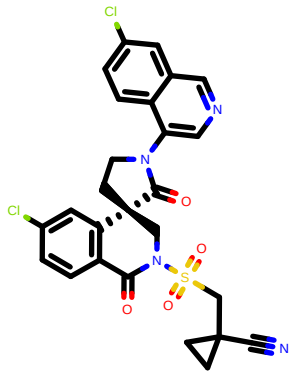
CID:	EDJ-MED-7e491f08-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(CC3(F)F)c5cncc6c5cccc6
RUN:	RUN1318
DDG (kcal/mol):	-2.18
dDDG (kcal/mol):	0.15

MAT-POS-be048f2c-7_1



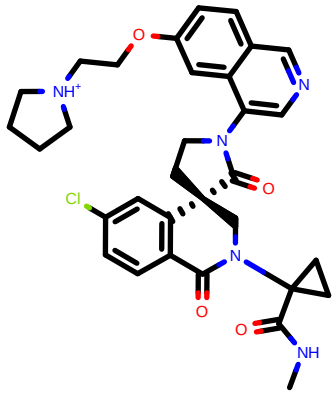
CID:	MAT-POS-be048f2c-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(Cc5c4cc(cc5)Cl)C(=O)c6ccnn6C7CC7
RUN:	RUN1300
DDG (kcal/mol):	-2.14
dDDG (kcal/mol):	0.15

EDJ-MED-9f4ac58c-1_1



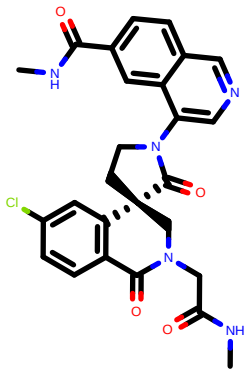
CID:	EDJ-MED-9f4ac58c-1_1
SMILES:	c1cc2c(cc1Cl)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1327
DDG (kcal/mol):	-2.05
dDDG (kcal/mol):	0.50

EDJ-MED-dfa1d800-1_1



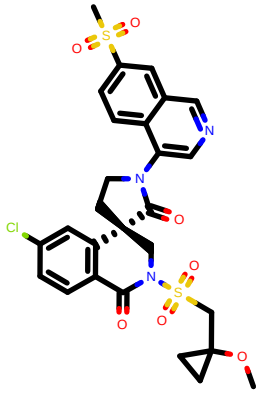
CID:	EDJ-MED-dfa1d800-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1413
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.39

MAT-POS-38eb6498-6_1



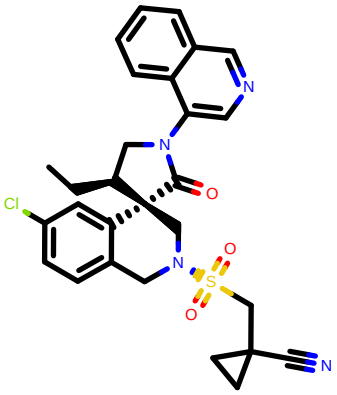
CID:	MAT-POS-38eb6498-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)C(=O)NC)c5cc(ccc5C1=O)Cl
RUN:	RUN1293
DDG (kcal/mol):	-2.04
dDDG (kcal/mol):	0.15

EDJ-MED-9f4ac58c-8_1



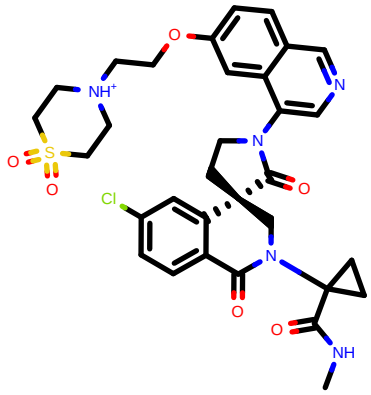
CID:	EDJ-MED-9f4ac58c-8_1
SMILES:	COC1(CC1)CS(=O)(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1396
DDG (kcal/mol):	-1.99
dDDG (kcal/mol):	0.40

MAT-POS-50a80394-2_4



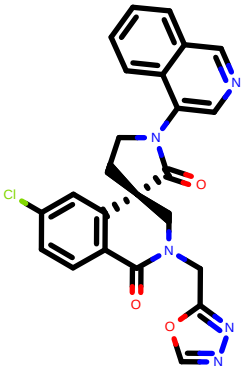
CID:	MAT-POS-50a80394-2_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN1348
DDG (kcal/mol):	-1.97
dDDG (kcal/mol):	0.58

EDJ-MED-dfa1d800-3_1



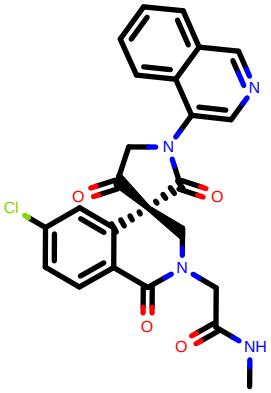
CID:	EDJ-MED-dfa1d800-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CCS(=O)(=O)CC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1459
DDG (kcal/mol):	-1.92
dDDG (kcal/mol):	0.29

PET-UNK-aa57768f-7_1



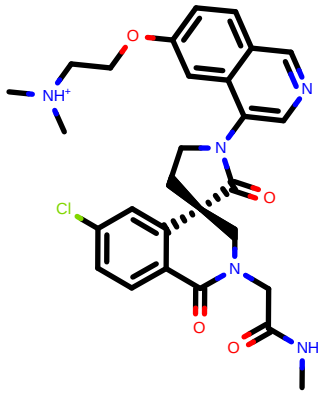
CID:	PET-UNK-aa57768f-7_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN1133
DDG (kcal/mol):	-1.90
dDDG (kcal/mol):	0.11

EDJ-MED-a12e3a20-2_1



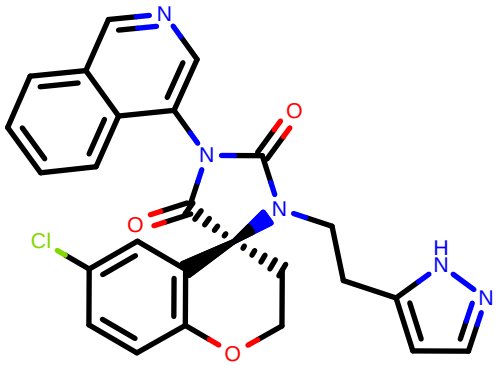
CID:	EDJ-MED-a12e3a20-2_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=O)CN(C2=O)c4cncc5c4cccc5
RUN:	RUN1140
DDG (kcal/mol):	-1.87
dDDG (kcal/mol):	0.12

EDJ-MED-b6c6ee2b-5_1



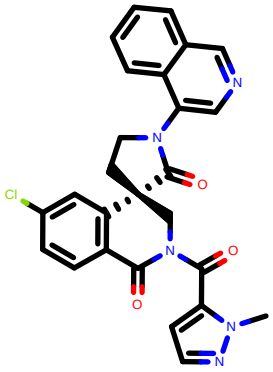
CID:	EDJ-MED-b6c6ee2b-5_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN1399
DDG (kcal/mol):	-1.85
dDDG (kcal/mol):	0.27

VLA-UNK-f702bf1c-1_1



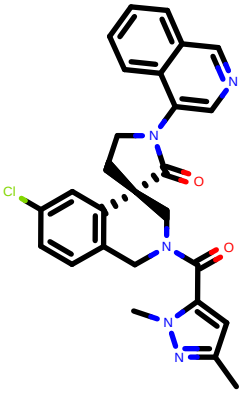
CID:	VLA-UNK-f702bf1c-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6ccn[nH]6
RUN:	RUN1164
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.12

EDJ-MED-cc48ee33-2_1



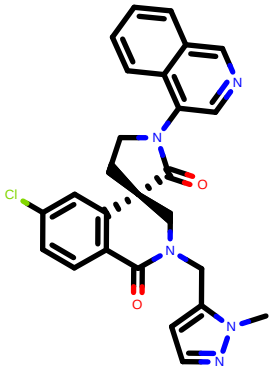
CID:	EDJ-MED-cc48ee33-2_1
SMILES:	Cn1c(ccn1)C(=O)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1243
DDG (kcal/mol):	-1.81
dDDG (kcal/mol):	0.14

EDJ-MED-cc48ee33-5_1



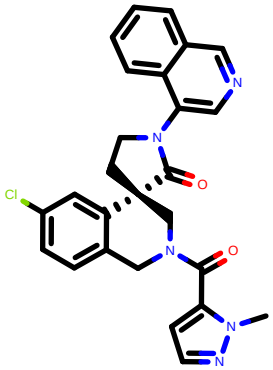
CID:	EDJ-MED-cc48ee33-5_1
SMILES:	Cc1cc(n(n1)C)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1250
DDG (kcal/mol):	-1.80
dDDG (kcal/mol):	0.12

EDJ-MED-cc48ee33-7_1



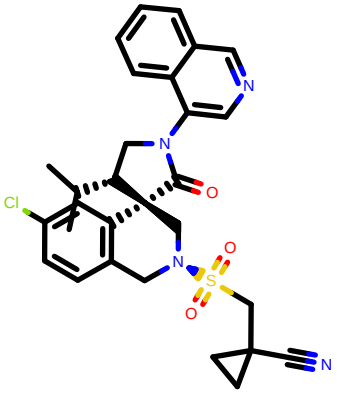
CID:	EDJ-MED-cc48ee33-7_1
SMILES:	Cn1c(ccn1)CN2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1182
DDG (kcal/mol):	-1.79
dDDG (kcal/mol):	0.19

EDJ-MED-cc48ee33-3_1



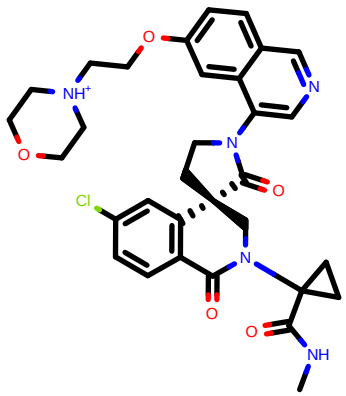
CID:	EDJ-MED-cc48ee33-3_1
SMILES:	Cn1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1185
DDG (kcal/mol):	-1.74
dDDG (kcal/mol):	0.13

MAT-POS-50a80394-3_3



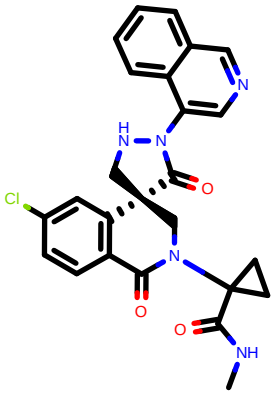
CID:	MAT-POS-50a80394-3_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1371
DDG (kcal/mol):	-1.71
dDDG (kcal/mol):	0.49

EDJ-MED-dfa1d800-2_1



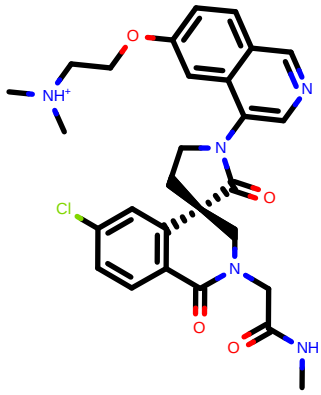
CID:	EDJ-MED-dfa1d800-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCOCC6)c7cc(ccc7C2=O)Cl
RUN:	RUN1435
DDG (kcal/mol):	-1.70
dDDG (kcal/mol):	0.36

EDJ-MED-fed7ac0b-2_1



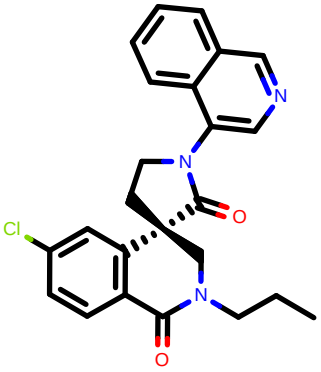
CID:	EDJ-MED-fed7ac0b-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CNN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1187
DDG (kcal/mol):	-1.65
dDDG (kcal/mol):	0.13

MAT-POS-38eb6498-4_1



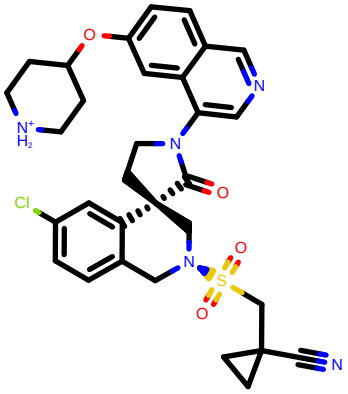
CID:	MAT-POS-38eb6498-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)OCC[NH+](C)C)c5cc(ccc5C1=O)Cl
RUN:	RUN1389
DDG (kcal/mol):	-1.62
dDDG (kcal/mol):	0.26

PET-UNK-aa57768f-9_1



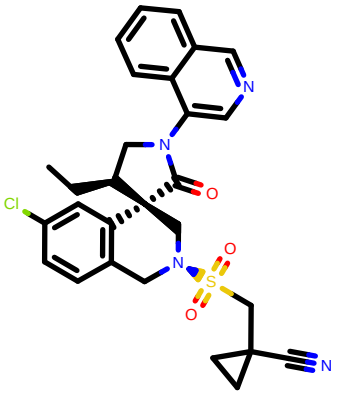
CID:	PET-UNK-aa57768f-9_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1032
DDG (kcal/mol):	-1.60
dDDG (kcal/mol):	0.10

EDJ-MED-ee81482e-4_2



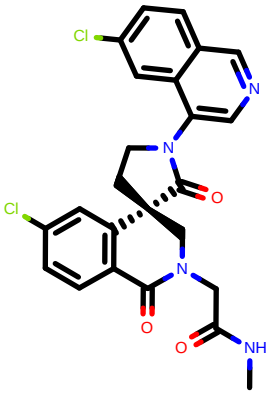
CID:	EDJ-MED-ee81482e-4_2
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1406
DDG (kcal/mol):	-1.55
dDDG (kcal/mol):	0.76

MAT-POS-50a80394-2_2



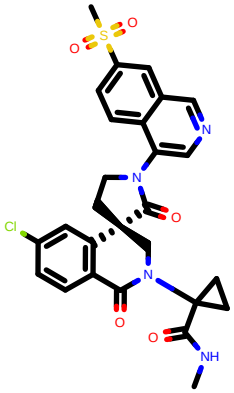
CID:	MAT-POS-50a80394-2_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1343
DDG (kcal/mol):	-1.49
dDDG (kcal/mol):	0.55

LUO-POS-8c3e556a-2_1



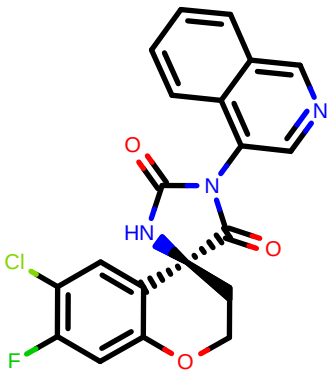
CID:	LUO-POS-8c3e556a-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1154
DDG (kcal/mol):	-1.47
dDDG (kcal/mol):	0.10

EDJ-MED-976a33d5-2_1



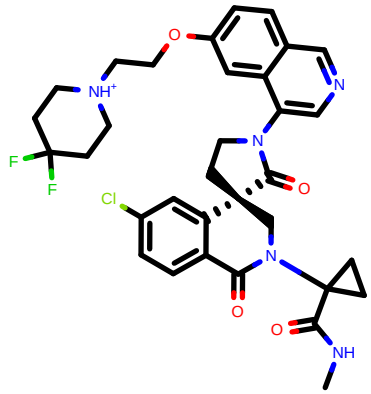
CID:	EDJ-MED-976a33d5-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4ccc(c5)S(=O)(=O)C)c6cc(ccc6C2=O)Cl
RUN:	RUN1368
DDG (kcal/mol):	-1.42
dDDG (kcal/mol):	0.19

VLA-UNK-3a43cd95-1_1



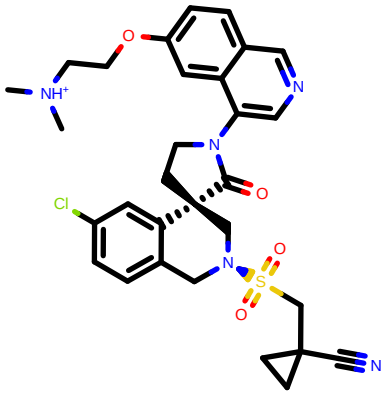
CID:	VLA-UNK-3a43cd95-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)F)Cl)NC3=O
RUN:	RUN1016
DDG (kcal/mol):	-1.40
dDDG (kcal/mol):	0.07

EDJ-MED-dfa1d800-4_1



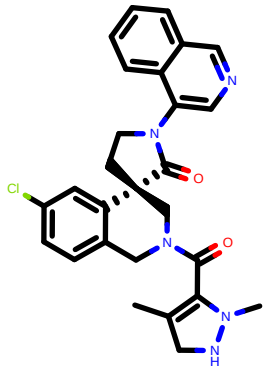
CID:	EDJ-MED-dfa1d800-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+]6CCC(CC6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN1457
DDG (kcal/mol):	-1.39
dDDG (kcal/mol):	0.34

LUO-POS-8484f2d3-1_1



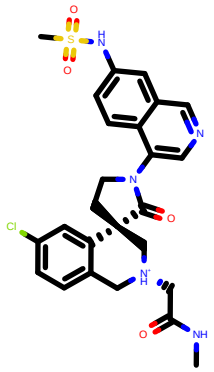
CID:	LUO-POS-8484f2d3-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1419
DDG (kcal/mol):	-1.37
dDDG (kcal/mol):	0.77

EDJ-MED-cc48ee33-4_1



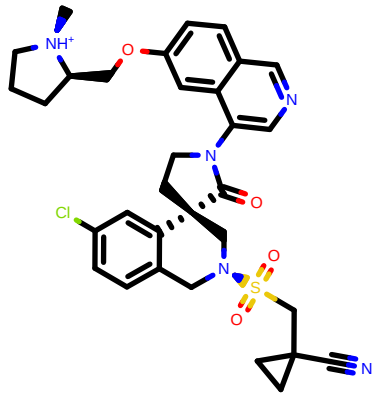
CID:	EDJ-MED-cc48ee33-4_1
SMILES:	Cc1cnn(c1C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl)C
RUN:	RUN1244
DDG (kcal/mol):	-1.29
dDDG (kcal/mol):	0.14

MAT-POS-b4d6b7fc-7_1



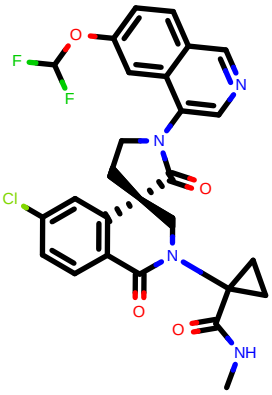
CID:	MAT-POS-b4d6b7fc-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN1266
DDG (kcal/mol):	-1.28
dDDG (kcal/mol):	0.26

MAT-POS-40ad851a-1_1



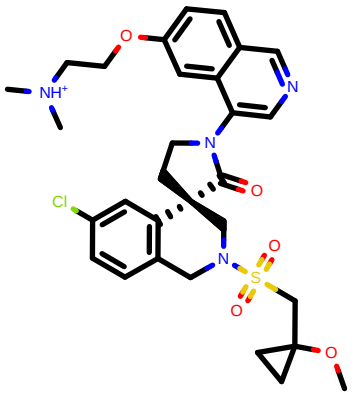
CID:	MAT-POS-40ad851a-1_1
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1438
DDG (kcal/mol):	-1.25
dDDG (kcal/mol):	0.66

EDJ-MED-5cd3920d-3_1



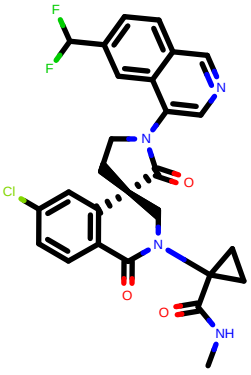
CID:	EDJ-MED-5cd3920d-3_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OC(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1395
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.16

MAT-POS-853c0ffa-10_2



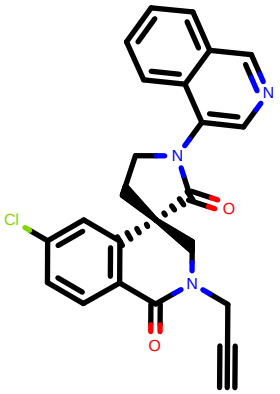
CID:	MAT-POS-853c0ffa-10_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN1412
DDG (kcal/mol):	-1.22
dDDG (kcal/mol):	0.53

EDJ-MED-5cd3920d-4_1



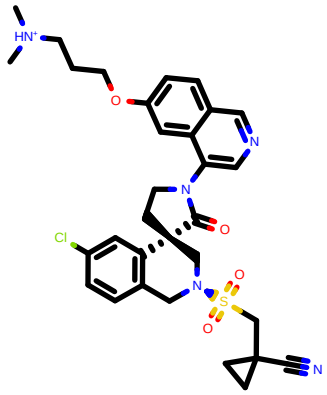
CID:	EDJ-MED-5cd3920d-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)C(F)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1352
DDG (kcal/mol):	-1.20
dDDG (kcal/mol):	0.15

PET-UNK-aa57768f-3_1



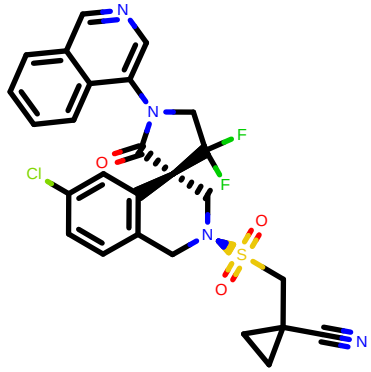
CID:	PET-UNK-aa57768f-3_1
SMILES:	C#CCN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1028
DDG (kcal/mol):	-1.19
dDDG (kcal/mol):	0.11

MAT-POS-40ad851a-4_1



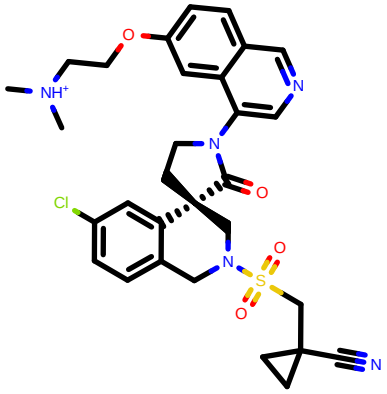
CID:	MAT-POS-40ad851a-4_1
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1428
DDG (kcal/mol):	-1.17
dDDG (kcal/mol):	0.68

EDJ-MED-7e491f08-1_2



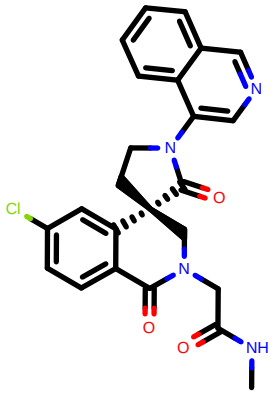
CID:	EDJ-MED-7e491f08-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN1350
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.74

LUO-POS-8484f2d3-1_2



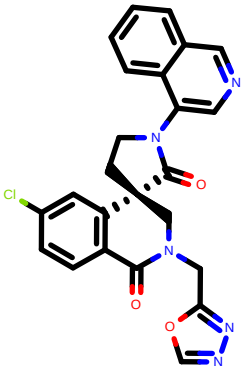
CID:	LUO-POS-8484f2d3-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1415
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.65

PET-UNK-14142a25-10_1



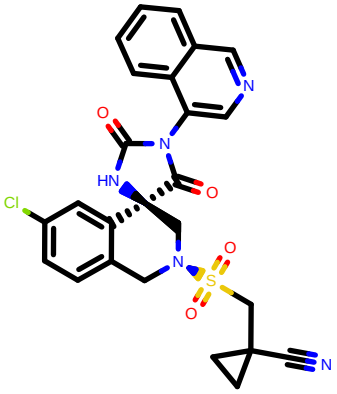
CID:	PET-UNK-14142a25-10_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1079
DDG (kcal/mol):	-1.14
dDDG (kcal/mol):	0.11

PET-UNK-aa57768f-1_1



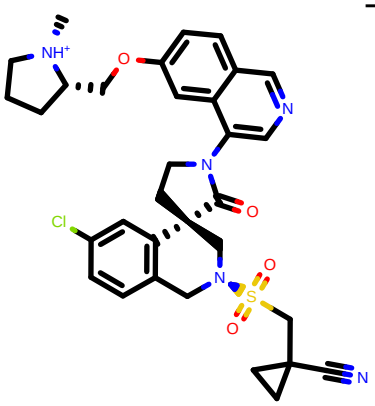
CID:	PET-UNK-aa57768f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)Cc6nnco6
RUN:	RUN1118
DDG (kcal/mol):	-1.13
dDDG (kcal/mol):	0.13

MAT-POS-c2d406ed-1_2



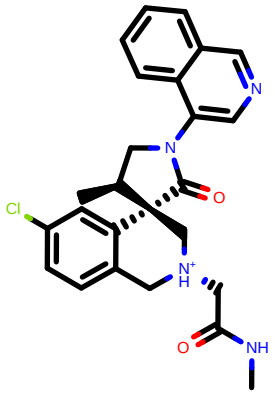
CID:	MAT-POS-c2d406ed-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN1284
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.25

MAT-POS-40ad851a-1_8



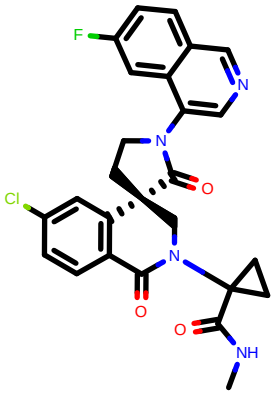
CID:	MAT-POS-40ad851a-1_8
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1443
DDG (kcal/mol):	-1.07
dDDG (kcal/mol):	0.78

MAT-POS-50a80394-4_2



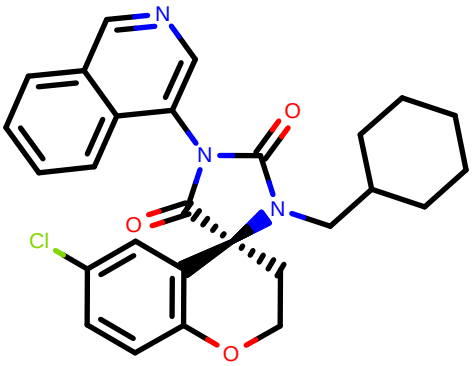
CID:	MAT-POS-50a80394-4_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1096
DDG (kcal/mol):	-1.06
dDDG (kcal/mol):	0.23

EDJ-MED-b6c6ee2b-7_1



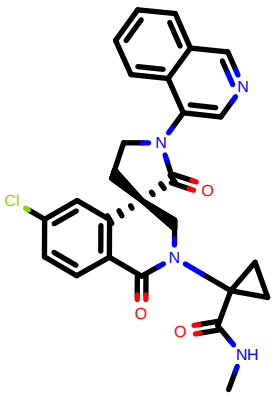
CID:	EDJ-MED-b6c6ee2b-7_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)F)c6cc(ccc6C2=O)Cl
RUN:	RUN1253
DDG (kcal/mol):	-1.04
dDDG (kcal/mol):	0.12

VLA-UCB-34f3ed0c-14_1



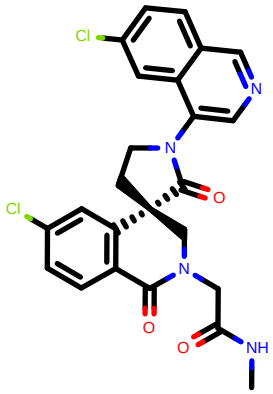
CID:	VLA-UCB-34f3ed0c-14_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN1148
DDG (kcal/mol):	-1.03
dDDG (kcal/mol):	0.14

EDJ-MED-976a33d5-1_1



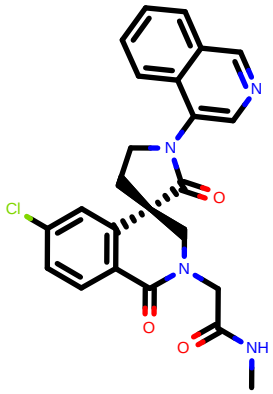
CID:	EDJ-MED-976a33d5-1_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1184
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.13

LUO-POS-8c3e556a-1_1



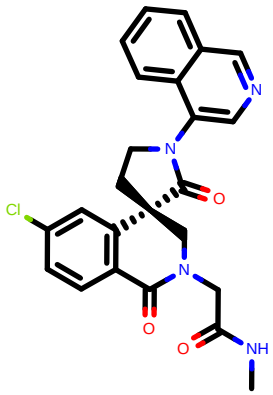
CID:	LUO-POS-8c3e556a-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1151
DDG (kcal/mol):	-1.01
dDDG (kcal/mol):	0.12

PET-UNK-14142a25-1_1



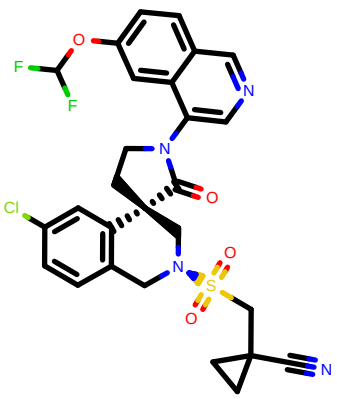
CID:	PET-UNK-14142a25-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1076
DDG (kcal/mol):	-0.98
dDDG (kcal/mol):	0.11

LUO-POS-9931618f-1_1



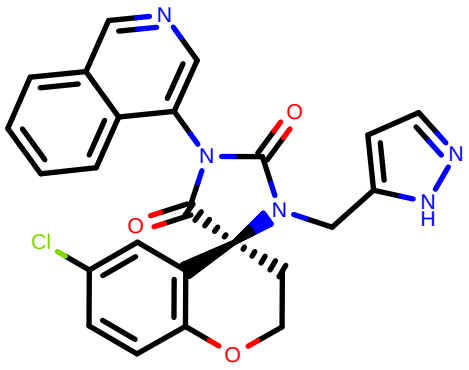
CID:	LUO-POS-9931618f-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1094
DDG (kcal/mol):	-0.96
dDDG (kcal/mol):	0.12

EDJ-MED-5cd3920d-1_2



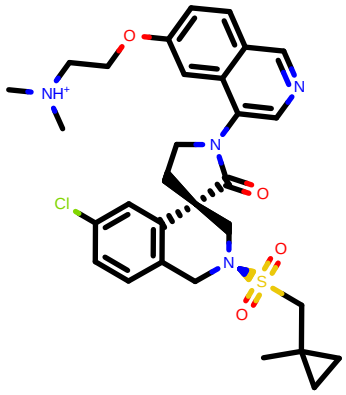
CID:	EDJ-MED-5cd3920d-1_2
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1402
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.47

VLA-UNK-f702bf1c-2_1



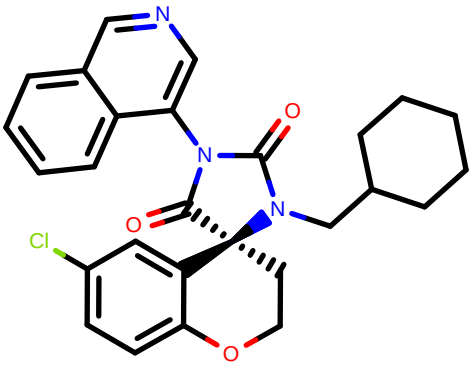
CID:	VLA-UNK-f702bf1c-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6ccn[nH]6
RUN:	RUN1110
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.12

MAT-POS-853c0ffa-19_1



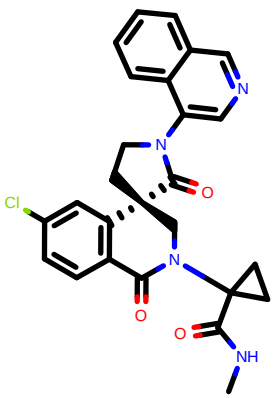
CID:	MAT-POS-853c0ffa-19_1
SMILES:	CC1(CC1)CS(=O)(=O)N@@[2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN1401
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.64

VLA-UNK-f702bf1c-6_1



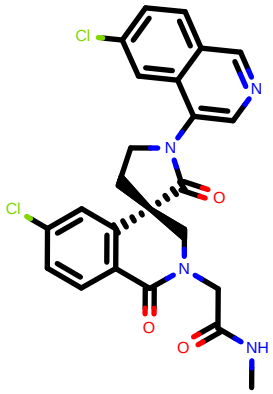
CID:	VLA-UNK-f702bf1c-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CC6CCCCC6
RUN:	RUN1155
DDG (kcal/mol):	-0.94
dDDG (kcal/mol):	0.15

MAT-POS-576f7758-2_1



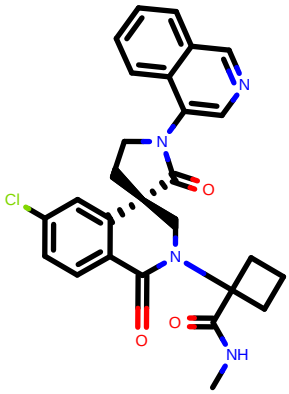
CID:	MAT-POS-576f7758-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1179
DDG (kcal/mol):	-0.93
dDDG (kcal/mol):	0.14

EDG-MED-b1ef7fe3-1_1



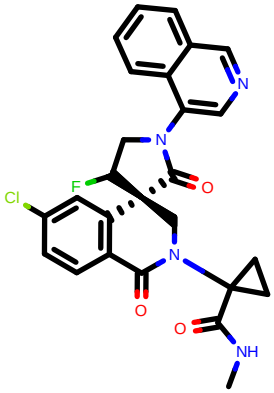
CID:	EDG-MED-b1ef7fe3-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1107
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.14

EDJ-MED-98c0a822-3_1



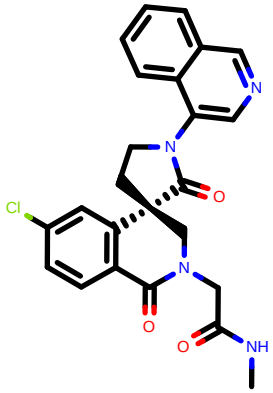
CID:	EDJ-MED-98c0a822-3_1
SMILES:	CNC(=O)C1(CCC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1246
DDG (kcal/mol):	-0.92
dDDG (kcal/mol):	0.20

EDJ-MED-fd8ed875-6_1



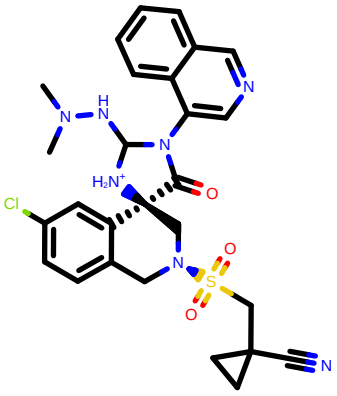
CID:	EDJ-MED-fd8ed875-6_1
SMILES:	CNC(=O)C1(CC1)N2C[C@@]3(c4cc(ccc4C2=O)Cl)C(=CN(C3=O)c5cncc6c5cccc6)F
RUN:	RUN1260
DDG (kcal/mol):	-0.90
dDDG (kcal/mol):	0.12

LUO-POS-9931618f-2_1



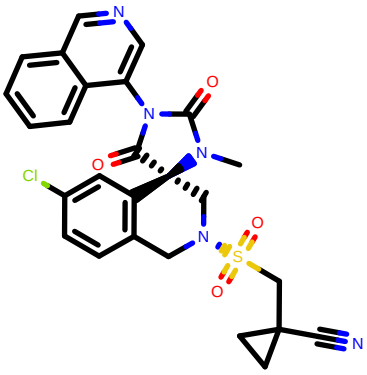
CID:	LUO-POS-9931618f-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1092
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.12

LUO-POS-b5068a05-1_2



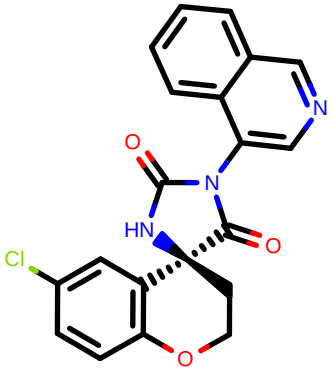
CID:	LUO-POS-b5068a05-1_2
SMILES:	C[NH+](C)NC1=N[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1398
DDG (kcal/mol):	-0.87
dDDG (kcal/mol):	0.27

MAT-POS-c2d406ed-2_2



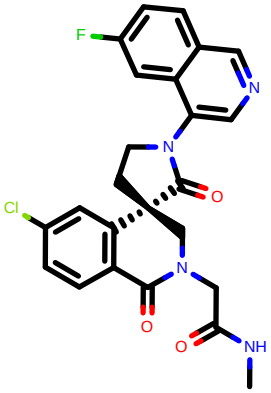
CID:	MAT-POS-c2d406ed-2_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1338
DDG (kcal/mol):	-0.86
dDDG (kcal/mol):	0.28

VLA-UNK-cf7facf1-1_1



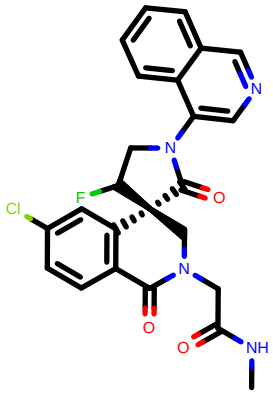
CID:	VLA-UNK-cf7facf1-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN996
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.05

EDG-MED-b1ef7fe3-2_1



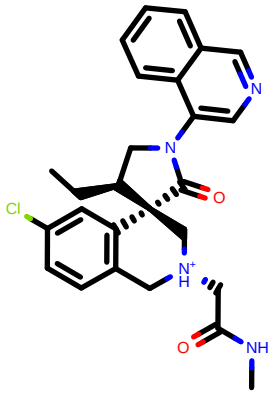
CID:	EDG-MED-b1ef7fe3-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1116
DDG (kcal/mol):	-0.84
dDDG (kcal/mol):	0.11

EDJ-MED-fd8ed875-5_1



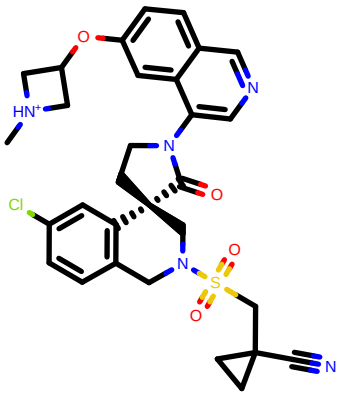
CID:	EDJ-MED-fd8ed875-5_1
SMILES:	CNC(=O)CN1C[C@@]2(c3cc(ccc3C1=O)Cl)C(=CN(C2=O)c4cncc5c4cccc5)F
RUN:	RUN1144
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.11

MAT-POS-50a80394-5_2



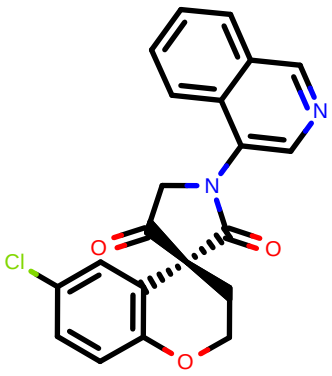
CID:	MAT-POS-50a80394-5_2
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1139
DDG (kcal/mol):	-0.83
dDDG (kcal/mol):	0.21

EDJ-MED-ee81482e-2_1



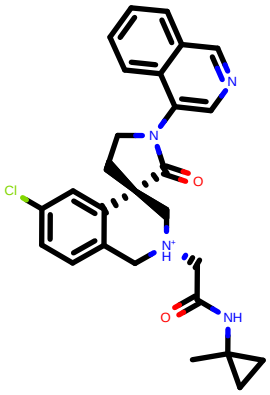
CID:	EDJ-MED-ee81482e-2_1
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1416
DDG (kcal/mol):	-0.82
dDDG (kcal/mol):	0.53

DAR-DIA-0f7b7cd9-9_1



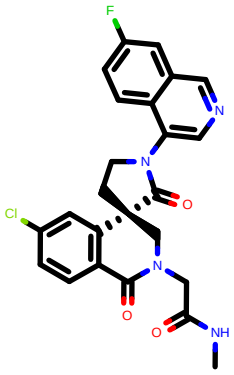
CID:	DAR-DIA-0f7b7cd9-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN1004
DDG (kcal/mol):	-0.81
dDDG (kcal/mol):	0.07

MAT-POS-69786b79-3_1



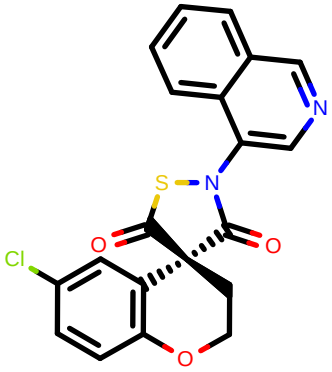
CID:	MAT-POS-69786b79-3_1
SMILES:	CC1(CC1)NC(=O)C[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1180
DDG (kcal/mol):	-0.79
dDDG (kcal/mol):	0.30

EDG-MED-b1ef7fe3-3_1



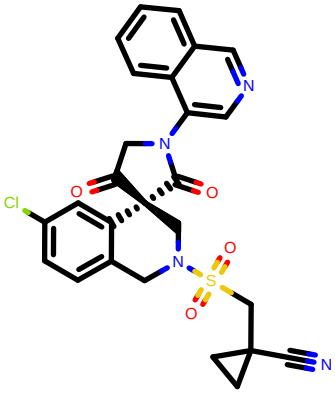
CID:	EDG-MED-b1ef7fe3-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1121
DDG (kcal/mol):	-0.78
dDDG (kcal/mol):	0.12

DAR-DIA-0f7b7cd9-8_1



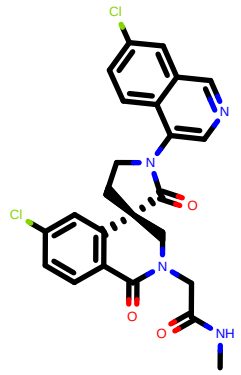
CID:	DAR-DIA-0f7b7cd9-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C(=O)S3
RUN:	RUN1002
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.07

EDJ-MED-a12e3a20-1_2



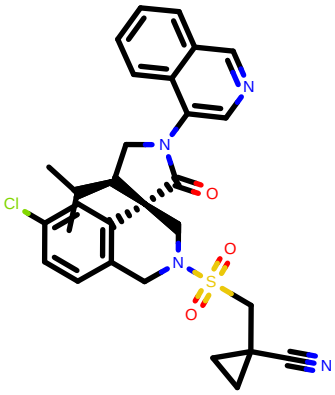
CID:	EDJ-MED-a12e3a20-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1306
DDG (kcal/mol):	-0.77
dDDG (kcal/mol):	0.46

EDG-MED-b1ef7fe3-4_1



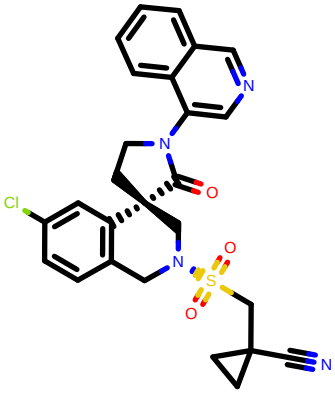
CID:	EDG-MED-b1ef7fe3-4_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3ccc(c4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1114
DDG (kcal/mol):	-0.73
dDDG (kcal/mol):	0.12

MAT-POS-50a80394-3_2



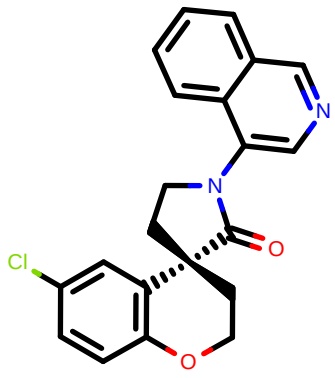
CID:	MAT-POS-50a80394-3_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1367
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.51

MIK-ENA-5d9157e9-2_2



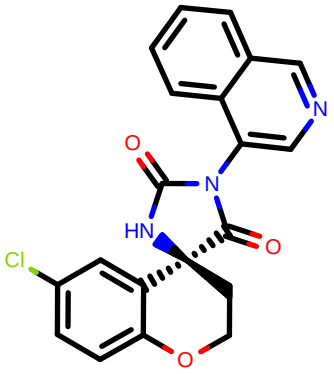
CID:	MIK-ENA-5d9157e9-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1240
DDG (kcal/mol):	-0.72
dDDG (kcal/mol):	0.49

EDJ-MED-159244ea-1_1



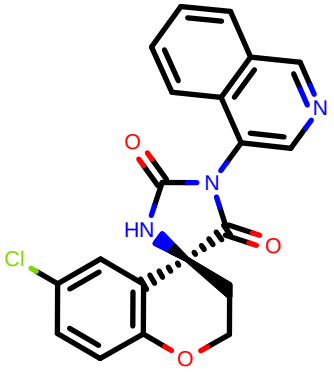
CID:	EDJ-MED-159244ea-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN982
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.06

VLA-UCB-29506327-1_1



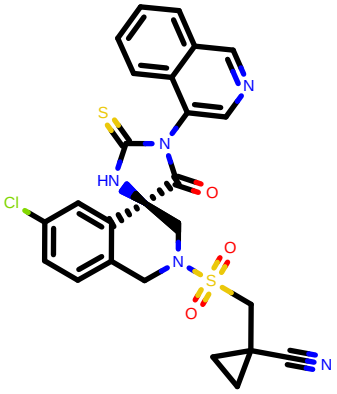
CID:	VLA-UCB-29506327-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1003
DDG (kcal/mol):	-0.71
dDDG (kcal/mol):	0.05

VLA-UCB-34f3ed0c-11_1



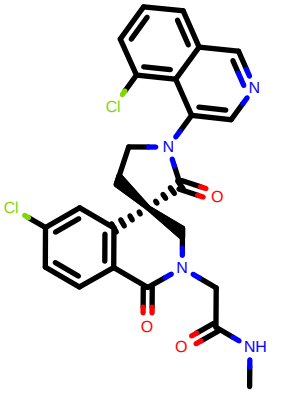
CID:	VLA-UCB-34f3ed0c-11_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1001
DDG (kcal/mol):	-0.70
dDDG (kcal/mol):	0.06

MAT-POS-c2d406ed-3_2



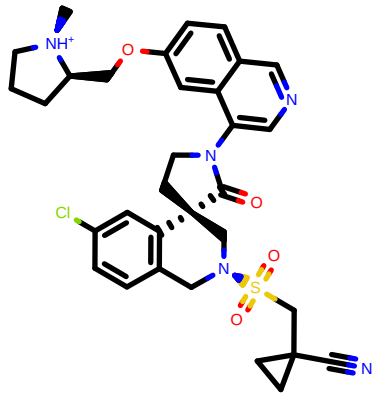
CID:	MAT-POS-c2d406ed-3_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN1299
DDG (kcal/mol):	-0.69
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-1_1



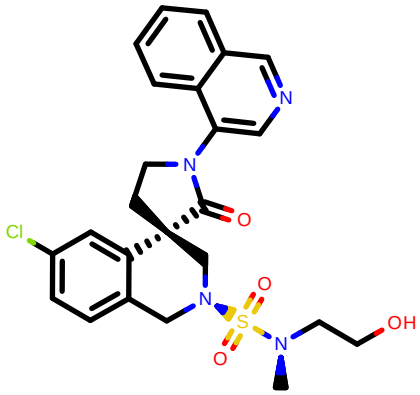
CID:	MAT-POS-853c0ffa-1_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1123
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.12

MAT-POS-40ad851a-1_5



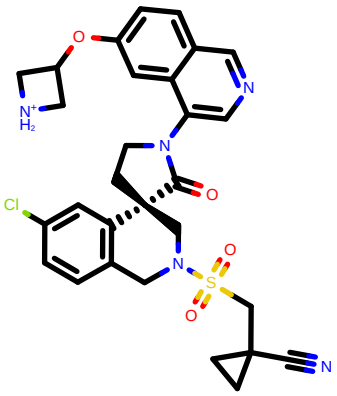
CID:	MAT-POS-40ad851a-1_5
SMILES:	C[N@@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1437
DDG (kcal/mol):	-0.68
dDDG (kcal/mol):	0.76

ALP-POS-ecbed2ba-19_3



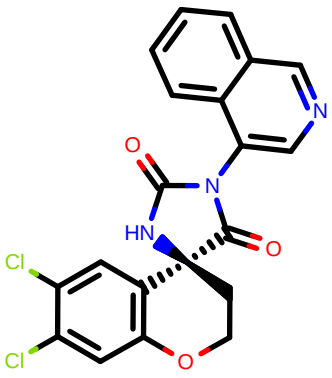
CID:	ALP-POS-ecbed2ba-19_3
SMILES:	C[N@@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1195
DDG (kcal/mol):	-0.66
dDDG (kcal/mol):	0.81

EDJ-MED-ee81482e-1_2



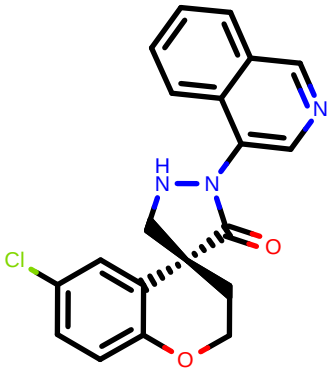
CID:	EDJ-MED-ee81482e-1_2
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1404
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.47

VLA-UNK-56836b69-2_1



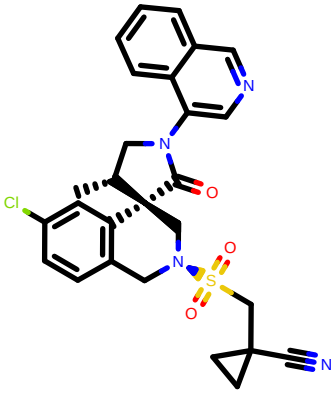
CID:	VLA-UNK-56836b69-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN1007
DDG (kcal/mol):	-0.62
dDDG (kcal/mol):	0.09

BEN-BAS-c2bc0d80-3_1



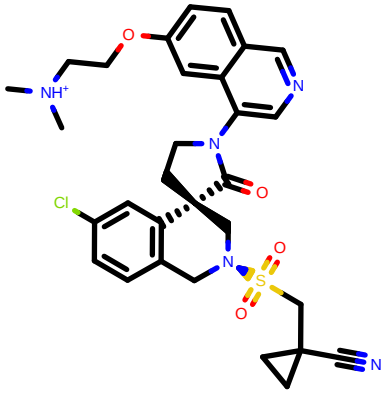
CID:	BEN-BAS-c2bc0d80-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)CN3
RUN:	RUN984
DDG (kcal/mol):	-0.61
dDDG (kcal/mol):	0.07

MAT-POS-50a80394-1_3



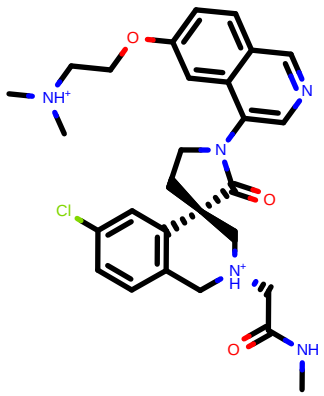
CID:	MAT-POS-50a80394-1_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1312
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.47

MAT-POS-38eb6498-1_1



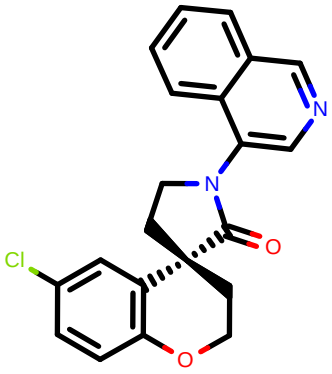
CID:	MAT-POS-38eb6498-1_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1414
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.58

MAT-POS-38eb6498-3_1



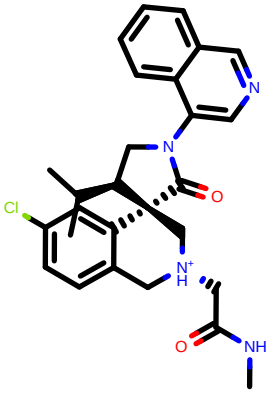
CID:	MAT-POS-38eb6498-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1353
DDG (kcal/mol):	-0.59
dDDG (kcal/mol):	0.35

MAT-POS-983b399a-1_1



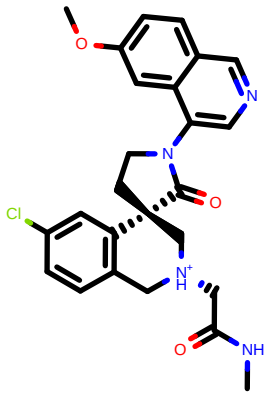
CID:	MAT-POS-983b399a-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN983
DDG (kcal/mol):	-0.56
dDDG (kcal/mol):	0.09

MAT-POS-50a80394-6_2



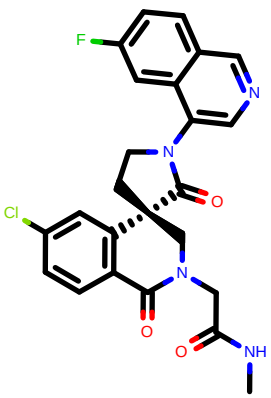
CID:	MAT-POS-50a80394-6_2
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1196
DDG (kcal/mol):	-0.55
dDDG (kcal/mol):	0.21

EDJ-MED-b6c6ee2b-2_1



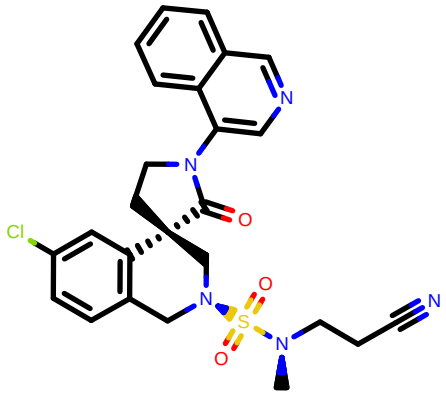
CID:	EDJ-MED-b6c6ee2b-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN1152
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.24

EDJ-MED-b6c6ee2b-6_1



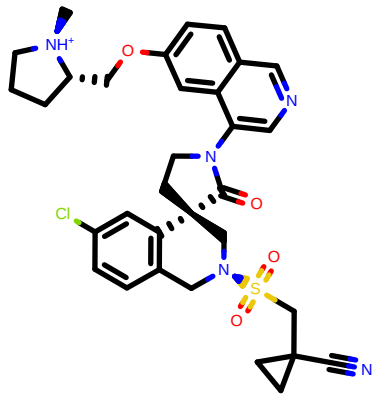
CID:	EDJ-MED-b6c6ee2b-6_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cc(cc4)F)c5cc(ccc5C1=O)Cl
RUN:	RUN1157
DDG (kcal/mol):	-0.52
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-16_4



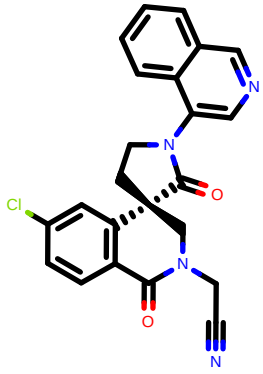
CID:	ALP-POS-ecbed2ba-16_4
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1232
DDG (kcal/mol):	-0.50
dDDG (kcal/mol):	0.73

MAT-POS-40ad851a-1_3



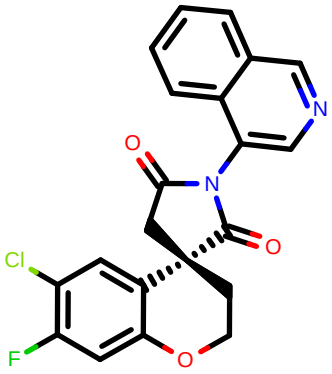
CID:	MAT-POS-40ad851a-1_3
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1436
DDG (kcal/mol):	-0.49
dDDG (kcal/mol):	0.85

PET-UNK-aa57768f-8_1



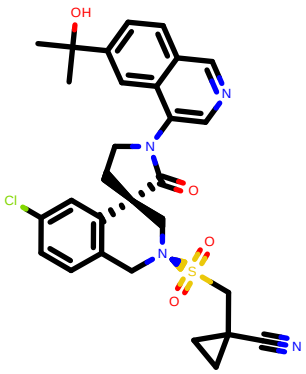
CID:	PET-UNK-aa57768f-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN1036
DDG (kcal/mol):	-0.47
dDDG (kcal/mol):	0.09

VLA-UNK-3a43cd95-3_1



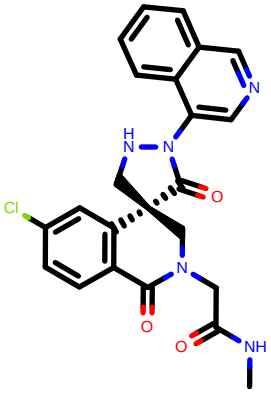
CID:	VLA-UNK-3a43cd95-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(c(c5)F)Cl
RUN:	RUN1012
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.05

MAT-POS-853c0ffa-11_1



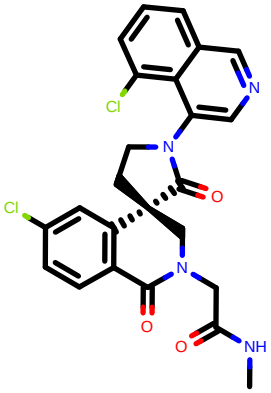
CID:	MAT-POS-853c0ffa-11_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1382
DDG (kcal/mol):	-0.46
dDDG (kcal/mol):	0.42

EDJ-MED-fed7ac0b-1_1



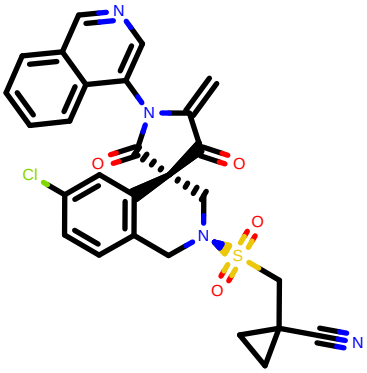
CID:	EDJ-MED-fed7ac0b-1_1
SMILES:	CNC(=O)CN1C[C@]2(CNN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1084
DDG (kcal/mol):	-0.43
dDDG (kcal/mol):	0.19

MAT-POS-1d5ab790-3_1



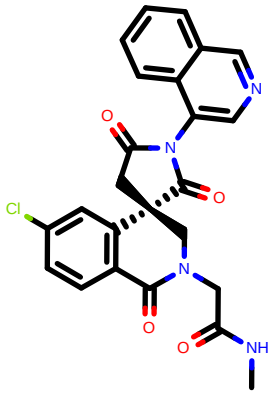
CID:	MAT-POS-1d5ab790-3_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3c(ccc4)Cl)c5cc(ccc5C1=O)Cl
RUN:	RUN1142
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.13

PET-UNK-94036022-6_2



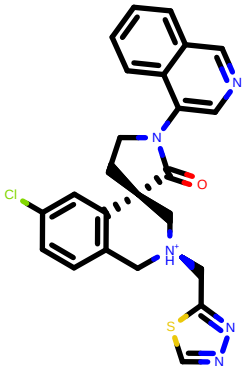
CID:	PET-UNK-94036022-6_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1356
DDG (kcal/mol):	-0.41
dDDG (kcal/mol):	0.56

LUO-POS-868e8996-7_1



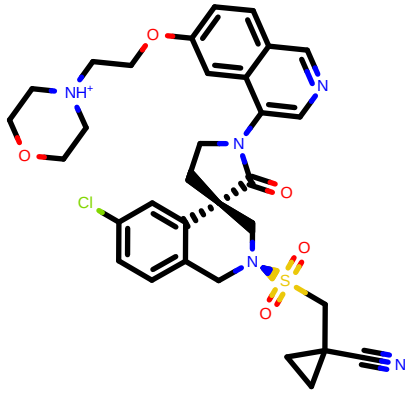
CID:	LUO-POS-868e8996-7_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1117
DDG (kcal/mol):	-0.40
dDDG (kcal/mol):	0.10

PET-UNK-7e9559de-4_2



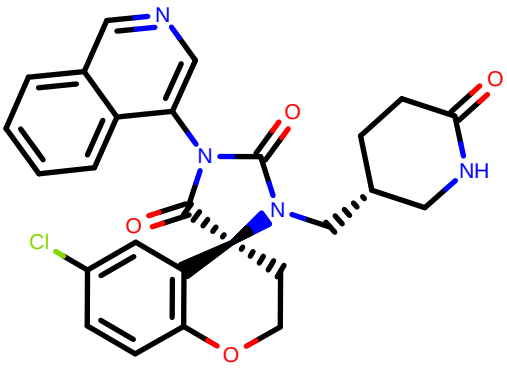
CID:	PET-UNK-7e9559de-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1090
DDG (kcal/mol):	-0.39
dDDG (kcal/mol):	0.15

EDJ-MED-468565e0-2_1



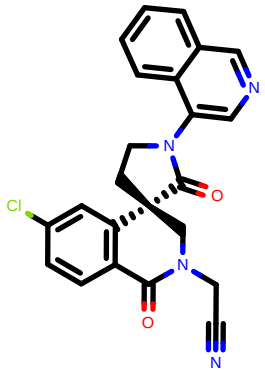
CID:	EDJ-MED-468565e0-2_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1444
DDG (kcal/mol):	-0.35
dDDG (kcal/mol):	0.68

VLA-UNK-f702bf1c-5_1



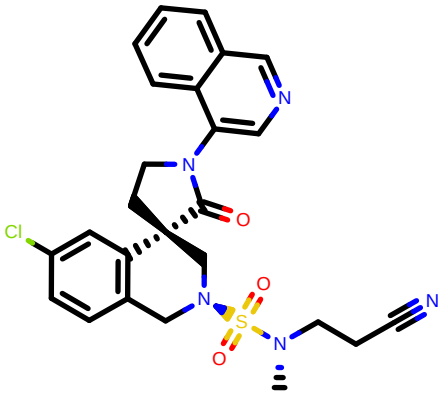
CID:	VLA-UNK-f702bf1c-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CCC(=O)NC6
RUN:	RUN1201
DDG (kcal/mol):	-0.34
dDDG (kcal/mol):	0.19

PET-UNK-aa57768f-2_1



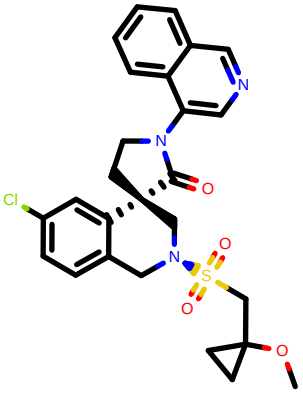
CID:	PET-UNK-aa57768f-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CN(C(=O)c5c4cc(cc5)Cl)CC#N
RUN:	RUN1034
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.09

ALP-POS-ecbed2ba-16_1



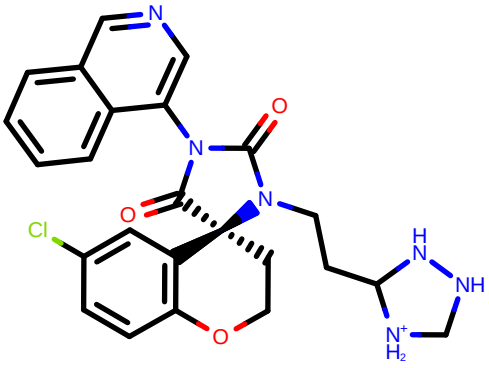
CID:	ALP-POS-ecbed2ba-16_1
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1230
DDG (kcal/mol):	-0.33
dDDG (kcal/mol):	0.35

ALP-POS-ecbed2ba-6_1



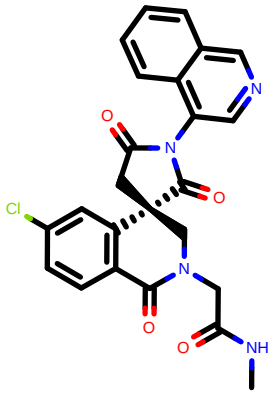
CID:	ALP-POS-ecbed2ba-6_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1217
DDG (kcal/mol):	-0.31
dDDG (kcal/mol):	0.34

VLA-UNK-f702bf1c-8_1



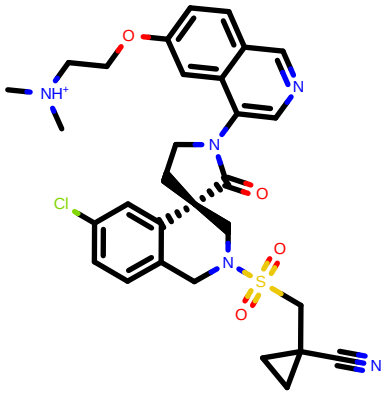
CID:	VLA-UNK-f702bf1c-8_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCc6[nH]ncn6
RUN:	RUN1166
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.19

LUO-POS-868e8996-8_1



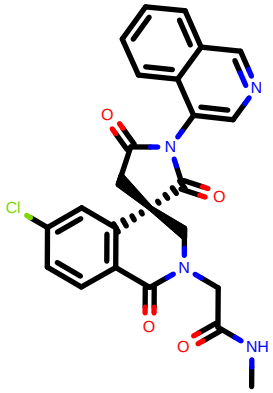
CID:	LUO-POS-868e8996-8_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1119
DDG (kcal/mol):	-0.30
dDDG (kcal/mol):	0.11

LUO-POS-8484f2d3-2_1



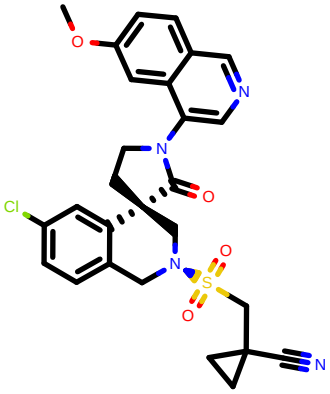
CID:	LUO-POS-8484f2d3-2_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1411
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.50

MAT-POS-1bed62cf-2_1



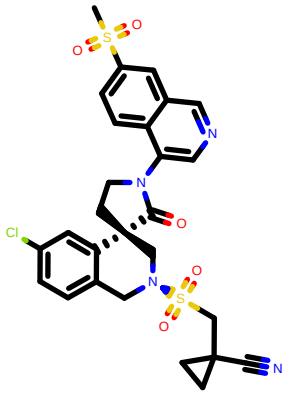
CID:	MAT-POS-1bed62cf-2_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1109
DDG (kcal/mol):	-0.29
dDDG (kcal/mol):	0.09

EDJ-MED-b6c6ee2b-3_2



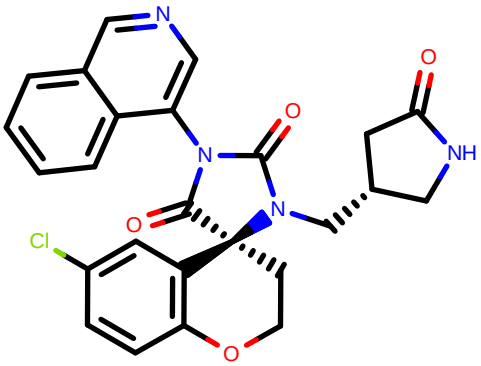
CID:	EDJ-MED-b6c6ee2b-3_2
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1351
DDG (kcal/mol):	-0.27
dDDG (kcal/mol):	0.57

MAT-POS-853c0ffa-15_1



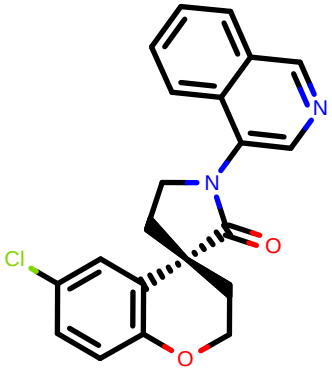
CID:	MAT-POS-853c0ffa-15_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1375
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.46

VLA-UNK-f702bf1c-4_1



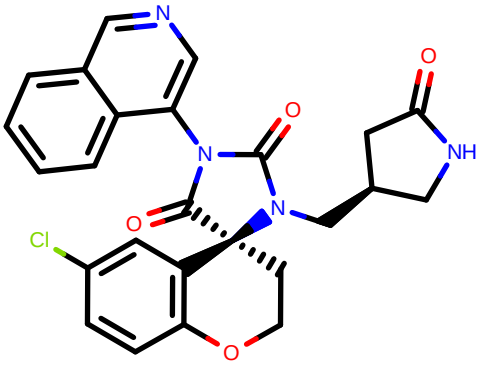
CID:	VLA-UNK-f702bf1c-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@@H]6CC(=O)NC6
RUN:	RUN1163
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.16

ALP-POS-477dc5b7-4_1



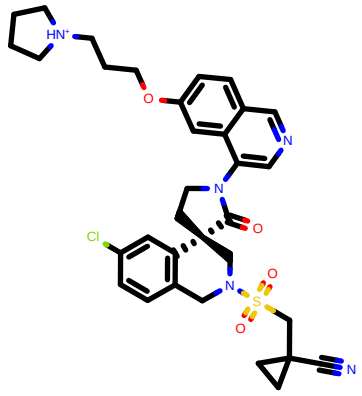
CID:	ALP-POS-477dc5b7-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN980
DDG (kcal/mol):	-0.24
dDDG (kcal/mol):	0.09

VLA-UNK-f702bf1c-4_2



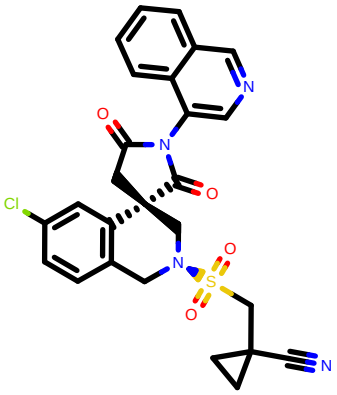
CID:	VLA-UNK-f702bf1c-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CC(=O)NC6
RUN:	RUN1161
DDG (kcal/mol):	-0.23
dDDG (kcal/mol):	0.17

MAT-POS-40ad851a-5_1



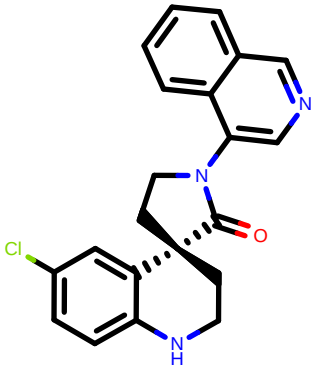
CID:	MAT-POS-40ad851a-5_1
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1456
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.68

LUO-POS-868e8996-10_1



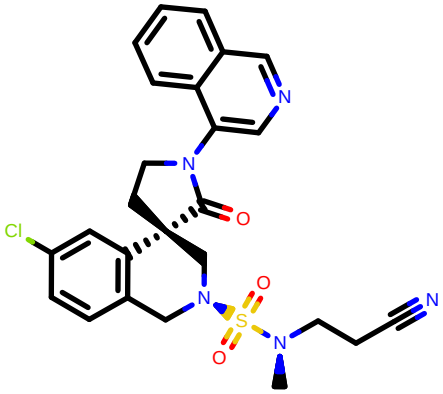
CID:	LUO-POS-868e8996-10_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1270
DDG (kcal/mol):	-0.21
dDDG (kcal/mol):	0.34

DAR-DIA-6be260fc-5_1



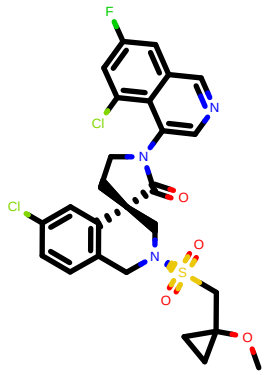
CID:	DAR-DIA-6be260fc-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCNc5c4cc(cc5)Cl
RUN:	RUN978
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.14

ALP-POS-ecbed2ba-16_3



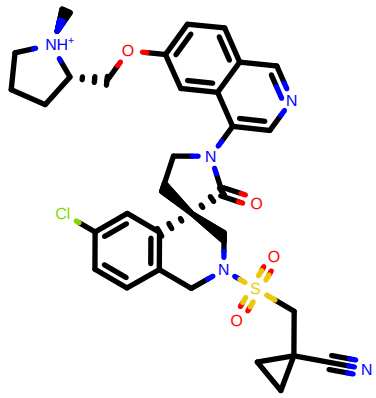
CID:	ALP-POS-ecbed2ba-16_3
SMILES:	C[N@@](CCC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1231
DDG (kcal/mol):	-0.19
dDDG (kcal/mol):	0.65

MAT-POS-853c0ffa-8_2



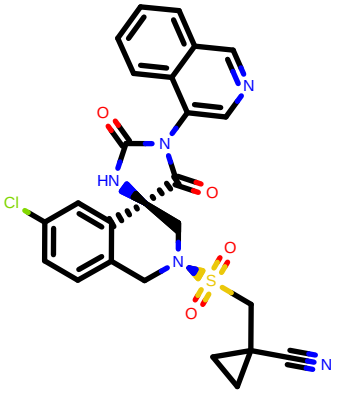
CID:	MAT-POS-853c0ffa-8_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1335
DDG (kcal/mol):	-0.18
dDDG (kcal/mol):	0.36

MAT-POS-40ad851a-1_7



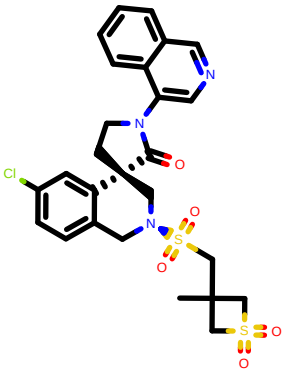
CID:	MAT-POS-40ad851a-1_7
SMILES:	C[N@@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1451
DDG (kcal/mol):	-0.15
dDDG (kcal/mol):	0.97

MAT-POS-c2d406ed-1_1



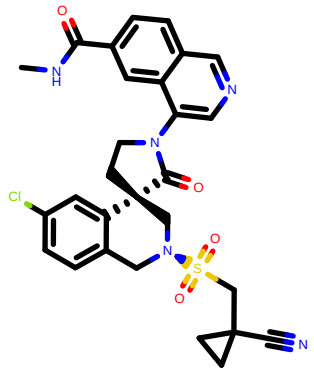
CID:	MAT-POS-c2d406ed-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=O
RUN:	RUN1294
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.22

ALP-POS-ecbed2ba-1_2



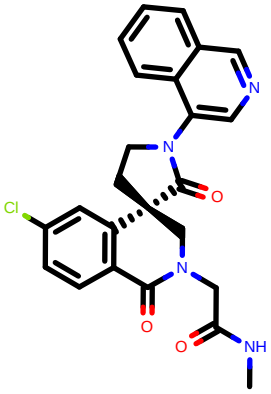
CID:	ALP-POS-ecbed2ba-1_2
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1334
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.54

MAT-POS-38eb6498-2_2



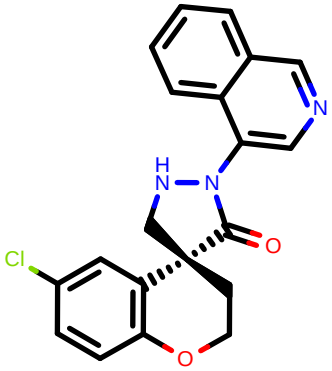
CID:	MAT-POS-38eb6498-2_2
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1385
DDG (kcal/mol):	-0.12
dDDG (kcal/mol):	0.63

EDJ-MED-fd8ed875-3_1



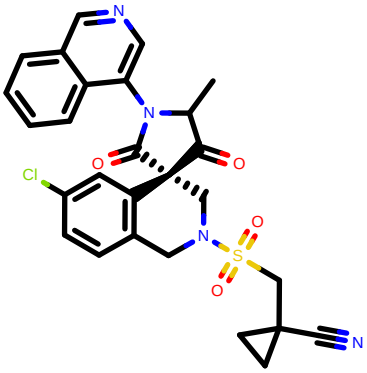
CID:	EDJ-MED-fd8ed875-3_1
SMILES:	CNC(=O)CN1C[C@]2(C=CN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1089
DDG (kcal/mol):	-0.10
dDDG (kcal/mol):	0.13

BRU-THA-73c97d88-1_1



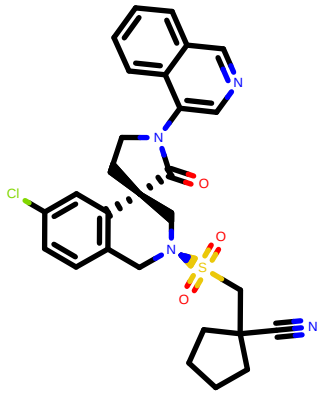
CID:	BRU-THA-73c97d88-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)C=N3
RUN:	RUN987
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.06

PET-UNK-94036022-13_2



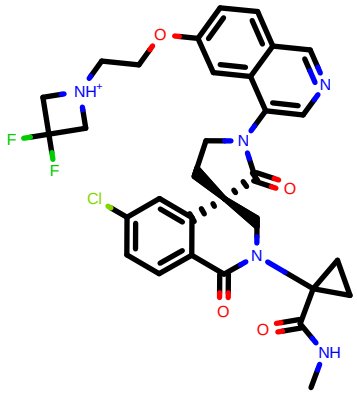
CID:	PET-UNK-94036022-13_2
SMILES:	C=C1C(=O)[C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1360
DDG (kcal/mol):	-0.05
dDDG (kcal/mol):	0.63

ALP-POS-ecbed2ba-15_1



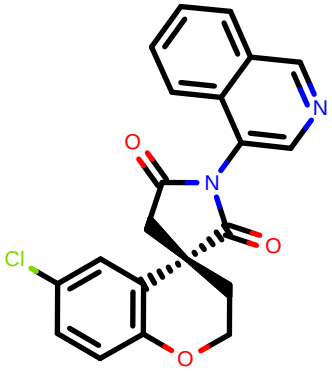
CID:	ALP-POS-ecbed2ba-15_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN1332
DDG (kcal/mol):	-0.03
dDDG (kcal/mol):	0.43

EDJ-MED-dfa1d800-5_1



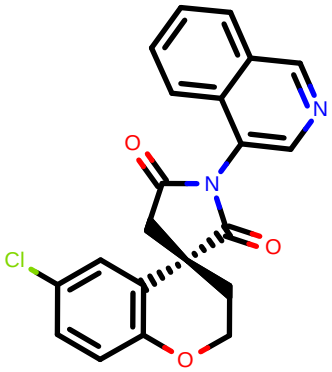
CID:	EDJ-MED-dfa1d800-5_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cc(cc5)OCCN6CC(C6)(F)F)c7cc(ccc7C2=O)Cl
RUN:	RUN1433
DDG (kcal/mol):	-0.01
dDDG (kcal/mol):	0.31

VLA-UCB-50c39ae8-2_1



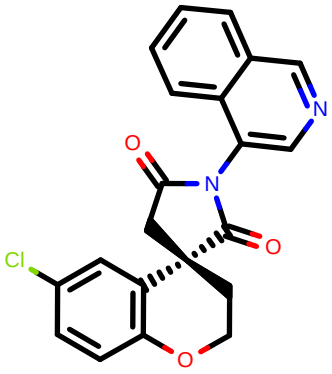
CID:	VLA-UCB-50c39ae8-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN992
DDG (kcal/mol):	-0.00
dDDG (kcal/mol):	0.00

BEN-BAS-c2bc0d80-6_1



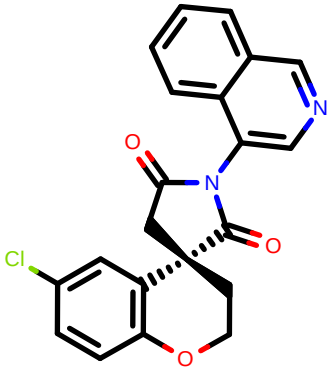
CID:	BEN-BAS-c2bc0d80-6_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN994
DDG (kcal/mol):	-0.00
dDDG (kcal/mol):	0.00

VLA-UCB-05e51b3f-5_1



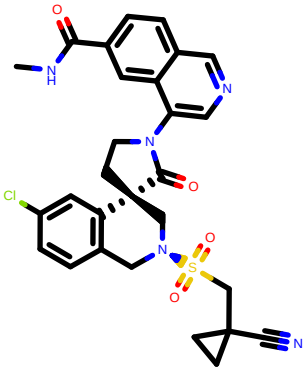
CID:	VLA-UCB-05e51b3f-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN991
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

MAT-POS-94643566-1_1



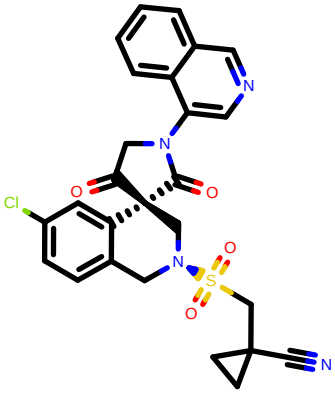
CID:	MAT-POS-94643566-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)CCOc5c4cc(cc5)Cl
RUN:	RUN995
DDG (kcal/mol):	0.00
dDDG (kcal/mol):	0.00

MAT-POS-38eb6498-2_1



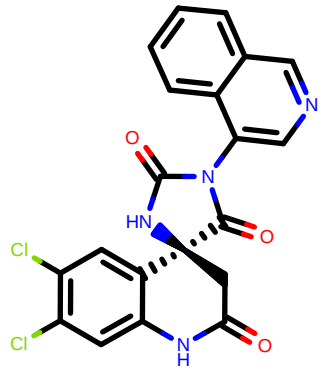
CID:	MAT-POS-38eb6498-2_1
SMILES:	CNC(=O)c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1384
DDG (kcal/mol):	0.01
dDDG (kcal/mol):	0.43

EDJ-MED-a12e3a20-1_1



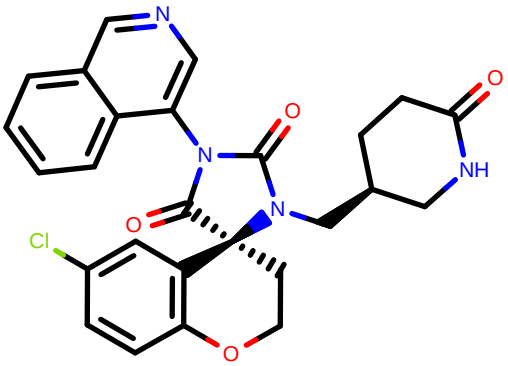
CID:	EDJ-MED-a12e3a20-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC(=O)[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1301
DDG (kcal/mol):	0.04
dDDG (kcal/mol):	0.56

VLA-UNK-56836b69-5_1



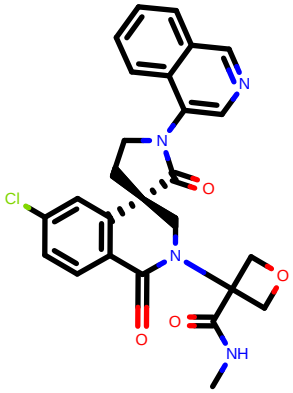
CID:	VLA-UNK-56836b69-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CC(=O)Nc5c4cc(c(c5)Cl)Cl)NC3=O
RUN:	RUN1017
DDG (kcal/mol):	0.10
dDDG (kcal/mol):	0.11

VLA-UNK-f702bf1c-5_2



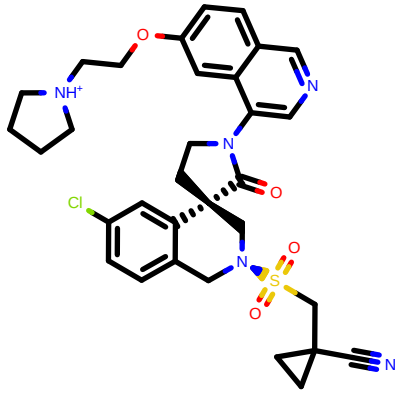
CID:	VLA-UNK-f702bf1c-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)C[C@H]6CCC(=O)NC6
RUN:	RUN1202
DDG (kcal/mol):	0.13
dDDG (kcal/mol):	0.15

EDJ-MED-98c0a822-4_1



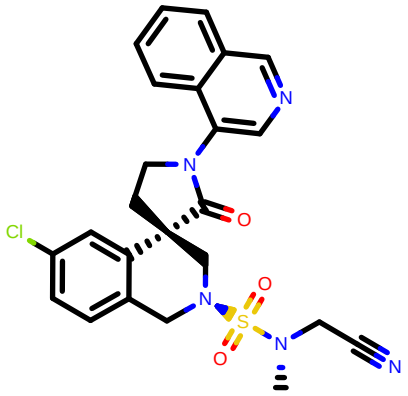
CID:	EDJ-MED-98c0a822-4_1
SMILES:	CNC(=O)C1(COC1)N2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1247
DDG (kcal/mol):	0.15
dDDG (kcal/mol):	0.14

EDJ-MED-468565e0-1_1



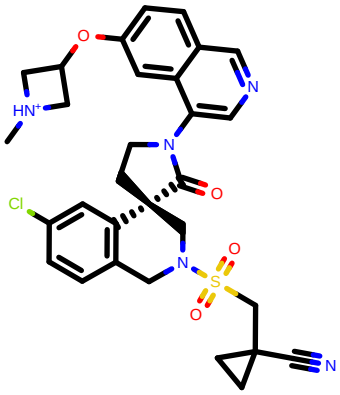
CID:	EDJ-MED-468565e0-1_1
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1446
DDG (kcal/mol):	0.16
dDDG (kcal/mol):	0.74

ALP-POS-ecbed2ba-17_2



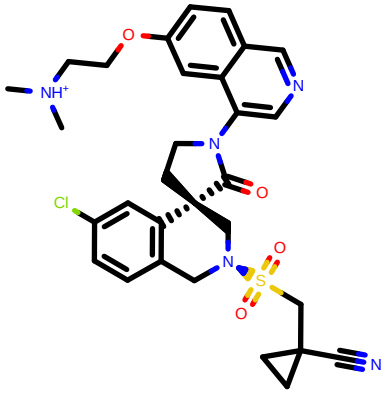
CID:	ALP-POS-ecbed2ba-17_2
SMILES:	C[N@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1172
DDG (kcal/mol):	0.20
dDDG (kcal/mol):	0.26

EDJ-MED-ee81482e-2_2



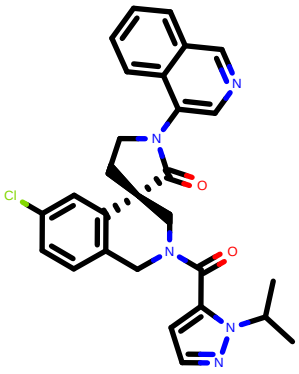
CID:	EDJ-MED-ee81482e-2_2
SMILES:	C[NH+]1CC(C1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1417
DDG (kcal/mol):	0.21
dDDG (kcal/mol):	0.55

MAT-POS-853c0ffa-9_2



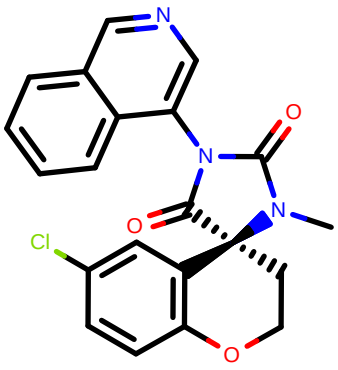
CID:	MAT-POS-853c0ffa-9_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1410
DDG (kcal/mol):	0.21
dDDG (kcal/mol):	0.81

MAT-POS-be048f2c-6_1



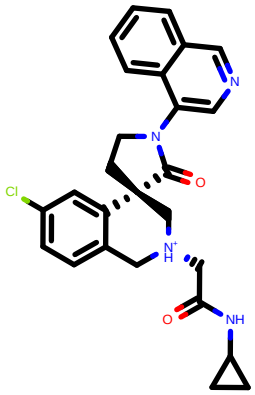
CID:	MAT-POS-be048f2c-6_1
SMILES:	CC(C)n1c(ccn1)C(=O)N2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1305
DDG (kcal/mol):	0.22
dDDG (kcal/mol):	0.23

BEN-BAS-c2bc0d80-7_1



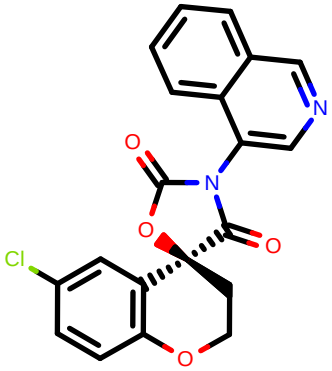
CID:	BEN-BAS-c2bc0d80-7_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(cc3)Cl)c4cncc5c4cccc5
RUN:	RUN1008
DDG (kcal/mol):	0.27
dDDG (kcal/mol):	0.07

MAT-POS-69786b79-2_1



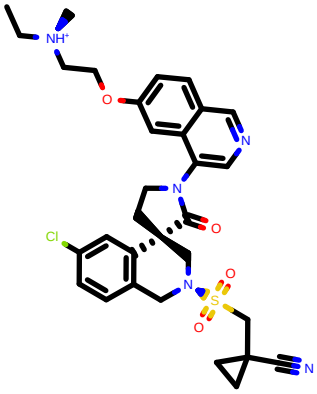
CID:	MAT-POS-69786b79-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN1135
DDG (kcal/mol):	0.27
dDDG (kcal/mol):	0.29

MAT-POS-ec6d90b7-2_1



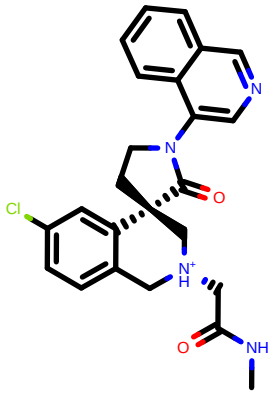
CID:	MAT-POS-ec6d90b7-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN1000
DDG (kcal/mol):	0.30
dDDG (kcal/mol):	0.03

MAT-POS-40ad851a-2_3



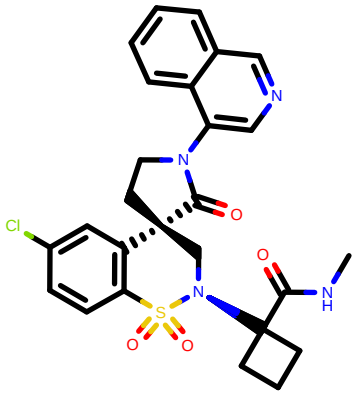
CID:	MAT-POS-40ad851a-2_3
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1424
DDG (kcal/mol):	0.31
dDDG (kcal/mol):	0.85

LUO-POS-868e8996-11_1



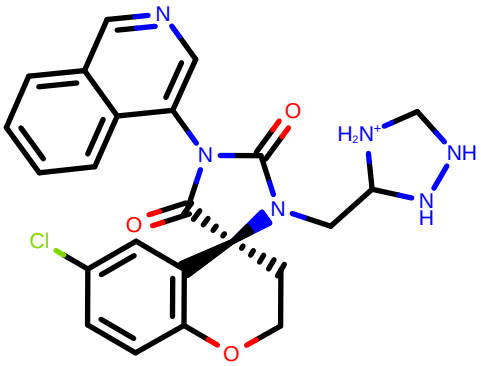
CID:	LUO-POS-868e8996-11_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1055
DDG (kcal/mol):	0.31
dDDG (kcal/mol):	0.24

EDJ-MED-98c0a822-1_2



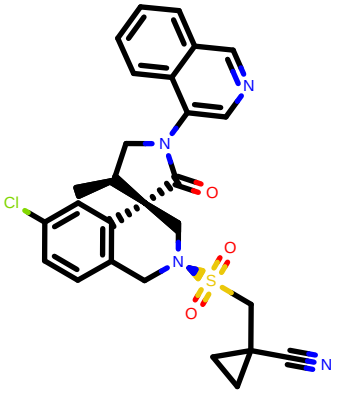
CID:	EDJ-MED-98c0a822-1_2
SMILES:	CNC(=O)C1(CCC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1304
DDG (kcal/mol):	0.31
dDDG (kcal/mol):	0.44

VLA-UNK-f702bf1c-3_1



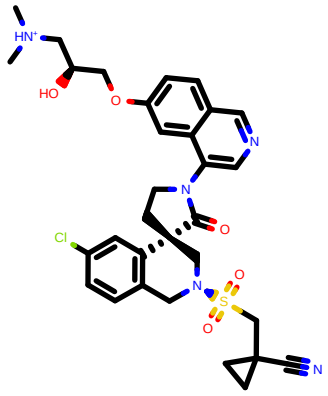
CID:	VLA-UNK-f702bf1c-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)Cc6[nH]ncn6
RUN:	RUN1111
DDG (kcal/mol):	0.36
dDDG (kcal/mol):	0.15

MAT-POS-50a80394-1_4



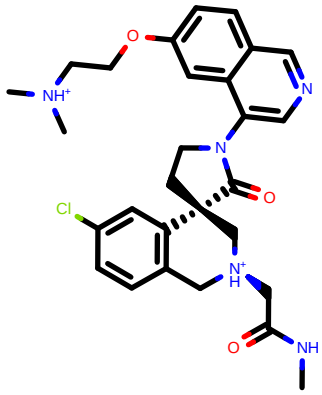
CID:	MAT-POS-50a80394-1_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1317
DDG (kcal/mol):	0.36
dDDG (kcal/mol):	0.43

EDJ-MED-ee81482e-3_1



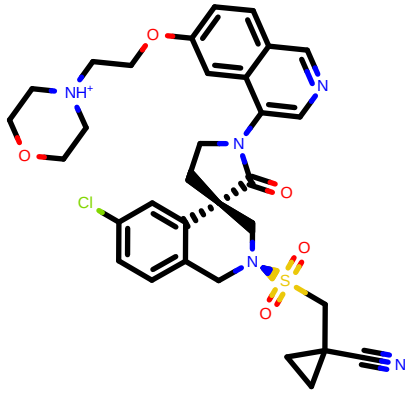
CID:	EDJ-MED-ee81482e-3_1
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1426
DDG (kcal/mol):	0.36
dDDG (kcal/mol):	0.74

EDJ-MED-b6c6ee2b-1_2



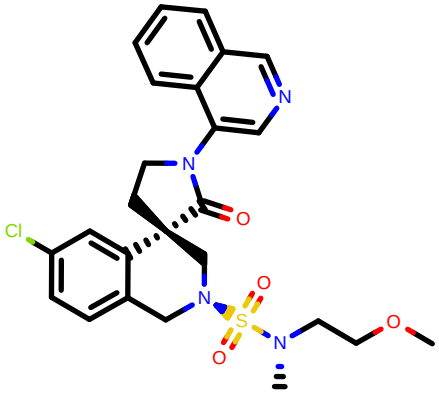
CID:	EDJ-MED-b6c6ee2b-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1369
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.40

EDJ-MED-468565e0-2_2



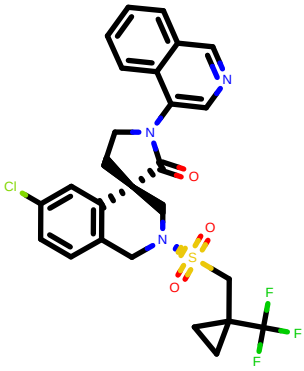
CID:	EDJ-MED-468565e0-2_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCOCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1455
DDG (kcal/mol):	0.38
dDDG (kcal/mol):	0.77

ALP-POS-ecbed2ba-21_1



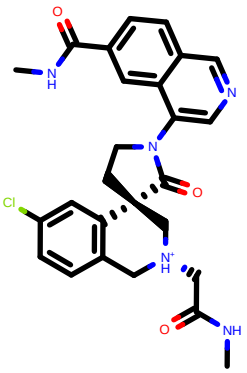
CID:	ALP-POS-ecbed2ba-21_1
SMILES:	C[N@@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1235
DDG (kcal/mol):	0.39
dDDG (kcal/mol):	0.29

EDJ-MED-5cd3920d-6_2



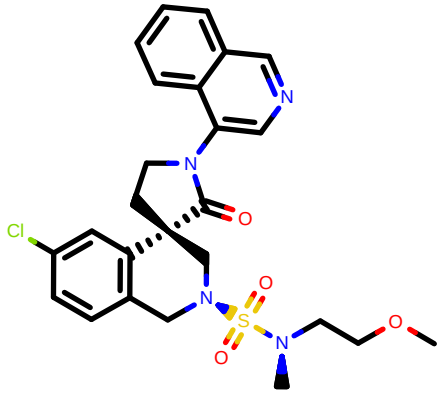
CID:	EDJ-MED-5cd3920d-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN1344
DDG (kcal/mol):	0.39
dDDG (kcal/mol):	0.55

MAT-POS-38eb6498-5_1



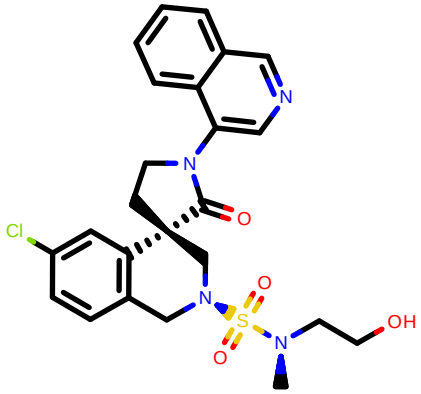
CID:	MAT-POS-38eb6498-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN1239
DDG (kcal/mol):	0.40
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-21_4



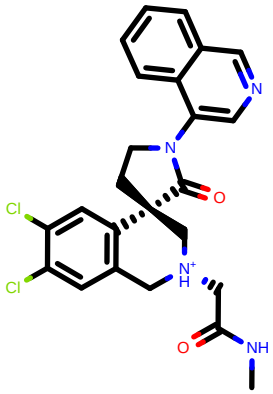
CID:	ALP-POS-ecbed2ba-21_4
SMILES:	C[N@](CCOC)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1241
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.56

ALP-POS-ecbed2ba-19_4



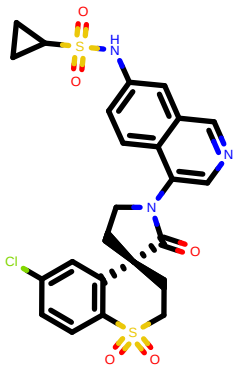
CID:	ALP-POS-ecbed2ba-19_4
SMILES:	C[N@](CCO)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1193
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.84

ALP-POS-afe0272e-1_1



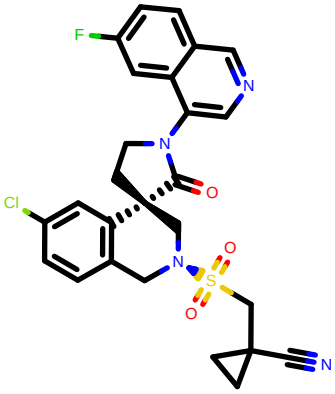
CID:	ALP-POS-afe0272e-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN1081
DDG (kcal/mol):	0.41
dDDG (kcal/mol):	0.29

EDJ-MED-ede5c6cb-2_1



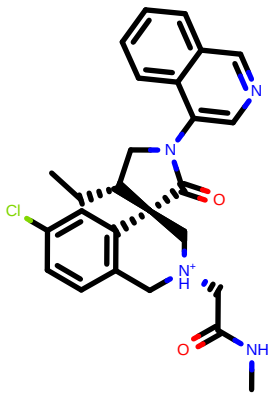
CID:	EDJ-MED-ede5c6cb-2_1
SMILES:	c1cc2c(cc1NS(=O)(=O)C3CC3)cncc2N4CC[C@@]5(C4=O)CCS(=O)(=O)c6c5cc(cc6)Cl
RUN:	RUN1263
DDG (kcal/mol):	0.42
dDDG (kcal/mol):	0.21

MAT-POS-853c0ffa-13_1



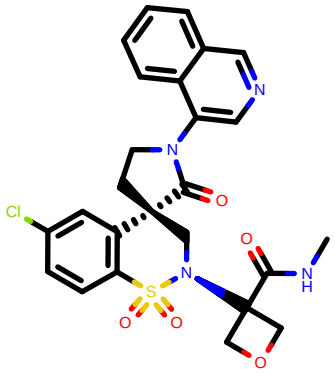
CID:	MAT-POS-853c0ffa-13_1
SMILES:	c1cc2cncc(c2cc1F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1278
DDG (kcal/mol):	0.45
dDDG (kcal/mol):	0.38

MAT-POS-50a80394-5_1



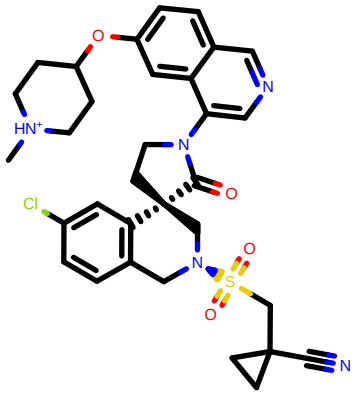
CID:	MAT-POS-50a80394-5_1
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1146
DDG (kcal/mol):	0.45
dDDG (kcal/mol):	0.22

EDJ-MED-98c0a822-2_1



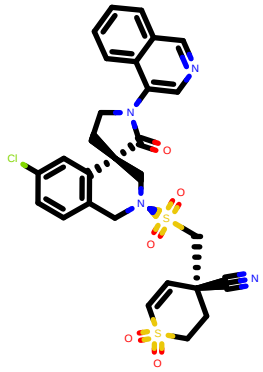
CID:	EDJ-MED-98c0a822-2_1
SMILES:	CNC(=O)C1(COC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1307
DDG (kcal/mol):	0.46
dDDG (kcal/mol):	0.29

LUO-POS-d1147590-1_2



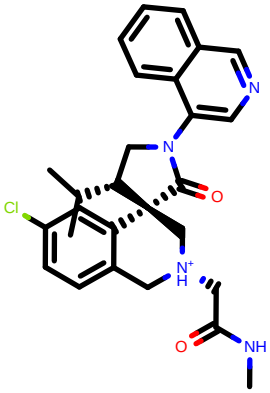
CID:	LUO-POS-d1147590-1_2
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1450
DDG (kcal/mol):	0.46
dDDG (kcal/mol):	0.69

ALP-POS-ecbed2ba-2_1



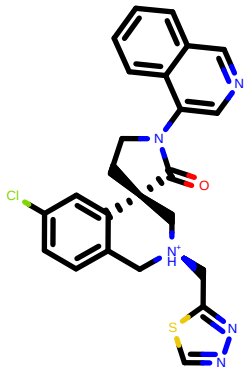
CID:	ALP-POS-ecbed2ba-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN1393
DDG (kcal/mol):	0.47
dDDG (kcal/mol):	0.50

MAT-POS-50a80394-6_1



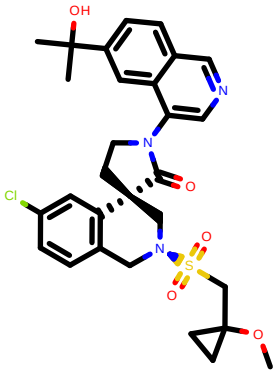
CID:	MAT-POS-50a80394-6_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1194
DDG (kcal/mol):	0.47
dDDG (kcal/mol):	0.22

MAT-POS-96396902-1_2



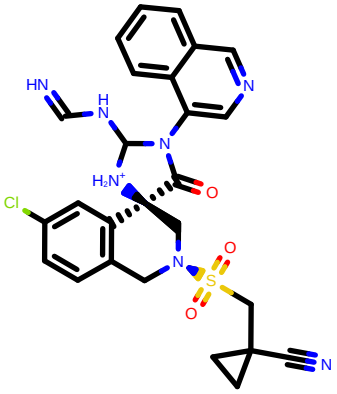
CID:	MAT-POS-96396902-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1099
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.19

MAT-POS-853c0ffa-12_1



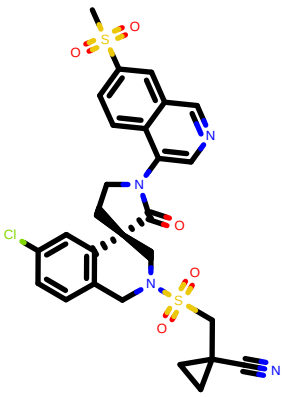
CID:	MAT-POS-853c0ffa-12_1
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN1383
DDG (kcal/mol):	0.48
dDDG (kcal/mol):	0.44

LUO-POS-b5068a05-2_1



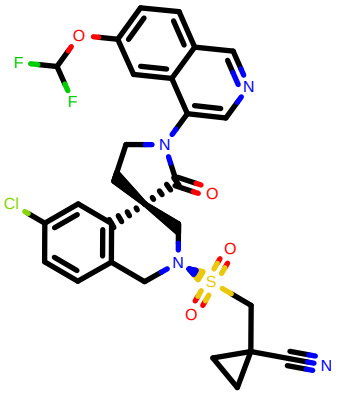
CID:	LUO-POS-b5068a05-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN1379
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.31

MAT-POS-853c0ffa-15_2



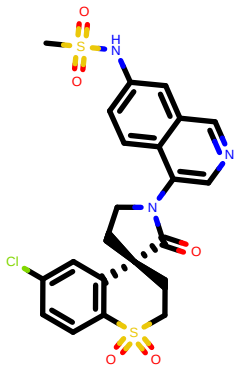
CID:	MAT-POS-853c0ffa-15_2
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1377
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.51

EDJ-MED-5cd3920d-1_1



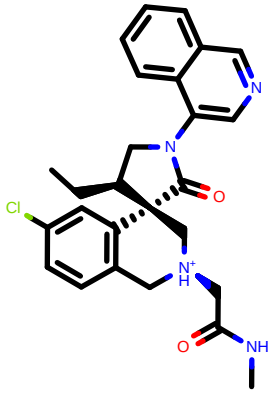
CID:	EDJ-MED-5cd3920d-1_1
SMILES:	c1cc2cncc(c2cc1OC(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1397
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.39

EDJ-MED-94fddcec-7_1



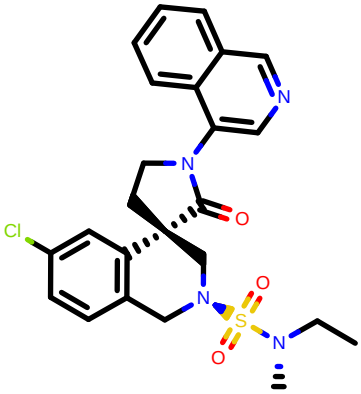
CID:	EDJ-MED-94fddcec-7_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1124
DDG (kcal/mol):	0.49
dDDG (kcal/mol):	0.18

MAT-POS-50a80394-5_4



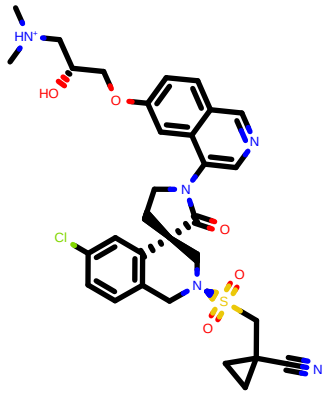
CID:	MAT-POS-50a80394-5_4
SMILES:	CC[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1149
DDG (kcal/mol):	0.50
dDDG (kcal/mol):	0.21

ALP-POS-ecbed2ba-18_4



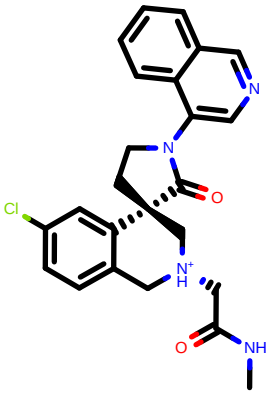
CID:	ALP-POS-ecbed2ba-18_4
SMILES:	CC[N@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1130
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.53

EDJ-MED-ee81482e-3_2



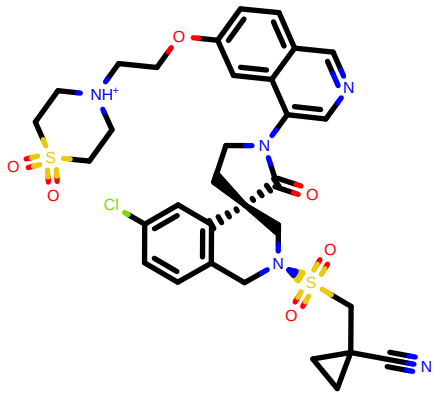
CID:	EDJ-MED-ee81482e-3_2
SMILES:	C[NH+](C)C[C@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1429
DDG (kcal/mol):	0.51
dDDG (kcal/mol):	0.63

MAT-POS-c7726e07-5_1



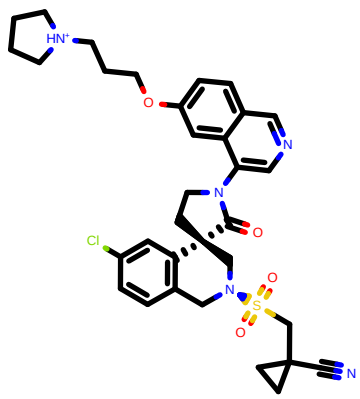
CID:	MAT-POS-c7726e07-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1051
DDG (kcal/mol):	0.52
dDDG (kcal/mol):	0.26

EDJ-MED-468565e0-3_2



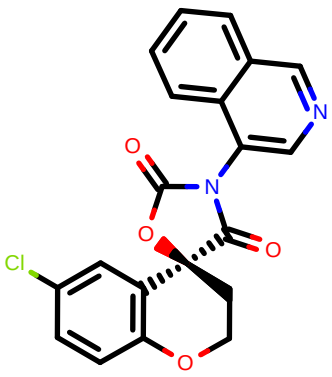
CID:	EDJ-MED-468565e0-3_2
SMILES:	c1cc2cncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1458
DDG (kcal/mol):	0.53
dDDG (kcal/mol):	0.73

MAT-POS-40ad851a-5_2



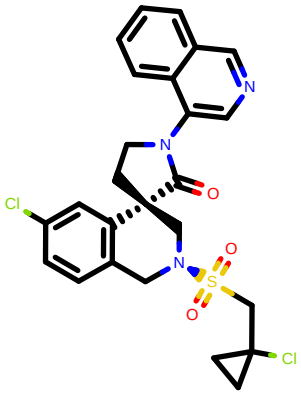
CID:	MAT-POS-40ad851a-5_2
SMILES:	c1cc2cncc(c2cc1OCCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1447
DDG (kcal/mol):	0.54
dDDG (kcal/mol):	0.87

MAT-POS-90505e2b-1_1



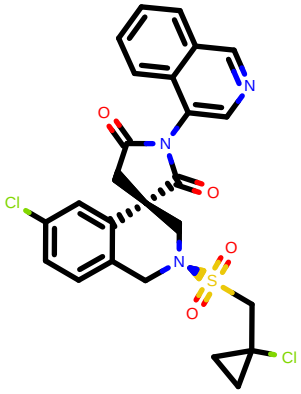
CID:	MAT-POS-90505e2b-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN997
DDG (kcal/mol):	0.55
dDDG (kcal/mol):	0.03

PET-UNK-94036022-10_1



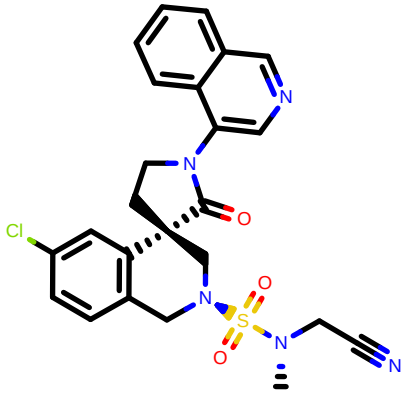
CID:	PET-UNK-94036022-10_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1199
DDG (kcal/mol):	0.57
dDDG (kcal/mol):	0.28

PET-UNK-94036022-12_1



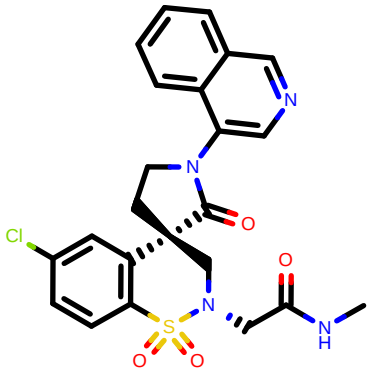
CID:	PET-UNK-94036022-12_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1262
DDG (kcal/mol):	0.57
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-17_4



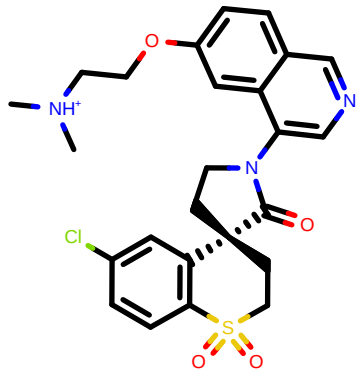
CID:	ALP-POS-ecbed2ba-17_4
SMILES:	C[N@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1176
DDG (kcal/mol):	0.58
dDDG (kcal/mol):	0.67

ALP-POS-4483ae88-2_2



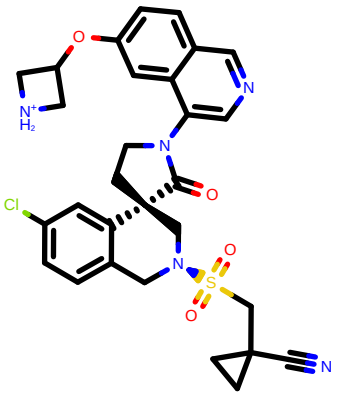
CID:	ALP-POS-4483ae88-2_2
SMILES:	CNC(=O)C[N@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN1120
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.21

EDJ-MED-d4864bdc-4_1



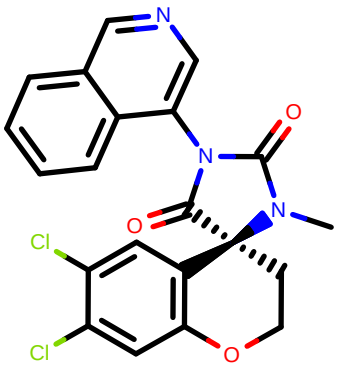
CID:	EDJ-MED-d4864bdc-4_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1203
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.28

EDJ-MED-ee81482e-1_1



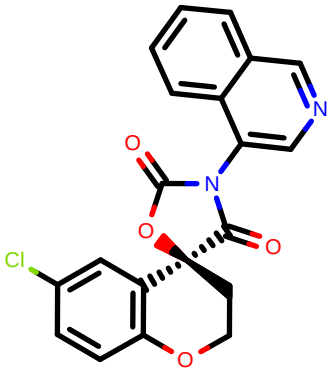
CID:	EDJ-MED-ee81482e-1_1
SMILES:	c1cc2cncc(c2cc1OC3C[NH2+]C3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1407
DDG (kcal/mol):	0.59
dDDG (kcal/mol):	0.59

VLA-UNK-56836b69-3_1



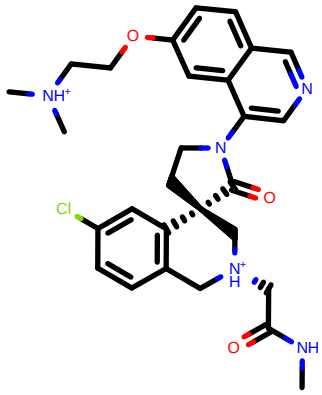
CID:	VLA-UNK-56836b69-3_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12CCOc3c2cc(c(c3)Cl)Cl)c4cncc5c4cccc5
RUN:	RUN1011
DDG (kcal/mol):	0.60
dDDG (kcal/mol):	0.09

MAT-POS-ec6d90b7-1_1



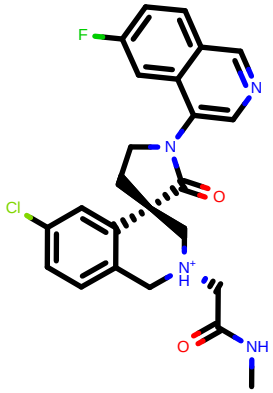
CID:	MAT-POS-ec6d90b7-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)OC3=O
RUN:	RUN998
DDG (kcal/mol):	0.61
dDDG (kcal/mol):	0.03

EDJ-MED-b6c6ee2b-1_1



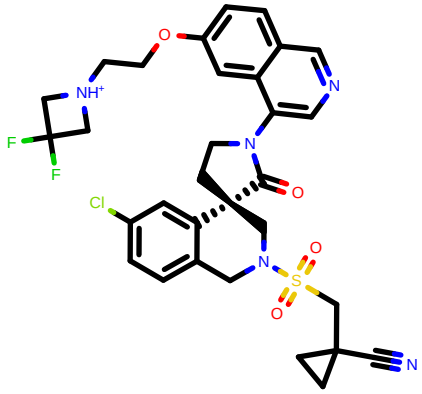
CID:	EDJ-MED-b6c6ee2b-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1357
DDG (kcal/mol):	0.62
dDDG (kcal/mol):	0.44

LUO-POS-b4dec3be-1_1



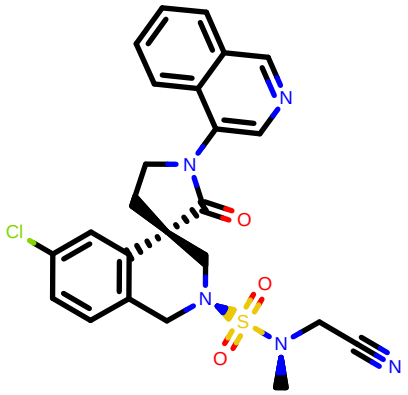
CID:	LUO-POS-b4dec3be-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1097
DDG (kcal/mol):	0.62
dDDG (kcal/mol):	0.24

EDJ-MED-468565e0-5_2



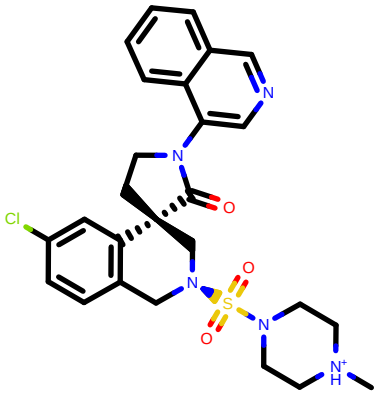
CID:	EDJ-MED-468565e0-5_2
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1441
DDG (kcal/mol):	0.65
dDDG (kcal/mol):	0.69

ALP-POS-ecbed2ba-17_3



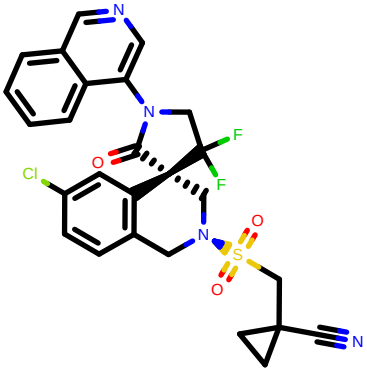
CID:	ALP-POS-ecbed2ba-17_3
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1181
DDG (kcal/mol):	0.66
dDDG (kcal/mol):	0.54

LUO-POS-ed2cfb03-1_2



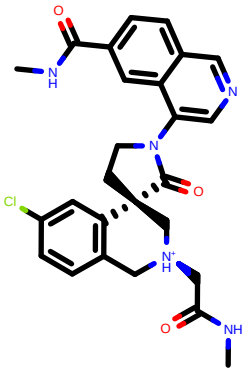
CID:	LUO-POS-ed2cfb03-1_2
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1321
DDG (kcal/mol):	0.66
dDDG (kcal/mol):	0.81

EDJ-MED-7e491f08-1_1



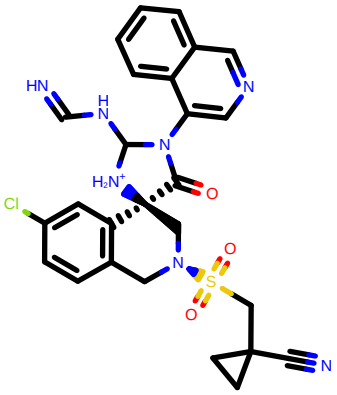
CID:	EDJ-MED-7e491f08-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4ccc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)(F)F
RUN:	RUN1347
DDG (kcal/mol):	0.66
dDDG (kcal/mol):	0.47

MAT-POS-38eb6498-5_2



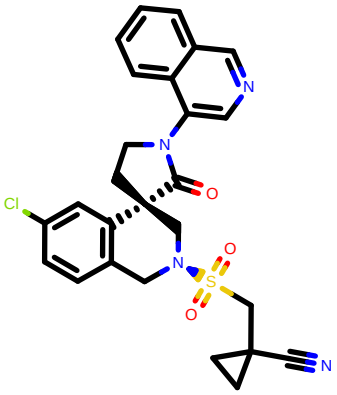
CID:	MAT-POS-38eb6498-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)C(=O)NC)Cl
RUN:	RUN1251
DDG (kcal/mol):	0.67
dDDG (kcal/mol):	0.24

LUO-POS-b5068a05-2_2



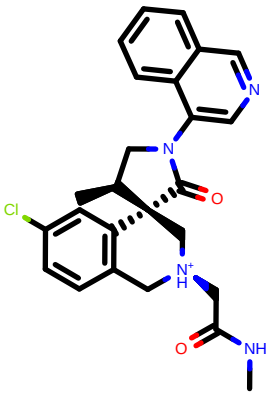
CID:	LUO-POS-b5068a05-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)N=C3NC#N
RUN:	RUN1386
DDG (kcal/mol):	0.69
dDDG (kcal/mol):	0.39

EDJ-MED-8bb691af-6_1



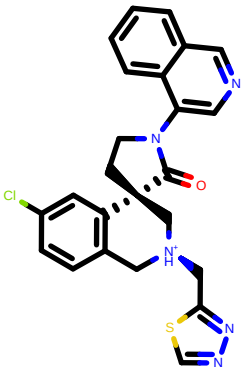
CID:	EDJ-MED-8bb691af-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1207
DDG (kcal/mol):	0.71
dDDG (kcal/mol):	0.28

MAT-POS-50a80394-4_4



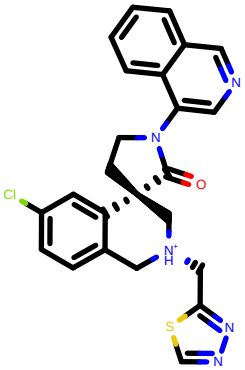
CID:	MAT-POS-50a80394-4_4
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1098
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.22

PET-UNK-7e9559de-1_2



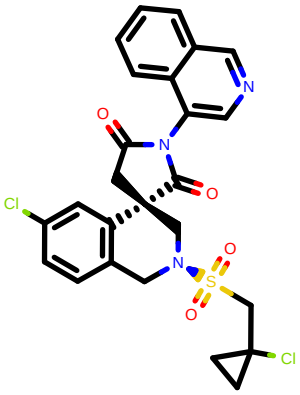
CID:	PET-UNK-7e9559de-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1091
DDG (kcal/mol):	0.72
dDDG (kcal/mol):	0.18

MAT-POS-96396902-1_1



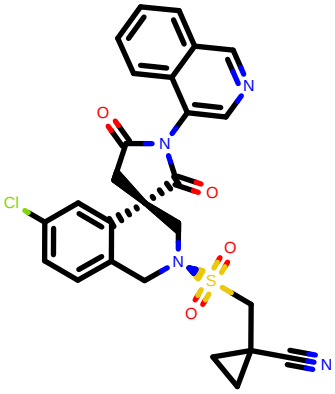
CID:	MAT-POS-96396902-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1100
DDG (kcal/mol):	0.74
dDDG (kcal/mol):	0.19

PET-UNK-94036022-5_1



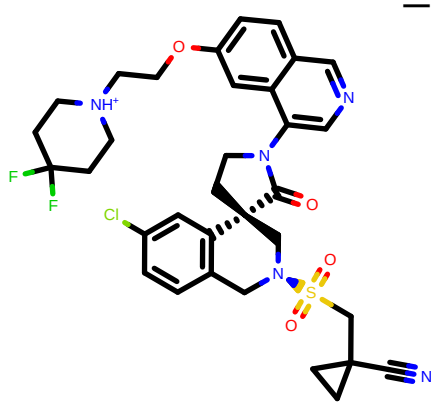
CID:	PET-UNK-94036022-5_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1254
DDG (kcal/mol):	0.75
dDDG (kcal/mol):	0.30

MAT-POS-1bed62cf-1_1



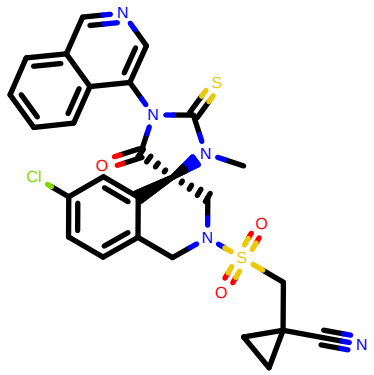
CID:	MAT-POS-1bed62cf-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1265
DDG (kcal/mol):	0.76
dDDG (kcal/mol):	0.26

EDJ-MED-468565e0-4_1



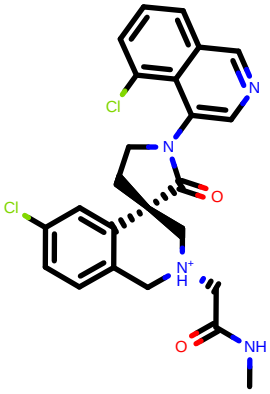
CID:	EDJ-MED-468565e0-4_1
SMILES:	c1cc2ncc(c2cc1OCC[NH+]3CCC(CC3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1460
DDG (kcal/mol):	0.77
dDDG (kcal/mol):	0.80

MAT-POS-c2d406ed-4_2



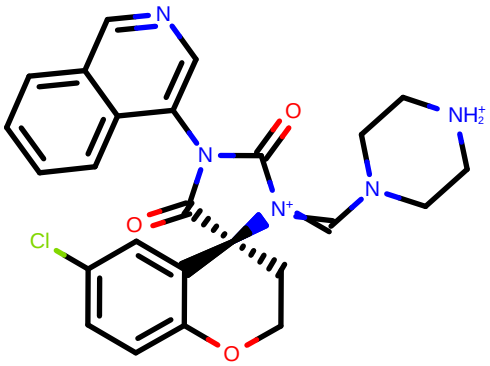
CID:	MAT-POS-c2d406ed-4_2
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1342
DDG (kcal/mol):	0.78
dDDG (kcal/mol):	0.48

MAT-POS-1d5ab790-2_1



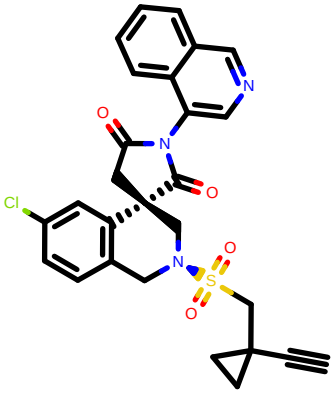
CID:	MAT-POS-1d5ab790-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1082
DDG (kcal/mol):	0.78
dDDG (kcal/mol):	0.24

VLA-UCB-34f3ed0c-15_1



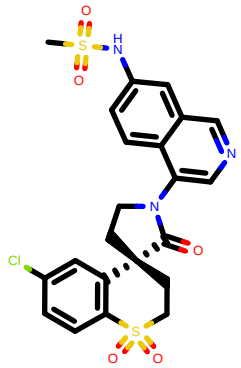
CID:	VLA-UCB-34f3ed0c-15_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CN6CC[NH2+]CC6
RUN:	RUN1162
DDG (kcal/mol):	0.79
dDDG (kcal/mol):	0.40

PET-UNK-94036022-4_1



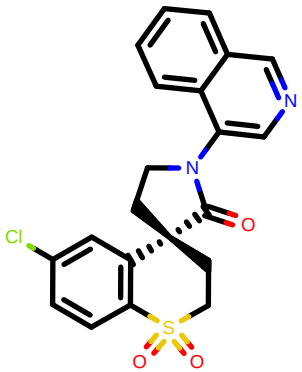
CID:	PET-UNK-94036022-4_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1310
DDG (kcal/mol):	0.83
dDDG (kcal/mol):	0.27

EDJ-MED-ede5c6cb-1_1



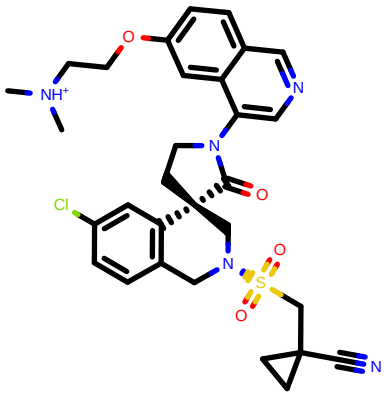
CID:	EDJ-MED-ede5c6cb-1_1
SMILES:	CS(=O)(=O)Nc1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1150
DDG (kcal/mol):	0.83
dDDG (kcal/mol):	0.20

EDJ-MED-d4864bdc-3_1



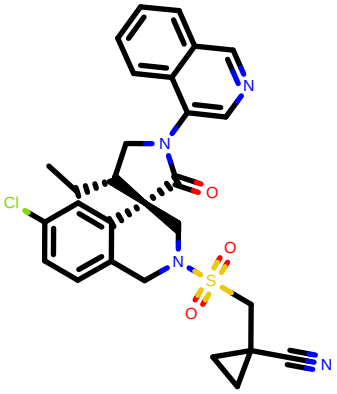
CID:	EDJ-MED-d4864bdc-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1009
DDG (kcal/mol):	0.86
dDDG (kcal/mol):	0.14

MAT-POS-38eb6498-1_2



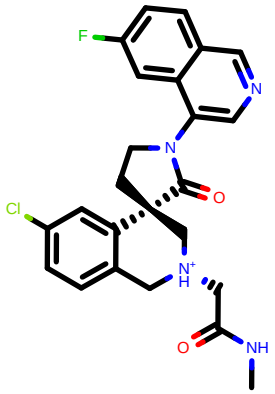
CID:	MAT-POS-38eb6498-1_2
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1418
DDG (kcal/mol):	0.87
dDDG (kcal/mol):	0.80

MAT-POS-50a80394-2_3



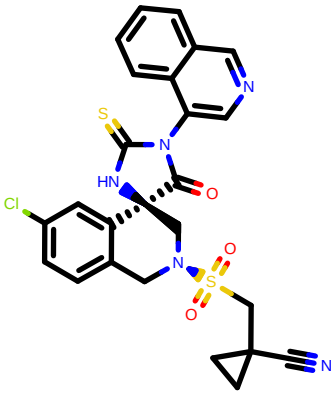
CID:	MAT-POS-50a80394-2_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1340
DDG (kcal/mol):	0.88
dDDG (kcal/mol):	0.72

LUO-POS-b4dec3be-2_1



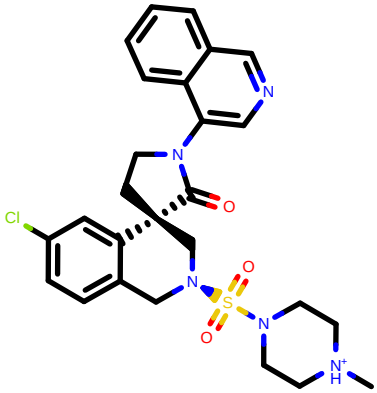
CID:	LUO-POS-b4dec3be-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1104
DDG (kcal/mol):	0.88
dDDG (kcal/mol):	0.27

MAT-POS-c2d406ed-3_1



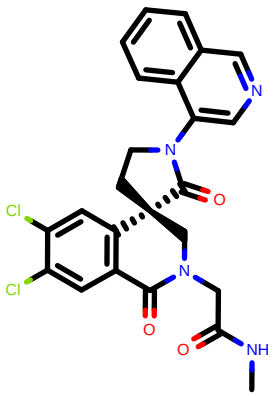
CID:	MAT-POS-c2d406ed-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)NC3=S
RUN:	RUN1298
DDG (kcal/mol):	0.89
dDDG (kcal/mol):	0.25

LUO-POS-ed2cfb03-1_1



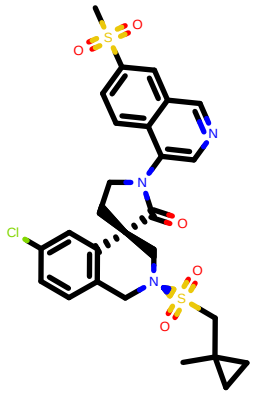
CID:	LUO-POS-ed2cfb03-1_1
SMILES:	C[NH+]1CCN(CC1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1319
DDG (kcal/mol):	0.89
dDDG (kcal/mol):	0.33

ALP-POS-afe0272e-2_1



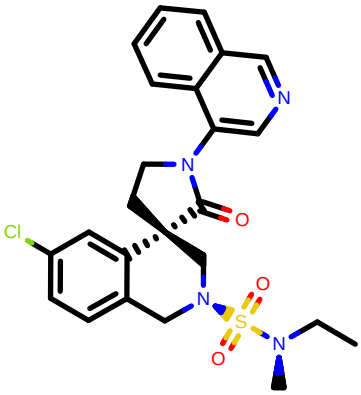
CID:	ALP-POS-afe0272e-2_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(c(cc5C1=O)Cl)Cl
RUN:	RUN1138
DDG (kcal/mol):	0.92
dDDG (kcal/mol):	0.16

MAT-POS-853c0ffa-22_1



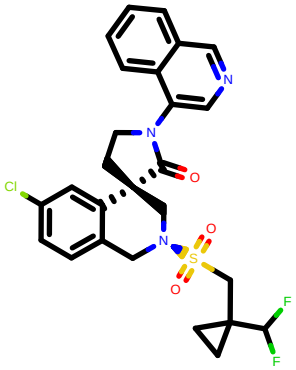
CID:	MAT-POS-853c0ffa-22_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1361
DDG (kcal/mol):	0.95
dDDG (kcal/mol):	0.52

ALP-POS-ecbed2ba-18_3



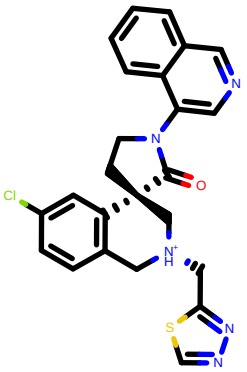
CID:	ALP-POS-ecbed2ba-18_3
SMILES:	CC[N@@](C)S(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1128
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.32

EDJ-MED-5cd3920d-5_2



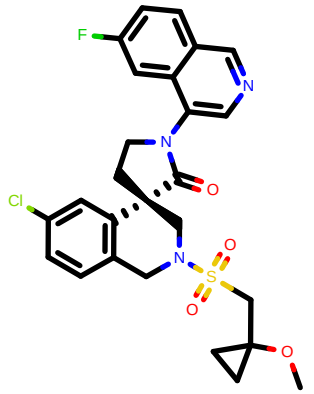
CID:	EDJ-MED-5cd3920d-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN1320
DDG (kcal/mol):	0.96
dDDG (kcal/mol):	0.54

PET-UNK-7e9559de-4_1



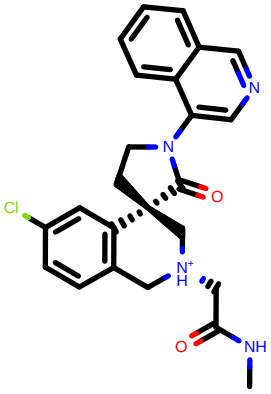
CID:	PET-UNK-7e9559de-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1088
DDG (kcal/mol):	0.98
dDDG (kcal/mol):	0.18

MAT-POS-853c0ffa-14_2



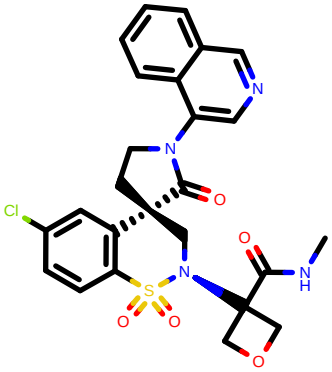
CID:	MAT-POS-853c0ffa-14_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1283
DDG (kcal/mol):	0.99
dDDG (kcal/mol):	0.44

MAT-POS-c7726e07-6_1



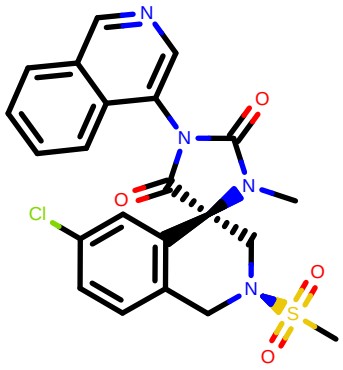
CID:	MAT-POS-c7726e07-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1052
DDG (kcal/mol):	1.00
dDDG (kcal/mol):	0.26

EDJ-MED-98c0a822-2_2



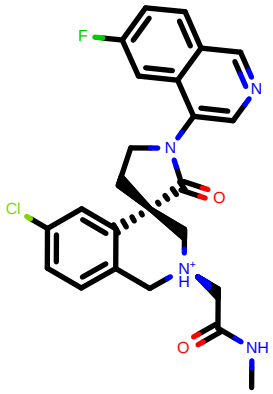
CID:	EDJ-MED-98c0a822-2_2
SMILES:	CNC(=O)C1(COC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1308
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.28

MAT-POS-2e8b2191-8_2



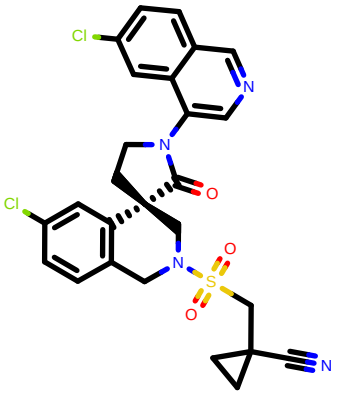
CID:	MAT-POS-2e8b2191-8_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1069
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.11

MAT-POS-b4d6b7fc-5_2



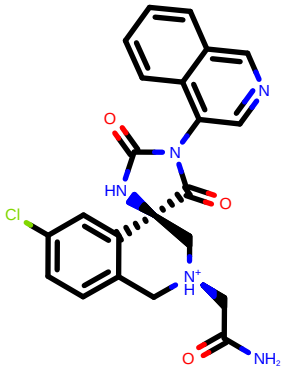
CID:	MAT-POS-b4d6b7fc-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1077
DDG (kcal/mol):	1.01
dDDG (kcal/mol):	0.19

EDJ-MED-b6c6ee2b-4_2



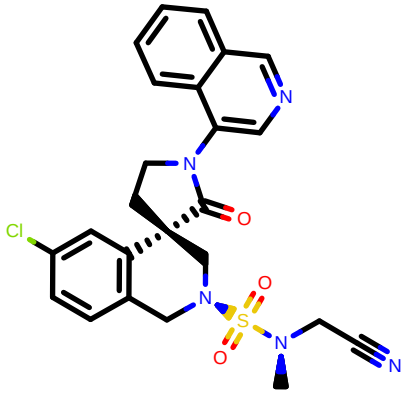
CID:	EDJ-MED-b6c6ee2b-4_2
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1309
DDG (kcal/mol):	1.02
dDDG (kcal/mol):	0.50

VLA-MRT-a639d434-2_2



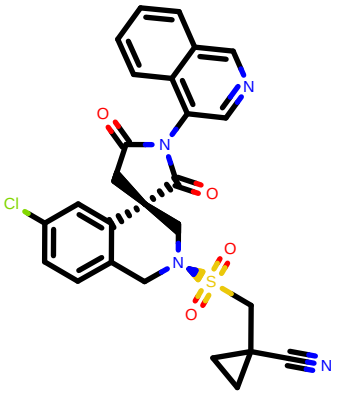
CID:	VLA-MRT-a639d434-2_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1041
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-17_1



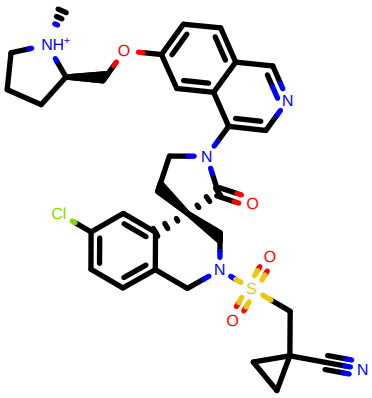
CID:	ALP-POS-ecbed2ba-17_1
SMILES:	C[N@@](CC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1175
DDG (kcal/mol):	1.03
dDDG (kcal/mol):	0.24

LUO-POS-868e8996-9_1



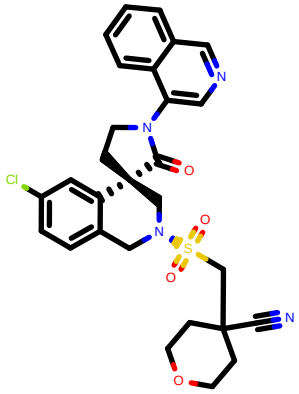
CID:	LUO-POS-868e8996-9_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1269
DDG (kcal/mol):	1.04
dDDG (kcal/mol):	0.35

MAT-POS-40ad851a-1_6



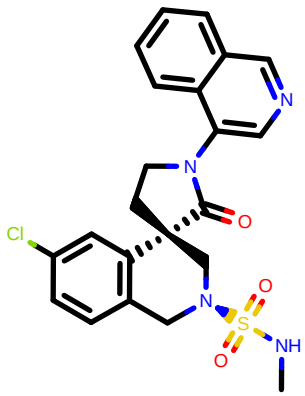
CID:	MAT-POS-40ad851a-1_6
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1445
DDG (kcal/mol):	1.05
dDDG (kcal/mol):	0.91

ALP-POS-ecbed2ba-11_2



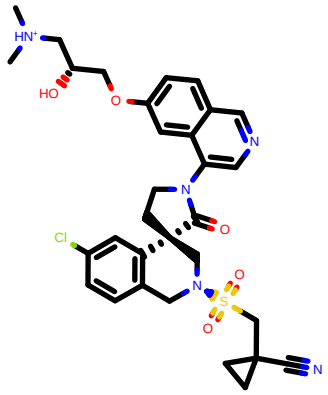
CID:	ALP-POS-ecbed2ba-11_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN1362
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.50

LUO-POS-ed2cfb03-2_1



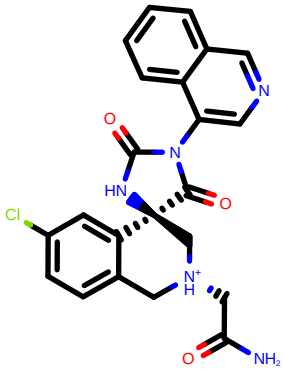
CID:	LUO-POS-ed2cfb03-2_1
SMILES:	CNS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1070
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.20

EDJ-MED-ee81482e-3_4



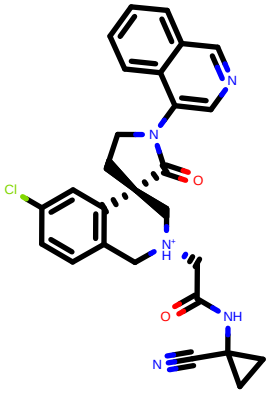
CID:	EDJ-MED-ee81482e-3_4
SMILES:	C[NH+](C)C[C@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1431
DDG (kcal/mol):	1.07
dDDG (kcal/mol):	0.85

VLA-MRT-a639d434-2_1



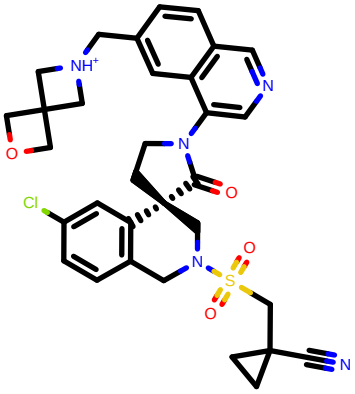
CID:	VLA-MRT-a639d434-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1039
DDG (kcal/mol):	1.10
dDDG (kcal/mol):	0.20

MAT-POS-69786b79-4_1



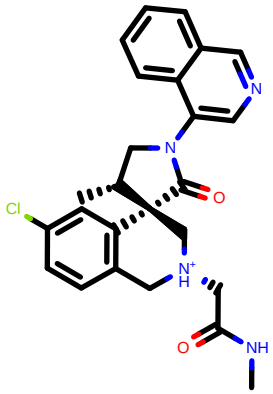
CID:	MAT-POS-69786b79-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN1242
DDG (kcal/mol):	1.14
dDDG (kcal/mol):	0.30

EDJ-MED-ee81482e-5_2



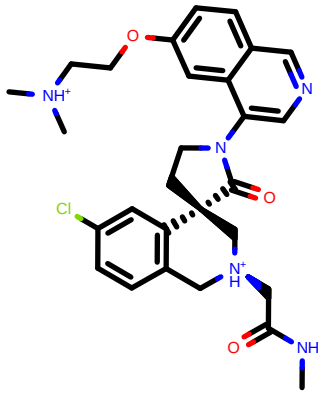
CID:	EDJ-MED-ee81482e-5_2
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@](Cc7c6cc(cc7)Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN1434
DDG (kcal/mol):	1.16
dDDG (kcal/mol):	0.57

MAT-POS-50a80394-4_1



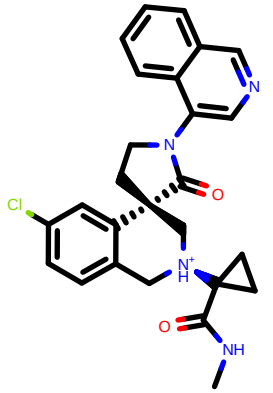
CID:	MAT-POS-50a80394-4_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1095
DDG (kcal/mol):	1.17
dDDG (kcal/mol):	0.18

MAT-POS-38eb6498-3_2



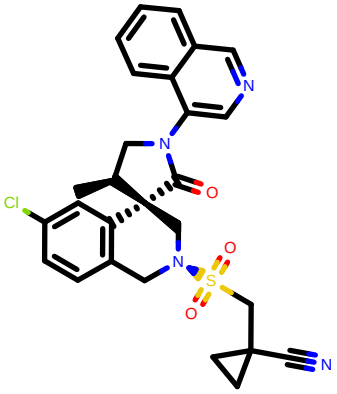
CID:	MAT-POS-38eb6498-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OCC[NH+](C)C)Cl
RUN:	RUN1364
DDG (kcal/mol):	1.18
dDDG (kcal/mol):	0.46

ALP-POS-ecbed2ba-7_2



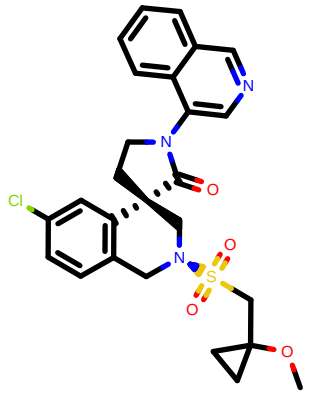
CID:	ALP-POS-ecbed2ba-7_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1113
DDG (kcal/mol):	1.18
dDDG (kcal/mol):	0.17

MAT-POS-50a80394-1_2



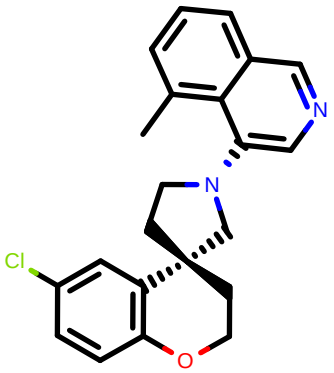
CID:	MAT-POS-50a80394-1_2
SMILES:	C[C@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1313
DDG (kcal/mol):	1.19
dDDG (kcal/mol):	0.39

ALP-POS-ecbed2ba-6_2



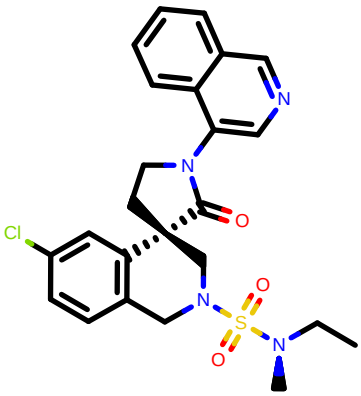
CID:	ALP-POS-ecbed2ba-6_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1210
DDG (kcal/mol):	1.19
dDDG (kcal/mol):	0.41

EDJ-MED-a6bab6fb-1_1



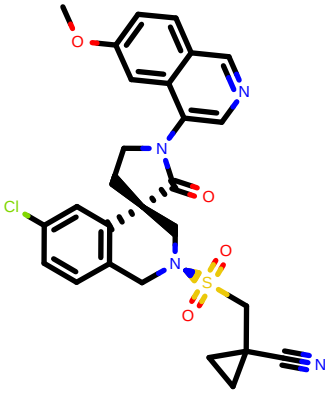
CID:	EDJ-MED-a6bab6fb-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN990
DDG (kcal/mol):	1.20
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-18_2



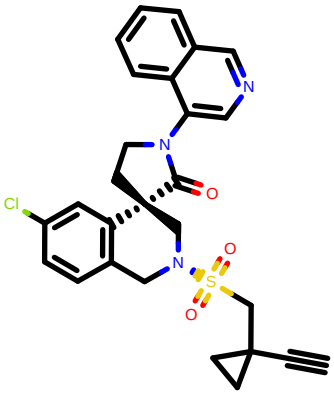
CID:	ALP-POS-ecbed2ba-18_2
SMILES:	CC[N@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1126
DDG (kcal/mol):	1.20
dDDG (kcal/mol):	0.32

EDJ-MED-b6c6ee2b-3_1



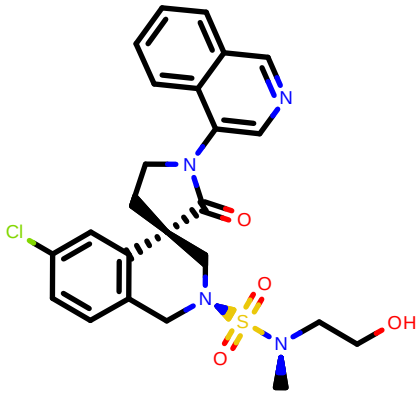
CID:	EDJ-MED-b6c6ee2b-3_1
SMILES:	COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1346
DDG (kcal/mol):	1.21
dDDG (kcal/mol):	0.61

PET-UNK-94036022-2_2



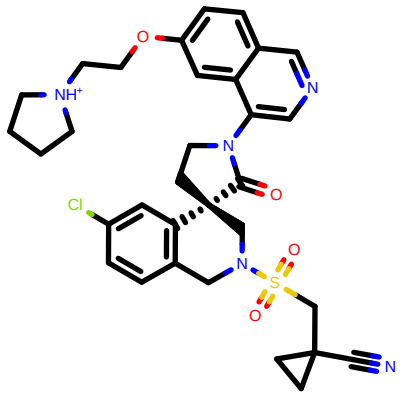
CID:	PET-UNK-94036022-2_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1257
DDG (kcal/mol):	1.24
dDDG (kcal/mol):	0.35

ALP-POS-ecbed2ba-19_1



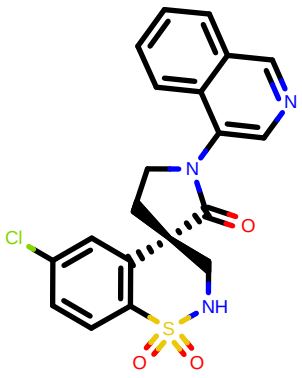
CID:	ALP-POS-ecbed2ba-19_1
SMILES:	C[N@@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1183
DDG (kcal/mol):	1.27
dDDG (kcal/mol):	0.36

EDJ-MED-468565e0-1_2



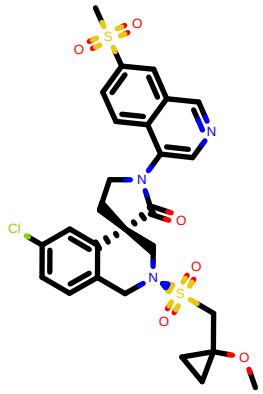
CID:	EDJ-MED-468565e0-1_2
SMILES:	c1cc2cncc(c2cc1OCC[NH+]3CCCC3)N4CC[C@@]5(C4=O)C[N@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1453
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.78

ALP-POS-4483ae88-1_1



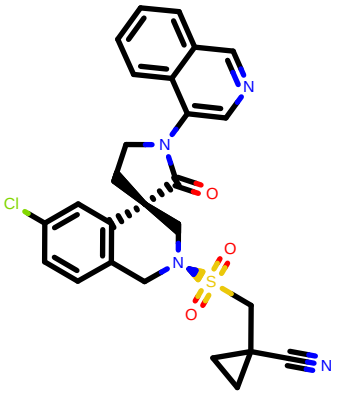
CID:	ALP-POS-4483ae88-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1025
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.11

MAT-POS-853c0ffa-16_1



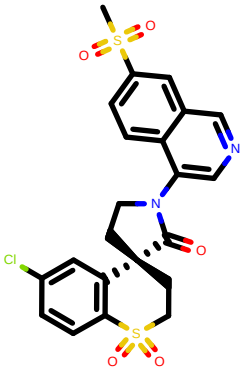
CID:	MAT-POS-853c0ffa-16_1
SMILES:	COC1(CC1)CS(=O)(=O)N@@[2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1374
DDG (kcal/mol):	1.30
dDDG (kcal/mol):	0.48

ALP-POS-ecbed2ba-4_1



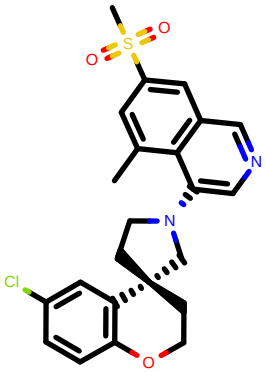
CID:	ALP-POS-ecbed2ba-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1215
DDG (kcal/mol):	1.31
dDDG (kcal/mol):	0.35

EDJ-MED-94fddcec-5_1



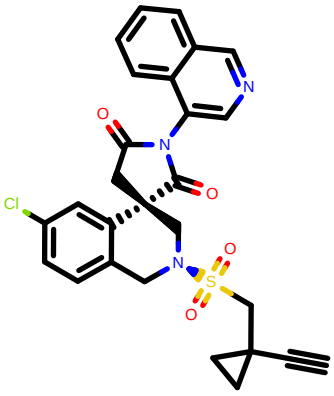
CID:	EDJ-MED-94fddcec-5_1
SMILES:	CS(=O)(=O)c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1075
DDG (kcal/mol):	1.31
dDDG (kcal/mol):	0.18

EDJ-MED-d7486dd1-1_1



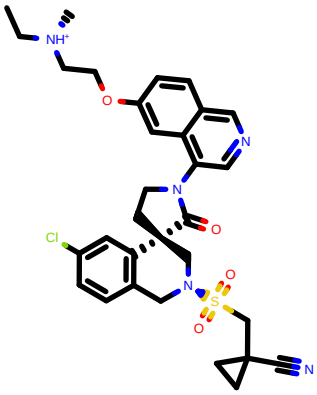
CID:	EDJ-MED-d7486dd1-1_1
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1027
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.12

PET-UNK-94036022-11_1



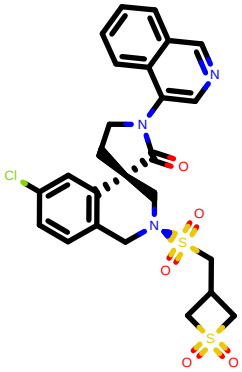
CID:	PET-UNK-94036022-11_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1325
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.25

MAT-POS-40ad851a-2_4



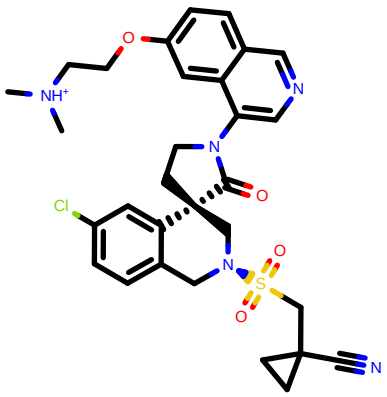
CID:	MAT-POS-40ad851a-2_4
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1423
DDG (kcal/mol):	1.33
dDDG (kcal/mol):	0.73

ALP-POS-ecbed2ba-5_2



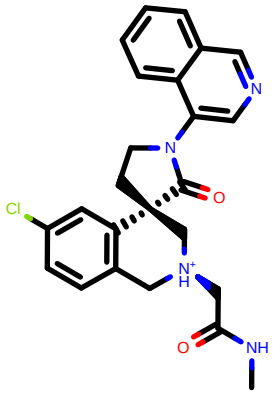
CID:	ALP-POS-ecbed2ba-5_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN1288
DDG (kcal/mol):	1.34
dDDG (kcal/mol):	0.52

MAT-POS-853c0ffa-9_1



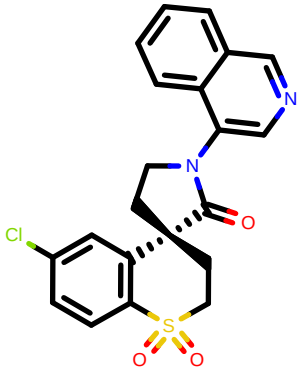
CID:	MAT-POS-853c0ffa-9_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1409
DDG (kcal/mol):	1.35
dDDG (kcal/mol):	0.52

LUO-POS-868e8996-12_2



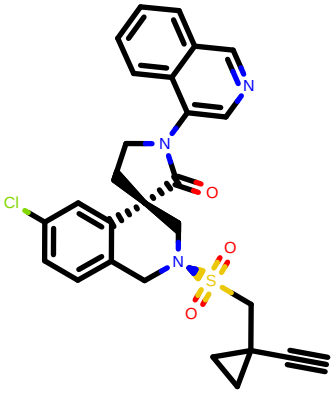
CID:	LUO-POS-868e8996-12_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1057
DDG (kcal/mol):	1.35
dDDG (kcal/mol):	0.21

ALP-POS-41e2080f-1_1



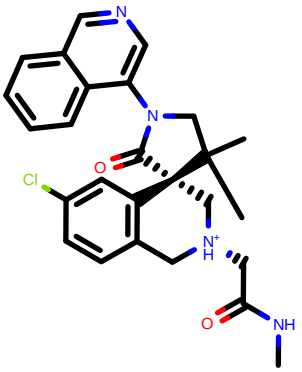
CID:	ALP-POS-41e2080f-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1020
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.14

PET-UNK-94036022-2_1



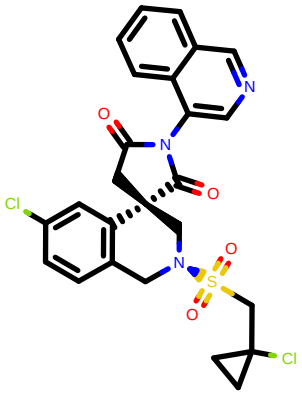
CID:	PET-UNK-94036022-2_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1258
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.28

MAT-POS-50a80394-7_1



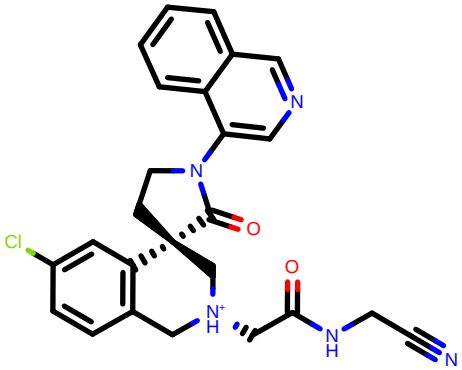
CID:	MAT-POS-50a80394-7_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN1143
DDG (kcal/mol):	1.36
dDDG (kcal/mol):	0.22

PET-UNK-94036022-5_2



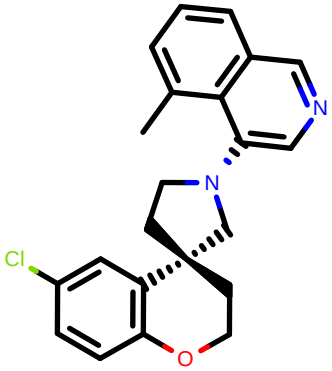
CID:	PET-UNK-94036022-5_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1256
DDG (kcal/mol):	1.38
dDDG (kcal/mol):	0.33

ALP-POS-ecbed2ba-14_1



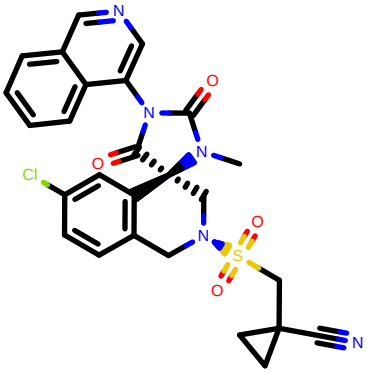
CID:	ALP-POS-ecbed2ba-14_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN1127
DDG (kcal/mol):	1.40
dDDG (kcal/mol):	0.24

EDJ-MED-a6bab6fb-1_2



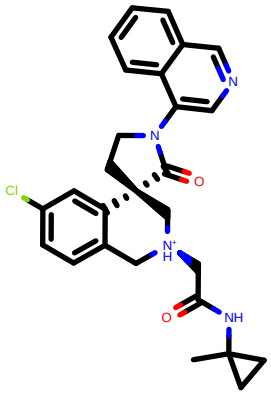
CID:	EDJ-MED-a6bab6fb-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN979
DDG (kcal/mol):	1.41
dDDG (kcal/mol):	0.09

MAT-POS-c2d406ed-2_1



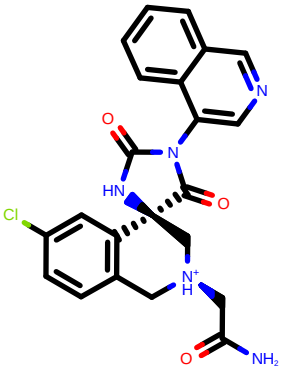
CID:	MAT-POS-c2d406ed-2_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5ncc6c5cccc6
RUN:	RUN1336
DDG (kcal/mol):	1.42
dDDG (kcal/mol):	0.23

MAT-POS-69786b79-3_2



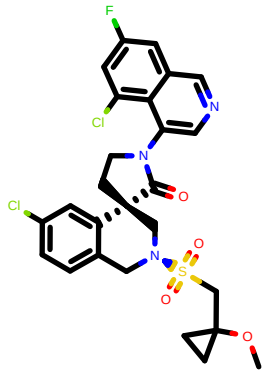
CID:	MAT-POS-69786b79-3_2
SMILES:	CC1(CC1)NC(=O)C[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1191
DDG (kcal/mol):	1.42
dDDG (kcal/mol):	0.24

VLA-MRT-8c78ee15-4_2



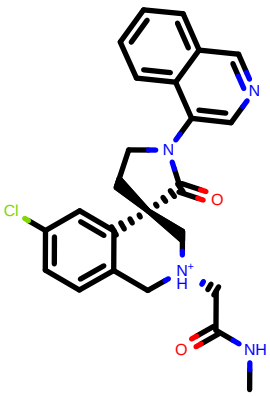
CID:	VLA-MRT-8c78ee15-4_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1038
DDG (kcal/mol):	1.43
dDDG (kcal/mol):	0.18

MAT-POS-853c0ffa-8_1



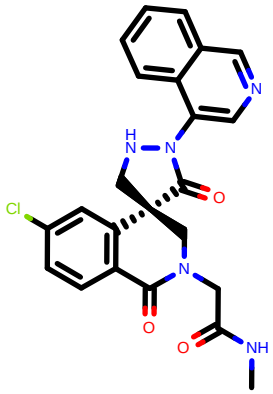
CID:	MAT-POS-853c0ffa-8_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1331
DDG (kcal/mol):	1.47
dDDG (kcal/mol):	0.38

LUO-POS-868e8996-12_1



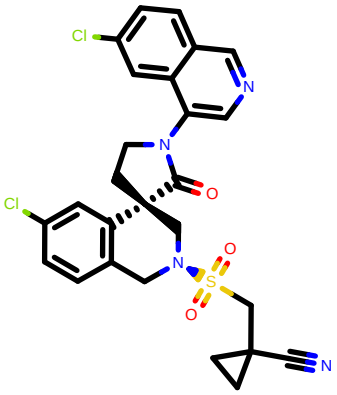
CID:	LUO-POS-868e8996-12_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1053
DDG (kcal/mol):	1.48
dDDG (kcal/mol):	0.23

EDJ-MED-fed7ac0b-4_1



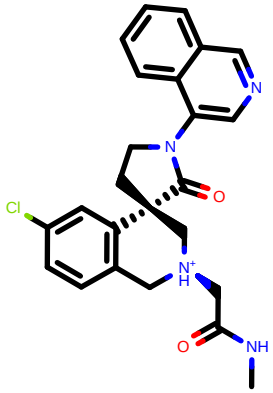
CID:	EDJ-MED-fed7ac0b-4_1
SMILES:	CNC(=O)CN1C[C@]2(C=NN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1080
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.16

EDJ-MED-b6c6ee2b-4_1



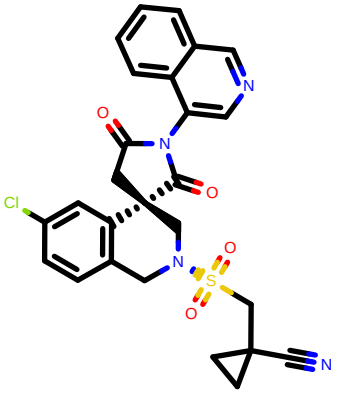
CID:	EDJ-MED-b6c6ee2b-4_1
SMILES:	c1cc2cncc(c2cc1Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1303
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.33

MAT-POS-c7726e07-6_2



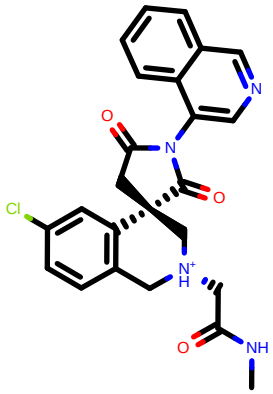
CID:	MAT-POS-c7726e07-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1056
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.21

LUO-POS-868e8996-10_2



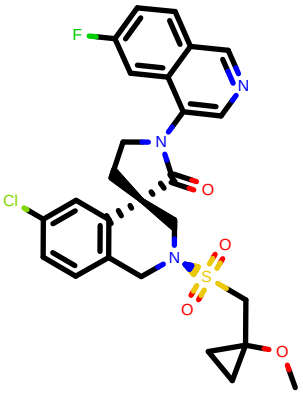
CID:	LUO-POS-868e8996-10_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1271
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.43

MAT-POS-1bed62cf-3_1



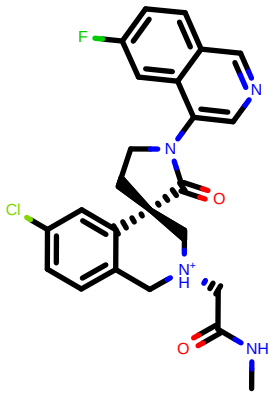
CID:	MAT-POS-1bed62cf-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1072
DDG (kcal/mol):	1.49
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-14_1



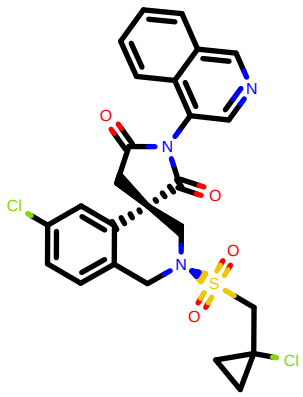
CID:	MAT-POS-853c0ffa-14_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1281
DDG (kcal/mol):	1.51
dDDG (kcal/mol):	0.29

MAT-POS-b4d6b7fc-5_1



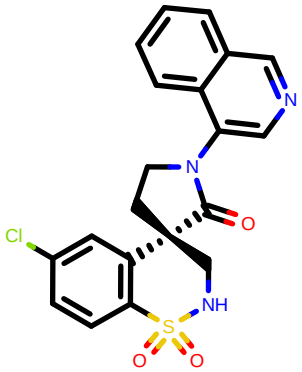
CID:	MAT-POS-b4d6b7fc-5_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1073
DDG (kcal/mol):	1.52
dDDG (kcal/mol):	0.27

PET-UNK-94036022-12_2



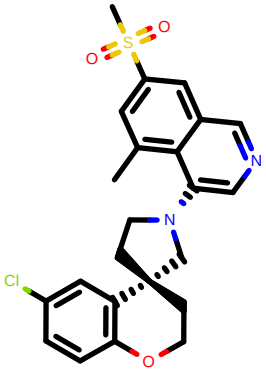
CID:	PET-UNK-94036022-12_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1264
DDG (kcal/mol):	1.52
dDDG (kcal/mol):	0.34

EDJ-MED-f9b78f78-4_1



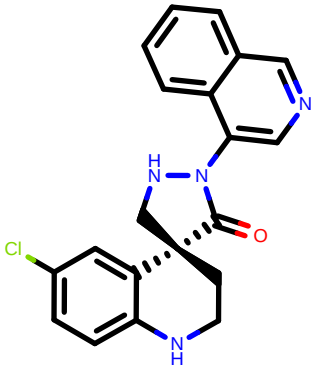
CID:	EDJ-MED-f9b78f78-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CNS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1026
DDG (kcal/mol):	1.53
dDDG (kcal/mol):	0.15

EDJ-MED-d7486dd1-1_2



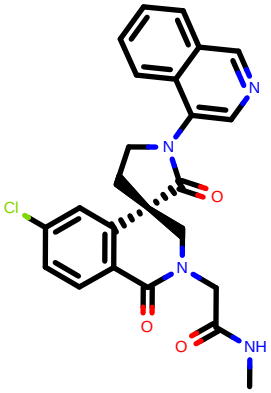
CID:	EDJ-MED-d7486dd1-1_2
SMILES:	Cc1cc(cc2c1c(cnc2)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1030
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.11

BRU-THA-55eab31a-1_1



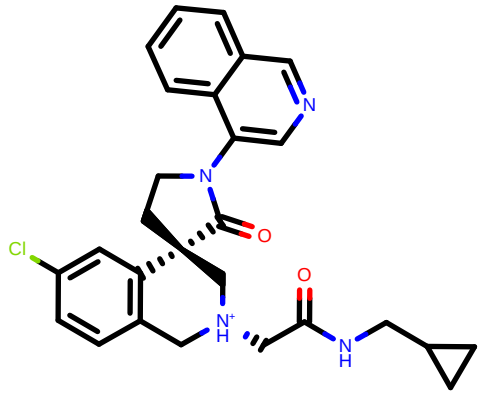
CID:	BRU-THA-55eab31a-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCNc5c4cc(cc5)Cl)C=N3
RUN:	RUN993
DDG (kcal/mol):	1.54
dDDG (kcal/mol):	0.16

EDJ-MED-8bb691af-8_1



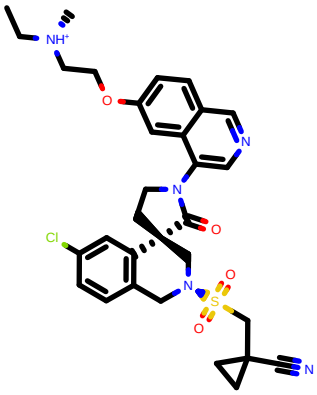
CID:	EDJ-MED-8bb691af-8_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1065
DDG (kcal/mol):	1.55
dDDG (kcal/mol):	0.17

ALP-POS-ecbed2ba-12_1



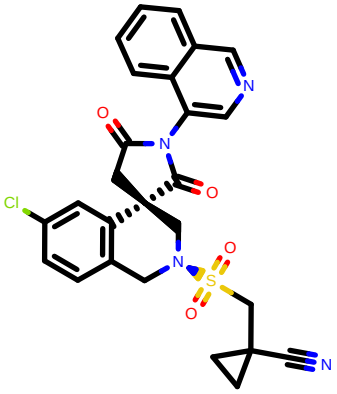
CID:	ALP-POS-ecbed2ba-12_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN1178
DDG (kcal/mol):	1.55
dDDG (kcal/mol):	0.27

MAT-POS-40ad851a-2_2



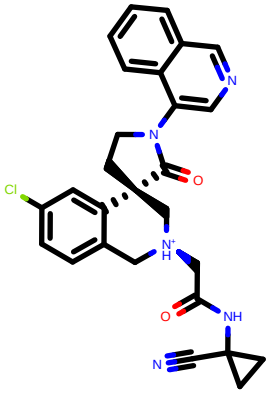
CID:	MAT-POS-40ad851a-2_2
SMILES:	CC[N@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1425
DDG (kcal/mol):	1.56
dDDG (kcal/mol):	0.70

LUO-POS-868e8996-9_2



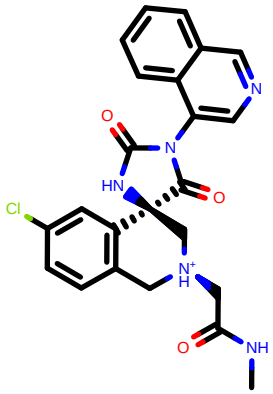
CID:	LUO-POS-868e8996-9_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1267
DDG (kcal/mol):	1.58
dDDG (kcal/mol):	0.43

MAT-POS-69786b79-4_2



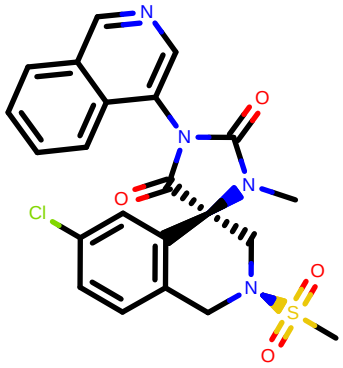
CID:	MAT-POS-69786b79-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6(CC6)C#N
RUN:	RUN1249
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.24

VLA-MRT-a639d434-1_2



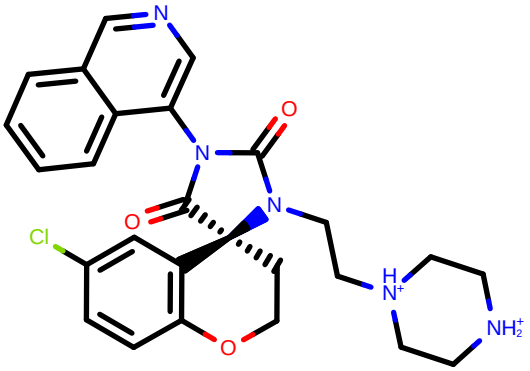
CID:	VLA-MRT-a639d434-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1071
DDG (kcal/mol):	1.59
dDDG (kcal/mol):	0.19

EDJ-MED-7587a9ee-1_2



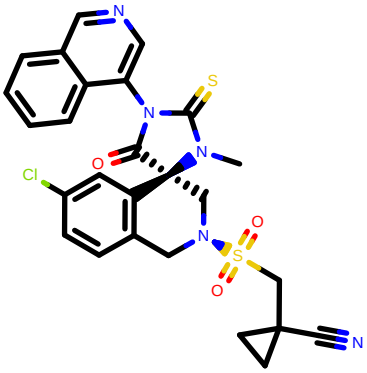
CID:	EDJ-MED-7587a9ee-1_2
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1060
DDG (kcal/mol):	1.60
dDDG (kcal/mol):	0.12

VLA-UNK-f702bf1c-7_1



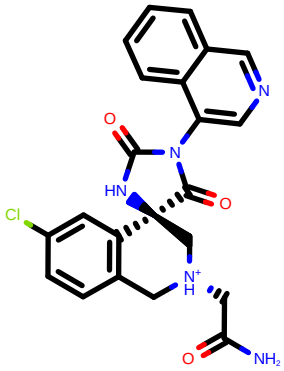
CID:	VLA-UNK-f702bf1c-7_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(CCOc5c4cc(cc5)Cl)N(C3=O)CCN6CC[NH2+]CC6
RUN:	RUN1204
DDG (kcal/mol):	1.62
dDDG (kcal/mol):	0.18

MAT-POS-c2d406ed-4_1



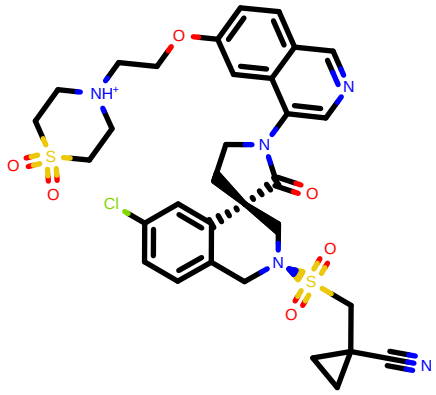
CID:	MAT-POS-c2d406ed-4_1
SMILES:	CN1C(=S)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1339
DDG (kcal/mol):	1.62
dDDG (kcal/mol):	0.31

VLA-MRT-8c78ee15-4_1



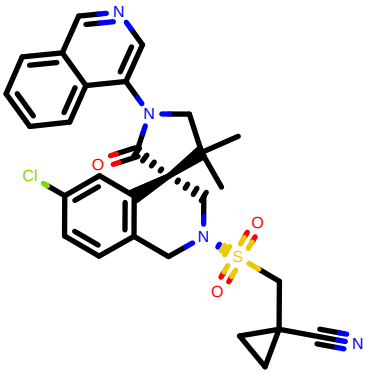
CID:	VLA-MRT-8c78ee15-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)N)NC3=O
RUN:	RUN1037
DDG (kcal/mol):	1.65
dDDG (kcal/mol):	0.21

EDJ-MED-468565e0-3_1



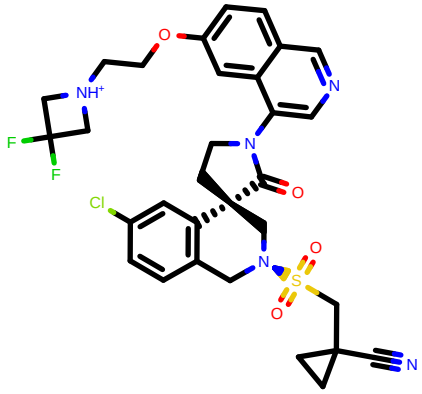
CID:	EDJ-MED-468565e0-3_1
SMILES:	c1cc2cncc(c2cc1OCCN3CCS(=O)(=O)CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1448
DDG (kcal/mol):	1.66
dDDG (kcal/mol):	0.85

MAT-POS-50a80394-8_2



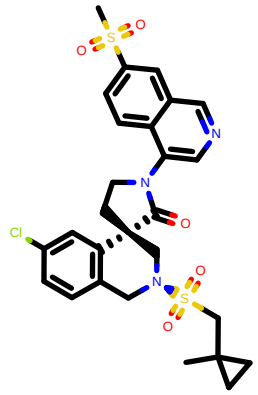
CID:	MAT-POS-50a80394-8_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN1341
DDG (kcal/mol):	1.67
dDDG (kcal/mol):	0.79

EDJ-MED-468565e0-5_1



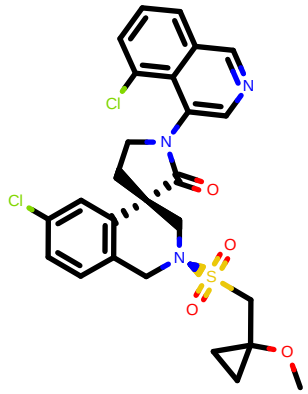
CID:	EDJ-MED-468565e0-5_1
SMILES:	c1cc2cncc(c2cc1OCCN3CC(C3)(F)F)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1449
DDG (kcal/mol):	1.68
dDDG (kcal/mol):	0.63

MAT-POS-853c0ffa-22_2



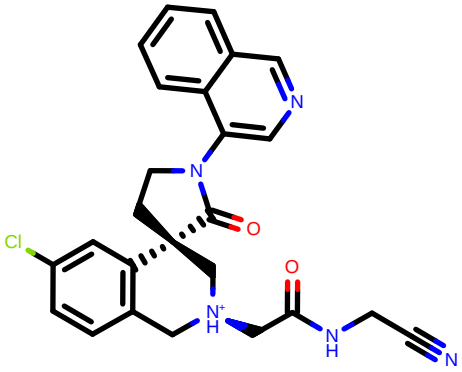
CID:	MAT-POS-853c0ffa-22_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1363
DDG (kcal/mol):	1.68
dDDG (kcal/mol):	0.57

MAT-POS-853c0ffa-7_1



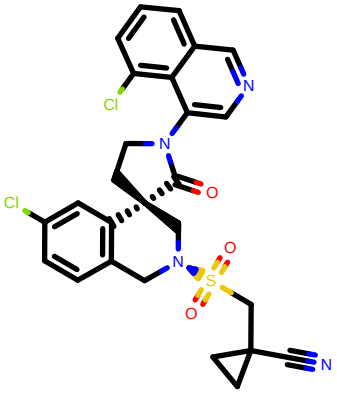
CID:	MAT-POS-853c0ffa-7_1
SMILES:	COC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1275
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.35

ALP-POS-ecbed2ba-14_2



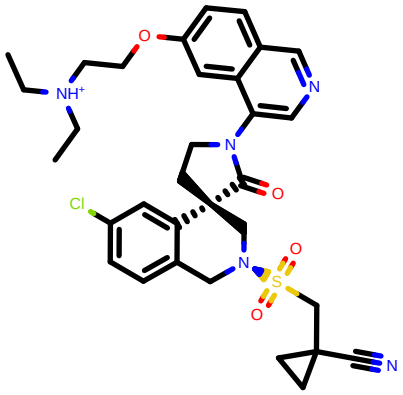
CID:	ALP-POS-ecbed2ba-14_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC#N
RUN:	RUN1115
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.23

MAT-POS-853c0ffa-5_1



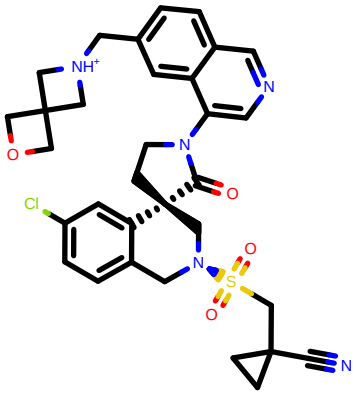
CID:	MAT-POS-853c0ffa-5_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1273
DDG (kcal/mol):	1.69
dDDG (kcal/mol):	0.38

MAT-POS-40ad851a-3_1



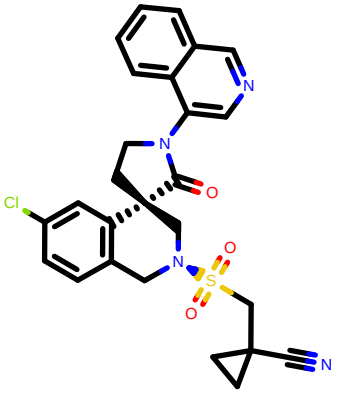
CID:	MAT-POS-40ad851a-3_1
SMILES:	CC[NH+](CC)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1442
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.84

EDJ-MED-ee81482e-5_1



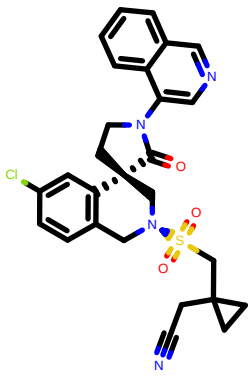
CID:	EDJ-MED-ee81482e-5_1
SMILES:	c1cc2cncc(c2cc1C[NH+]3CC4(C3)COC4)N5CC[C@@]6(C5=O)C[N@@](Cc7c6cc(cc7)Cl)S(=O)(=O)CC8(CC8)C#N
RUN:	RUN1432
DDG (kcal/mol):	1.70
dDDG (kcal/mol):	0.63

MIK-ENA-5d9157e9-2_1



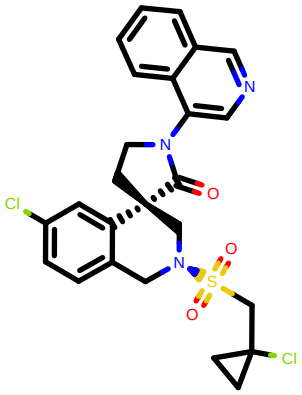
CID:	MIK-ENA-5d9157e9-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1238
DDG (kcal/mol):	1.71
dDDG (kcal/mol):	0.57

ALP-POS-ecbed2ba-22_1



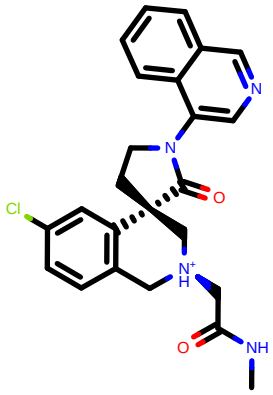
CID:	ALP-POS-ecbed2ba-22_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)CC#N
RUN:	RUN1292
DDG (kcal/mol):	1.73
dDDG (kcal/mol):	0.42

PET-UNK-94036022-3_1



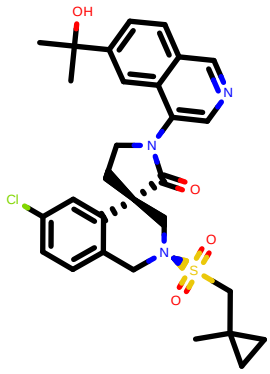
CID:	PET-UNK-94036022-3_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1200
DDG (kcal/mol):	1.73
dDDG (kcal/mol):	0.25

EDJ-MED-8bb691af-4_2



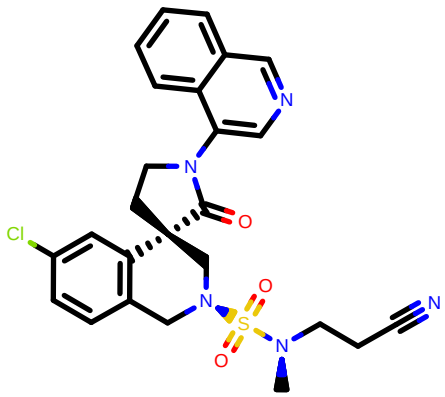
CID:	EDJ-MED-8bb691af-4_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1043
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.21

MAT-POS-853c0ffa-20_1



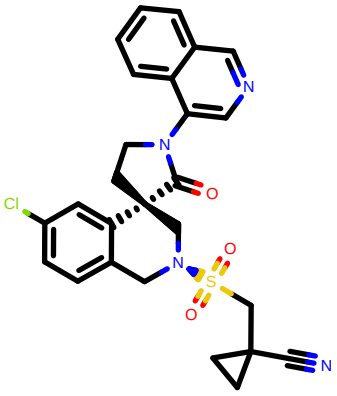
CID:	MAT-POS-853c0ffa-20_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(cc6)C(C)(C)O)Cl
RUN:	RUN1365
DDG (kcal/mol):	1.74
dDDG (kcal/mol):	0.57

ALP-POS-ecbed2ba-16_2



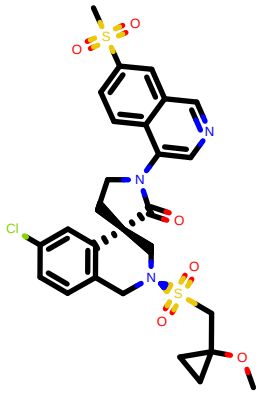
CID:	ALP-POS-ecbed2ba-16_2
SMILES:	C[N@](CCC#N)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1223
DDG (kcal/mol):	1.78
dDDG (kcal/mol):	0.31

MIK-ENA-5d9157e9-1_1



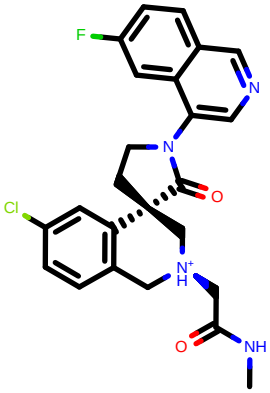
CID:	MIK-ENA-5d9157e9-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1236
DDG (kcal/mol):	1.78
dDDG (kcal/mol):	0.46

MAT-POS-853c0ffa-16_2



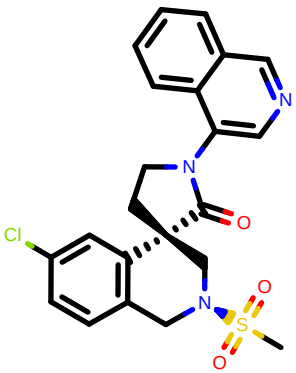
CID:	MAT-POS-853c0ffa-16_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5ccc(c6)S(=O)(=O)C)Cl
RUN:	RUN1381
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.48

LUO-POS-b4dec3be-1_2



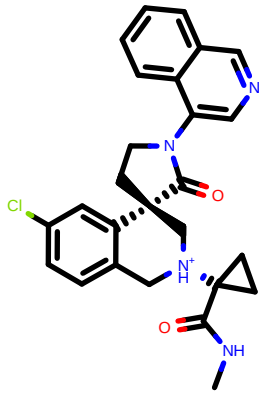
CID:	LUO-POS-b4dec3be-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1103
DDG (kcal/mol):	1.79
dDDG (kcal/mol):	0.19

EDJ-MED-7587a9ee-3_1



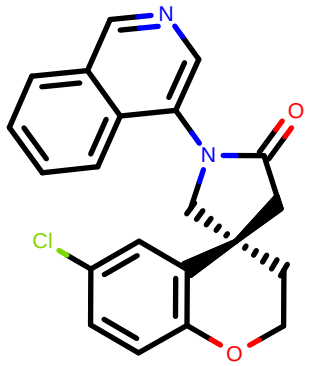
CID:	EDJ-MED-7587a9ee-3_1
SMILES:	CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1024
DDG (kcal/mol):	1.80
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-7_1



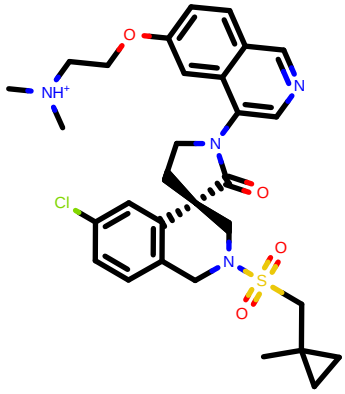
CID:	ALP-POS-ecbed2ba-7_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1122
DDG (kcal/mol):	1.81
dDDG (kcal/mol):	0.26

MAT-POS-983b399a-3_1



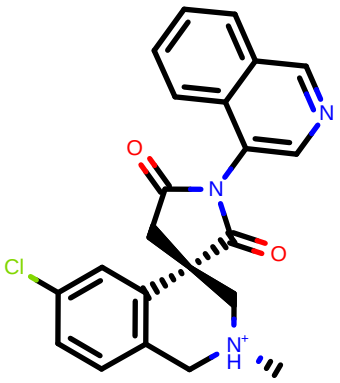
CID:	MAT-POS-983b399a-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN999
DDG (kcal/mol):	1.81
dDDG (kcal/mol):	0.08

MAT-POS-853c0ffa-19_2



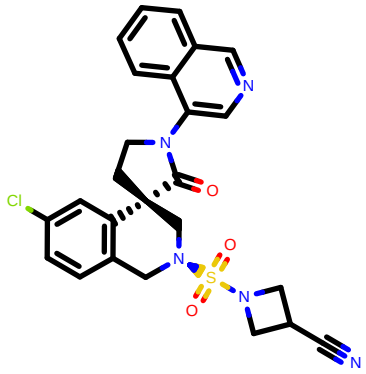
CID:	MAT-POS-853c0ffa-19_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)OCC[NH+](C)C)Cl
RUN:	RUN1400
DDG (kcal/mol):	1.82
dDDG (kcal/mol):	0.52

JOH-MSK-51c67e7d-2_1



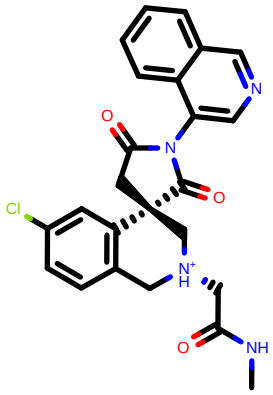
CID:	JOH-MSK-51c67e7d-2_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1019
DDG (kcal/mol):	1.82
dDDG (kcal/mol):	0.15

ALP-POS-ecbed2ba-9_1



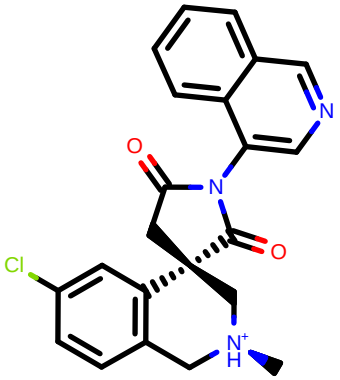
CID:	ALP-POS-ecbed2ba-9_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN1222
DDG (kcal/mol):	1.82
dDDG (kcal/mol):	0.61

JOH-MSK-1f2dff76-1_1



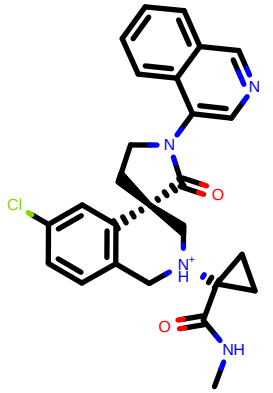
CID:	JOH-MSK-1f2dff76-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1101
DDG (kcal/mol):	1.86
dDDG (kcal/mol):	0.22

JOH-MSK-51c67e7d-2_2



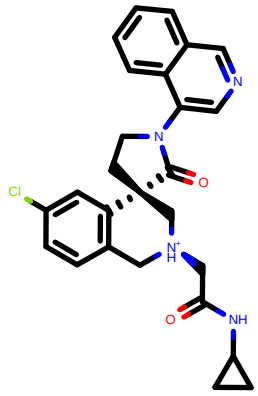
CID:	JOH-MSK-51c67e7d-2_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1022
DDG (kcal/mol):	1.86
dDDG (kcal/mol):	0.10

MAT-POS-69786b79-1_1



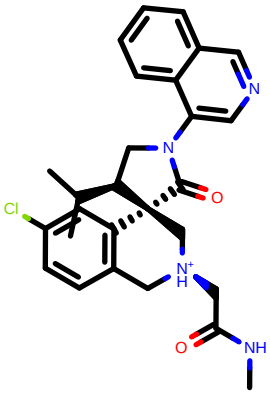
CID:	MAT-POS-69786b79-1_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1131
DDG (kcal/mol):	1.88
dDDG (kcal/mol):	0.23

MAT-POS-69786b79-2_2



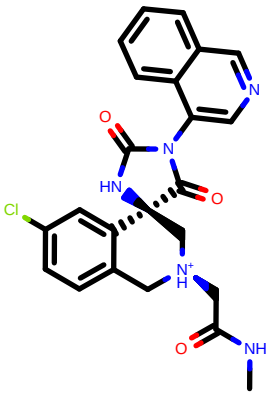
CID:	MAT-POS-69786b79-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC6CC6
RUN:	RUN1136
DDG (kcal/mol):	1.88
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-6_4



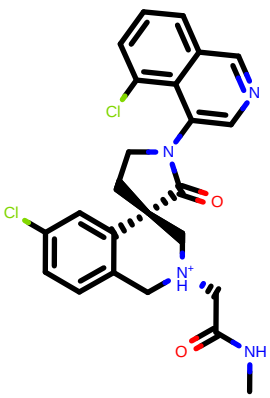
CID:	MAT-POS-50a80394-6_4
SMILES:	CC(C)[C@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1188
DDG (kcal/mol):	1.90
dDDG (kcal/mol):	0.27

VLA-MRT-8c78ee15-3_2



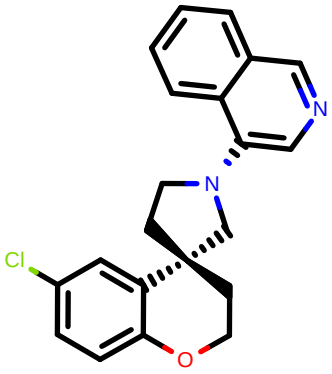
CID:	VLA-MRT-8c78ee15-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1067
DDG (kcal/mol):	1.90
dDDG (kcal/mol):	0.24

MAT-POS-b4d6b7fc-6_1



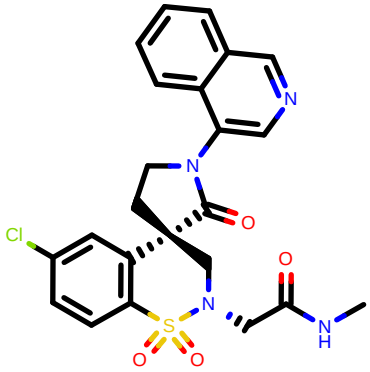
CID:	MAT-POS-b4d6b7fc-6_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1074
DDG (kcal/mol):	1.92
dDDG (kcal/mol):	0.19

MAT-POS-983b399a-2_2



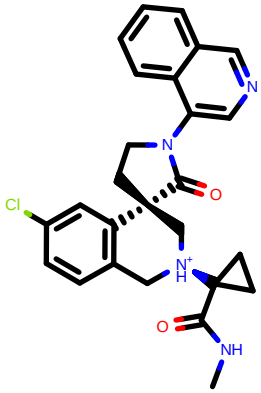
CID:	MAT-POS-983b399a-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN974
DDG (kcal/mol):	1.95
dDDG (kcal/mol):	0.08

ALP-POS-4483ae88-2_1



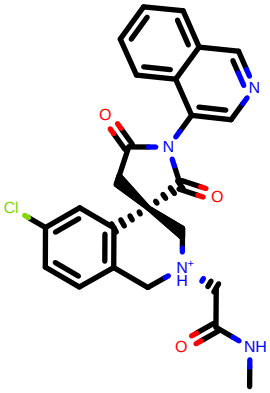
CID:	ALP-POS-4483ae88-2_1
SMILES:	CNC(=O)C[N@@]1C[C@]2(CCN(C2=O)c3cncc4c3cccc4)c5cc(ccc5S1(=O)=O)Cl
RUN:	RUN1112
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.22

MAT-POS-576f7758-1_2



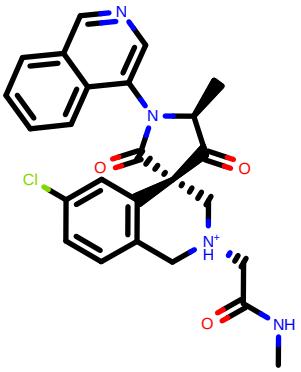
CID:	MAT-POS-576f7758-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1141
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.19

JOH-MSK-1f2dff76-2_1



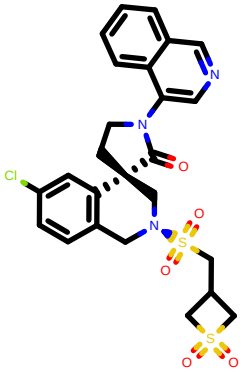
CID:	JOH-MSK-1f2dff76-2_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1105
DDG (kcal/mol):	1.96
dDDG (kcal/mol):	0.27

PET-UNK-94036022-7_1



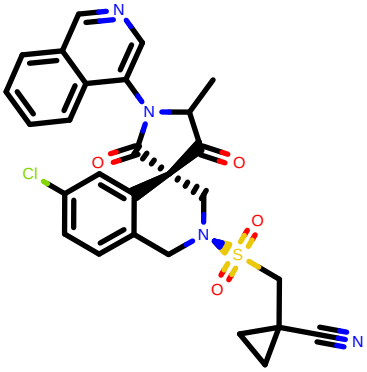
CID:	PET-UNK-94036022-7_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1156
DDG (kcal/mol):	1.97
dDDG (kcal/mol):	0.28

ALP-POS-ecbed2ba-5_1



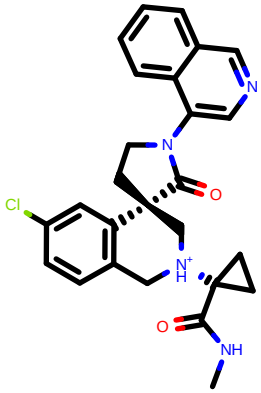
CID:	ALP-POS-ecbed2ba-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6CS(=O)(=O)C6
RUN:	RUN1282
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.88

PET-UNK-94036022-13_1



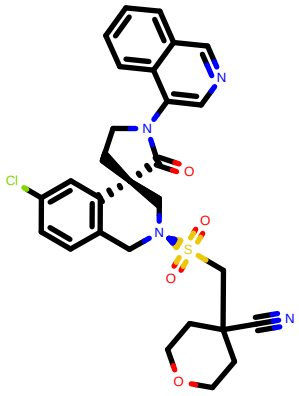
CID:	PET-UNK-94036022-13_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1358
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.37

MAT-POS-576f7758-1_1



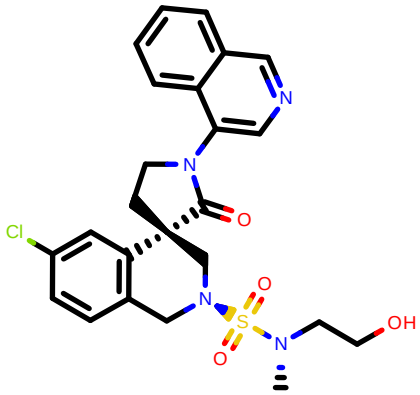
CID:	MAT-POS-576f7758-1_1
SMILES:	CNC(=O)C1(CC1)[N@@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1137
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-11_1



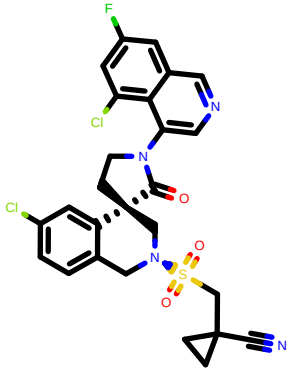
CID:	ALP-POS-ecbed2ba-11_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCOCC6)C#N
RUN:	RUN1355
DDG (kcal/mol):	1.99
dDDG (kcal/mol):	0.73

ALP-POS-ecbed2ba-19_2



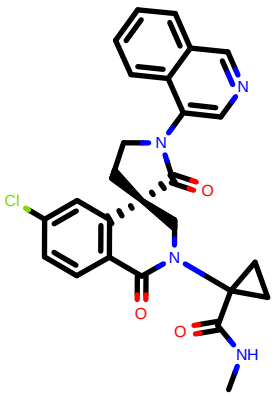
CID:	ALP-POS-ecbed2ba-19_2
SMILES:	C[N@](CCO)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1189
DDG (kcal/mol):	2.01
dDDG (kcal/mol):	0.54

MAT-POS-853c0ffa-6_2



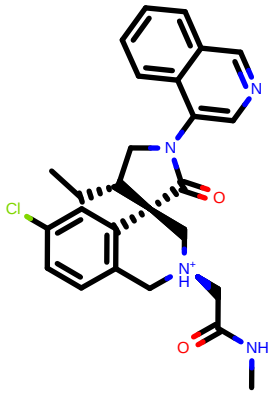
CID:	MAT-POS-853c0ffa-6_2
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1328
DDG (kcal/mol):	2.01
dDDG (kcal/mol):	0.65

EDJ-MED-fd8ed875-4_1



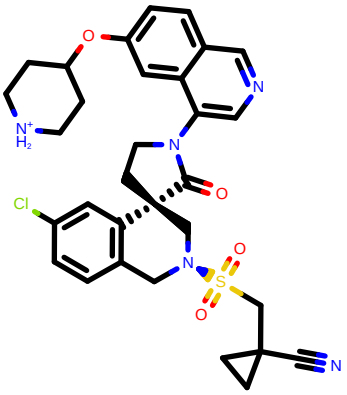
CID:	EDJ-MED-fd8ed875-4_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(C=CN(C3=O)c4cncc5c4cccc5)c6cc(ccc6C2=O)Cl
RUN:	RUN1186
DDG (kcal/mol):	2.01
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-5_3



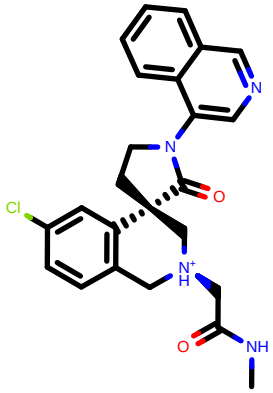
CID:	MAT-POS-50a80394-5_3
SMILES:	CC[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1147
DDG (kcal/mol):	2.02
dDDG (kcal/mol):	0.25

EDJ-MED-ee81482e-4_1



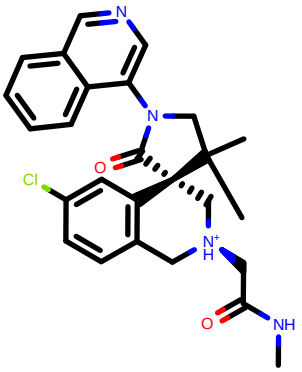
CID:	EDJ-MED-ee81482e-4_1
SMILES:	c1cc2cncc(c2cc1OC3CC[NH2+]CC3)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1421
DDG (kcal/mol):	2.03
dDDG (kcal/mol):	0.54

MAT-POS-c7726e07-5_2



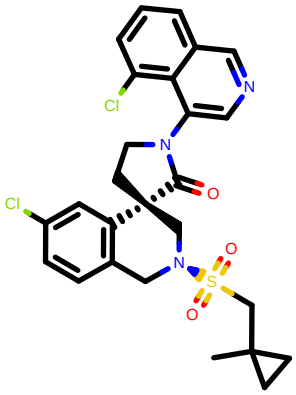
CID:	MAT-POS-c7726e07-5_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1048
DDG (kcal/mol):	2.04
dDDG (kcal/mol):	0.21

MAT-POS-50a80394-7_2



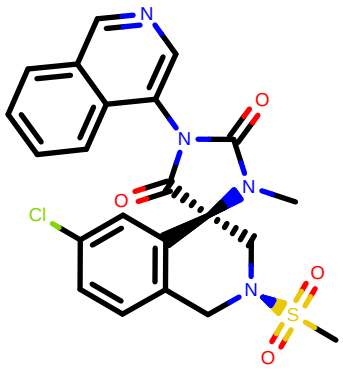
CID:	MAT-POS-50a80394-7_2
SMILES:	CC1(CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5)C
RUN:	RUN1153
DDG (kcal/mol):	2.04
dDDG (kcal/mol):	0.24

MAT-POS-853c0ffa-17_1



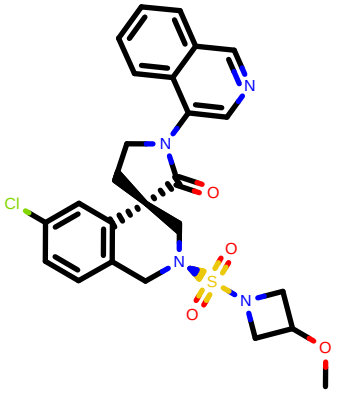
CID:	MAT-POS-853c0ffa-17_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1206
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.36

MAT-POS-2e8b2191-8_1



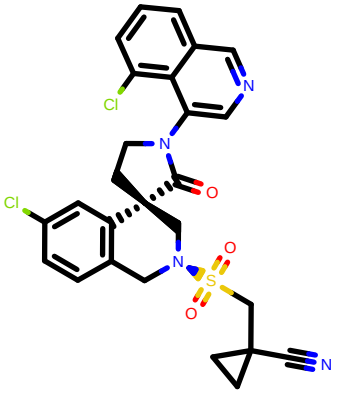
CID:	MAT-POS-2e8b2191-8_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1061
DDG (kcal/mol):	2.05
dDDG (kcal/mol):	0.12

ALP-POS-ecbed2ba-10_1



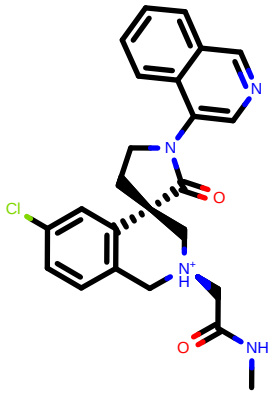
CID:	ALP-POS-ecbed2ba-10_1
SMILES:	COC1CN(C1)S(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1225
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.44

MAT-POS-1d5ab790-1_2



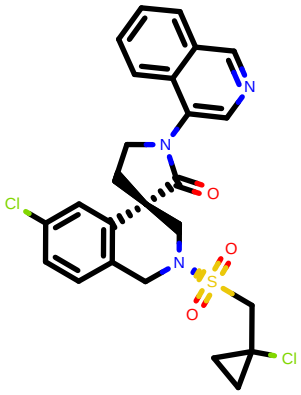
CID:	MAT-POS-1d5ab790-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1295
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.50

LUO-POS-868e8996-11_2



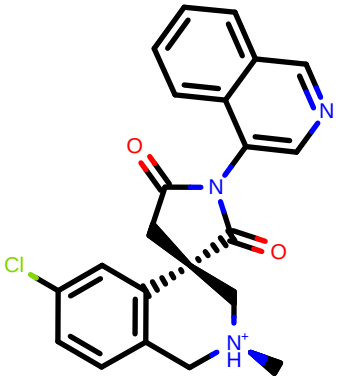
CID:	LUO-POS-868e8996-11_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1058
DDG (kcal/mol):	2.07
dDDG (kcal/mol):	0.22

PET-UNK-94036022-3_2



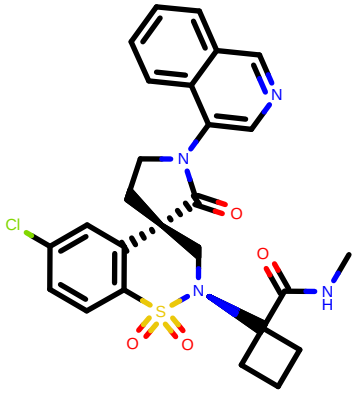
CID:	PET-UNK-94036022-3_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1198
DDG (kcal/mol):	2.09
dDDG (kcal/mol):	0.32

JOH-MSK-51c67e7d-1_2



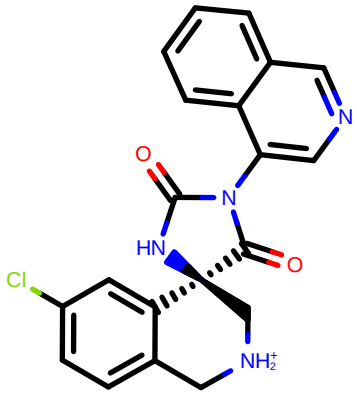
CID:	JOH-MSK-51c67e7d-1_2
SMILES:	C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1021
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.10

EDJ-MED-98c0a822-1_1



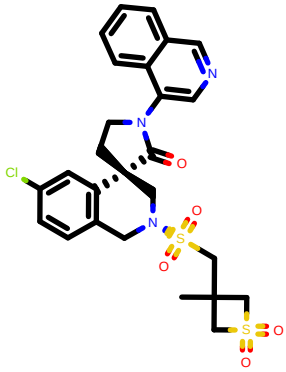
CID:	EDJ-MED-98c0a822-1_1
SMILES:	CNC(=O)C1(CCC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1302
DDG (kcal/mol):	2.10
dDDG (kcal/mol):	0.37

VLA-MRT-8c78ee15-1_1



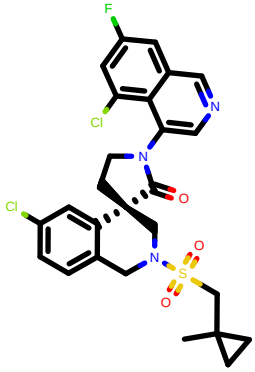
CID:	VLA-MRT-8c78ee15-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1005
DDG (kcal/mol):	2.12
dDDG (kcal/mol):	0.20

ALP-POS-ecbed2ba-1_1



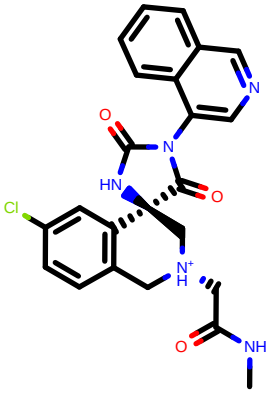
CID:	ALP-POS-ecbed2ba-1_1
SMILES:	CC1(CS(=O)(=O)C1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1329
DDG (kcal/mol):	2.15
dDDG (kcal/mol):	0.72

MAT-POS-853c0ffa-18_2



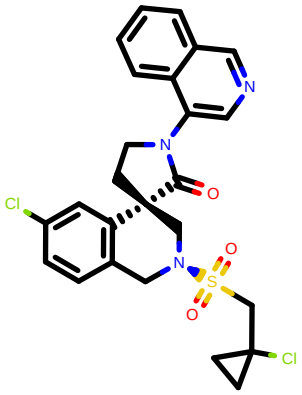
CID:	MAT-POS-853c0ffa-18_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1280
DDG (kcal/mol):	2.16
dDDG (kcal/mol):	0.45

VLA-MRT-a639d434-1_1



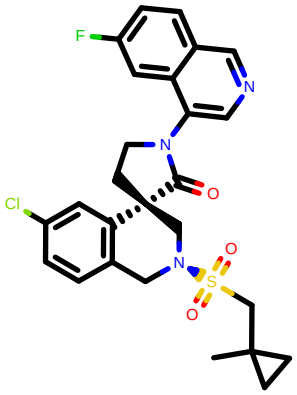
CID:	VLA-MRT-a639d434-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1062
DDG (kcal/mol):	2.16
dDDG (kcal/mol):	0.22

PET-UNK-94036022-10_2



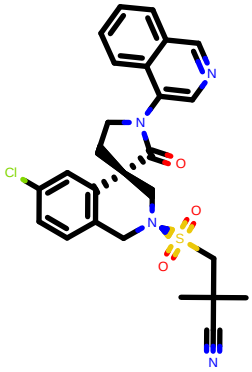
CID:	PET-UNK-94036022-10_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)Cl
RUN:	RUN1190
DDG (kcal/mol):	2.18
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-21_1



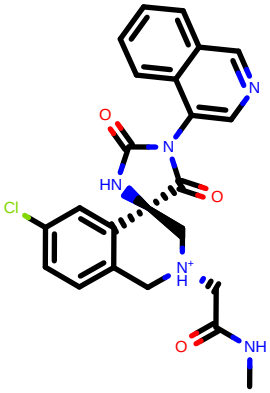
CID:	MAT-POS-853c0ffa-21_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1212
DDG (kcal/mol):	2.19
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-13_1



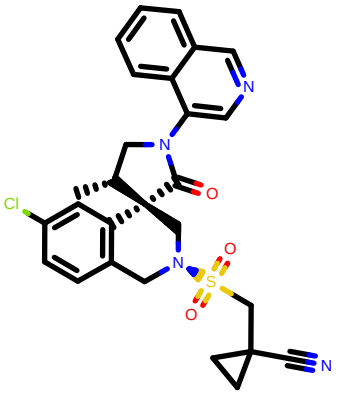
CID:	ALP-POS-ecbed2ba-13_1
SMILES:	CC(C)(CS(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN1228
DDG (kcal/mol):	2.21
dDDG (kcal/mol):	0.46

VLA-MRT-8c78ee15-3_1



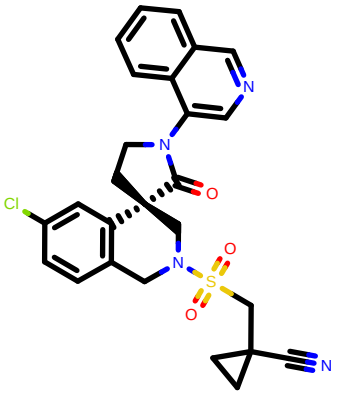
CID:	VLA-MRT-8c78ee15-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@@]3(C1)C(=O)N(C(=O)N3)c4cncc5c4cccc5)Cl
RUN:	RUN1064
DDG (kcal/mol):	2.21
dDDG (kcal/mol):	0.24

MAT-POS-50a80394-1_1



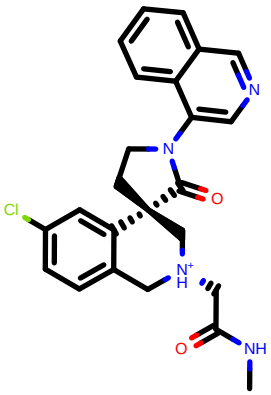
CID:	MAT-POS-50a80394-1_1
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1311
DDG (kcal/mol):	2.22
dDDG (kcal/mol):	0.58

MIK-ENA-5d9157e9-1_2



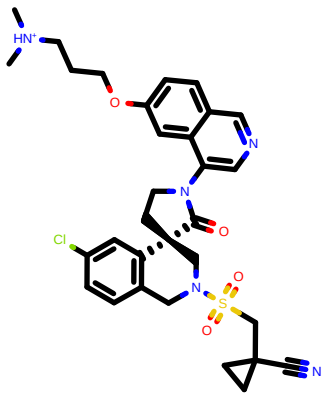
CID:	MIK-ENA-5d9157e9-1_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1233
DDG (kcal/mol):	2.25
dDDG (kcal/mol):	0.50

EDJ-MED-8bb691af-4_1



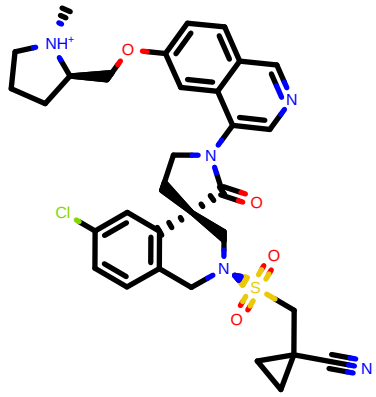
CID:	EDJ-MED-8bb691af-4_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1045
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.27

MAT-POS-40ad851a-4_2



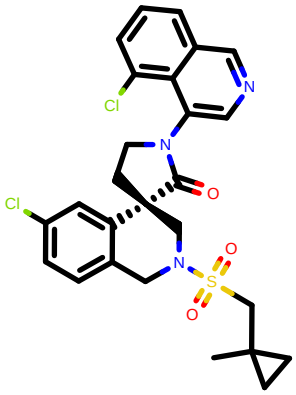
CID:	MAT-POS-40ad851a-4_2
SMILES:	C[NH+](C)CCCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1427
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.64

MAT-POS-40ad851a-1_2



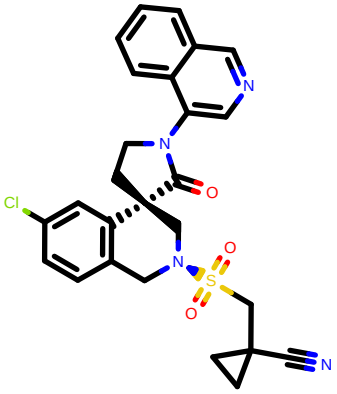
CID:	MAT-POS-40ad851a-1_2
SMILES:	C[N@H+]1CCC[C@@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1454
DDG (kcal/mol):	2.30
dDDG (kcal/mol):	0.65

MAT-POS-853c0ffa-17_2



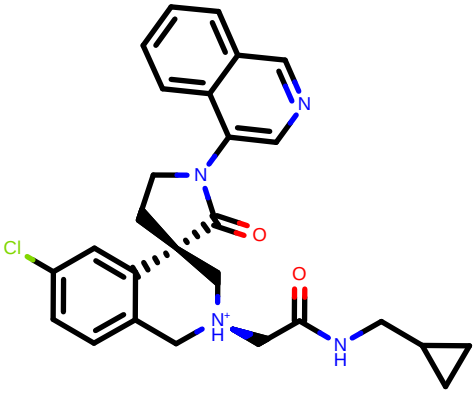
CID:	MAT-POS-853c0ffa-17_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1211
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.36

ALP-POS-ecbed2ba-4_2



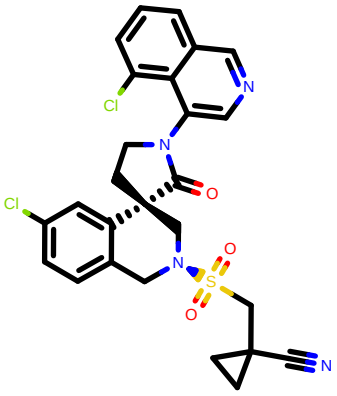
CID:	ALP-POS-ecbed2ba-4_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1214
DDG (kcal/mol):	2.31
dDDG (kcal/mol):	0.66

ALP-POS-ecbed2ba-12_2



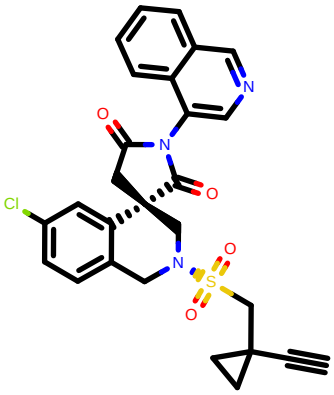
CID:	ALP-POS-ecbed2ba-12_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NCC6CC6
RUN:	RUN1177
DDG (kcal/mol):	2.32
dDDG (kcal/mol):	0.22

MAT-POS-1d5ab790-1_1



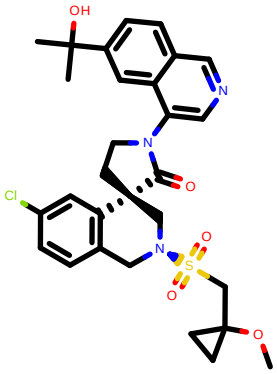
CID:	MAT-POS-1d5ab790-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1290
DDG (kcal/mol):	2.32
dDDG (kcal/mol):	0.53

PET-UNK-94036022-4_2



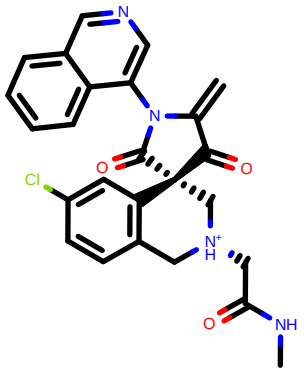
CID:	PET-UNK-94036022-4_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1323
DDG (kcal/mol):	2.32
dDDG (kcal/mol):	0.37

MAT-POS-853c0ffa-12_2



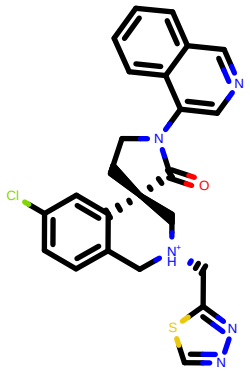
CID:	MAT-POS-853c0ffa-12_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC)O
RUN:	RUN1378
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.67

PET-UNK-94036022-14_1



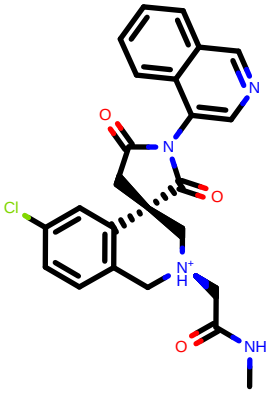
CID:	PET-UNK-94036022-14_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1158
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.34

PET-UNK-7e9559de-1_1



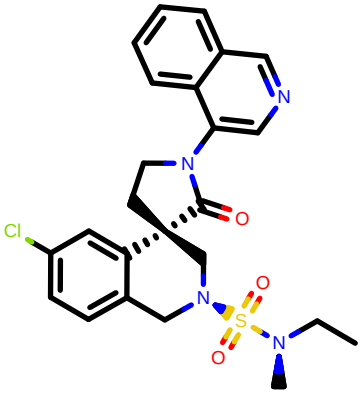
CID:	PET-UNK-7e9559de-1_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@H+](Cc5c4cc(cc5)Cl)Cc6nncs6
RUN:	RUN1087
DDG (kcal/mol):	2.33
dDDG (kcal/mol):	0.20

MAT-POS-1bed62cf-3_2



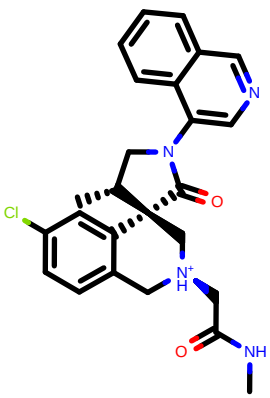
CID:	MAT-POS-1bed62cf-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1068
DDG (kcal/mol):	2.37
dDDG (kcal/mol):	0.18

ALP-POS-ecbed2ba-18_1



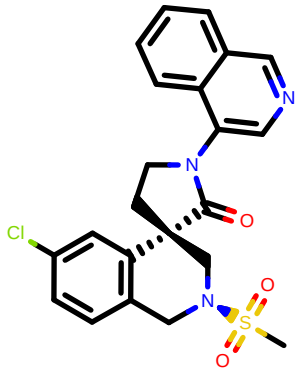
CID:	ALP-POS-ecbed2ba-18_1
SMILES:	CC[N@@](C)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1125
DDG (kcal/mol):	2.41
dDDG (kcal/mol):	0.30

MAT-POS-50a80394-4_3



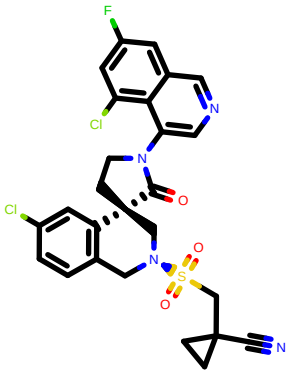
CID:	MAT-POS-50a80394-4_3
SMILES:	C[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1093
DDG (kcal/mol):	2.42
dDDG (kcal/mol):	0.23

EDJ-MED-7587a9ee-3_2



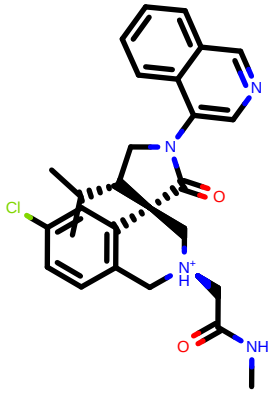
CID:	EDJ-MED-7587a9ee-3_2
SMILES:	CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1023
DDG (kcal/mol):	2.43
dDDG (kcal/mol):	0.22

MAT-POS-853c0ffa-6_1



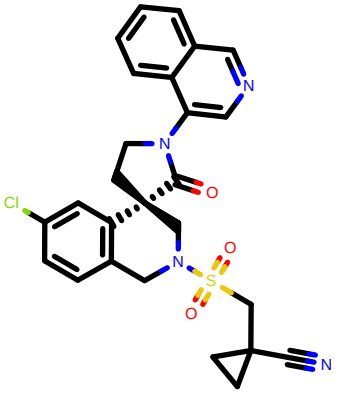
CID:	MAT-POS-853c0ffa-6_1
SMILES:	c1cc2c(cc1Cl)[C@@]3(CCN(C3=O)c4cncc5c4c(cc(c5)F)Cl)C[N@@](C2)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1324
DDG (kcal/mol):	2.44
dDDG (kcal/mol):	0.69

MAT-POS-50a80394-6_3



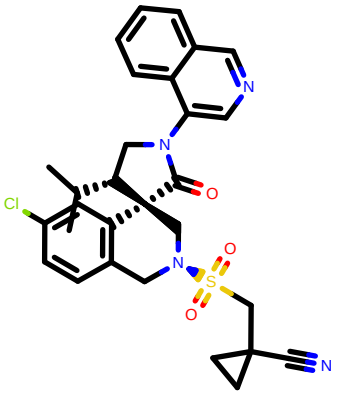
CID:	MAT-POS-50a80394-6_3
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@H+](Cc3c2cc(cc3)Cl)CC(=O)NC)c4cncc5c4cccc5
RUN:	RUN1197
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.30

EDJ-MED-8bb691af-6_2



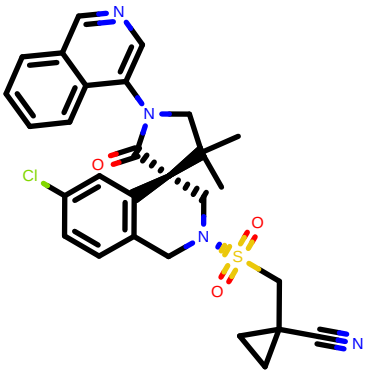
CID:	EDJ-MED-8bb691af-6_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1209
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.54

MAT-POS-50a80394-3_1



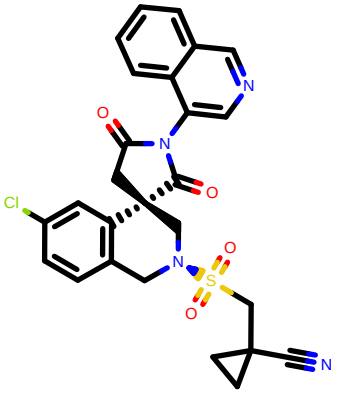
CID:	MAT-POS-50a80394-3_1
SMILES:	CC(C)[C@@H]1CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6
RUN:	RUN1359
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.59

MAT-POS-50a80394-8_1



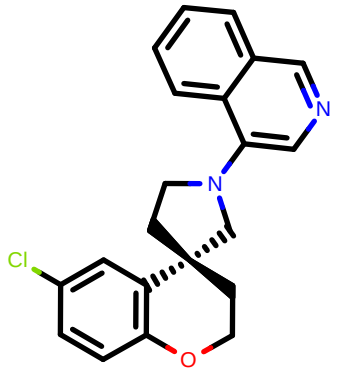
CID:	MAT-POS-50a80394-8_1
SMILES:	CC1(CN(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)c5cncc6c5cccc6)C
RUN:	RUN1345
DDG (kcal/mol):	2.45
dDDG (kcal/mol):	0.66

MAT-POS-1bed62cf-1_2



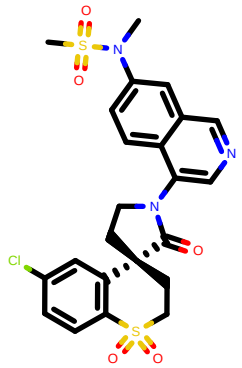
CID:	MAT-POS-1bed62cf-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1261
DDG (kcal/mol):	2.53
dDDG (kcal/mol):	0.46

EDJ-MED-159244ea-2_2



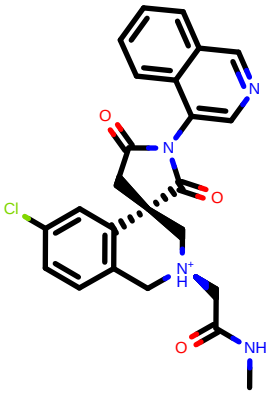
CID:	EDJ-MED-159244ea-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN976
DDG (kcal/mol):	2.53
dDDG (kcal/mol):	0.10

EDJ-MED-94fddcec-6_1



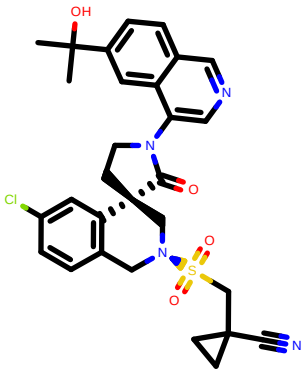
CID:	EDJ-MED-94fddcec-6_1
SMILES:	C[N@@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1171
DDG (kcal/mol):	2.54
dDDG (kcal/mol):	0.26

JOH-MSK-1f2dff76-1_2



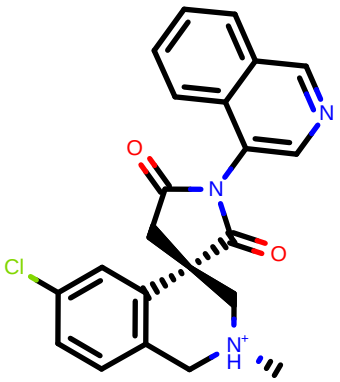
CID:	JOH-MSK-1f2dff76-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1106
DDG (kcal/mol):	2.55
dDDG (kcal/mol):	0.19

MAT-POS-853c0ffa-11_2



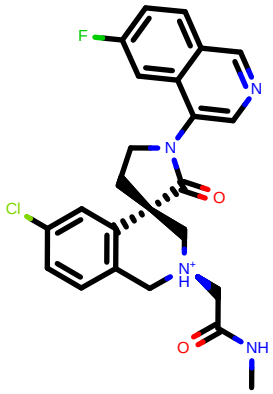
CID:	MAT-POS-853c0ffa-11_2
SMILES:	CC(C)(c1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1387
DDG (kcal/mol):	2.56
dDDG (kcal/mol):	0.75

JOH-MSK-51c67e7d-1_1



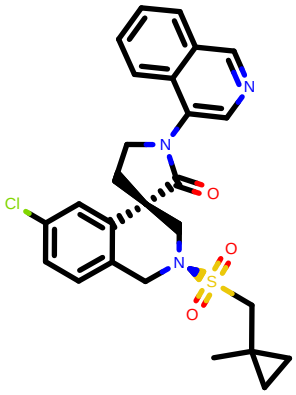
CID:	JOH-MSK-51c67e7d-1_1
SMILES:	C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1018
DDG (kcal/mol):	2.59
dDDG (kcal/mol):	0.19

LUO-POS-b4dec3be-2_2



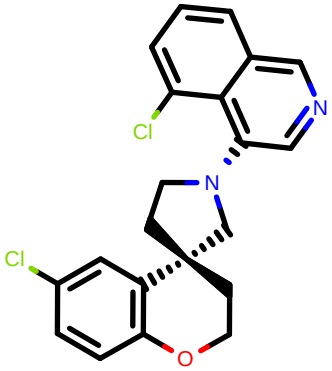
CID:	LUO-POS-b4dec3be-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)F)Cl
RUN:	RUN1102
DDG (kcal/mol):	2.61
dDDG (kcal/mol):	0.24

ALP-POS-ecbed2ba-3_2



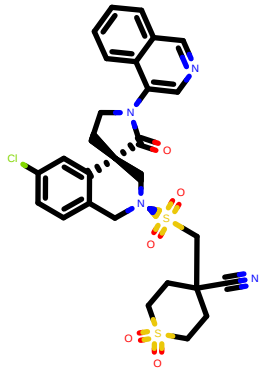
CID:	ALP-POS-ecbed2ba-3_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1174
DDG (kcal/mol):	2.63
dDDG (kcal/mol):	0.39

EDJ-MED-e78d5f1a-1_2



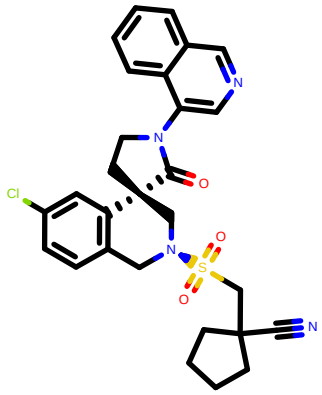
CID:	EDJ-MED-e78d5f1a-1_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN988
DDG (kcal/mol):	2.68
dDDG (kcal/mol):	0.10

ALP-POS-ecbed2ba-2_2



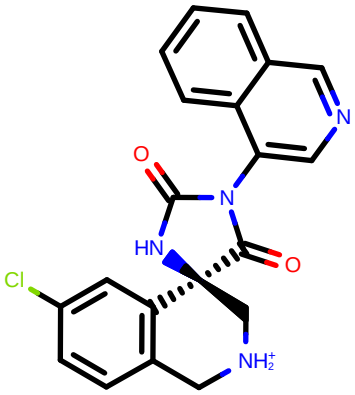
CID:	ALP-POS-ecbed2ba-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCS(=O)(=O)CC6)C#N
RUN:	RUN1388
DDG (kcal/mol):	2.70
dDDG (kcal/mol):	0.47

ALP-POS-ecbed2ba-15_2



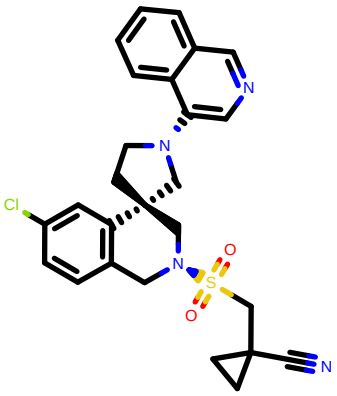
CID:	ALP-POS-ecbed2ba-15_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCCC6)C#N
RUN:	RUN1333
DDG (kcal/mol):	2.70
dDDG (kcal/mol):	0.47

VLA-MRT-8c78ee15-2_1



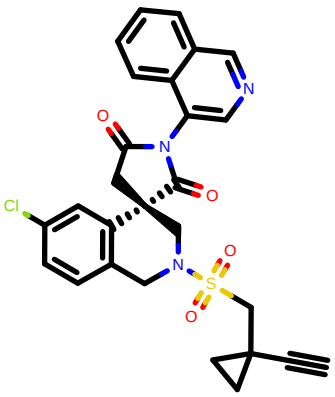
CID:	VLA-MRT-8c78ee15-2_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1010
DDG (kcal/mol):	2.70
dDDG (kcal/mol):	0.20

EDJ-MED-8bb691af-2_4



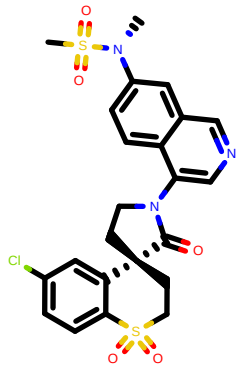
CID:	EDJ-MED-8bb691af-2_4
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1170
DDG (kcal/mol):	2.71
dDDG (kcal/mol):	0.46

PET-UNK-94036022-11_2



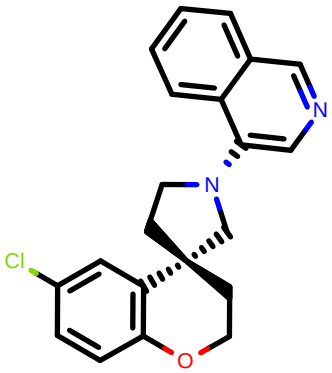
CID:	PET-UNK-94036022-11_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CC(=O)N(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1315
DDG (kcal/mol):	2.71
dDDG (kcal/mol):	0.35

EDJ-MED-94fddcec-6_2



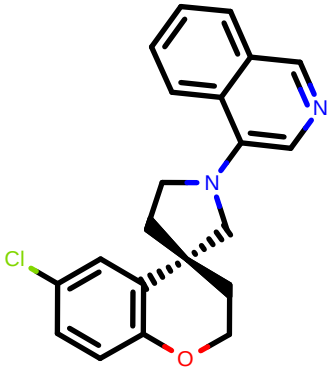
CID:	EDJ-MED-94fddcec-6_2
SMILES:	C[N@](c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl)S(=O)(=O)C
RUN:	RUN1169
DDG (kcal/mol):	2.73
dDDG (kcal/mol):	0.22

EDJ-MED-159244ea-2_1



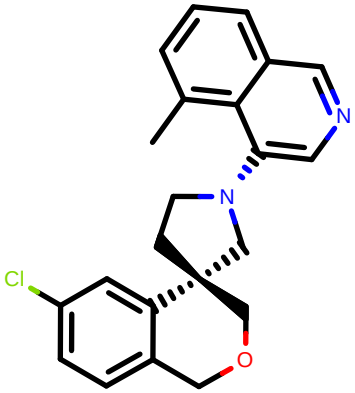
CID:	EDJ-MED-159244ea-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN977
DDG (kcal/mol):	2.75
dDDG (kcal/mol):	0.09

MAT-POS-983b399a-2_1



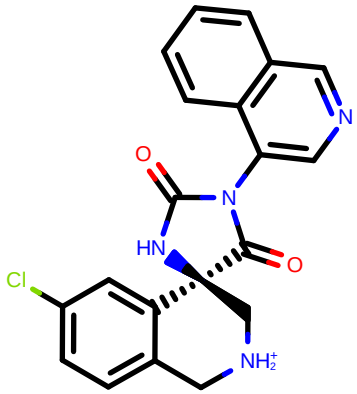
CID:	MAT-POS-983b399a-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN975
DDG (kcal/mol):	2.79
dDDG (kcal/mol):	0.09

EDJ-MED-f3cfbbb5-1_2



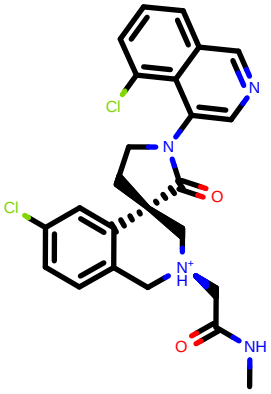
CID:	EDJ-MED-f3cfbbb5-1_2
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN986
DDG (kcal/mol):	2.80
dDDG (kcal/mol):	0.10

VLA-MRT-a639d434-3_1



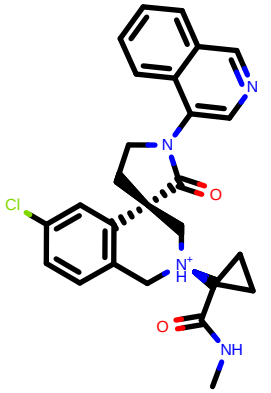
CID:	VLA-MRT-a639d434-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[NH2+]Cc5c4cc(cc5)Cl)NC3=O
RUN:	RUN1013
DDG (kcal/mol):	2.82
dDDG (kcal/mol):	0.21

MAT-POS-1d5ab790-2_2



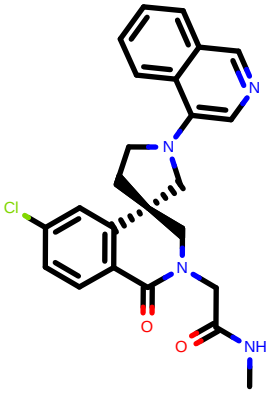
CID:	MAT-POS-1d5ab790-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1086
DDG (kcal/mol):	2.83
dDDG (kcal/mol):	0.26

MAT-POS-69786b79-1_2



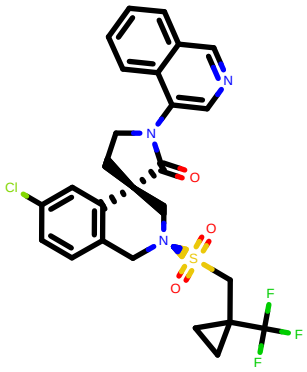
CID:	MAT-POS-69786b79-1_2
SMILES:	CNC(=O)C1(CC1)[N@H+]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1134
DDG (kcal/mol):	2.88
dDDG (kcal/mol):	0.24

EDJ-MED-8bb691af-7_2



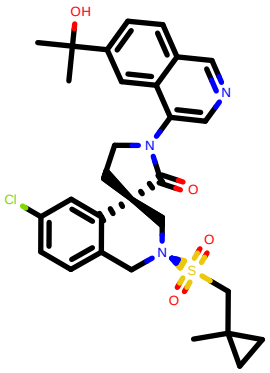
CID:	EDJ-MED-8bb691af-7_2
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1044
DDG (kcal/mol):	2.88
dDDG (kcal/mol):	0.15

EDJ-MED-5cd3920d-6_1



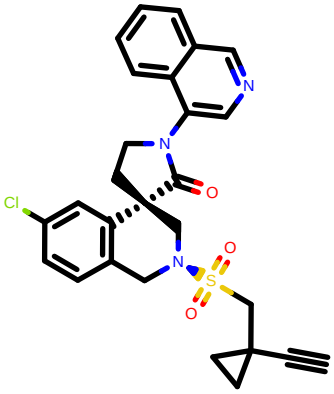
CID:	EDJ-MED-5cd3920d-6_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4ccc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)(F)F
RUN:	RUN1349
DDG (kcal/mol):	2.91
dDDG (kcal/mol):	0.44

MAT-POS-853c0ffa-20_2



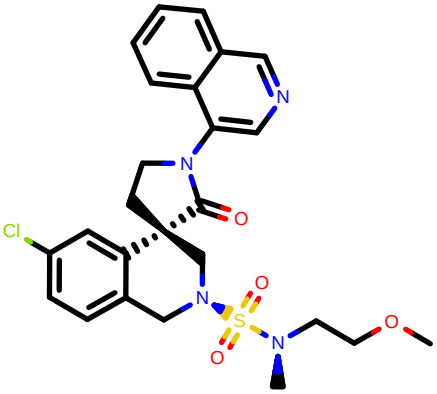
CID:	MAT-POS-853c0ffa-20_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)C(C)(C)O)Cl
RUN:	RUN1366
DDG (kcal/mol):	2.93
dDDG (kcal/mol):	0.47

PET-UNK-94036022-9_1



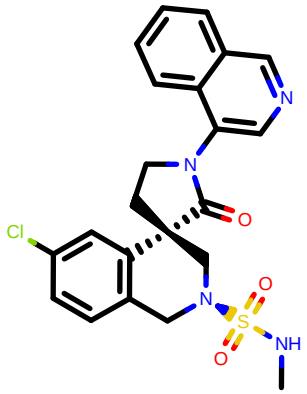
CID:	PET-UNK-94036022-9_1
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1248
DDG (kcal/mol):	2.94
dDDG (kcal/mol):	0.34

ALP-POS-ecbed2ba-21_2



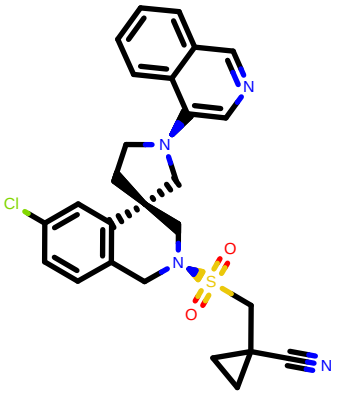
CID:	ALP-POS-ecbed2ba-21_2
SMILES:	C[N@](CCOC)S(=O)(=O)[N@@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1237
DDG (kcal/mol):	2.97
dDDG (kcal/mol):	0.37

LUO-POS-ed2cfb03-2_2



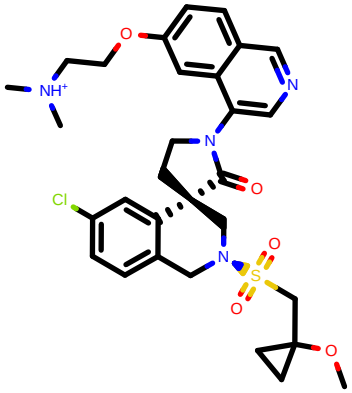
CID:	LUO-POS-ed2cfb03-2_2
SMILES:	CNS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1063
DDG (kcal/mol):	2.98
dDDG (kcal/mol):	0.55

EDJ-MED-8bb691af-2_3



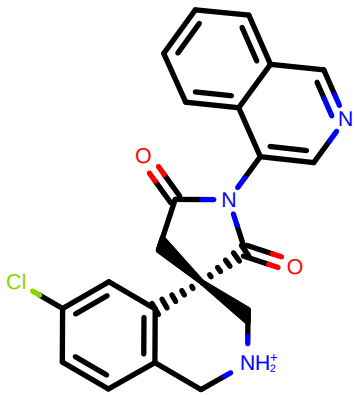
CID:	EDJ-MED-8bb691af-2_3
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1167
DDG (kcal/mol):	2.99
dDDG (kcal/mol):	0.42

MAT-POS-853c0ffa-10_1



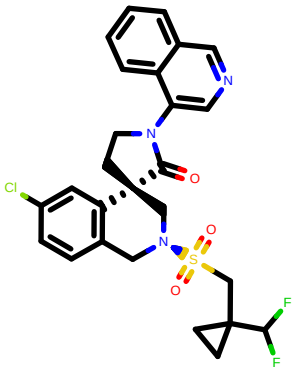
CID:	MAT-POS-853c0ffa-10_1
SMILES:	C[NH+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)OC
RUN:	RUN1408
DDG (kcal/mol):	3.00
dDDG (kcal/mol):	0.60

JOH-MSK-1f2dff76-4_1



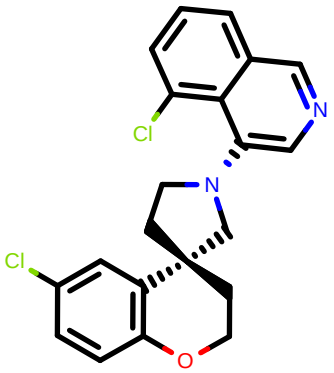
CID:	JOH-MSK-1f2dff76-4_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN1006
DDG (kcal/mol):	3.02
dDDG (kcal/mol):	0.14

EDJ-MED-5cd3920d-5_1



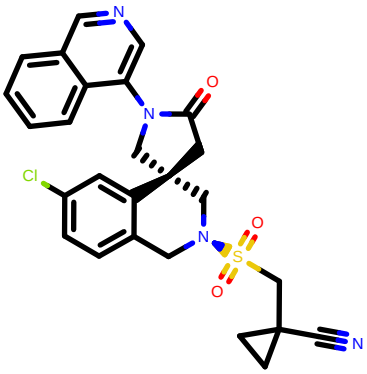
CID:	EDJ-MED-5cd3920d-5_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C(F)F
RUN:	RUN1316
DDG (kcal/mol):	3.07
dDDG (kcal/mol):	0.46

EDJ-MED-e78d5f1a-1_1



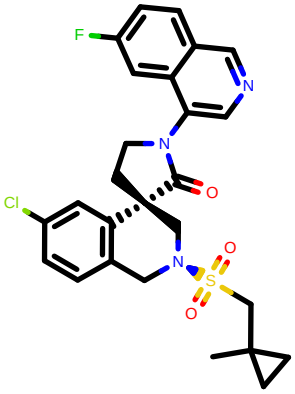
CID:	EDJ-MED-e78d5f1a-1_1
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3)CCOc5c4cc(cc5)Cl
RUN:	RUN989
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.11

EDJ-MED-8bb691af-5_2



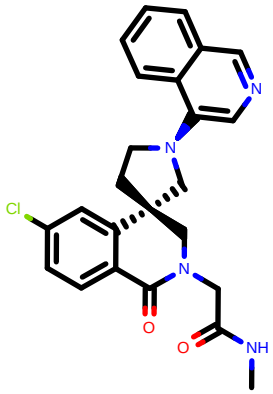
CID:	EDJ-MED-8bb691af-5_2
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1208
DDG (kcal/mol):	3.08
dDDG (kcal/mol):	0.46

MAT-POS-853c0ffa-21_2



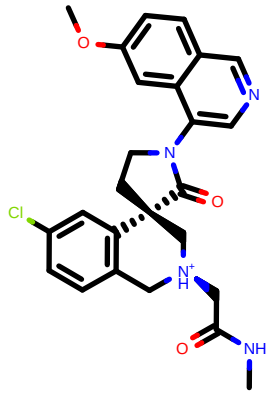
CID:	MAT-POS-853c0ffa-21_2
SMILES:	CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cc(cc6)F)Cl
RUN:	RUN1216
DDG (kcal/mol):	3.10
dDDG (kcal/mol):	0.39

EDJ-MED-8bb691af-7_1



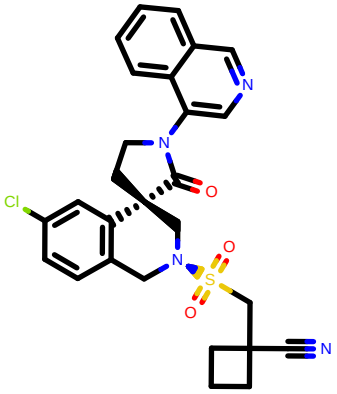
CID:	EDJ-MED-8bb691af-7_1
SMILES:	CNC(=O)CN1C[C@]2(CCN(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1047
DDG (kcal/mol):	3.10
dDDG (kcal/mol):	0.14

EDJ-MED-b6c6ee2b-2_2



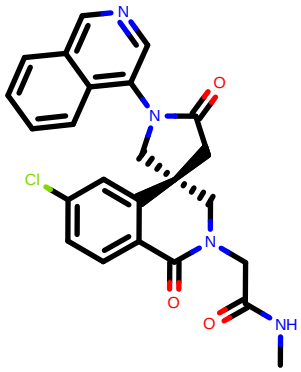
CID:	EDJ-MED-b6c6ee2b-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cc(cc5)OC)Cl
RUN:	RUN1145
DDG (kcal/mol):	3.11
dDDG (kcal/mol):	0.25

ALP-POS-ecbed2ba-8_1



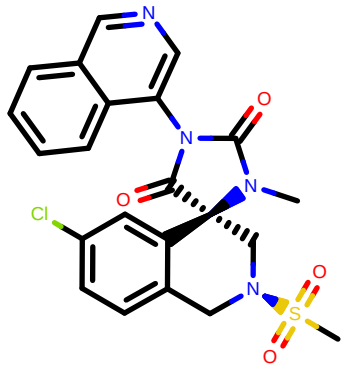
CID:	ALP-POS-ecbed2ba-8_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N
RUN:	RUN1286
DDG (kcal/mol):	3.11
dDDG (kcal/mol):	0.49

EDJ-MED-8bb691af-9_1



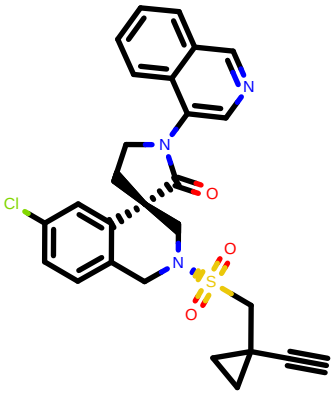
CID:	EDJ-MED-8bb691af-9_1
SMILES:	CNC(=O)CN1C[C@]2(CC(=O)N(C2)c3cncc4c3cccc4)c5cc(ccc5C1=O)Cl
RUN:	RUN1066
DDG (kcal/mol):	3.12
dDDG (kcal/mol):	0.13

EDJ-MED-7587a9ee-1_1



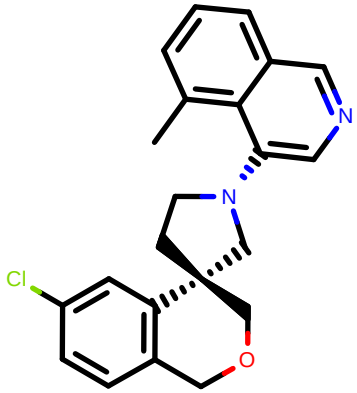
CID:	EDJ-MED-7587a9ee-1_1
SMILES:	CN1C(=O)N(C(=O)[C@@]12C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)C)c4cncc5c4cccc5
RUN:	RUN1059
DDG (kcal/mol):	3.14
dDDG (kcal/mol):	0.15

PET-UNK-94036022-9_2



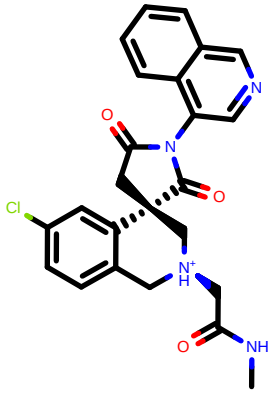
CID:	PET-UNK-94036022-9_2
SMILES:	C#CC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1259
DDG (kcal/mol):	3.17
dDDG (kcal/mol):	0.51

EDJ-MED-f3cfbbb5-1_1



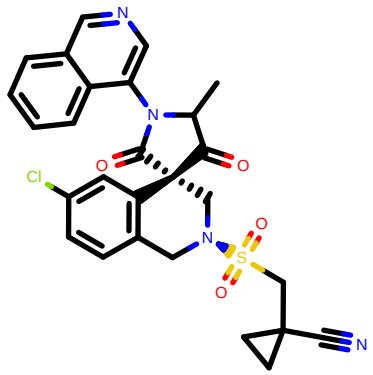
CID:	EDJ-MED-f3cfbbb5-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)COCc5c4cc(cc5)Cl
RUN:	RUN985
DDG (kcal/mol):	3.17
dDDG (kcal/mol):	0.12

JOH-MSK-1f2dff76-2_2



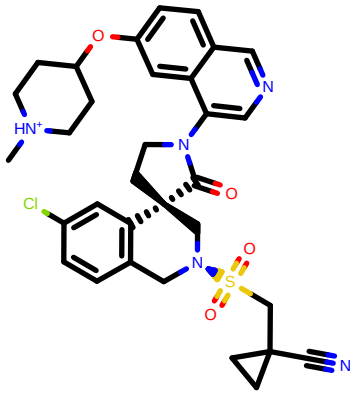
CID:	JOH-MSK-1f2dff76-2_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1108
DDG (kcal/mol):	3.19
dDDG (kcal/mol):	0.19

PET-UNK-94036022-6_1



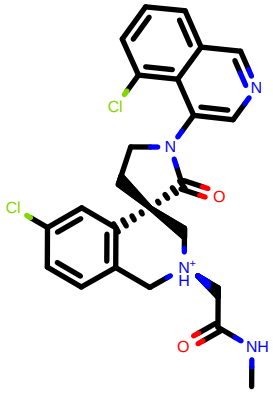
CID:	PET-UNK-94036022-6_1
SMILES:	C=C1C(=O)[C@]2(C[N@@](Cc3c2cc(cc3Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1354
DDG (kcal/mol):	3.20
dDDG (kcal/mol):	0.55

LUO-POS-d1147590-1_1



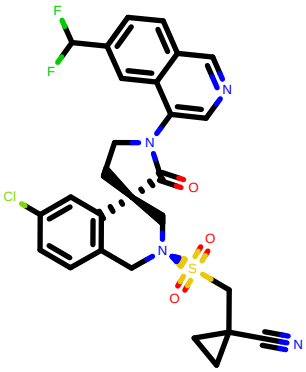
CID:	LUO-POS-d1147590-1_1
SMILES:	C[NH+]1CCC(CC1)Oc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1452
DDG (kcal/mol):	3.23
dDDG (kcal/mol):	0.73

MAT-POS-b4d6b7fc-6_2



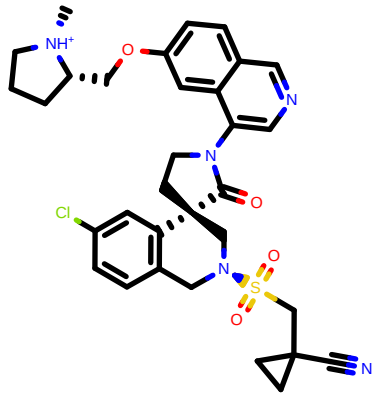
CID:	MAT-POS-b4d6b7fc-6_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4c(ccc5)Cl)Cl
RUN:	RUN1078
DDG (kcal/mol):	3.26
dDDG (kcal/mol):	0.23

EDJ-MED-5cd3920d-2_2



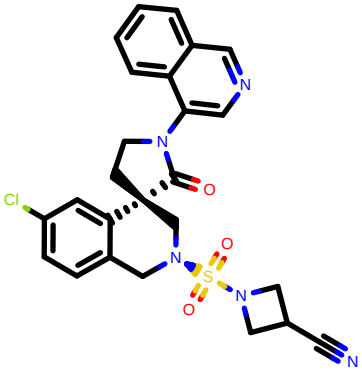
CID:	EDJ-MED-5cd3920d-2_2
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1373
DDG (kcal/mol):	3.28
dDDG (kcal/mol):	0.58

MAT-POS-40ad851a-1_4



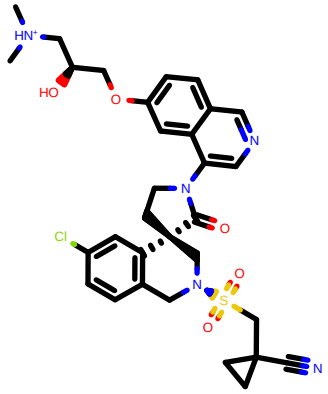
CID:	MAT-POS-40ad851a-1_4
SMILES:	C[N@H+]1CCC[C@H]1COc2ccc3cncc(c3c2)N4CC[C@@]5(C4=O)C[N@@](Cc6c5cc(cc6)Cl)S(=O)(=O)CC7(CC7)C#N
RUN:	RUN1439
DDG (kcal/mol):	3.35
dDDG (kcal/mol):	0.65

ALP-POS-ecbed2ba-9_2



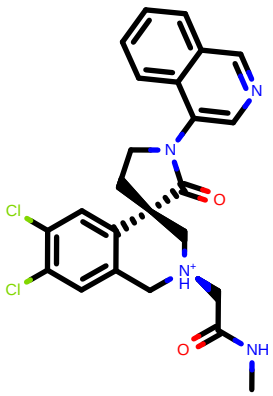
CID:	ALP-POS-ecbed2ba-9_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CC(C6)C#N
RUN:	RUN1213
DDG (kcal/mol):	3.36
dDDG (kcal/mol):	0.76

EDJ-MED-ee81482e-3_3



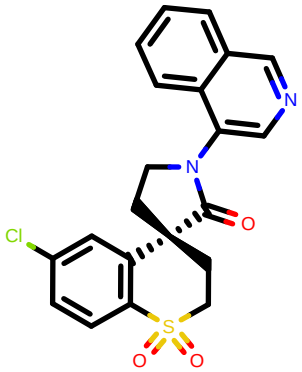
CID:	EDJ-MED-ee81482e-3_3
SMILES:	C[NH+](C)C[C@@H](COc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)O
RUN:	RUN1430
DDG (kcal/mol):	3.36
dDDG (kcal/mol):	0.88

ALP-POS-afe0272e-1_2



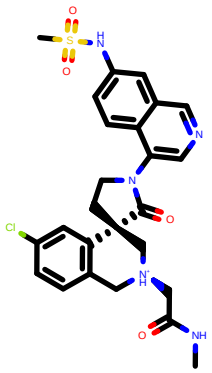
CID:	ALP-POS-afe0272e-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2cc(c(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)Cl
RUN:	RUN1085
DDG (kcal/mol):	3.38
dDDG (kcal/mol):	0.32

EDJ-MED-94fddcec-4_1



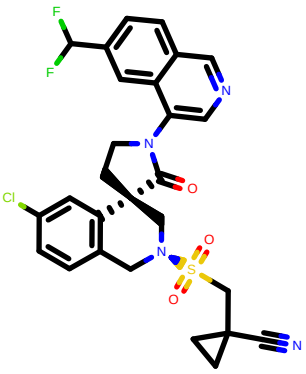
CID:	EDJ-MED-94fddcec-4_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)CCS(=O)(=O)c5c4cc(cc5)Cl
RUN:	RUN1015
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.15

MAT-POS-b4d6b7fc-7_2



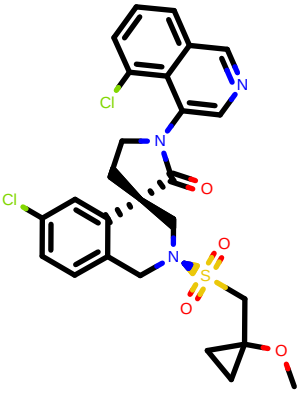
CID:	MAT-POS-b4d6b7fc-7_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4ccc(c5)NS(=O)(=O)C)Cl
RUN:	RUN1296
DDG (kcal/mol):	3.39
dDDG (kcal/mol):	0.33

EDJ-MED-5cd3920d-2_1



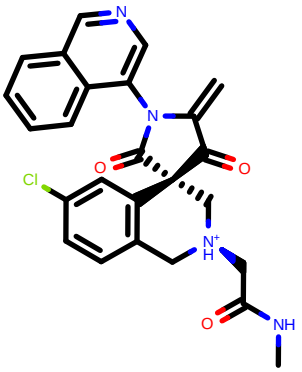
CID:	EDJ-MED-5cd3920d-2_1
SMILES:	c1cc2cncc(c2cc1C(F)F)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1370
DDG (kcal/mol):	3.41
dDDG (kcal/mol):	0.34

MAT-POS-853c0ffa-7_2



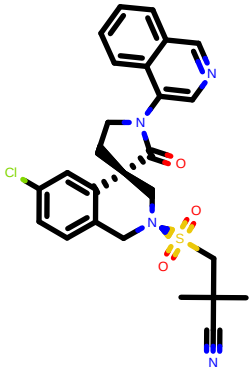
CID:	MAT-POS-853c0ffa-7_2
SMILES:	COC1(CC1)CS(=O)(=O)[N@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(ccc6)Cl)Cl
RUN:	RUN1276
DDG (kcal/mol):	3.50
dDDG (kcal/mol):	0.38

PET-UNK-94036022-7_2



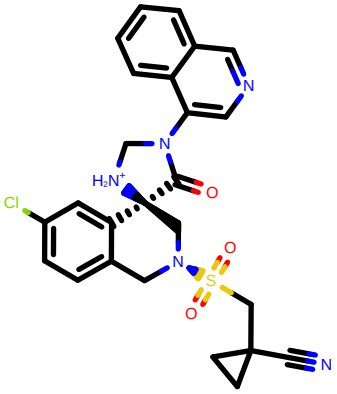
CID:	PET-UNK-94036022-7_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1159
DDG (kcal/mol):	3.52
dDDG (kcal/mol):	0.26

ALP-POS-ecbed2ba-13_2



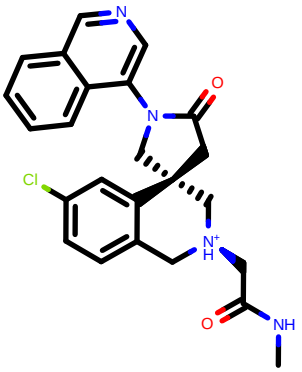
CID:	ALP-POS-ecbed2ba-13_2
SMILES:	CC(C)(CS(=O)(=O)[N@]1Cc2ccc(cc2[C@]3(C1)CCN(C3=O)c4cncc5c4cccc5)Cl)C#N
RUN:	RUN1220
DDG (kcal/mol):	3.53
dDDG (kcal/mol):	0.56

EDG-MED-00af8776-1_1



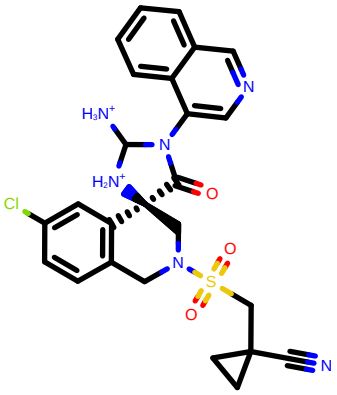
CID:	EDG-MED-00af8776-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1221
DDG (kcal/mol):	3.60
dDDG (kcal/mol):	0.32

EDJ-MED-8bb691af-3_2



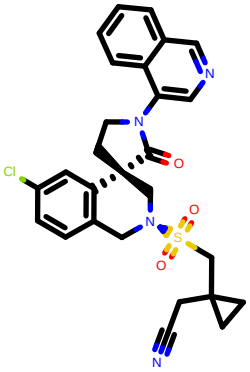
CID:	EDJ-MED-8bb691af-3_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1042
DDG (kcal/mol):	3.65
dDDG (kcal/mol):	0.22

LUO-POS-eaf50f21-1_2



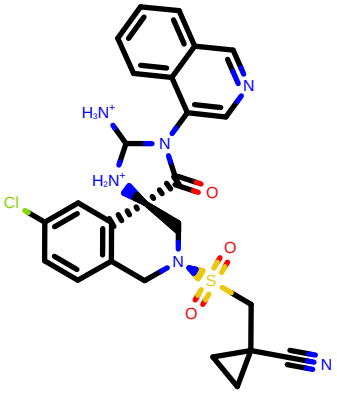
CID:	LUO-POS-eaf50f21-1_2
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)[NH+]=C3N
RUN:	RUN1326
DDG (kcal/mol):	3.65
dDDG (kcal/mol):	0.43

ALP-POS-ecbed2ba-22_2



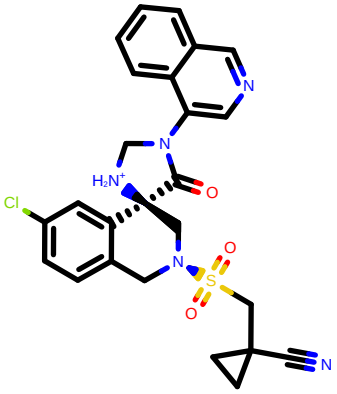
CID:	ALP-POS-ecbed2ba-22_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)CC#N
RUN:	RUN1285
DDG (kcal/mol):	3.72
dDDG (kcal/mol):	0.46

LUO-POS-eaf50f21-1_1



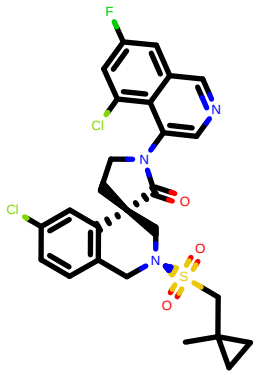
CID:	LUO-POS-eaf50f21-1_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)[C@@]4(C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N)[NH+]=C3N
RUN:	RUN1322
DDG (kcal/mol):	3.75
dDDG (kcal/mol):	0.35

EDG-MED-0c930815-1_2



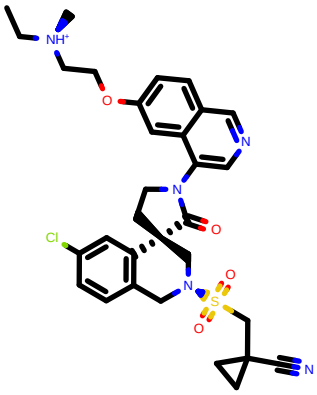
CID:	EDG-MED-0c930815-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1218
DDG (kcal/mol):	3.78
dDDG (kcal/mol):	0.41

MAT-POS-853c0ffa-18_1



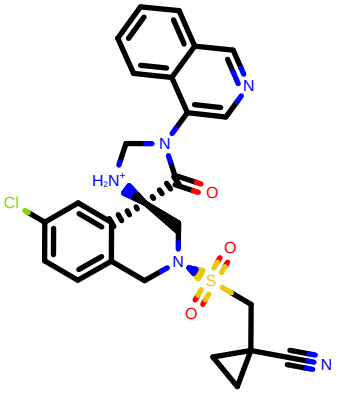
CID:	MAT-POS-853c0ffa-18_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5c(cc(c6)F)Cl)Cl
RUN:	RUN1287
DDG (kcal/mol):	3.80
dDDG (kcal/mol):	0.30

MAT-POS-40ad851a-2_1



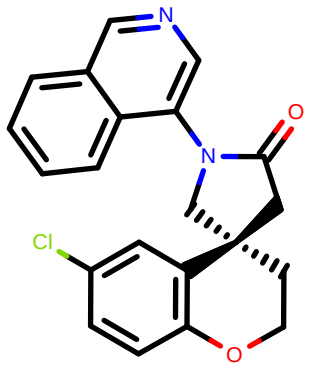
CID:	MAT-POS-40ad851a-2_1
SMILES:	CC[N@@H+](C)CCOc1ccc2cncc(c2c1)N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1422
DDG (kcal/mol):	3.80
dDDG (kcal/mol):	0.64

EDG-MED-b6bce001-1_1



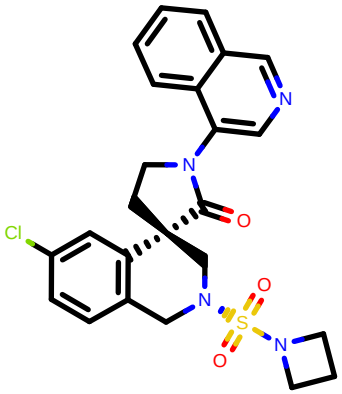
CID:	EDG-MED-b6bce001-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1229
DDG (kcal/mol):	3.84
dDDG (kcal/mol):	0.30

EDJ-MED-159244ea-3_1



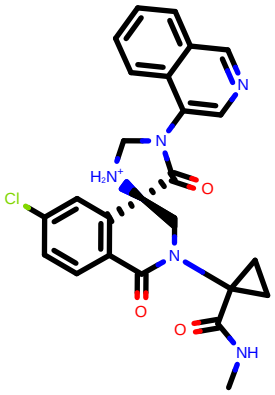
CID:	EDJ-MED-159244ea-3_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@@]4(CCOc5c4cc(cc5)Cl)CC3=O
RUN:	RUN981
DDG (kcal/mol):	3.91
dDDG (kcal/mol):	0.08

ALP-POS-ecbed2ba-20_2



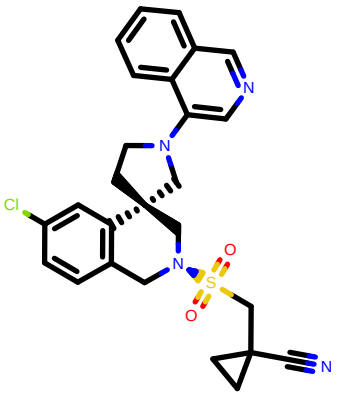
CID:	ALP-POS-ecbed2ba-20_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN1129
DDG (kcal/mol):	3.99
dDDG (kcal/mol):	0.66

EDJ-MED-fd8ed875-2_1



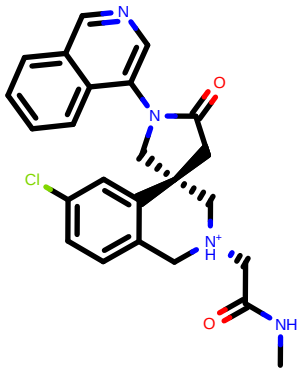
CID:	EDJ-MED-fd8ed875-2_1
SMILES:	CNC(=O)C1(CC1)N2C[C@]3(c4cc(ccc4C2=O)Cl)C(=O)N(C=[NH+]3)c5cncc6c5cccc6
RUN:	RUN1192
DDG (kcal/mol):	4.02
dDDG (kcal/mol):	0.16

EDJ-MED-8bb691af-2_1



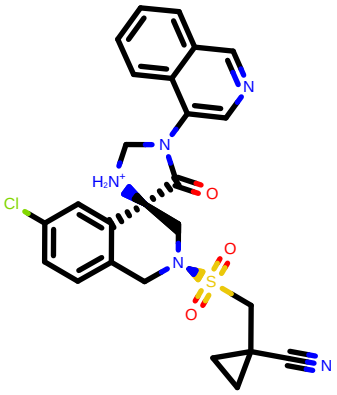
CID:	EDJ-MED-8bb691af-2_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1165
DDG (kcal/mol):	4.03
dDDG (kcal/mol):	0.36

EDJ-MED-8bb691af-3_1



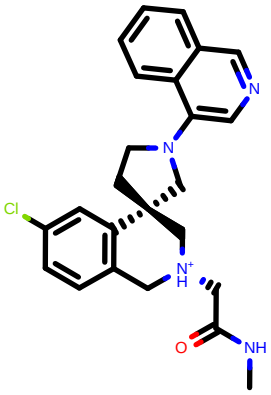
CID:	EDJ-MED-8bb691af-3_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CC(=O)N(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1040
DDG (kcal/mol):	4.03
dDDG (kcal/mol):	0.24

EDG-MED-00af8776-1_2



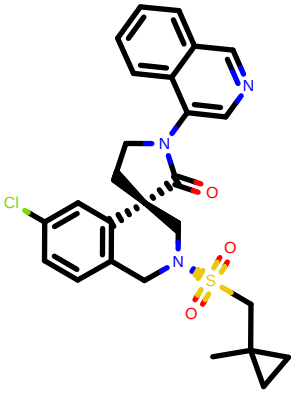
CID:	EDG-MED-00af8776-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1224
DDG (kcal/mol):	4.03
dDDG (kcal/mol):	0.44

EDJ-MED-8bb691af-1_1



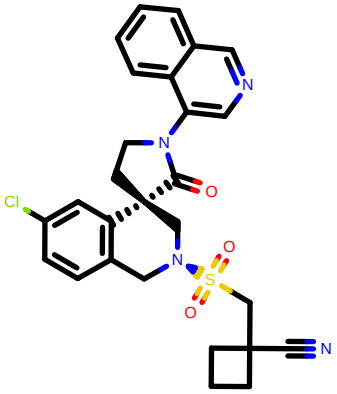
CID:	EDJ-MED-8bb691af-1_1
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1029
DDG (kcal/mol):	4.04
dDDG (kcal/mol):	0.23

ALP-POS-ecbed2ba-3_1



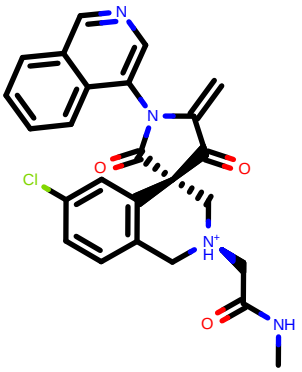
CID:	ALP-POS-ecbed2ba-3_1
SMILES:	CC1(CC1)CS(=O)(=O)[N@@]2Cc3ccc(cc3[C@]4(C2)CCN(C4=O)c5cncc6c5cccc6)Cl
RUN:	RUN1173
DDG (kcal/mol):	4.11
dDDG (kcal/mol):	0.30

ALP-POS-ecbed2ba-8_2



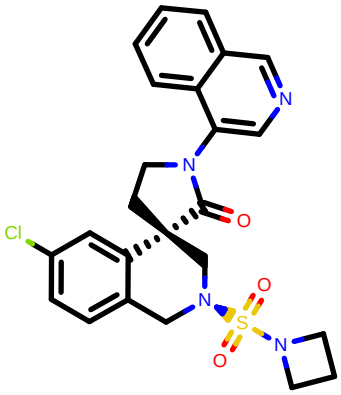
CID:	ALP-POS-ecbed2ba-8_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CCC6)C#N
RUN:	RUN1279
DDG (kcal/mol):	4.13
dDDG (kcal/mol):	0.63

PET-UNK-94036022-14_2



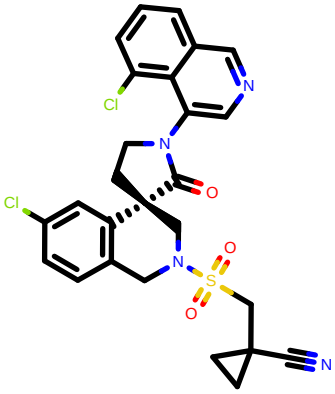
CID:	PET-UNK-94036022-14_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)C(=O)C(=C)N(C3=O)c4cncc5c4cccc5)Cl
RUN:	RUN1160
DDG (kcal/mol):	4.13
dDDG (kcal/mol):	0.21

ALP-POS-ecbed2ba-20_1



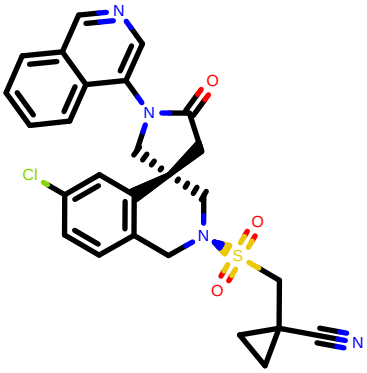
CID:	ALP-POS-ecbed2ba-20_1
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)N6CCC6
RUN:	RUN1132
DDG (kcal/mol):	4.17
dDDG (kcal/mol):	0.65

MAT-POS-853c0ffa-5_2



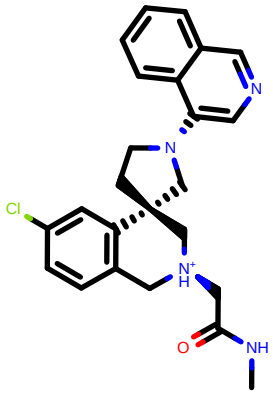
CID:	MAT-POS-853c0ffa-5_2
SMILES:	c1cc2cncc(c2c(c1)Cl)N3CC[C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1274
DDG (kcal/mol):	4.18
dDDG (kcal/mol):	0.54

EDJ-MED-8bb691af-5_1



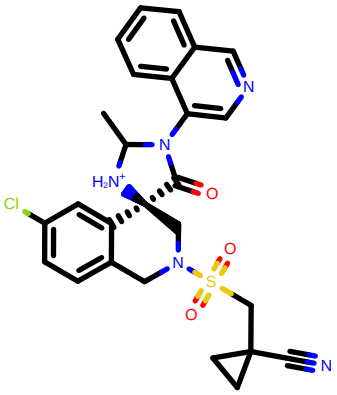
CID:	EDJ-MED-8bb691af-5_1
SMILES:	c1ccc2c(c1)cncc2N3C[C@]4(CC3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1205
DDG (kcal/mol):	4.23
dDDG (kcal/mol):	0.36

EDJ-MED-8bb691af-1_2



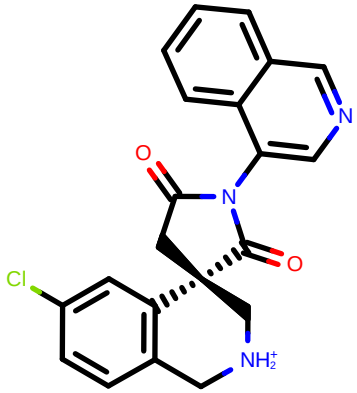
CID:	EDJ-MED-8bb691af-1_2
SMILES:	CNC(=O)C[N@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1031
DDG (kcal/mol):	4.33
dDDG (kcal/mol):	0.23

EDG-MED-b6bce001-2_2



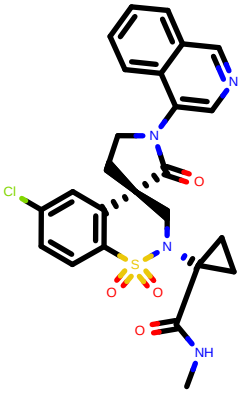
CID:	EDG-MED-b6bce001-2_2
SMILES:	CC1=[NH+][C@]2(C[N@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1291
DDG (kcal/mol):	4.34
dDDG (kcal/mol):	0.39

JOH-MSK-1f2dff76-3_1



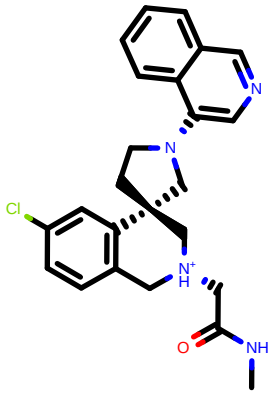
CID:	JOH-MSK-1f2dff76-3_1
SMILES:	c1ccc2c(c1)cncc2N3C(=O)C[C@@]4(C3=O)C[NH2+]Cc5c4cc(cc5)Cl
RUN:	RUN1014
DDG (kcal/mol):	4.35
dDDG (kcal/mol):	0.18

EDJ-MED-976a33d5-3_1



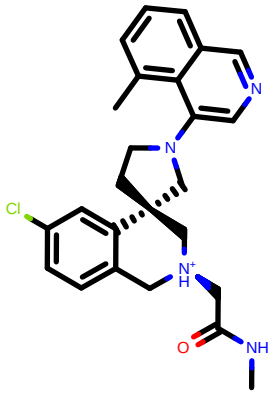
CID:	EDJ-MED-976a33d5-3_1
SMILES:	CNC(=O)C1(CC1)[N@@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1245
DDG (kcal/mol):	4.41
dDDG (kcal/mol):	0.59

EDJ-MED-8bb691af-1_3



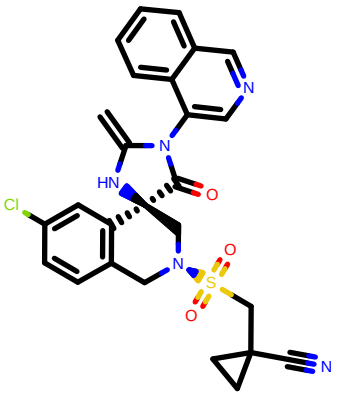
CID:	EDJ-MED-8bb691af-1_3
SMILES:	CNC(=O)C[N@@H+]1Cc2ccc(cc2[C@]3(C1)CCN(C3)c4cncc5c4cccc5)Cl
RUN:	RUN1033
DDG (kcal/mol):	4.60
dDDG (kcal/mol):	0.21

EDJ-MED-3656d29d-1_4



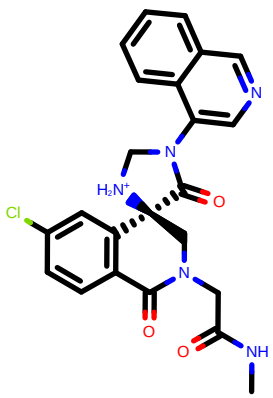
CID:	EDJ-MED-3656d29d-1_4
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1050
DDG (kcal/mol):	4.66
dDDG (kcal/mol):	0.19

EDG-MED-b6bce001-2_1



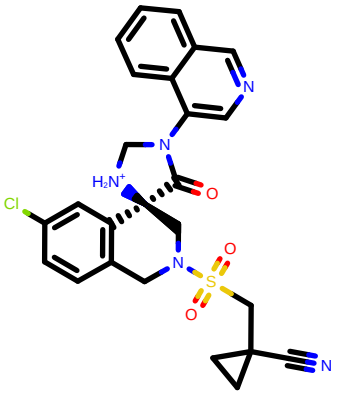
CID:	EDG-MED-b6bce001-2_1
SMILES:	CC1=[NH+][C@]2(C[N@@](Cc3c2cc(cc3)Cl)S(=O)(=O)CC4(CC4)C#N)C(=O)N1c5cncc6c5cccc6
RUN:	RUN1289
DDG (kcal/mol):	5.03
dDDG (kcal/mol):	0.37

EDJ-MED-fd8ed875-1_1



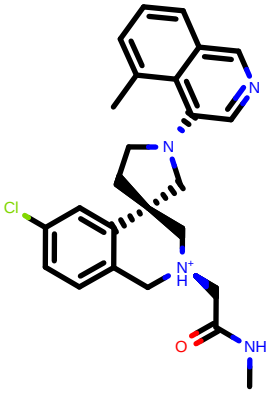
CID:	EDJ-MED-fd8ed875-1_1
SMILES:	CNC(=O)CN1C[C@]2(c3cc(ccc3C1=O)Cl)C(=O)N(C=[NH+]2)c4cncc5c4cccc5
RUN:	RUN1083
DDG (kcal/mol):	5.09
dDDG (kcal/mol):	0.13

EDG-MED-b6bce001-1_2



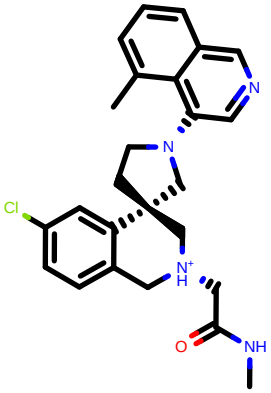
CID:	EDG-MED-b6bce001-1_2
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1226
DDG (kcal/mol):	5.13
dDDG (kcal/mol):	0.52

EDJ-MED-3656d29d-1_3



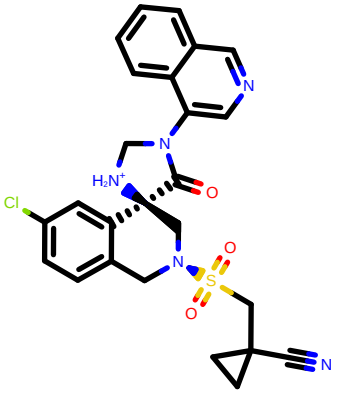
CID:	EDJ-MED-3656d29d-1_3
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1054
DDG (kcal/mol):	5.15
dDDG (kcal/mol):	0.22

EDJ-MED-3656d29d-1_1



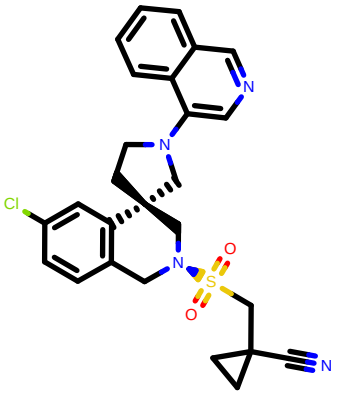
CID:	EDJ-MED-3656d29d-1_1
SMILES:	Cc1cccc2c1c(cnc2)N3CC[C@@]4(C3)C[N@@H+](Cc5c4cc(cc5)Cl)CC(=O)NC
RUN:	RUN1049
DDG (kcal/mol):	5.20
dDDG (kcal/mol):	0.22

EDG-MED-0c930815-1_1



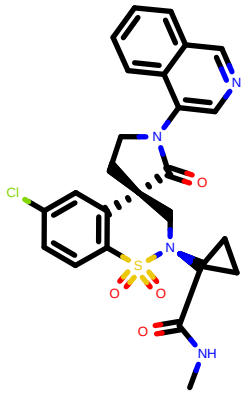
CID:	EDG-MED-0c930815-1_1
SMILES:	c1ccc2c(c1)cncc2N3C=[NH+][C@@]4(C3=O)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1219
DDG (kcal/mol):	5.35
dDDG (kcal/mol):	0.35

EDJ-MED-8bb691af-2_2



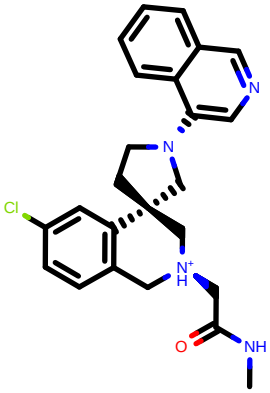
CID:	EDJ-MED-8bb691af-2_2
SMILES:	c1ccc2c(c1)cncc2N3CC[C@@]4(C3)C[N@@](Cc5c4cc(cc5)Cl)S(=O)(=O)CC6(CC6)C#N
RUN:	RUN1168
DDG (kcal/mol):	5.55
dDDG (kcal/mol):	0.37

EDJ-MED-976a33d5-3_2



CID:	EDJ-MED-976a33d5-3_2
SMILES:	CNC(=O)C1(CC1)[N@]2C[C@]3(CCN(C3=O)c4cncc5c4cccc5)c6cc(ccc6S2(=O)=O)Cl
RUN:	RUN1255
DDG (kcal/mol):	5.66
dDDG (kcal/mol):	0.57

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:	RUN1035
DDG (kcal/mol):	5.72
dDDG (kcal/mol):	0.24